Analysis of nonlinear diffusion equations of second and fourth order

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Abstract

Due to the ongoing miniaturization of semiconductor devices, quantum effects play a more and more dominant role. Usually, quantum phenomena are modeled by using kinetic equations, but sometimes a fluid-dynamical description presents several advantages; for example the better tractability from a numerical point of view and the assignation of boundary conditions. In the following work we study three fluid-type nonlinear partial differential equations of the second and fourth order; these models are related to the modeling of semiconductor devices. The first part concerns the study of a fully implicit semidiscretization in time and of the long-time asymptotics of a Fokker-Planck equation of degenerate type. The second part is devoted to the study of a quantum hydrodynamic model in one space dimension and the asymptotic decay of the model is formally shown. In the last section of the work existence and long-time behaviour of a nonlinear fourth-order parabolic equation (reduced quantum drift-diffusion model) in one space dimension are proved and some numerical examples are given.

Contents

Chapter 1

Introductory Overview

In the following we shall deal with the study of several nonlinear partial differential equations of second and fourth order, describing different diffusion phenomena and related to the modeling of semiconductor devices. In this sense it is possible to divide this work into three independent parts:

I. The study of a Fokker-Planck equation.

II. The investigation of stationary solutions to a quantum hydrodynamic model.

III. The study of a reduced quantum drift-diffusion model.

The modern computer and telecommunication industry relies heavily on the use of semiconductors devices. The reason of the rapid development and success in the semiconductor technology is refereed to the ongoing devices miniaturization. The microelectronics industry produces very miniaturized components with small characteristic length scale, like tunneling diodes, which have a structure of only few nanometer length. In such components quantum phenomena become no more negligible, even sometimes predominant and the physical phenomena have to be described by quantum mechanics equations.

A semiconductor device needs an *input* (generally light or electronic signal) and produces an *output* (light or electronic signal); the device is connected to the electric circuit by contacts at which a voltage is applied. We are interesting in devices which produce electric signals, for example current of electrons generated by the applied potential. In this case the relation between the *input* (applied voltage) and the *output* (current through one contact) is a curve (not necessary a function) called *current-voltage characteristic*.

Depending on the devices structure, the transport of particles can be very different, due to several physical phenomena, like drift, diffusion, scattering and quantum effects. The more appropriate way to describe a large number of particles flowing through a device is a kinetic or a fluid-dynamic type description. On the other hand, electrons are in a semiconductor crystal quantum objects, for which a wave-like description using the Schrődinger equation seems to be necessary. Therefore there are several mathematical models, which are able to describe particular phenomena in particular devices. These models vary for complexity and for mathematical properties and build a hierarchy, in which three classes can be distinguishes: kinetic models, fluid-dynamical models and quantum models.

In a quantum dynamical view, each single electron is interpreted as a wave; the motion of an electron ensemble of M particles in a vacuum under the influence of a (real-valued) electrostatic potential V is described by the *wave* function $\psi(x,t)$, solution to the *Schrödinger equation*

$$i\epsilon\frac{\partial\psi}{\partial t} = -\frac{\epsilon^2}{2}\sum_{j=1}^{M}\Delta_{x_j}\psi - V(x,t)\psi, \quad x\in\mathbb{R}^{dM},\ t>0. \tag{1.0.1}$$

The letter i denotes the complex unit and ϵ the scaled Planck constant. Another equivalent formulation to the Schrödinger description of the motion of an electron ensemble is given by the kinetic (Wigner) formulation. Let $\psi(x,t)$ be a solution to (1.0.1); we define the *density matrix*

$$\rho(r,s,t) := \overline{\psi(r,t)}\psi(s,t), \quad r,\ s\in\mathbb{R}^{dM},\ t>0.$$

The *Wigner function* has been introduced by Wigner (1932), defined as

$$w(x,k,t) := \frac{1}{(2\pi)^{dM}}\int_{\mathbb{R}^{dM}}\rho(x+\frac{\epsilon}{2}\eta, x-\frac{\epsilon}{2}\eta, t)e^{i\eta\cdot k}d\eta,$$

and formally solves the following equation

$$\frac{\partial w}{\partial t} + k\cdot\nabla_x w - \Theta[V]w = 0, \quad x,\ k\in\mathbb{R}^{dM},\ t>0, \tag{1.0.2}$$

where (x,k) are the position-momentum variables; $\Theta[V]$ is a pseudo-differential operator [**71**], defined as

$$\begin{aligned}(\theta[V])(w)(x,k,t) \quad = \quad & \frac{1}{(2\pi)^{dM}}\int_{\mathbb{R}^{dM}}\int_{\mathbb{R}^{dM}}\frac{i}{\epsilon}\Big[V\Big(x+\frac{\epsilon}{2}\eta,t\Big) - V\Big(x-\frac{\epsilon}{2}\eta,t\Big)\Big]\\ & \times w(x,k',t)e^{i(k-k')\cdot\eta}dk'\,d\eta,\end{aligned}$$

applied to the electrostatic potential V, which is usually self-consistent and given by the *Poisson equation*

$$-\lambda^2\Delta V = n - C(x), \tag{1.0.3}$$

where λ is the semiconductor permittivity, $C(x)$ a positive function describing the concentration of the fixed charge background ions in the semiconductor crystal and n the particle density, defined as $n(x,t) := \int_{\mathbb{R}^d} w(x,k,t)\, dk$.
In the mathematical modeling for semiconductor devices it is necessary to take into account also the physical effects coming from short-range particle interactions, like collisions of electrons with other electrons or with the crystal lattice. In particular, in semiconductor crystals there are three main scattering phenomena: electron-phonon scattering, ionized impurity scattering and carrier-carrier scattering. Collision effects can be described at the kinetic level by the Wigner-Fokker-Planck equation

$$(1.0.4) \qquad \frac{\partial w}{\partial t} + k \cdot \nabla_x w - \Theta[V]w = Q(w), \quad (x,k) \in \mathbb{R}^{2d},\ t > 0.$$

The term $Q(w)$ is called *collision operator*; it models the interaction of the electrons with the phonons of the crystal lattice (oscillators) and has the form

$$(1.0.5) \qquad Q(w) = \alpha \Delta_k w + \frac{1}{\tau}\mathrm{div}_k(kw) + \beta \mathrm{div}_x(\nabla_k w) + \nu \Delta_x w,$$

with α, β, τ and ν positive constants. The model (1.0.4), (1.0.5) governs the dynamical evolution of an electron ensemble in the single-particle Hartree approximation interacting dissipatively with an idealized heat bath consisting of an ensemble of harmonic oscillators and modeling the semiconductor lattice. Problem (1.0.4), (1.0.5) has been derived in [**20, 35**] and studied in [**7, 8, 9**].
Due to the nonlinearities and to the high number of independent variables, the mathematical analysis of kinetic models can be very complicated. Simpler macroscopic models have been derived from (1.0.4); these models describe the evolution of macroscopic quantities, like electron and hole density. One of the advantages of a fluid-dynamical description concerns numerical simulations, which require in this case less computation power. Moreover, as semiconductor devices are modeled in a bounded domain, it is easier to find physically relevant boundary conditions for macroscopic variables then for wave or for the Wigner function, for which the natural physical setting is based on an unbounded domain.
The particle density $n(x,t)$ and the current density $J(x,t)$ are defined respectively as the zeroth and first moment of the Wigner function

$$n(x,t) := \int_{\mathbb{R}^d} w(x,k,t)\, dk, \quad J(x,t) := \int_{\mathbb{R}^d} kw(x,k,t)\, dk,$$

and macroscopic equations are derived from (1.0.4) using the *moment method*. We multiply (1.0.4) by 1 and k and after integration over $k \in \mathbb{R}^d$, we get the so-called moment equations

$$
\begin{aligned}
(1.0.6)\quad & \frac{\partial\langle w\rangle}{\partial t} + \mathrm{div}\langle kw\rangle = \nu\Delta\langle w\rangle,\\
& \frac{\partial\langle kw\rangle}{\partial t} + \mathrm{div}\langle k\otimes kw\rangle - \langle w\rangle\nabla V = -\frac{\langle kw\rangle}{\tau} - \beta\mathrm{div}\langle w\rangle + \nu\Delta\langle kw\rangle,
\end{aligned}
$$

where $\langle g(k)\rangle := \int_{\mathbb{R}^d} g(k)\, dk$. The goal of this method is to express each term of the above system of equations in term of the moments $\langle w\rangle$ and $\langle kw\rangle$. The main difficulties arise now from the flux $\langle k\otimes kw\rangle$, which cannot be rewritten with help of the first and second order moment. Therefore a *closure condition* is needed. As in the case of the classical kinetic theory, we achieve the closure condition by assuming as in [**40**] that the Wigner function w is close to a wave function displaces equilibrium density such that

$$
w(x,k,t) = w_{\mathrm{eq}}(x, k - u(x,t), t),
$$

where $u(x,t)$ is some group velocity,

$$
\begin{aligned}
(1.0.7)\qquad w_{\mathrm{eq}} = A(x,t)\mathrm{exp}\Big(-\frac{|k|^2}{2T} + \frac{V}{T}\Big)\Big[1 + \epsilon^2\Big(\frac{1}{8T^2}\Delta_x V \\
+ \frac{1}{24T^3}|\nabla_x V|^2 - \frac{1}{24T^3}\sum_{i,j=1}^{d} k_i k_j \frac{\partial^2 V}{\partial x_i\partial x_j}\Big) + O(\epsilon^4)\Big],
\end{aligned}
$$

and T is the electron temperature. The function (1.0.7) is derived from an $O(\epsilon^4)$ approximation of the thermal equilibrium density first given by Wigner [**79**]. The function $A(x,t)$ is assumed to be slowly varying in x and t. Then the first moments are $\langle w\rangle = n$ and $\langle kw\rangle = J$ and

$$
(1.0.8)\quad \langle k\otimes kw\rangle = \frac{J\otimes J}{n} + nT\mathrm{Id} - \frac{\epsilon^2}{12T}n(\nabla\otimes\nabla)V + O(\epsilon^4).
$$

The formula (1.0.7) implies that n equals $e^{V/T}$ times a constant, up to the term of order $O(\epsilon^2)$, and therefore, if the temperature is slowly varying,

$$
\frac{\partial^2 \log n}{\partial x_i\partial x_j} = \frac{1}{T}\frac{\partial^2 V}{\partial x_i\partial x_j} + O(\epsilon^2).
$$

Using this condition we can replace all second derivatives of V by second derivatives of $\log n$, making an error of order $O(\epsilon^4)$. This yields to the *viscous quantum hydrodynamic equations*

$$
\begin{aligned}
(1.0.9)\qquad & \frac{\partial n}{\partial t} + \mathrm{div}J = \nu\Delta n, \quad x\in\mathbb{R}^d,\ t>0,\\
& \frac{\partial J}{\partial t} + \mathrm{div}\left(\frac{J\otimes J}{n}\right) + \nabla(nT) + n\nabla V - \frac{\epsilon^2}{2}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\frac{J}{\tau} + \nu\Delta J,
\end{aligned}
$$

where the electrostatic potential V is self-consistent and given by (1.0.3). The above system consists in conservation laws for the particle and for the current density. The quantum term $\frac{\epsilon^2}{2}n\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$ can be interpreted as a quantum self-potential term with the Bohm potential $\frac{\Delta\sqrt{n}}{\sqrt{n}}$ or as the divergence of the pressure tensor $P = \frac{\epsilon^2}{4}n(\nabla \otimes \nabla)\log n$. The terms $\frac{J}{\tau}$, $\nu\Delta n$ and $\nu\Delta J$ model interactions of the electrons with the phonons of the semiconductor crystal lattice. The term nT describes the pressure tensor. In the literature we can find several assumptions for the temperature T; the function T can be assumed to be constant, a function of the particle density $T(n)$, as in the fluid-dynamical case, or described by an additional equation. In this last case, the additional equation can be derived from the Wigner equation (1.0.4) by a moment method, similar as above, multiplying (1.0.4) by the second moment $\frac{1}{2}|k|^2$ and integrating oder $k \in \mathbb{R}^d$. In the following we consider the temperature as a function of the particle density $T = T(n)$. Setting $\nu = 0$ in (1.0.9) we get the so-called inviscid *quantum hydrodynamic model*.

We perform now in the inviscid quantum hydrodynamic model the following diffusion scaling: in (1.0.9) with $\nu = 0$ we substitute t by t/τ and J by $J\tau$, where τ is the relaxation time constant. After scaling we obtain

$$\tau\frac{\partial n}{\partial t} + \tau \mathrm{div} J = 0, \quad x \in \mathbb{R}^d,\ t > 0, \tag{1.0.10}$$
$$\tau^2\frac{\partial J}{\partial t} + \tau^2 \mathrm{div}\left(\frac{J \otimes J}{n}\right) + \nabla(nT(n)) + n\nabla V - \frac{\epsilon^2}{2}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -J.$$

If the constant τ is small, then the above system describes a situation for large time-scale and small current density. Computing formally the limit $\tau \to 0$ in (1.0.10), the *quantum drift-diffusion model* is derived

$$\frac{\partial n}{\partial t} + \mathrm{div} J = 0, \tag{1.0.11}$$
$$J = -\nabla(nT(n)) - n\nabla V + \frac{\epsilon^2}{2}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right).$$

The model consists in nonlinear continuity equation for the particle density; the current density J is given by the sum of the diffusion current $\nabla nT(n)$ and of the drift current nE, where E is the sum of the electrostatic potential field with a quantum term, $E = \nabla\left(V - \frac{\epsilon^2}{2}\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$.
For vanishing scaled Planck constant $\epsilon = 0$ we obtain the classical *drift-diffusion model*

$$\frac{\partial n}{\partial t} + \mathrm{div} J = 0, \quad J_0 = -\nabla(nT(n)) - n\nabla V. \tag{1.0.12}$$

Recently another derivation of the quantum drift-diffusion model has been presented [**32**]; the model is derived from the Wigner equation (1.0.4) with a BGK-collision operator via a moment method and using as closure condition the *entropy minimization principle*. Let

$$Q(w) := M[w] - w$$

be the collision operator, where τ is the relaxation time and $M[w]$ the quantum Maxwellian. The function $M[w]$ is defined as a minimizer of a quantum entropy, subject to the constraint of a given particle density. More precisely, we introduce the free energy functional

$$H(w) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} w\left(\mathrm{Ln}\, w - 1 + \frac{|k|^2}{2} - V(x)\right)\frac{dx\, dk}{(2\pi\epsilon^d)}.$$

The "quantum logarithm" operator Ln is defined as $\mathrm{Ln}(w) = W(\log W^{-1}(w))$, where W is the Wigner transform and W^{-1} the inverse (also called Weyl's quantization) defined as

$$(W^{-1}[w])\phi(x) = \int_{\mathbb{R}^{2d}} w\left(\frac{x+y}{2}, k, t\right)\phi(y)e^{ik(x-y)}\,\frac{dkdy}{(2\pi\epsilon^d)},$$

for suitable $\phi(x)$. The quantum Maxwellian $M[w]$ is assumed to be the minimizer of $H(w)$ under the constraint of given particle density, more precisely

$$H(M[w]) = \min\left\{H(w) \mid \int_{\mathbb{R}^d} w(x,k)\, dk = n(x), \quad \forall x \in \mathbb{R}^d\right\}.$$

The quantum drift diffusion equations come now from a diffusion limit; we rescale (1.0.4) in time, replacing t by t/δ and $Q(w)$ by $Q(w)/\delta$. This yields

$$\delta\frac{\partial w_\delta}{\partial t} + k\cdot\nabla_x w_\delta - \Theta[V]w_\delta = \frac{1}{\delta}(M[w_\delta] - w_\delta), \quad (x,k)\in\mathbb{R}^{2d},\ t>0.$$

It can be proved that $w_\delta \longrightarrow w_0$ as $\delta \rightarrow 0$ and the functions $n := \int_{\mathbb{R}^d} w_0\, dk$ and $P := \int_{\mathbb{R}^d} k\otimes k\; w_0\, dk$ satisfy the equations

$$\frac{\partial n}{\partial t} + \mathrm{div}J = 0, \quad J = \mathrm{div}P - n\nabla V. \tag{1.0.13}$$

Taking now an approximation of the function w_0 (Chapman-Enskog method), which yields

$$J = J_0 + O(\epsilon^4),$$

equations (1.0.13) can be rewritten as

$$\frac{\partial n}{\partial t} + \mathrm{div}J = 0, \quad J_0 = -\nabla n - n\nabla V + \frac{\epsilon^2}{6}n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right),$$

with constant temperature $T = 1$. Note that the Bohm potential in the above equation has been derived by a factor 3 compared to the expression in (1.0.11). The physical explanation of this discrepancy has not been found.

1.1 Short summary of part I

The first part of the work concerns the analysis of a fully implicit semidiscretization in time and the long-time behaviour of equations of the form

$$\frac{\partial n}{\partial t} + \mathrm{div} J = 0, \quad x \in \Omega \subset \mathbb{R}^d,\ t > 0, \tag{1.1.1}$$

where the current density J is given by

$$J = -\nabla f(n) - n\nabla V, \tag{1.1.2}$$

with n the electron density and V the electrostatic potential. The function $f(n)$ describes the particle pressure and it is given by $f(n) = n\,T(n)$, with $T(n)$ the temperature. If $f'(0) = 0$, the diffusion term in parabolic equations like (1.1.1), (1.1.2) becomes of degenerate type.

The family of equations (1.1.1), (1.1.2) include drift-diffusion type models (1.0.12), where the potential is given by the Poisson equation, nonlinear Fokker-Planck equations, where $V(x)$ is assumed to be confined and general nonlinear diffusion equations, where $V(x) \equiv 0$.

The existence analysis of (1.1.1), (1.1.2) with a confining potential or in case $V \equiv 0$ is done in [**25, 75**]. The fine description of long-time asymptotics for nonlinear diffusion equations like (1.1.1), (1.1.2) has attracted in the last years many mathematicians; the interest on this problem is based on a bring-up of new ideas coming from different communities: the entropy approach from kinetic theory, having its roots in the famous H-Theorem for the Boltzmann equation [**27, 65**], the optimal mass transport theory, giving a geometric point of view of these equations [**66, 26, 2, 3**] and variational techniques related to new Gagliardo-Nirenberg inequalities [**36**].

Nonlinear diffusion equations without confinement, $V(x) \equiv 0$, are expected to diffuse as $t \to \infty$, and thus, solutions vanish as $t \to \infty$ with an expansion of their support or their tails depending whether the diffusion is slow or fast. On the contrary, nonlinear Fokker-Planck equations are expected to stabilize towards a steady state n_∞, defined by setting the flux to zero $\nabla V + \nabla h(n_\infty) = 0$, where $h(n) := \int_1^n \frac{f'(s)}{s}\, ds$. A rigorous proof of this stabilization was done in [**25**] in L^1 by using an entropy-entropy production approach. The stationary state was characterized as the unique minimizer in the space of integrable functions with given mass of a suitable functional that we call entropy. This entropy functional was then proved to be a Lyapunov functional for the equation and thus, the study of its evolution gave the desired convergence rate. We refer to [**27, 25, 65**] for details. Moreover, generalized Log-Sobolev inequalities were obtained in [**25**] relating the entropy to the entropy production.

Equations like (1.1.1), (1.1.2), either with $V \equiv 0$ or $V \neq 0$, share remarkable properties with respect to Wasserstein distances for probability measures. This remarkable property of the family of equations (1.1.1), (1.1.2) is that assuming that $V(x)$ is convex, their flow map is a global contraction for the 2-Wasserstein distance [**66, 26, 2, 3**]. Moreover, in the one dimensional case equations (1.1.1), (1.1.2) under the convexity assumption on $V(x)$, are contractions for all Wasserstein distances [**28, 23**].
Nonlinear Fokker-Planck equations with confining potential $V(x) = \frac{1}{2}|x|^2$ and nonlinearity $f(n) = n^m$ are equivalent through an explicit change of variables to the nonlinear diffusion equation with $V(x) \equiv 0$ and $f(n) = n^m$ and therefore, the study of their long-time behaviour is equivalent too. In fact, the stabilization towards equilibrium of the nonlinear Fokker-Planck equation translates into a self-similar behavior as $t \to \infty$ for the nonlinear diffusion equation, in the sense that all solutions resemble a self-similar profile as $t \to \infty$. This self-similar profile is the well-known Barenblatt profile for homogenous nonlinear diffusions.

In Chapter 2 we analyze the semidiscretization based on the implicit Euler scheme of nonlinear Fokker-Planck equation (1.1.1), (1.1.2) with confining potential in a bounded domain.
In [**10**] the large time behaviour for an implicit semidiscretization in time of (1.1.1), (1.1.2) in the whole space with $f(n) = n$ and confining potential is studied. We shall recall that the analytical methods used in [**10**] for the linear case are not helpful if $f(n)$ is of degenerate type; since the staedy-state in the linear case $f(n) = n$ is strictly positive, given by $n_\infty := e^{-V}$, weighted Sobolev spaces like $L^2(n_\infty^{-1})$, equipped with the inner product $\langle n_1, n_2 \rangle_{n_\infty^{-1}} := \int_{\mathbb{R}^d} \frac{n_1 n_2}{n_\infty}\, dx$, can be defined and some property like conservation of mass can be easily proved. But the most important difference between the linear and the degenerate case consists on the treatment of the convection term $n\nabla V$; since, if $f(n) = n$, the staedy-state is given by $n_\infty = e^{-V}$, the current density $J = \nabla f(n) + n\nabla V$ can be rewritten as $J = n_\infty \nabla \left(\frac{n}{n_\infty}\right)$, which simplifies the analysis considerable.
The implicit Euler scheme for (1.1.1), (1.1.2) in case of degenerate diffusion term in the whole space has not yet been investigated.
We will show moreover that the semidiscretization of (1.1.1), (1.1.2) preserves the non-increasing behaviour of the entropy functional.
In section 2.2 we deal with the long-time behaviour of (1.1.1), (1.1.2) in case $V \equiv 0$ and $f(n) = n^m$. More precisely, the contractivity of Wasserstein distances in one space dimension is used to obtain a bound on the expansion rate of the support of solutions. It is well known that the degeneracy at level $n = 0$ of the diffusivity $D(n) = mn^{m-1}$ causes the phenomena called *finite speed of propagation*. This means that the support of the solution $n(\cdot, t)$

to (1.1.1), (1.1.2) is a bounded set for all $t \geq 0$. In fact it can be proved that the solution $n(x,t)$ as $t \to +\infty$ converges to the Barenblatt function with the same mass as the initial data. This result is already known since the work of J.L. Vázquez [**74**], but here we will give a alternative and very simple proof of the *finite propagation* property, by using mass transportation techniques.
Although several qualitative properties of the solutions for general nonlinear diffusion equations have been obtained [**57**], there is no result concerning asymptotic profiles of general diffusion equations except in the case of power-like behavior for small values of n.

1.2 Short summary of part II

In this part of the work we investigate the one-dimensional stationary solution of the *viscous* quantum hydrodynamic model

$$\begin{aligned} &n_t + J_x = \nu n_{xx}, \\ &J_t + \left(\frac{J^2}{n}\right)_x + Tn_x - nV_x - \frac{\epsilon^2}{2} n \left(\frac{\sqrt{n}_{xx}}{\sqrt{n}}\right)_x = -\frac{J}{\tau} + \nu J_{xx}, \\ &\lambda^2 V_{xx} = n - C(x) \quad x \in (0,1),\ t > 0, \end{aligned} \tag{1.2.1}$$

with boundary conditions

$$n(0) = n(1) = 1, \quad n_x(0) = n_x(1) = 0, \quad V(0) = V_0, \quad J(0) = J_0,$$

where $n(x,t)$ describes the electron density, $J(x,t)$ the current density and $V(x,t)$ the electrostatic potential. The function $C(x)$ describes the concentration of fixed background charges. The physical constants are the (scaled) Planck constant ϵ, the Debye length λ, the (scaled) temperature T supposed to be constant, the positive constant ν called *viscosity* and the (scaled) momentum relaxation time τ. This model can be derived by a moment method [**40**], similarly as in the case of the quantum hydrodynamic model, from a Wigner-Fokker-Planck equation (1.0.4) with a collision operator of the form (1.0.5).
Concerning the mathematical analysis of the stationary inviscid quantum hydrodynamic model ((1.2.1) with $\nu = 0$), many results are available [**44, 49, 39, 81**]. It has been shown (in one and several space dimensions) that there exists a weak solution to (1.2.1) with $\nu = 0$ (and for various choices of the boundary conditions), if a subsonic-type condition of the form

$$\frac{J_0}{n} < \sqrt{T + \frac{\varepsilon^2}{4}} \quad \text{in } (0,1), \tag{1.2.2}$$

is satisfied, i.e., if the current density is small enough. (Recall that an Euler flow is called subsonic if $J_0/n < \sqrt{T}$.) Moreover, for special boundary conditions, it has been proved [**39**] that the quantum hydrodynamic equations do *not* possess a weak solution if the current density is sufficiently large. The main difficulty in the existence analysis (besides of the mathematical treatment of the third-order quantum term) is the convection term $(J^2/n)_x$. In fact (see [**39**]) this term may force the particle density to cavitate if the current density is large enough. Without this term, the stationary equations (still with $\nu = 0$) become the quantum drift-diffusion model for which a solution exists for any data [**15**]. The third-order quantum term possesses a regularizing effect since the condition (1.2.2) allows for slightly "supersonic" flows [**44**].

The question arises if, as in the case of the *classical* hydrodynamic equations, the viscous terms $\nu\Delta n$ and $\nu\Delta J$ regularize the equations in such a way that the existence of solutions can be proved for all values of the current densities. In this work we give a partial answer to this question.

More precisely, we prove the existence of classical solutions if the following "weakly supersonic" condition holds:

$$\frac{J_0}{n} < \frac{1}{\sqrt{2}}\sqrt{T + \frac{\varepsilon^2}{16} + \frac{\nu}{\tau}} \quad \text{in } (0,1). \tag{1.2.3}$$

Thus, the current density is allowed to be large if either the viscosity ν is large or the (scaled) relaxation time is small enough. The reason for this restriction comes from the fact that, roughly speaking, the viscous term νJ_{xx} can be reformulated (up to a factor) as the third-order quantum term. In fact, integrating $J_x = \nu n_{xx}$ and using the boundary condition for J we obtain $J = \nu n_x + J_0$, which gives

$$\left(\frac{J^2}{n}\right)_x - \nu J_{xx} = -2\nu^2 n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x + \left(\frac{J_0^2}{n}\right)_x + 2\nu J_0(\log n)_{xx},$$

and therefore, we can reformulate equation (1.2.1) formally as

$$\begin{aligned}\left(\frac{J_0^2}{n}\right)_x + \left(T + \frac{\nu}{\tau}\right)n_x - nV_x \quad &- \quad \left(2\nu^2 + \frac{\varepsilon^2}{2}\right)n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x \\ &= \quad -\frac{J_0}{\tau} - 2J_0\nu(\log n)_{xx}.\end{aligned} \tag{1.2.4}$$

This formulation shows that the viscous terms indeed regularize the equations (as the coefficient of the quantum term becomes larger) but there is still a convection term which may force the solutions to cavitate for large values of the current density J_0. (Unfortunately, the method in [**39**] cannot be applied to prove this conjecture rigorously.) Thus we expect a similar restriction on the current density as (1.2.2), but allowing for larger current densities. However, for sufficiently large ν/τ, we can allow for "supersonic" current densities $J_0/n > \sqrt{T + \epsilon^2/4}$. We also remark that the above argument only holds in one space dimension. For the multi-dimensional problem, no results are available. This situation is similar to the inviscid quantum hydrodynamic equations, where mathematical results are essentially only available in one space dimension (except [**49**]).

In order to prove the existence of solutions to (1.2.4), we rewrite (1.2.4) as a fourth-order equation and employ the technique of exponential transformation of variables $n = e^u$ as in [**44**] (first used in [**18**]). The existence of a weak solution $u \in H^2(0,1)$ provides a weak solution $n = e^u$ which is *strictly positive*. Notice that maximum principle arguments can generally be *not* applied to third- or fourth-order equations, and therefore, the exponential transformation of variables circumvents this fact to prove positive lower bounds for the particle density. As a second result we prove the uniqueness of stationary solutions of (1.2.1) in one space dimension for sufficiently small parameters ν, ϵ and J_0. In semiconductor problems it is well known that uniqueness of solutions can only be expected for sufficiently small current densities since there are devices based on multiple solutions.

Using $u = \log n$ as a test function in the weak formulation of the fourth-order equation, we obtain the estimate

$$\left(\nu^2 + \frac{\epsilon^2}{4}\right)\|u_{xx}\|_{L^2} + \left(T + \frac{\nu}{\tau}\right)\|u_x\|_{L^2} \le K, \tag{1.2.5}$$

where $K > 0$ is a constant not depending on u, ν or ϵ (see Lemma 3.6). This inequality is the key estimate of chapter 3. It provides an H^1 bound for u independently of ν and ϵ. This allows to perform the inviscid limit $\nu \to 0$ and the semiclassical limit $\epsilon \to 0$. These limits as well as the combined limit $\nu^2 + \epsilon^2 \to 0$ are shown in Section 3.3.

A numerical study of the viscous quantum hydrodynamic model, including the asymptotic behavior of the solutions for small parameters (ν and ϵ), is published in [**55, 52**].

In Section 3.4 the long-time asymptotics of solutions to (1.2.1) in one space dimension towards the so-called thermal equilibrium state (no current flow) is studied. Special thermal equilibrium functions are given by $n = 1$, $J = 0$ and $V = 0$ in $\Omega = (0,1)$ and we prove that any strong solution of (1.2.1) with initial data $n(\cdot,t) = n_I$ and $J(\cdot,t) = J_I$ and boundary conditions

$$n = 1 \qquad n_x = 0 \qquad V = 0, \qquad \text{on} \quad \partial\Omega \times \quad (0,\infty)$$
$$\int_{\partial\Omega} J\left[J_x\left(\frac{\epsilon^2}{4\nu} + \nu\right) - \frac{1}{2}J^2\right](\cdot,t)ds = 0 \qquad t > 0$$

converges exponentially fast to the unique thermal equilibrium state $(n, J, V) = (1, 0, 0)$.
For the proof we assume, but we have not proved yet, that the system (1.2.1) has a global in time solution. The result of global in time existence presents several difficulties; the main one concerns the effective current density $J - \nu n_x$, which is not constant anymore, contrary to the stationary case. Therefore the idea to rewrite the system as one equation for the particle density is not useful. We can expect to get local-in-time existence of solutions, or "small" solutions globally in time, starting with initial data near the thermal equilibrium; these results can be proved by a Galarkin method, which yields existence of solutions by standard ODE methods. The main question arises now if the particle density becomes zero at a certain time and if the linear physical viscosity terms $\nu\Delta n$ and $\nu\Delta J$ are enough to prevent the function n to cavitate. No results are available in the literature.
The proof of the exponential decay to the thermal equilibrium is based on the entropy/entropy dissipation method, which is applied here for the first time to a third-order equation. Let

$$E(t) := \int_0^1 \left[\frac{\epsilon^2}{2}(\sqrt{n})_x^2 + T(n(\log n - 1) + 1) + \frac{\lambda^2}{2}V_x^2 + \frac{1}{2}\frac{J^2}{n} \right](x,t)dx \geq 0,$$

be the *free energy functional*, consisting on quantum energy, thermodynamical entropy, electric energy and kinetic energy of the system; the idea is to derive an inequality of the form

$$E(t) + \int_0^t \int_0^1 P(x,t)dxds \leq E(0),$$

where the entropy dissipation rate $P(x,t)$ depends on the variables and his derivatives. We show that:

$$\int_0^1 P(x,t)dx \geq \gamma E(t)$$

for some $\gamma > 0$ and thus Gronwall's lemma implies:

$$E(t) \leq E(0)e^{-\gamma t}, \qquad t \geq 0.$$

Finally Poincaré inequality gives convergence rate of (n, J, V) to the thermal equilibrium.

1.3 Short summary of part III

The third part of this work concerns the analysis of a simplified transient quantum drift diffusion model (1.0.11).

The mathematical analysis and the numerical understanding of (1.0.11) in the stationary case is now in a rather advanced state. The stationary problem has been solved in [**15**], thermal equilibrium problem in [**72**] and a generalized Gummel iteration for an efficient numerical treatment in the one dimensional space has been developed in [**68**].
Concerning the transient case, only partial results are known. The crucial problem in the analysis comes from the fourth-order nature of the system. In order to understand better the influence of the fourth order term, we studied a simplified model: setting vanishing temperature and zero electric field in (1.0.11), the system can be rewritten as a fourth-order parabolic equation for the particle density. In one space dimension, assuming smooth nonvacum solutions, the Bohm potential differential operator $\left(n\left((\sqrt{n})_{xx}/\sqrt{n}\right)_x\right)_x$ can be equivalently rewritten as $(n(\log n)_{xx})_{xx}$ and system (1.0.11) reduces to the nonlinear fourth order parabolic problem

$$\partial_t n + (n(\log n)_{xx})_{xx} = 0, \quad n(\cdot, 0) = n_I(\cdot). \tag{1.3.1}$$

Equation (1.3.1) also arises as a scaling limit in the study of interface fluctuations in a certain spin system [**34**]. In quantum semiconductor modeling, Dirichlet-Neumann boundary conditions of the type

$$n(0,t) = n(1,t) = 1, \quad n_x(0,t) = n_x(1,t) = 0, \quad t > 0, \tag{1.3.2}$$

have been employed to model resonant tunneling diodes in $\Omega = (0,1)$ [**53**]. The existence of global weak solutions to (1.3.1)-(1.3.2) has been proved in [**54**].
The boundary conditions (1.3.2) simplify the analysis of (1.3.1) considerably. Indeed, one of the main ideas of the existence proof is to employ an exponential transformation of variables, $n = e^y$. In the new variable y, the boundary conditions are homogeneous. Thus, using, for instance, the test function y in the weak formulation of (1.3.1), no integrals with boundary data appear.
The boundary conditions (1.3.2) follow from physical considerations like the charge neutrality at the boundary contacts, i.e. $n - C = 0$ at $x = 0, 1$, where $C = C(x)$ models fixed background charges. Numerical results show that the Neumann boundary conditions for the density n should be non-homogeneous for ultra-small semiconductor devices (see Section 4 in [**67**]). Moreover, when the values of the doping profile $C(x)$ are different at the contacts, the Dirichlet boundary conditions satisfy $n(0,t) \neq n(1,t)$. Therefore, we wish to study the more general *non-homogeneous* boundary conditions

$$n(0,t) = n_0, \quad n(1,t) = n_1, \quad n_x(0,t) = w_0, \quad n_x(1,t) = w_1, \quad t > 0, \tag{1.3.3}$$

where n_0, $n_1 > 0$ and w_0, $w_1 \in \mathbb{R}$. The treatment of this non-homogeneities is also interesting from a mathematical point of view. Indeed, almost all results for (1.3.1) (and for related fourth-order equations like the thin-film model [**16**]) are shown only for periodic or no-flux boundary conditions or for whole-space problems, in order to avoid integrals with boundary data and to use conservation of mass property $\int_\Omega n(x,t)\,dx = \int_\Omega n_I(x)\,dx$ for all $t > 0$. In this work, we show how to deal with non-homogeneous boundary conditions for equation (1.3.1).

More precisely, we show (i) the existence and uniqueness of a classical positive solution n_∞ to the stationary problem corresponding to (1.3.1), (ii) the existence of global nonnegative weak solutions $n(\cdot,t)$ to the transient problem (1.3.1), (1.3.3), and (iii) the exponential convergence of $n(\cdot,t)$ to its steady state n_∞ as $t \to \infty$ in the L^1 norm, under the assumption that the boundary data is such that $\log n_\infty$ is concave. The long-time behavior is illustrated by numerical experiments. Notice that this is the first result of the *stationary* problem corresponding to (1.3.1) in the literature (if (1.3.2) or periodic boundary conditions are assumed, the steady state is constant). We also remark that the Wasserstein techniques of [**41**] cannot be applied to (1.3.1), (1.3.3) since this technique relies on the conservation of the L^1 norm which is not the case here. The long-time behavior of solutions to (1.3.1) has been studied for periodic boundary conditions [**19, 37**] and for the boundary conditions (1.3.2) [**56**]. In particular, it could be shown that the solutions converge exponentially fast to its (constant) steady state. The decay rate has been numerically computed in [**24**]. No results are available up to now for the case of the non-homogenous boundary conditions (1.3.3).

The first main result is the existence and uniqueness of stationary solutions needed in the existence proof for the transient problem. The existence proof is based on a fixed-point argument and appropriate *a priori* estimates, using heavily the structure of the equation and the one-dimensionality. More precisely, we perform the exponential transformation $n = e^y$ and write the equation in $(n(\log n)_{xx})_{xx} = 0$ as $y_{xx} = (ax+b)e^{-y}$ for some a, $b \in \mathbb{R}$. The key point is to derive uniform bounds on a and b. This implies a uniform H^1 bound for y and, in view of the one-dimensionality, a uniform L^∞ bound for $y = \log n$, hence showing the positivity of n. For the uniqueness we employ a monotonicity property of the operator $\sqrt{n} \mapsto -(n(\log n)_{xx})_{xx}/(2\sqrt{n})$ for suitable functions n (the monotonicity property has been first observed in [**54**]).

The second main result is the existence of solutions to the transient problem. For the proof of this result we semi-discretize (1.3.1) in time and solve at each time step a nonlinear elliptic problem. The main difficulty is to obtain uniform estimates. The idea of [**54**] is to derive these estimates from a special Lyapunov functional,

$$E_1(t) = \int_0^1 \left(\frac{n}{n_\infty} - \log \frac{n}{n_\infty} \right) dx,$$

which is also called an "entropy" functional. Indeed, a formal computation (made precise in Section 4.2) shows that

$$\frac{dE_1}{dt} + \int_0^1 (\log n)_{xx}^2 dx = \int_0^1 n(\log n)_{xx} \left(\frac{1}{n_\infty}\right)_{xx} dx, \tag{1.3.4}$$

implying that E_1 is nonincreasing if $(1/n_\infty)_{xx} = 0$, which is the case in [**54**] where $n_\infty =$ const. holds. However, in the general case $(1/n_\infty)_{xx} \neq 0$, the right-hand side of (1.3.4) still needs to be estimated.

The key idea is to employ the *new* "entropy"

$$E_2(t) = \int_0^1 (\sqrt{n} - \sqrt{n_\infty})^2 dx.$$

A formal computation yields

$$\frac{dE_2}{dt} + 2\int_0^1 \left(\sqrt[4]{\frac{n_\infty}{n}}(\sqrt{n})_{xx} - \sqrt[4]{\frac{n}{n_\infty}}(\sqrt{n_\infty})_{xx}\right)^2 dx = 0. \tag{1.3.5}$$

With this estimate the right-hand side of (1.3.4) can be treated. Indeed, the above entropy production integral allows to find the bound

$$\int_0^1 \left(\sqrt{n}(\log n)_{xx}^2 + (\sqrt[8]{n})_x^4\right) dx \leq c, \tag{1.3.6}$$

for some constant $c > 0$ only depending on the boundary data; see Lemma 4.8 for details. Then, using Young's inequality, the right-hand side of (1.3.4) is bounded from above by

$$\int_0^1 \sqrt{n}(\log n)_{xx}^2 dx + \|1/n_\infty^2\|_{W^{2,\infty}(0,1)} \int_0^1 n^{3/2} dx,$$

which is bounded in view of (1.3.6). We stress the fact that this idea is new in the literature.

The above estimates are only valid if n is nonnegative. However, no maximum principle is generally available for fourth-order equations. We prove the nonnegativity property by employing the same idea as in the stationary case: after introducing an exponential variable $n = e^y$, we obtain a uniform H^2 bound by (1.3.4) and (1.3.6) and hence an L^∞ bound for $y = \log n$, which shows that n is positive. Letting the parameter of the time discretization tend to zero, we conclude the nonnegativity of n.

We notice that, interestingly, the new entropy E_2 is connected with the monotonicity property of $\sqrt{n} \mapsto -(n(\log n)_{xx})_{xx}/(2\sqrt{n})$ since the proof of this property also relies on the estimate (1.3.5) (see Lemma 2.3 in [**54**] and (4.1.7) below).

The physical (relative) entropy

$$E_3(t) = \int_0^1 \left(n \log \frac{n}{n_\infty} - n + n_\infty \right) dx$$

is still another Lyapunov functional. It is used in the proof of the long-time behavior of solutions, which is our final main result:

$$\|n(\cdot, t) - n_\infty\|_{L^1(0,1)} \leq ce^{-\lambda t}, \quad t > 0,$$

where c, $\lambda > 0$ are constants only depending on the boundary and initial data. In order to prove this result, we take formally the time derivative of the relative entropy E_3. It can be shown (see Section 4.3 for details) that the assumption $(\log n_\infty)_{xx} \leq 0$ allows to derive

$$\frac{dE_3}{dt} + P \leq 0,$$

where $P \geq 0$ denotes the entropy production term involving second derivatives of n. This term can be estimated similarly as in [**56**] in terms of the entropy yielding

$$\frac{dE_3}{dt} + 2\lambda E_3 \leq 0,$$

for some $\lambda > 0$. Gronwall's inequality implies the exponential convergence in terms of the relative entropy. A Csiszar-Kullback-type inequality then gives the assertion. The assumption on the concavity of $\log n_\infty$ can be slightly relaxed (see Remark 4.15).

Chapter 2

Semidiscretization and long-time asymptotics of nonlinear diffusion equations

In this chapter we deal with long-time asymptotics of nonlinear second-order diffusion equations of the form

$$\begin{aligned} \frac{\partial n}{\partial t} + \mathrm{div} J &= 0, \quad J = -\nabla f(n) - n\nabla V, \quad x \in \Omega, t > 0, \\ n(\cdot, t) &= n_I(\cdot), \end{aligned}$$

where Ω is either a smooth bounded domain or $\Omega = \mathbb{R}^d$ and $V(x)$ is a confining potential.

In section 2.1 we prove the well-posedness of a semidiscretization in time of the above equations with a diffusion term $f(n)$ of degenerate type in a bounded domain, based on the implicit Euler scheme. Moreover it will be shown that this numerical scheme preserves the non-increasing behaviour of the entropy and numerical examples are given, in one and more space dimension.

In section 2.2 mass transportation methods are used to obtain a bound on the expansion rate of the support of solutions in case $V \equiv 0$.

2.1 Semidiscretization of a nonlinear diffusion equation and numerical examples

We divide the time interval $(0, T]$ for some $T > 0$ in N subintervals $(t_{k-1}, t_k]$, with $k = 1, \ldots, N$, where $0 = t_0 < \cdots < t_N = T$. Define $\tau_k = t_k - t_{k-1} > 0$

and $\tau = \max\{t_k : k = 1, \dots, N\}$. We assume that $\tau \to 0$ as $N \to +\infty$. For given $k \in \{1, \dots, N\}$ and $0 \le n_{k-1} \in L^2(\Omega)$ we solve the semi-discrete problem

$$\frac{n_k - n_{k-1}}{\tau_k} = \operatorname{div}(n_k \nabla V + \nabla f(n_k)), \quad x \in \Omega \subset \mathbb{R}^d, \tag{2.1.1}$$

$$n_0 = n_I, \tag{2.1.2}$$

$$n_k \frac{\partial V}{\partial \nu} + \frac{\partial f(n_k)}{\partial \nu} = 0, \quad x \in \partial\Omega. \tag{2.1.3}$$

Under the assumptions:
(F1) $f : [0, +\infty) \to \mathbb{R}$ is continuous, strictly increasing such that $f(0) = 0$, $f'(0) = 0$ and f^{-1} Hölder function of order θ,
(F2) let $F(n) := \int_0^n f(s)\, ds$, then $(F^{-1} \circ f)(s)$ is a concave function for all $s \ge 0$,
(F3) there exists a positive constant c, not depending on n, such that $f(n) \le c(F^{-1} \circ f \circ F)(n)$ for all $n \ge 0$,
(F4) there exists a positive constant A such that $nf(n) - F(n) \le AF(n)$,
(V1) V is uniformly convex function i.e. $D^2V(x) \ge \alpha\mathrm{Id}$ and $V(x) \longrightarrow +\infty$ as $|x| \longrightarrow +\infty$,
(I1) the function n_I is nonnegative and bounded,
we show the following results

2.1 Theorem. *For each $k = 1, \dots, N$ there exists a nonnegative weak solution $n_k \in L^2(\Omega)$ with $f(n_k) \in H^1(\Omega)$ of (2.1.1)-(2.1.3) fulfilling*

$$\begin{aligned} \int_\Omega \nabla\psi \cdot \nabla f(n_k)\, dx &= -\int_\Omega n_k \nabla\psi \cdot \nabla V\, dx \\ &\quad - \frac{1}{\tau_k} \int_\Omega \psi(n_k - n_{k-1})\, dx, \end{aligned} \tag{2.1.4}$$

for all $\psi \in H^1(\Omega)$.

2.2 Theorem. *For $k = 1, \dots, N$ let n_k be a recursively defined nonnegative weak solution of (2.1.1)-(2.1.3) in the sense of Theorem 2.1. There exists a nonnegative function $n \in L^\infty(0, T, L^\infty(\Omega))$ with $f(n) \in L^2(0, T, H^1(\Omega))$ and $\partial_t u \in L^2(0, T, (H^1(\Omega))^*)$ such that $n_k \rightharpoonup n$ in $L^2(\Omega)$, $f(n_k) \rightharpoonup f(n)$ in $H^1(\Omega)$ if $\tau_k \to 0$, fulfilling*

$$\int_0^T \langle n_t, \Phi \rangle_{H^{1*}, H^1}\, dt = -\int_0^T \int_\Omega \nabla\Phi \cdot (n\nabla V + \nabla f(n))\, dxdt,$$

for all $\Phi \in C^\infty(\Omega \times [0, T])$, where $(H^1)^*$ denotes the dual space of H^1, and $n(\cdot, t) = n_I$ in the sense of $(H^1)^*$.

The proof of Theorem 2.1 is based on a Leray-Schauder fixed-point argument; the main point of the problem lies in the proof of nonnegativity for the function n_k. Maximum principles, like Stampacchia's methods, require test functions of type $(n_k - M)^+ := \max\{(n_k - M), 0\}$; in our case this method can be used only after an appropriates regularization of the function n_k. Instead of that, we solved this problem using another approach, more precisely by showing a L^1-comparison-type principle, from which the non-negativity and the L^∞-estimate for the function n_k can be directly derived. The proof of Theorem 2.2 follows from a-priori estimates and compactness results.

2.3 Remark. The assumptions (F2)-(F4) are needed for technical reasons; functions satisfying (F2)-(F4) are for example $f(n) = n^m$ and $f(n) = n^q + n^m$, m, $q > 1$.

2.1.1 A-Priori estimates

In this section we derive a priori estimates for the sequence $\{n^{(N)}\}_{N\in\mathbb{N}}$, defined as $n^{(N)}(x,t) := n_k(x)$ if $t \in (t_{k-1}, t_k]$ and $x \in \Omega$.

2.4 Lemma. (L^1-estimate, conservation of mass)
For $k = 1, \ldots, N$ let n_k be a recursively defined nonnegative weak solution of (2.1.1)-(2.1.3) in the sense of Theorem 2.1. It holds

$$\int_\Omega n_k\, dx = \int_\Omega n_I\, dx. \tag{2.1.5}$$

Proof. Take $\phi = 1$ as test function in (2.1.4). □

2.5 Lemma. *Let n_I, $\hat{n}_I$ satisfy (I1) and for $k = 1, \ldots, N$ let n_k, $\hat{n}_k$ be recursively defined nonnegative weak solutions in the sense of Theorem 2.1 of*

$$\frac{n_k - n_{k-1}}{\tau_k} = div\,(n_k \nabla V + \nabla f(n_k)), \quad n_0 = n_I \text{ in } \Omega$$
$$\frac{\hat{n}_k - \hat{n}_{k-1}}{\tau_k} = div\,(\hat{n}_k \nabla V + \nabla f(\hat{n}_k)), \quad \hat{n}_0 = \hat{n}_I \text{ in } \Omega$$

respectively, with boundary conditions (2.1.3). It holds

$$\int_\Omega (n_k - \hat{n}_k)^+ (f(n_k) - f(\hat{n}_k))^+\, dx \le \int_\Omega (n_{k-1} - \hat{n}_{k-1})^+ (f(n_k) - f(\hat{n}_k))^+\, dx. \tag{2.1.6}$$

Proof. We consider the difference of the weak formulation for n_k and $\hat{n}_k$ with test function $\psi := (f(n_k) - f(\hat{n}_k))\text{sign}^+_\delta(f(n_k) - f(\hat{n}_k))$, defined as follows

$$\text{sign}^+_\delta(s) = \begin{cases} 1 & \text{if } s \geq \delta \\ 0 & \text{if } s \leq 0 \\ \frac{e+1}{e-1}\left(\frac{2e^{s/\delta}}{e^{s/\delta}+1} - 1\right) & \text{otherwise.} \end{cases} \tag{2.1.7}$$

It is easy to see that $\text{sign}^+_\delta(s) \to \text{sign}^+(s)$ when $\delta \to 0$, where

$$\text{sign}^+(s) = \begin{cases} 1 & \text{if } s > 0 \\ 0 & \text{if } s \leq 0, \end{cases}$$

and that

$$\text{sign}^{+\prime}_\delta(s) = \frac{e+1}{(e-1)\delta}\frac{2e^{s/\delta}}{e^{2s/\delta} + 1 + 2e^{s/\delta}} \leq \frac{e+1}{2(e-1)\delta}, \tag{2.1.8}$$

if $0 \leq s \leq \delta$. Note that the test function ψ defined as above belongs to $H^1(\Omega)$, since

$$\begin{aligned} \|\psi\|_{H^1(\Omega)} &\leq \|f(n_k) - f(\hat{n}_k)\|_{L^2(\Omega)} \\ &+ \|\nabla(f(n_k) - f(\hat{n}_k))\|_{L^2(\Omega)}(1 + \delta\, \text{sign}^{+\prime}_\delta(f(n_k) - f(\hat{n}_k))) \\ &\leq c\|f(n_k) - f(\hat{n}_k)\|_{H^1(\Omega)}. \end{aligned}$$

It holds

$$\begin{aligned} &\int_\Omega (n_k - \hat{n}_k)(f(n_k) - f(\hat{n}_k))\, \text{sign}^+_\delta(f(n_k) - f(\hat{n}_k))\, dx \\ &\quad - \int_\Omega (n_{k-1} - \hat{n}_{k-1})(f(n_k) - f(\hat{n}_k))\, \text{sign}^+_\delta(f(n_k) - f(\hat{n}_k))\, dx \\ &= -\tau_k \int_\Omega (n_k - \hat{n}_k)(f(n_k) - f(\hat{n}_k))\nabla\text{sign}^+_\delta(f(n_k) - f(\hat{n}_k)) \cdot \nabla V\, dx \\ &\quad - \tau_k \int_\Omega (n_k - \hat{n}_k)\text{sign}^+_\delta(f(n_k) - f(\hat{n}_k))\nabla(f(n_k) - f(\hat{n}_k)) \cdot \nabla V\, dx \\ &\quad - \tau_k \int_\Omega \nabla\text{sign}^+_\delta(f(n_k) - f(\hat{n}_k)) \cdot \nabla(f(n_k) - f(\hat{n}_k))\, dx \\ &\quad - \tau_k \int_\Omega \text{sign}^+_\delta(f(n_k) - f(\hat{n}_k))|\nabla(f(n_k) - f(\hat{n}_k))|^2\, dx \end{aligned}$$

$$=: I_1 + I_2 + I_3 + I_4. \tag{2.1.9}$$

Assumption **(F1)** and (2.1.8) imply that

$$\begin{aligned} I_1 + I_2 &\leq c\tau_k\delta^{\theta+1} \int_\Omega (\text{sign}^+_\delta)'(f(n_k) - f(\hat{n}_k))\nabla(f(n_k) - f(\hat{n}_k)) \cdot \nabla V\, dx \\ &\quad + \tau_k\delta^\theta \int_\Omega \int_\Omega |\nabla(f(n_k) - f(\hat{n}_k)) \cdot \nabla V|\, dx \\ &\leq c\tau_k\delta^\theta \int_\Omega |\nabla(f(n_k) - f(\hat{n}_k)) \cdot \nabla V|\, dx, \end{aligned}$$

where c does not depend on δ and $I_1 + I_2 \to 0$ as $\delta \to 0$. From (2.1.9) we get

$$\begin{aligned}
&\int_\Omega (n_k - \hat{n}_k)(f(n_k) - f(\hat{n}_k)) \operatorname{sign}_\delta^+(f(n_k) - f(\hat{n}_k))\, dx \\
&\quad - \int_\Omega (n_{k-1} - \hat{n}_{k-1})(f(n_k) - f(\hat{n}_k)) \operatorname{sign}_\delta^+(f(n_k) - f(\hat{n}_k))\, dx \\
&\le c\tau_k \delta^\theta \int_\Omega |\nabla(f(n_k) - f(\hat{n}_k)) \cdot \nabla V|\, dx \\
&\quad - \tau_k \int_\Omega (\operatorname{sign}_\delta^+ + \operatorname{sign}_\delta^{+'})(f(n_k) - f(\hat{n}_k))|\nabla(f(n_k) - f(\hat{n}_k))|^2\, dx \\
&\le c\tau_k \delta^\theta \int_\Omega |\nabla(f(n_k) - f(\hat{n}_k)) \cdot \nabla V|\, dx.
\end{aligned}$$

Passing to the limit $\delta \to 0$ it follows

$$\begin{aligned}
&\int_\Omega (n_k - \hat{n}_k)(f(n_k) - f(\hat{n}_k)) \operatorname{sign}^+(f(n_k) - f(\hat{n}_k))\, dx \\
\le &\int_\Omega (n_{k-1} - \hat{n}_{k-1})(f(n_k) - f(\hat{n}_k)) \operatorname{sign}^+(f(n_k) - f(\hat{n}_k))\, dx.
\end{aligned}$$

For the assertion it is sufficiently to prove now that

$$\int_\Omega (n_{k-1} - \hat{n}_{k-1})^+ (f(n_k) - f(\hat{n}_k))^+\, dx \ge \int_\Omega (n_{k-1} - \hat{n}_{k-1})(f(n_k) - f(\hat{n}_k))^+\, dx.$$

But this is obvious in both cases $\operatorname{sign}^+(f(n_k) - f(\hat{n}_k)) = 0$ and $\operatorname{sign}^+(f(n_k) - f(\hat{n}_k)) = 1$. □

2.6 Corollary. *For $k = 1, \ldots, N$ let n_k be a recursively defined nonnegative weak solution in the sense of Theorem 2.1 of (2.1.1)-(2.1.3). There exists a constant c, depending only on the initial data n_I such that*

$$\|n_k\|_{L^\infty(\Omega)} \le c.$$

Proof. We claim that there exists a function $\bar{n} \ge n_I$, solution of

$$\bar{n}\nabla V + \nabla f(\bar{n}) = 0. \tag{2.1.10}$$

Indeed, define $h(n) := \int_1^n \frac{f'(s)}{s}\, ds$. The function $\bar{n}(x) := h^{-1}(C - V(x))$ solves (2.1.10) and we can choose C large enough such that $n_I \le \bar{n}$ in Ω. Note that $\bar{n}$ solves problem (2.1.1) with $n_0 = \bar{n}$. Using (2.1.6), it holds that

$$\int_\Omega (n_k - \bar{n})^+ (f(n_k) - f(\bar{n}))^+\, dx \le 0$$

and the corollary follows. □

2.7 Lemma. *For $k = 1, ..., N$ let n_k be a recursively defined nonnegative weak solution of (2.1.1)-(2.1.3). It holds*

$$\sum_{i=1}^{N} \tau_i \|f(n_i)\|^2_{H^1(\Omega)} \, dx \leq c(n_I, V, T).$$

Proof. We define the function $G(s) := sf(s) - F(s)$ and consider the following difference:

$$\begin{aligned}
&\int_\Omega [F(n_k) - F(n_{k-1})] \, dx = \int_\Omega \left[\int_{n_{k-1}}^{n_k} f(s) \, ds \right] \, dx \leq \int_\Omega (n_k - n_{k-1}) f(n_k) \, dx \\
&= -\tau_k \int_\Omega n_k \nabla f(n_k) \cdot \nabla V \, dx - \tau_k \int_\Omega |\nabla f(n_k)|^2 \, dx \\
&= -\tau_k \int_\Omega \nabla G(n_k) \cdot \nabla V \, dx - \tau_k \int_\Omega |\nabla f(n_k)|^2 \, dx \\
&= -\tau_k \int_\Omega \operatorname{div}(G(n_k) \nabla V) \, dx + \tau_k \int_\Omega G(n_k) \Delta V \, dx - \tau_k \int_\Omega |\nabla f(n_k)|^2 \, dx \\
&\leq \tau_k \int_\Omega G(n_k) \Delta V \, dx - \tau_k \int_\Omega |\nabla f(n_k)|^2 \, dx \\
&\leq \tau_k \|\Delta V\|_{L^\infty(\Omega)} A \int_\Omega F(n_k) \, dx - \tau_k \int_\Omega |\nabla f(n_k)|^2 \, dx,
\end{aligned}$$

using **(F4)** and the fact that $G \frac{\partial V}{\partial \nu} \geq 0$ on $\partial\Omega$ because of the convexity of V and $G(s) \geq 0$ for $s \geq 0$. This implies

$$(1 - \tau_k \|\Delta V\|_{L^\infty(\Omega)} A) \int_\Omega F(n_k) \, dx + \tau_k \int_\Omega |\nabla f(n_k)|^2 \, dx \leq \int_\Omega F(n_{k-1}) \, dx.$$

Summing up the above inequality, we obtain

$$\begin{aligned}
(1 - \tau \|\Delta V\|_{L^\infty(\Omega)} A)^k \int_\Omega F(n_k) \, dx + \sum_{i=1}^{k} \frac{\tau_i}{(1 - \tau \|\Delta V\|_{L^\infty(\Omega)} A)^{i-1}} \int_\Omega |\nabla f(n_i)|^2 \, dx& \\
\leq \int_\Omega F(n_I) \, dx&,
\end{aligned}$$

where $\tau := \max_{i=1,...,k} \tau_i$. Using the fact that $\frac{1}{(1-ax)} \leq e^{2ax}$ for ax positive and sufficiently small, it holds

$$\int_\Omega F(n_k) \, dx \leq e^{cT}, \quad \sum_{i=1}^{k} \tau_i \int_\Omega |\nabla f(n_i)|^2 \, dx \leq e^{cT}, \tag{2.1.11}$$

where c is a positive constant, depending only on $\|\Delta V\|_{L^\infty(\Omega)}$ and A.
Taking now into account assumption **(F3)**, we get

$$\int_\Omega f(n_k) \, dx \leq c \int_\Omega (F^{-1} \circ f \circ F)(n_k) \, dx \leq c \left(F^{-1} \circ f \left(\int_\Omega F(n_k) \, dx \right) \right) \leq c,$$

using **(F2)**, Jensen's inequality and the fact that f and F^{-1} are continuous functions. The Poincare inequality

$$\sum_{i=1}^{k} \tau_i \|f(n_i) - \int_\Omega f(n_i)\, dx\|^2_{H^1(\Omega)} \leq \sum_{i=1}^{k} \tau_i \|\nabla f(n_i)\|^2_{L^2(\Omega)},$$

and (2.1.11) finish the proof. □

2.1.2 Existence

2.8 Lemma. *Let $0 \leq n_{\epsilon,k-1} \in L^2(\Omega)$, $\sigma \in [0,1]$ and $0 \leq f(n_{\epsilon,k}) \in H^1(\Omega)$, $0 \leq n_{\epsilon,k} \in L^2(\Omega)$ satisfy*

$$\begin{aligned}\int_\Omega \nabla\psi \cdot \nabla f(n_{\epsilon,k})\, dx \;=\; &-\; \sigma \int_\Omega n_{\epsilon,k} \nabla\psi \cdot \nabla V\, dx \;-\; \frac{\sigma}{\tau_k} \int_\Omega \psi (n_{\epsilon,k} - n_{\epsilon,k-1})\, dx \\ &-\; \epsilon \int_\Omega \psi f(n_{\epsilon,k})\, dx,\end{aligned}$$

for all $\psi \in H^1(\Omega)$. It holds

$$\sum_{i=1}^{N} \tau_i \|f(n_{\epsilon,i})\|_{H^1(\Omega)} \leq e^{cT}, \tag{2.1.12}$$

where c depends only on the initial datum n_I.

Proof. Following the calculations as in Lemma 2.7, it is easy to show that

$$\begin{aligned}&\int_\Omega [F(n_{\epsilon,k}) - F(n_{k-1})]\, dx + \frac{\tau_k}{\sigma} \int_\Omega |\nabla f(n_{\epsilon,k})|^2\, dx + \frac{\tau_k}{\sigma}\epsilon \int_\Omega f(n_{\epsilon,k})^2\, dx \\ &\leq \tau_k \|\Delta V\|_{L^\infty(\Omega)} A \int_\Omega F(n_{\epsilon,k})\, dx,\end{aligned}$$

using assumption (F4). Therefore, summing up in k, we obtain

$$\begin{aligned}&(1 - \tau\|\Delta V\|_{L^\infty(\Omega)} A)^k \int_\Omega F(n_{\epsilon,k})\, dx \\ &+ \sum_{i=1}^{k} \tau_i \left(\int_\Omega |\nabla f(n_{\epsilon,i})|^2\, dx + \epsilon \int_\Omega f(n_{\epsilon,i})^2\, dx \right) \\ &\leq \int_\Omega F(n_I)\, dx.\end{aligned}$$

where $\tau := \min_{i=1,..,k} \tau_i$, which implies

$$\int_\Omega F(n_k)\, dx \leq e^{cT}.$$

Now, again from **(F3)**, it holds

$$\int_\Omega f(n_{\epsilon,k})\,dx \le c\int_\Omega (F^{-1}\circ f\circ F)(n_{\epsilon,k})\,dx \le c\left(F^{-1}\circ f\left(\int_\Omega F(n_{\epsilon,k})\,dx\right)\right) \le c,$$

using Jensen's inequality and the fact that f and F^{-1} are continuous functions. Finally, the Poincare inequality

$$\sum_{i=1}^k \tau_i \| f(n_{\epsilon,i}) - \int_\Omega f(n_{\epsilon,i})\,dx\|^2_{H^1(\Omega)} \le \sum_{i=1}^k \tau_i \|\nabla f(n_{\epsilon,i})\|^2_{L^2(\Omega)},$$

proves the lemma. □

Proof of Theorem 2.1. We employ the Leray-Schauder theorem. Let $k = 1,\dots,N$ be fixed and assume that $0 \le n_{k-1} \in L^2(\Omega)$. Moreover, let $w \in L^2(\Omega)$ and $\sigma \in [0,1]$ be given and consider the problem

$$\begin{aligned}\int_\Omega \nabla\psi\cdot\nabla\mathcal{F}_\epsilon\,dx \;&=\; -\sigma\int_\Omega f^{-1}(w^+)\nabla\psi\cdot\nabla V\,dx\\ &- \frac{\sigma}{\tau_k}\int_\Omega \psi(f^{-1}(w^+) - n_{k-1})\,dx - \epsilon\int_\Omega \psi\mathcal{F}_\epsilon\,dx,\end{aligned} \tag{2.1.13}$$

where $w^+ := \max(w,0)$ and $\psi \in H^1(\Omega)$.
Note that, thanks to the Hölder continuity property of f^{-1}, the second and third integral in the above equation are well-defined. Indeed, it holds, for all $w \in L^2(\Omega)$

$$\int_\Omega |f^{-1}(w^+)|^2\,dx = \int_\Omega |f^{-1}(w^+) - f^{-1}(0)|^2\,dx \le c\int_\Omega |w^+|^{2\theta}\,dx,$$

using the fact that $f^{-1}(0) = 0$.
Problem (2.1.13) has a unique solution $\mathcal{F}_\epsilon \in H^1(\Omega)$. Therefore the operator $S : L^2(\Omega)\times[0,1] \longrightarrow L^2(\Omega)$ given by $S(w,\sigma) = \mathcal{F}_\epsilon$ is well defined.
It is easy to see that S is continuous, compact and $S(w,0) = 0$ for all $w \in L^2(\Omega)$. Let $\mathcal{F}_\epsilon \in H^1(\Omega)$ be a fixed-point of S, i.e. $S(\mathcal{F}_\epsilon,\sigma) = \mathcal{F}_\epsilon$ for $\sigma \in [0,1]$. We claim that $\mathcal{F}_\epsilon \ge 0$ a.e. Indeed, taking $\psi = \mathcal{F}_\epsilon{}^- := \min(0,\mathcal{F}_\epsilon)$ as test function, we get

$$\begin{aligned}\int_\Omega |\nabla\mathcal{F}_\epsilon{}^-|^2\,dx &= -\sigma\int_\Omega f^{-1}(\mathcal{F}_\epsilon{}^+)\nabla\mathcal{F}_\epsilon{}^-\cdot\nabla V\,dx\\ -\frac{\sigma}{\tau_k}\int_\Omega \mathcal{F}_\epsilon{}^-(f^{-1}(\mathcal{F}_\epsilon{}^+) - n_{k-1})\,dx &- \epsilon\int_\Omega \mathcal{F}_\epsilon{}^-\mathcal{F}_\epsilon\,dx\\ &= \frac{\sigma}{\tau_k}\int_\Omega \mathcal{F}_\epsilon{}^- n_{k-1}\,dx - \epsilon\int_\Omega \mathcal{F}_\epsilon{}^{-2}\,dx \le 0.\end{aligned}$$

Moreover, from Lemma 2.8 we can conclude that there exists a constant $C > 0$ independent of σ such that $\|\mathcal{F}_\epsilon\|_{H^1(\Omega)} \leq C$ for all $\mathcal{F}_\epsilon$ such that $S(\mathcal{F}_\epsilon, \sigma) = \mathcal{F}_\epsilon$.
The Leray-Schauder theorem implies that the map $S(\cdot, 1)$ has at least one fixed point, denoted again by $\mathcal{F}_\epsilon$, which is nonnegative and solves

$$\begin{aligned} \int_\Omega \nabla\psi \cdot \nabla\mathcal{F}_\epsilon \, dx &= -\int_\Omega n_\epsilon \nabla\psi \cdot \nabla V \, dx \\ &- \frac{1}{\tau_k}\int_\Omega \psi(n_\epsilon - n_{k-1}) \, dx - \epsilon \int_\Omega \psi\mathcal{F}_\epsilon \, dx, \end{aligned} \tag{2.1.14}$$

for all $\psi \in H^1(\Omega)$, with $n_\epsilon := f^{-1}(\mathcal{F}_\epsilon(x))$.
The set of functions $\{\mathcal{F}_\epsilon\}$ fulfills inequality (2.1.12). Therefore there exists a subsequence, denoted again with $\{\mathcal{F}_\epsilon\}$, weakly convergent in $H^1(\Omega)$ to $\mathcal{F}$ when $\epsilon \to 0$. Moreover, from inequality (2.1.12), using again the Hölder-continuity property of f^{-1}, it holds

$$\int_\Omega |n_\epsilon|^2 \, dx \leq c \int_\Omega |\mathcal{F}_\epsilon|^{2\theta} \, dx \leq c\left(1 + \int_\Omega |\mathcal{F}_\epsilon|^2 \, dx\right) \leq c,$$

where $n_\epsilon(x) := f^{-1}(\mathcal{F}_\epsilon(x))$. This implies the existence of a subsequence, denoted again by n_ϵ such that $n_\epsilon \rightharpoonup n$ weakly in $L^2(\Omega)$ when $\epsilon \to 0$. Passing to the limit $\epsilon \to 0$ in (2.1.14) it is easy to see that $\mathcal{F}$ and n satisfy the problem

$$\begin{aligned} \int_\Omega \nabla\psi \cdot \nabla\mathcal{F} \, dx &= -\int_\Omega n \nabla\psi \cdot \nabla V \, dx \\ &- \frac{1}{\tau_k}\int_\Omega \psi(n - n_{k-1}) \, dx - \epsilon \int_\Omega \psi\mathcal{F} \, dx. \end{aligned}$$

It remains to prove that $\mathcal{F} = f(n)$. From the compact embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$ it follows that $\mathcal{F}_\epsilon(x) \to \mathcal{F}$ in $L^2(\Omega)$ and a.e.. Using the continuity property of f^{-1}, it holds $n_\epsilon = f^{-1}(\mathcal{F}_\epsilon) \to f^{-1}(\mathcal{F})$ a.e., which means $n = f^{-1}(\mathcal{F})$. This implies that n and $f(n)$ satisfy (2.1.4). □

Let $n^{(N)}$ be defined by $n^{(N)}(x,t) := n_k(x)$ if $t \in (t_{k-1}, t_k]$, $x \in \Omega$ and σ_N be the shift operator defined as $(\sigma_N(n^{(N)}))(\cdot, t) := n_{k-1}$ for $t \in (t_{k-1}, t_k]$.

Proof of Theorem 2.2. From Corollary 2.6 and Lemma 2.7 it immediately follows that the sequence $(n^{(N)})_{N\in\mathbb{N}}$ and $(f(n^{(N)}))_{N\in\mathbb{N}}$ are bounded in $L^\infty(0,T;L^\infty(\Omega))$ and $L^2(0,T;H^1(\Omega))$ respectively. Thus there exist subsequences, again denoted by $(n^{(N)})$ and $(f(n^{(N)}))$ such that for $N \to +\infty$

$$n^{(N)} \rightharpoonup n \quad \text{weakly in } L^p(0,T;L^p(\Omega)) \quad \forall\, 1 < p < +\infty, \tag{2.1.15}$$

$$f(n^{(N)}) \rightharpoonup \bar{f} \quad \text{weakly in } L^2(0,T;H^1(\Omega)). \tag{2.1.16}$$

From (2.1.1) it holds

$$\begin{aligned} &\frac{1}{\tau}\|n^{(N)} - \sigma_N(n^{(N)})\|_{L^2(0,T;(H^1(\Omega))^*)} \\ &= \| \sup_{\|v\|_{H^1(\Omega)}=1} \langle \mathrm{div}(n^{(N)}\nabla V + \nabla f(n^{(N)})), v\rangle_{H^{1*},H^1} \|_{L^2(0,T)} \\ &\leq \| \sup_{\|v\|_{H^1(\Omega)}=1} \left[- \int_\Omega (n^{(N)}\nabla V \cdot \nabla v + \nabla v \cdot \nabla f(n^{(N)}))\, dx \right] \|_{L^2(0,T)} \leq C, \end{aligned}$$

using (2.1.3), which implies for $N \to +\infty$ (maybe for a subsequence)

$$\frac{1}{\tau}(n^{(N)} - \sigma_N(n^{(N)})) \rightharpoonup n_t \text{ weakly in } L^2(0,T,(H^1(\Omega))^*). \tag{2.1.17}$$

Note that Corollary 2.6 and Lemma 2.7 imply also that $(n^{(N)})_{N\in\mathbb{N}}$ is uniformly bounded in $L^2(0,T;W_p^s(\Omega))$ with $0 < s < 1$, $p \geq 2$ (see [**29**]).
It holds $W_p^s(\Omega) \hookrightarrow W_p^{s'}(\Omega) \hookrightarrow L^2(\Omega) \hookrightarrow (H^1(\Omega))^*$, $s' < s$, with compact injection from $W_p^s(\Omega)$ into $W_p^{s'}(\Omega)$. From Aubin's lemma it follows

$$n^{(N)} \to n \quad \text{strongly in } L^2(0,T;W_p^{s'}(\Omega)) \quad \text{for } N \to +\infty,$$

and maybe for a subsequence

$$n^{(N)} \to n \quad \text{a.e.} \quad \text{for } N \to +\infty. \tag{2.1.18}$$

The above convergence and the continuity assumption on f imply $f(n) = \bar{f}$.
Finally, from Corollary 2.6 we can conclude that $n \in L^\infty(0,T;L^\infty(\Omega))$.
The convergence results (2.1.15), (2.1.16) and (2.1.17) allow now to pass to the limit $N \to +\infty$ in the weak formulation of (2.1.1) to obtain a weak solution n and $f(n)$ of

$$n_t = \mathrm{div}(n\nabla V + \nabla f(n)), \quad \text{in } \Omega, \quad t > 0,$$

such that $n(\cdot,0) = n_I$ in the sense of $(H^1(\Omega))^*$. □

2.1.3 Numerical examples

The basic property of the numerical scheme (2.1.1)-(2.1.3) presented in the previous section is the decay of the relative entropy

$$E(n_k|n_\infty) := \int_\Omega [\phi(n) - \phi(n_\infty) - \phi'(n_\infty)(n - n_\infty)]\, dx, \tag{2.1.19}$$

where ϕ is a strictly convex function solving the problem

$$\phi''(n) = \frac{f'(n)}{n}, \quad \phi'(1) = 0, \quad \phi(0) = 0, \tag{2.1.20}$$

and $n_\infty := h^{-1}(C - V(x))$ the steady-state, where C is such that $\int_\Omega n_\infty \, dx = \int_\Omega n_I \, dx$.
Let us also remember that for general nonlinear Fokker-Planck equations the entropy

$$E(n_k) := \int_\Omega [n_k V(x) + \phi(n_k)] \, dx, \tag{2.1.21}$$

and the relative entropy (2.1.19) satisfy

$$E(n_k) - E(n_\infty) \geq E(n_k|n_\infty),$$

being equal if and only if n_∞ is positive everywhere (see [**25**, Proposition 5]). Moreover the difference can be explicitly written as

$$E(n_k) - E(n_\infty) - E(n_k|n_\infty) = \int_\Omega [V(x) + \phi'(n_\infty(x))](n_k - n_\infty)) \, dx. \tag{2.1.22}$$

2.9 Lemma. *For $k = 1, \ldots, N$ let n_k be a recursively defined nonnegative weak solution in the sense of Theorem 2.1 of (2.1.1)-(2.1.3). Assuming that*

$$\int_\Omega n_I |\nabla V + \nabla \phi'(n_I)|^2 \, dx < +\infty, \tag{2.1.23}$$

it holds

$$E(n_k) - E(n_\infty) \leq (E(n_I) - E(n_\infty))(1 + 2\alpha\Delta t)^{-k}, \quad k \in \mathbb{N}.$$

Proof. Here we give a formal proof of this lemma, based on the generalized Log-Sobolev inequality (see [**25**, Theorem 17]). Let

$$D(n_k) := \int_\Omega n_k |\nabla V + \nabla \phi'(n_k)|^2 \, dx,$$

be the entropy production for the functional $E(n_k|n_\infty)$ defined in (2.1.19). Then the generalized Log-Sobolev inequality asserts that

$$E(n_k|n_\infty) \leq E(n_k) - E(n_\infty) \leq \frac{1}{2\alpha} D(n_k) \quad \forall \, k \in \mathbb{N}, \tag{2.1.24}$$

using the uniform convexity of the potential V **(V1)**. From the convexity of ϕ, it follows

$$\begin{aligned}
E(n_k|n_\infty) &\geq \int_\Omega \phi'(n_{k+1})(n_k - n_{k+1}) + \phi(n_{k+1}) - \phi(n_\infty) - \phi'(n_\infty)(n_k - n_\infty) \, dx \\
&= \int_\Omega \phi(n_{k+1}) - \phi(n_\infty) - \phi'(n_\infty)(n_{k+1} - n_\infty) + \\
&\quad + \int_\Omega \phi'(n_\infty)(n_{k+1} - n_k) + \phi'(n_{k+1})(n_k - n_{k+1}) \, dx \\
&= E(n_{k+1}|n_\infty) + \int_\Omega [\phi'(n_\infty) - \phi'(n_{k+1})](n_{k+1} - n_k)) \, dx.
\end{aligned}$$

Now, using (2.1.22) we get

$$
\begin{aligned}
E(n_k) - E(n_\infty) &\geq E(n_{k+1}|n_\infty) + \int_\Omega [\phi'(n_\infty) - \phi'(n_{k+1})](n_{k+1} - n_k))\, dx \\
&\quad + \int_\Omega [V(x) + \phi'(n_\infty(x))](n_k - n_\infty))\, dx \\
&= E(n_{k+1}|n_\infty) - \int_\Omega [V(x) + \phi'(n_{k+1})](n_{k+1} - n_k))\, dx \\
&\quad + \int_\Omega [V(x) + \phi'(n_\infty(x))](n_k - n_\infty))\, dx + \int_\Omega \phi'(n_\infty)(n_{k+1} - n_k))\, dx \\
&\quad + \int_\Omega V(x)(n_{k+1} - n_k))\, dx \\
&= E(n_{k+1}|n_\infty) + \int_\Omega [V(x) + \phi'(n_\infty(x))](n_{k+1} - n_\infty))\, dx \\
&\quad - \int_\Omega [V(x) + \phi'(n_{k+1})](n_{k+1} - n_k))\, dx \\
&= E(n_{k+1}) - E(n_\infty) - \int_\Omega [V(x) + \phi'(n_{k+1})](n_{k+1} - n_k))\, dx.
\end{aligned}
$$

Therefore, from equation (2.1.1) and integrating by parts, we deduce

$$
\int_\Omega [V(x) + \phi'(n_{k+1})](n_{k+1} - n_k))\, dx = -\Delta t \int_\Omega n_{k+1} |\nabla V + \nabla \phi'(n_{k+1})|^2\, dx,
$$

and thus,

$$
E(n_k) - E(n_\infty) \geq E(n_{k+1}) - E(n_\infty) + \Delta t\, D(n_{k+1}).
$$

From inequality (2.1.24) it holds

$$
E(n_k) - E(n_\infty) \geq (1 + 2\alpha\Delta t)\,(E(n_{k+1}) - E(n_\infty)),
$$

and the theorem follows now recursively. □

We point out that the previous lemma was already observed in the linear case in [**10**] with a proof simplified by the fact $V(x) + \phi'(n_\infty(x)) = C$ for all $x \in \mathbb{R}^N$ for linear diffusions. It is the discrete version of the exponential decay with rate 2α in the continuous case obtained in [**25, 27**]. The rigorous proof of this lemma is done by approximations of the nonlinear function in the same spirit as in [**25**].

In the case of general nonlinear diffusion equations we have also a decay estimate for the corresponding entropy.

2.10 Corollary. *For $k = 1, \ldots, N$ let n_k be a recursively defined nonnegative weak solution in the sense of Theorem 2.1 of (2.1.1)-(2.1.3) with $V \equiv 0$,*

$f(n) = n^m$ and

$$\mathcal{E}(k) := \int_\Omega \phi(n_k(x))\, dx. \tag{2.1.25}$$

For all $k \in \mathbb{N}$ it holds

$$\mathcal{E}(k) \geq \mathcal{E}(k+1).$$

Let us show some numerical results related to problem (2.1.1) in the case $f(n) := n^m$ for some $m > 1$.

The porous medium equation.

We introduce the fully discretization of equation (2.1.1) with $V \equiv 0$ in a uniform grid using central finite differences in space to obtain:

$$\frac{n_k(i) - n_{k-1}(i)}{\Delta t} = D^+D^-(f(n_k(i))), \quad k \in \mathbb{N}, \quad i = 1, \ldots, M,$$

where D^+ and D^- are the standard forward and backward first order finite difference operators, defined for any discretized function $(z(i))_{i=1,\ldots,M}$ as follows

$$D^+z(i) := \frac{z(i+1) - z(i)}{\Delta x}, \quad i = 1, \ldots, M-1,$$
$$D^-z(i) := \frac{z(i) - z(i-1)}{\Delta x}, \quad i = 2, \ldots, M.$$

The resulting nonlinear system of equations is iteratively solved by Newton's method at each time step. Time stepping is set to constant.
Figure 2.1 shows numerical results for $f(n) := n^2$ with initial data

$$n_I(x) = \begin{cases} \frac{2[(4-x^2)-3.9\cos\left(\frac{\pi}{4}x\right)]}{\|2[(4-x^2)-3.9\cos\left(\frac{\pi}{4}x\right)]\|_{L^1(-2,2)}} & \text{if } -2 \leq x \leq 2, \\ 0 & \text{otherwise.} \end{cases} \tag{2.1.26}$$

Let us point out that the expected Barenblatt asymptotic profile

$$B(|x|, t) = t^{-\frac{d}{\lambda}} \left(C - \frac{(m-1)}{2m\lambda} |x|^2 t^{-\frac{2}{\lambda}} \right)_+^{\frac{1}{m-1}}, \tag{2.1.27}$$

is fixed by mass conservation

$$\int_{\mathbb{R}} B(|x|, t)\, dx = \int_{\mathbb{R}} n_I(x)\, dx.$$

(a) (b)

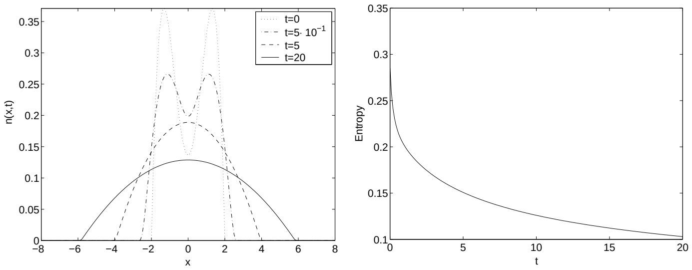


Figure 2.1: *Numerical results and entropy decay for (2.1.1) in case* $f(n) = n^2$ *and* $V \equiv 0$ *with initial condition (2.1.26) (a) Time evolution of* $n(x, t)$*, (b) Entropy evolution* $\mathcal{E}(t)$*.*

The results show the convergence to the selfsimilar profile given by the Barenblatt profile (2.1.27), where $\lambda := d(m-1)+2$ and $m = 2$ in this case, as $t \to \infty$ and the decreasing character of the entropy. Note that in this case the decay rate of the entropy is not exponential but rather algebraic. In fact, for the porous medium equation the entropy becomes the L^m of the solution that decays like $\frac{m-1}{m}\lambda$ due to the L^1-L^∞ effect [**11**] which asserts

$$\|n(\cdot, t)\|_{L^\infty(\mathbb{R}^d)} \leq C\, t^{-\frac{d}{d(m-1)+2}} \|n_I\|_{L^1(\mathbb{R}^d)}.$$

In figure 2.2 the numerical approximations of the two dimensional porous medium equation with $f(n) = n^3$ together with the entropy decay are plotted.

Nonlinear Fokker-Planck equation

This part of the work is devoted to the investigation of problem (2.1.1) in case $f(n) := n^m$, $m > 1$ and $V(x) := \frac{1}{2}x^2$. It is well known that a standard central finite differences fully discretized implicit Euler scheme for (2.1.1) does not give nice results. This is due to the fact that if $|V_x|$ assumes large values where the function n is small, the drift term nV_x becomes predominant with respect to the diffusion term $f(n)_{xx}$ will cause undesired oscillations and large negative values in the solution (see figure 2.3).

Therefore we follow the same scheme as in [**48**], used for a numerical approximation of the one dimensional transient drift-diffusion model for a bipolar semiconductor.

We recall briefly the most important steps. For the space discretization, we make use of a mixed exponential fitting method. The main idea con-

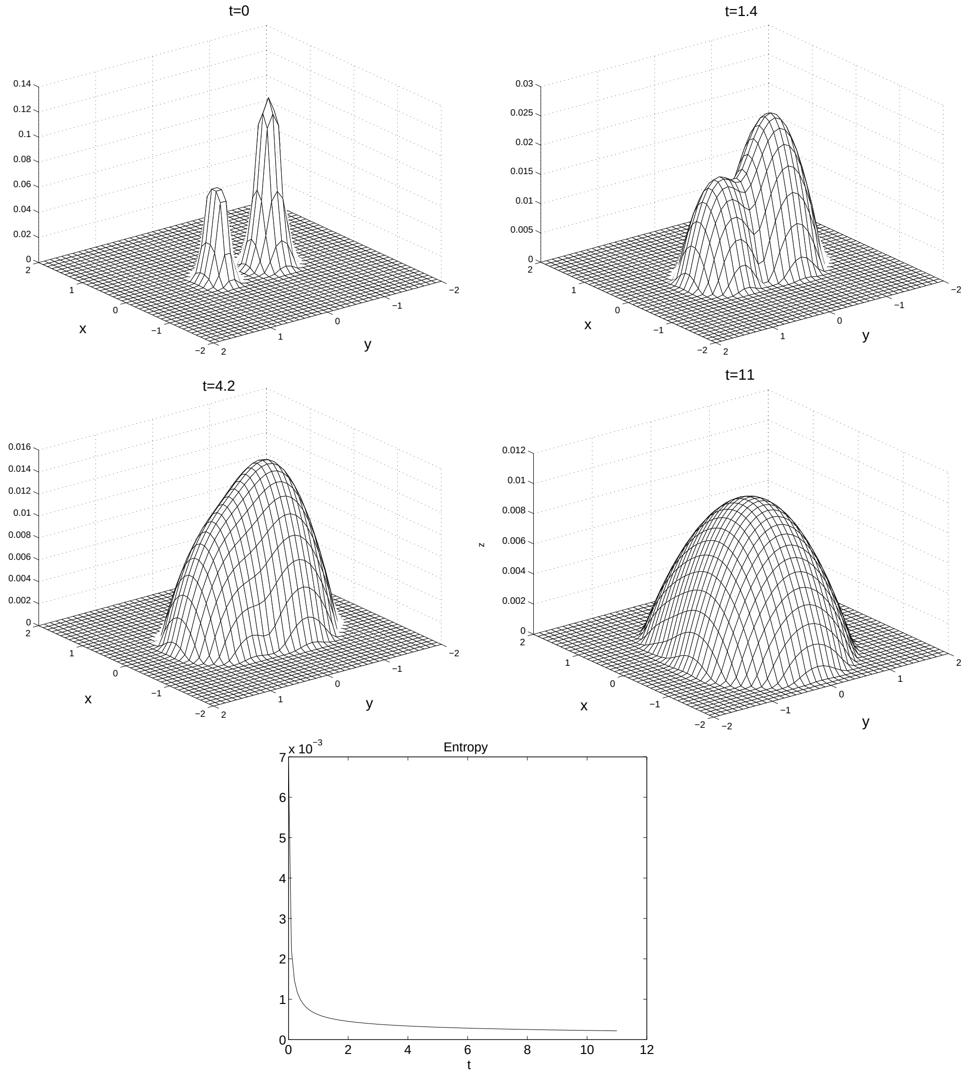


Figure 2.2: *Time evolution and Entropy decay of the 2D nonlinear diffusion equation (2.1.1) with $f(n) = n^3$ and $V \equiv 0$.*

sists to linearize at each time step the current of the equation assuming $f'(n(x,t_k)) \sim f'_k(x)$ is already known and rewrite the current term $J(x,t) := -(n(x,t)V_x(x) + f'_k(x)n_x(x,t))$ into an equation for the new variable $z := ne^{-V}$ in each spatial cell.

Let $x_i = i\Delta x$, where $i = 1, \ldots, M$ and $\Delta x > 0$, $I_i := (x_{i-1}, x_i]$ and $J_k(i)$, $n_k(i)$ and $V(i)$ be denote the approximative term on x_i at time $t_k := k\Delta t$. The method can be summarized in two main steps: (1) approximation of the diffusion term , (2) change of variable.

It makes physically sense to expect that, if the current density $\tilde{J}_k$ in the

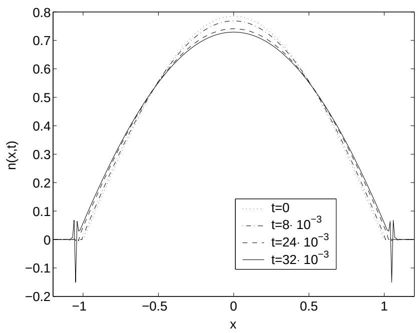


Figure 2.3: *Numerical results of (2.1.1) with central finite differences.*

interval I_i is positive, the flow is moving to the right direction and then the density valuated at the left $n_k(i-1)$ can be taken for the approximation of the coefficient of the diffusion term. More precisely

$$f'_k(i) := \begin{cases} f'(n_k(i-1)) & \text{if } \tilde{J}_k(i) > 0, \\ f'(n_k(i)) & \text{if } \tilde{J}_k(i) \le 0, \end{cases} \tag{2.1.28}$$

where we need an approximated value of the current $\tilde{J}_k(i)$ in I_i, for this, we take

$$\tilde{J}_k(i) := \begin{cases} 0 & \text{if} \quad n_k(i) = n_k(i-1) = 0, \\ \frac{-1}{\Delta x}\left[(\phi'(n_k(i)) - \phi'(n_k(i-1))) + (V(i) - V(i-1))\right] & \text{else.} \end{cases}$$

We define now a new variable

$$z_k := n_k \exp(V/f'_k(i)) \quad \text{in} \quad I_i.$$

Then the expression of the current on the interval I_i becomes

$$J_k \simeq -(f'_k(i)\exp(-V/f'_k(i))z_{k,x}))$$

and equation (2.1.1) can be rewritten as

$$\frac{1}{f'_k(i)}\exp(V/f'_k(i))J_k + z_{k,x} = 0 \quad \text{in} \quad I_i,$$
$$(J_k)_x = -\frac{1}{\Delta t}(n_{k+1} - n_k) \quad \text{in} \quad I_i.$$

We approximate now J_k and z_k as follows

$$J_k \in X_1 := \{\omega \in L^2(\Omega) \mid \omega(x) = a_i x + b_i,\ x \in I_i,\ i = 1, \dots, M\},$$
$$z_k \in X_0 := \{\xi \in L^2(\Omega) \mid \xi \text{ const. in } I_i,\ i = 1, \dots, M\},$$

and taking $\omega \in X_1$ and $\xi \in X_0$ as test functions for the above equations, the discrete system becomes

$$\sum_{i=1}^{M}\left(\int_{I_i}\frac{1}{f'_k(i)}\exp(V/f'_k(i))J_k\omega\,dx - \int_{I_i} z_k\omega_x\,dx + [u_k\exp(V/f'_k(i))\omega]_{x_{i-1}}^{x_i}\right) = 0,$$

$$\sum_{i=1}^{M}\left(\int_{I_i}(J_k)_x\xi \; + \int_{I_i}\frac{1}{\Delta t}(n_{k+1}-n_k)\xi\right) = 0.$$

We have now to approximate the last integrals. We choose $\xi = 1$ in I_i and $\xi = 0$ elsewhere as test function, getting in this way

$$J_k(i) - J_k(i-1) = -\frac{1}{\Delta t}\int_{I_i}(n_{k+1}-n_k).$$

The last integral is approximated as follows

$$\int_{I_i}(n_{k+1}-n_k) = \Delta x(n_{k+1}(i-1) - n_k(i-1)).$$

It remains to compute J_k; first we approximate $J_k(x) = J_k(i)$ if $x \in I_i$, then taking $\omega = 1$ in I_i and $\omega = 0$ elsewhere as test function, it holds

$$\int_{I_i}\frac{1}{f'_k(i)}\exp(V/f'_k(i))J_k(i)\,dx = -[n_k\exp(V/f'_k(i))]_{x_{i-1}}^{x_i},$$

which implies

$$\begin{aligned} J_k(i) = \;& -\left(\frac{V(i)-V(i-1)}{2}\coth\frac{V(i)-V(i-1)}{2f'_k(i)}\right)\frac{n_k(i)-n_k(i-1)}{\Delta x} \\ & - \frac{n_k(i)+n_k(i-1)}{2}\,\frac{V(i)-V(i-1)}{\Delta x}. \end{aligned}$$

This approximation for the flux is used in combination with an explicit Euler method

$$\frac{n_{k+1}(i)-n_k(i)}{\Delta t} = -\frac{1}{\Delta x}(J_k(i+1)-J_k(i)).$$

Since the approximation for the flux is conservative, it is clear that the L^1 norm of the solution will be preserved at the fully discrete level.
Figure 2.4 shows the evolution in time of (2.1.1) with $f(n) = n^2$. In this case the stationary-state of the problem with initial data

$$n_I(x) = \begin{cases} \frac{\pi}{4}\cos\left(\frac{\pi}{2}x\right) & \text{if } -1 \le x \le 1, \\ 0 & \text{otherwise,} \end{cases} \tag{2.1.29}$$

can be explicitly computed and given by

$$n_\infty(x) = \left(\frac{9^{1/3}}{4} - \frac{1}{4}x^2\right)_+^2. \tag{2.1.30}$$

Figure 2.4(b) shows that the relative entropy, defined as in (2.1.21), decays exponentially fast with rate -2.

(a) (b)

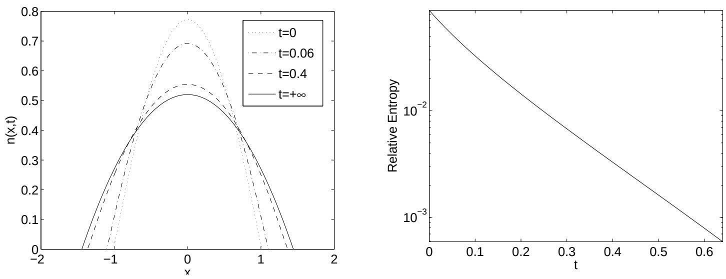


Figure 2.4: *Numerical results and entropy decay for (2.1.1) with initial condition (2.1.29) in the case $f(n) = n^2$: (a) Time evolution of $n(x,t)$, (b) Logarithmic plot of $E(n) - E(n_\infty)$.*

The numerical solution of (2.1.1) with initial condition

$$n_I(x) = \begin{cases} -\frac{13}{3}x^2 + \frac{5}{3}x & \text{if } -0.8 \le x \le -0.5, \\ -10x^2 - 14x - 4.8 & \text{if } -0.1 \le x \le 0.5, \\ 0 & \text{otherwise,} \end{cases} \tag{2.1.31}$$

in the case $f(n) = n^3$ is showed in figure 2.5. In this case the stationary solution is not explicit computed, but the convergence in time to a Barenblatt-type function is clear from the subplot 2.5(a). The relative entropy $E(n) - E(n_\infty)$ decreases numerically with constant rate -2 after a time interval, in which the decay is faster (figure 2.5(b)).

2.2 Evolution of the 1-D Wasserstein distances

We consider the problem

$$n_t = (n^m)_{xx}, \quad x \in \mathbb{R}, \quad t > 0, \quad m > 1, \tag{2.2.1}$$

$$n(x,0) = n_I(x), \quad x \in \mathbb{R}, \tag{2.2.2}$$

(a) (b)

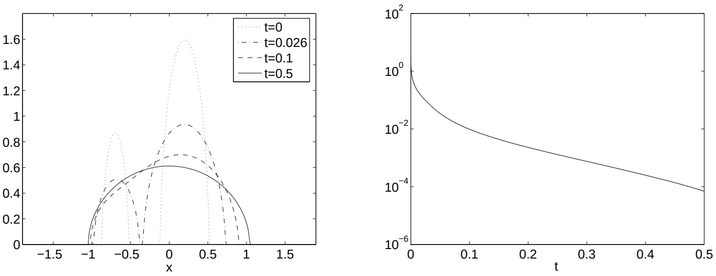


Figure 2.5: *Numerical results and entropy decay for (2.1.1) with initial condition (2.1.31) in the case $f(n) = n^3$: (a) Time Evolution of $n(x,t)$, (b) Logarithmic plot of $E(n) - E(n_\infty)$.*

where $n_I \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$, $\|n_I\|_{L^1(\mathbb{R})} = 1$, $n_I \geq 0$ and n_I is compactly supported.

Much is already known for problem (2.2.1), (2.2.2): see [**27, 57, 76, 74, 75**] and the references therein for existence, uniqueness and asymptotic behaviour results of the porous media equation. It also known that the degeneracy at level $n = 0$ of the diffusivity $D(n) = mn^{m-1}$ causes the phenomenon called *finite speed of propagation*. This means that the support of the solution $n(\cdot, t)$ to (2.2.1), (2.2.2) is a bounded set for all $t \geq 0$. In fact it can be proved that the solution $n(x,t)$ as $t \to +\infty$ converges to the Barenblatt *source-type* solution $B(|x|, t, C)$ with the same mass as the initial data.

In this paper we want to give a simple proof of the *finite propagation* property using mass transportation techniques. Precisely, we prove that the difference of support of two solutions of (2.2.1), (2.2.2) with different compactly supported initial conditions is a bounded in time function of a suitable Monge-Kantorovich related metric.

2.11 Theorem. *Let $n_1(x,t)$ and $n_2(x,t)$ be strong solutions of (2.2.1)-(2.2.2) with initial conditions $n_{I1}(x)$ and $n_{I2}(x)$ respectively, where $n_{Ii} \in L^1(\mathbb{R}) \cap L^\infty(\mathbb{R})$, $\|n_{Ii}\|_{L^1(\mathbb{R})} = 1$, $n_{Ii} \geq 0$ and n_{Ii} is compactly supported, $i = 1, 2$, and let $\Omega_i(t) = \{x \in \mathbb{R} / n_i(x,t) > 0\}$, $\quad i = 1, 2$.*
Let $\xi_i(t) = \inf[\Omega_i(t)]$, $\Xi_i(t) = \sup[\Omega_i(t)]$, for $t \geq 0$, $i = 1, 2$. Then

$$\max\{|\xi_1(t) - \xi_2(t)|, |\Xi_1(t) - \Xi_2(t)|\} \leq W_\infty(n_{I1}, n_{I2}), \quad \forall t \in [0, +\infty),$$

where $W_\infty(n_{I1}, n_{I2})$ is a constant, which depends only on the initial data n_{I1}, n_{I2} and is defined in (2.2.14).

The finite speed of propagation property follows by just taking as one of the solutions a time translation of the explicit Barenblatt solution which is known to have compact support expanding at the rate $t^{1/(m+1)}$.

Proof. Consider a sequence of functions $n_k \in C^\infty([0,+\infty)\times\mathbb{R})$, which are strong solutions (see [**75**]) of the problems P_k

$$n_t = (n^m)_{xx}, \quad x\in\mathbb{R}, \quad t>0, \quad m>1, \tag{2.2.3}$$

$$n(x,0) = n_{Ik}(x), \quad x\in\mathbb{R}, \tag{2.2.4}$$

where $n_{Ik}(x)$, $k\in\mathbb{N}$, is a sequence of bounded, integrable and strictly positive C^∞-smooth functions such that all their derivatives are bounded in $\mathbb{R}$, the condition $(m-1)(n_{Ik}^m)_{xx} \geq -a n_{Ik}$ holds for some constant $a>0$, and $n_{Ik}\to n_I$ in $L^1(\mathbb{R})$ if $k\to+\infty$. We may always do it in such a way that $\|n_{Ik}\|_{L^1(\mathbb{R})} = \|n_I\|_{L^1(\mathbb{R})}$ and $\|n_{Ik}\|_{L^\infty(\mathbb{R})} \leq \|n_I\|_{L^\infty(\mathbb{R})}$. From the L^1-contraction property it follows that $n_k \to n$ in $C([0,+\infty):L^1(\mathbb{R}))$ if $k\to+\infty$, where n is a strong solution of (2.2.1)-(2.2.2) (see [**75**], chapt. III).

This sequence of regularized solutions can be further approximated by a sequence of initial boundary value problems. We introduce a cutoff sequence $\theta_l \in C^\infty(\mathbb{R})$, $1<l\in\mathbb{N}$, with the following properties:

$$\theta_l(x) = 1 \quad \text{for} \quad |x| < l-1,$$

$$\theta_l(x) = 0 \quad \text{for} \quad |x|\geq l, \quad 0<\theta_l<1 \quad \text{for} \quad l-1<|x|<l.$$

The initial boundary value problem P_{kl}

$$n_t = (n^m)_{xx}, \quad x\in(-l,l), \quad t>0, \tag{2.2.5}$$

$$n(x,0) = n_{Ikl}(x) := \frac{n_{Ik}(x)\theta_l(x)}{\|n_{Ik}(x)\theta_l(x)\|_{L^1}}, \tag{2.2.6}$$

$$n(x,t) = 0 \quad \text{for} \quad |x| = l, \quad t\geq 0, \tag{2.2.7}$$

is mass preserving and has a unique solution $n_{kl}(x,t) \in C^\infty((0,+\infty)\times[-l,l]) \cap C([0,+\infty)\times[-l,l])$, strictly positive for $x\in(-l,l)$ and zero at the boundary (see [**75**], prop.6, chapt.II). Because $n_{Ikl} \longrightarrow n_{Ik}$ as $l\longrightarrow+\infty$, for all $k\in\mathbb{N}$, $n_{kl}\to n_k$ in $C([0,+\infty):L^1(\mathbb{R}))$ if $l\to+\infty$, where n_k is solution of the problem P_k.

Thanks to estimates independent of l for the moments of the solutions of the P_{kl} problems and passing to the limit in the corresponding inequalities, it can be easily shown that the solution $n_k(x,t)$ of (2.2.3)-(2.2.4) enjoys an important property. It holds

$$\int_{\mathbb{R}} |x|^p n_k(x,t)dx < +\infty, \quad \forall t\geq 0, \quad \forall p\in[1,+\infty). \tag{2.2.8}$$

We shall denote by $\mathbb{P}_p(\mathbb{R})$, with $p\in[1,+\infty)$, the set of all probability measures on $\mathbb{R}$ with finite moments of order p. Let $\Pi(\mu,\nu)$ be the set of all probability measures on $\mathbb{R}^2$ having μ, $\nu\in\mathbb{P}_p(\mathbb{R})$ as marginal distributions (see [**77**]). The Wasserstein p-distance between two probability measures $\mu, \nu \in \mathbb{P}_p(\mathbb{R})$ is defined as

$$(2.2.9)\quad W_p(\mu,\nu)^p := \inf_{\pi\in\Pi(\nu,\mu)} \int_{\mathbb{R}^2} |x-y|^p d\pi(x,y), \quad \forall p \in [1,+\infty).$$

W_p defines a metric on $\mathbb{P}_p(\mathbb{R})$ (see [**77**]). Bound (2.2.8) then shows that the Wasserstein p-distance between any two solutions which is initially finite, remains finite at any subsequent time.

Any probability measure μ on the real line can be described in terms of its *cumulative distribution function* $F(x) = \mu((-\infty, x])$ which is a right-continuous and non-decreasing function with $F(-\infty) = 0$ and $F(+\infty) = 1$. Then, the *generalized inverse* of F defined by $F^{-1}(\eta) = \inf\{x \in \mathbb{R}/F(x) > \eta\}$ is also a right-continuous and non-decreasing function on $[0,1]$.

Let $\mu,\ \nu \in \mathbb{P}_p(\mathbb{R})$ be probability measures and let $F(x)$, $G(x)$ be the respective distribution functions. On the real line (see [**77**]), the value of the Wasserstein p-distance $W_p(\mu,\nu)$ can be explicitly written in terms of the generalized inverse of the distribution functions,

$$(2.2.10)\quad W_p(\mu,\nu)^p = \int_0^1 |F^{-1}(\eta) - G^{-1}(\eta)|^p d\eta, \quad \forall p \in [1,+\infty).$$

Let $n_1(x,t)$, $n_2(x,t)$ be strong solutions of (2.2.1), (2.2.2) corresponding to initial conditions $n_{I1}(x)$ and $n_{I2}(x)$ respectively. We denote by $n_{1k}(x,t)$ and $n_{2k}(x,t)$ the strong solutions of (2.2.3), (2.2.4) with initial conditions $n_{I1k}(x)$ and $n_{I2k}(x)$ respectively, where $n_{Iik} \longrightarrow n_{Ii}$ in $L^1(\mathbb{R})$ for $i = 1,2$. Analogously, we consider the solutions $n_{1kl}(x,t)$ and $n_{2kl}(x,t)$ of the problems P_{kl} converging towards $n_{ik}(x,t)$ for $i = 1,2$ in $C([0,+\infty) : L^1(\mathbb{R}))$ as $l \to \infty$. Let $F_{ikl}(x,t)$ be the distribution functions of n_{ikl} for $i = 1,2$. A direct computation shows that $F_{ikl}^{-1}(\eta,t)$ solves the following equation

$$(2.2.11)\qquad \frac{\partial F_{ikl}^{-1}}{\partial t} = -\frac{\partial}{\partial \eta}\left(\left(\frac{\partial F_{ikl}^{-1}}{\partial \eta}\right)^{-m}\right), \quad i = 1,2,$$

for $t > 0$ and $\eta \in [0,1]$. Making use of equation (2.2.11), it is easy to prove that the Wasserstein p-distance

$$W_p(n_{1kl}, n_{2kl})(t) = \left\{\int_0^1 |F_{1kl}^{-1}(\eta,t) - F_{2kl}^{-1}(\eta,t)|^p d\eta\right\}^{\frac{1}{p}}, \quad \forall p \in [1,+\infty),$$

is a non-increasing in time function. In fact, for any given $p \geq 1$, integrating by parts one obtains

$$\frac{d}{dt}\int_0^1 |F_{1kl}^{-1}(\eta,t) - F_{2kl}^{-1}(\eta,t)|^p d\eta = p(p-1)\int_0^1 |F_{1kl}^{-1}(\eta,t) - F_{2kl}^{-1}(\eta,t)|^{p-2}$$
$$\times \left(F_{1kl}^{-1}(\eta,t)_\eta - F_{2kl}^{-1}(\eta,t)_\eta\right)\left[\left(F_{1kl}^{-1}(\eta,t)_\eta\right)^{-m} - \left(F_{2kl}^{-1}(\eta,t)_\eta\right)^{-m}\right] d\eta \leq 0$$

since the function x^{-m}, $m \geq 1$, is decreasing. Note that the boundary terms vanish due to the compact support of the solutions, which implies

$$\lim_{\eta \to 0^+} \left(F_{ikl}^{-1}(\eta,t)_\eta\right)^{-1} = \lim_{\eta \to 1^-} \left(F_{ikl}^{-1}(\eta,t)_\eta\right)^{-1} = 0 \qquad i = 1,2.$$

On the other hand, for all $p \in [1,+\infty)$,

$$W_p(n_{1kl}, n_{2kl}) \to W_p(n_{1k}, n_{2k}), \quad l \to +\infty, \tag{2.2.12}$$

$$W_p(n_{1k}, n_{2k}) \to W_p(n_1, n_2), \quad k \to +\infty. \tag{2.2.13}$$

This implies that $W_p(n_1,n_2) \leq W_p(n_{I1}, n_{I2})$, $\forall p \in [1,+\infty)$. Since the function $W_p(n_1,n_2)$ is increasing with respect to p, we can define the quantity

$$\begin{aligned} W_\infty(n_1,n_2) &:= \lim_{p \uparrow +\infty} W_p(n_1,n_2) \\ &= \sup_{\eta \in (0,1)} \operatorname{ess} |F_1^{-1}(\eta,t) - F_2^{-1}(\eta,t)|. \end{aligned} \tag{2.2.14}$$

Since $W_\infty(n_{I1}, n_{I2})$ is finite, we deduce easily that $W_\infty(n_1,n_2)$ is also a non-increasing in time function.
Note that the inverse function $F^{-1}(\eta)$ of a distribution $F(x) = \int_{-\infty}^{x} n(s)ds$, where $n(s)$ is a integrable compactly supported function, is continuous at the point $\eta = 0$ and $\eta = 1$. Thus we can justify the inequality

$$\begin{aligned} W_\infty(n_1,n_2) &= \sup_{\eta \in (0,1)} \operatorname{ess} |F_1^{-1}(\eta,t) - F_2^{-1}(\eta,t)| \\ &\geq \max\left\{|F_1^{-1}(0,t) - F_2^{-1}(0,t)|, |F_1^{-1}(1,t) - F_2^{-1}(1,t)|\right\} \\ &\geq \max\left\{|\xi_1(t) - \xi_2(t)|, |\Xi_1(t) - \Xi_2(t)|\right\}. \end{aligned} \tag{2.2.15}$$

□

We remark that the above arguments only hold in one space dimension due to the fact that only in this case one can express the p-Wasserstein distance in terms of pseudo-inverse distribution functions, as given in (2.2.10).

Figure 2.6 shows the evolution of the p-Wasserstein distance defined in (2.2.10) for several values of p between $n_1(x,t)$ and $n_2(x,t)$, solutions of (2.2.1), (2.2.2) with initial conditions (2.1.26) and (2.1.29) respectively, in case $m = 2$. The integral in (2.2.10) for the forthcoming tests is computed by numerical quadrature and we are using the fully discretized implicit Euler scheme described in subsection 2.1.

It is interesting to observe that although the distance between the solutions is only known to be a contraction, this distance is in fact decaying quickly as $t \to \infty$. Let us point out that the two initial data have zero center of mass and therefore are well centered. In fact, it is a conjecture to prove that there is a decay of the distance between the solutions when you fix the center of mass of the initial data. In the case of expansion rate of supports, this was already observed by J. L. Vázquez in [**74**].

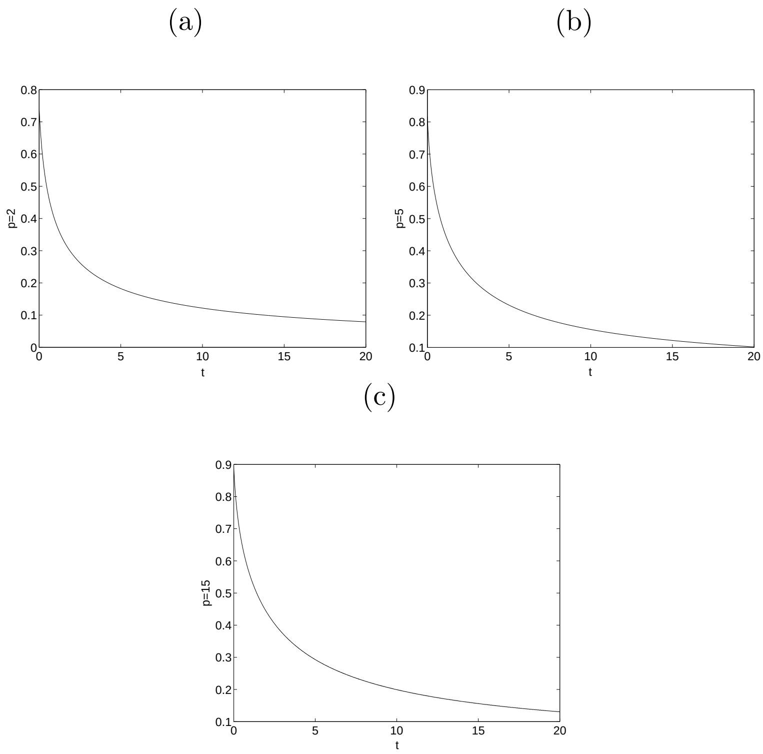


Figure 2.6: *Time evolution of the Wasserstein p-metric* $W_p(n_1, n_2)$*, where* $n_1(x,t)$ *and* $n_2(x,t)$ *are solutions of (2.2.1), (2.2.2) with* $m = 2$ *and initial conditions (2.1.26) and (2.1.29) respectively, in case (a)* $p = 2$*, (b)* $p = 5$*, (c)* $p = 15$*.*

Chapter 3

Analysis of the viscous quantum hydrodynamic equations

The objective of this chapter is the analysis to the one-dimensional stationary viscous quantum hydrodynamic model

$$J_x = \nu n_{xx}, \tag{3.0.1}$$

$$\left(\frac{J^2}{n}\right)_x + Tn_x - nV_x = \frac{\varepsilon^2}{2} n \left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x - \frac{J}{\tau} + \nu J_{xx}, \tag{3.0.2}$$

$$\lambda^2 V_{xx} = n - C(x) \quad \text{in } (0,1). \tag{3.0.3}$$

subject to the boundary conditions

$$n(0) = n(1) = 1, \quad n_x(0) = n_x(1) = 0, \quad V(0) = V_0, \tag{3.0.4}$$

$$J(0) = J_0, \quad V_0 = -\left(2\nu^2 + \frac{\varepsilon^2}{2}\right)(\sqrt{n})_{xx}(0) + \frac{J_0^2}{2}. \tag{3.0.5}$$

The last boundary condition can be interpreted as a Dirichlet condition for the Bohm potential at $x = 0$. Indeed, as the electrostatic potential is only defined up to an additive constant, this constant can be chosen such that $(\sqrt{n})_{xx}(0) = \alpha$ holds for any $\alpha \in \mathbb{R}$ (often $\alpha = 0$, see, e.g., [**53**]). Notice that we prescribe the current density but *not* the applied voltage $V(1) - V(0)$. Given J_0, the applied voltage can be computed from the solution of the above boundary-value problem, which gives a well-defined current-voltage characteristic.

Equations (3.0.1)-(3.0.3) can be derived from the Wigner-Fokker-Planck equations (1.0.4) with collision operator $Q(w)$ defined as (1.0.5) by a moment method, taking as closure condition an $O(\epsilon^4)$ approximation of the

thermal equilibrium density.
As we mention in the introduction, the system (3.0.1)-(3.0.3) can be reformulated as an elliptic fourth-order equation for the electron density n: after integration of (3.0.1) and substitution into (3.0.2) we obtain the expression (1.2.4). When we divide (1.2.4) by n and differentiate with respect to x, this equation is formally equivalent to

$$\begin{aligned} & -\left(2\nu^2+\frac{\varepsilon^2}{2}\right)\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_{xx}+\left(T+\frac{\nu}{\tau}\right)(\log n)_{xx} \\ & = \frac{n-C}{\lambda^2}+J_0^2\left(\frac{n_x}{n^3}\right)_x-2J_0\nu\left(\frac{1}{n}(\log n)_{xx}\right)_x-\frac{J_0}{\tau}\left(\frac{1}{n}\right)_x, \end{aligned} \tag{3.0.6}$$

using Poisson equation (3.0.3). The electrostatic potential can be recovered from (1.2.4), after division by n and integration:

$$\begin{aligned} V(x) & = -\left(2\nu^2+\frac{\varepsilon^2}{2}\right)\frac{(\sqrt{n})_{xx}}{\sqrt{n}}(x)+\left(T+\frac{\nu}{\tau}\right)\log n(x)+\frac{J_0^2}{2n(x)^2} \\ & \quad +\frac{J_0}{\tau}\int_0^x\frac{ds}{n(s)}+2J_0\nu\frac{n_x}{n^2}(x)+2J_0\nu\int_0^x\frac{n_x^2}{n^3}ds. \end{aligned} \tag{3.0.7}$$

The integration constant vanishes due to the boundary condition (3.0.5). The main difficulties in the analysis of equation like (3.0.6) are the mathematical treatment of the fourth and third order terms and the proof of positivity for the particle density. In this case the maximum principle is not available and other techniques are required. We note that the fourth-order term can be rewritten as

$$\left(n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x\right)_x=\frac{1}{2}(n(\log n)_{xx})_{xx}.$$

This reformulation suggests to introduce the exponential variable $n=e^u$; in fact in one space dimension an H^1 estimate for u yields L^∞ bound and hence positivity for the function n. Setting $n=e^u$ in (3.0.6) we arrive to the problem

$$\begin{aligned} & -\left(\nu^2+\frac{\varepsilon^2}{4}\right)\left(u_{xx}+\frac{u_x^2}{2}\right)_{xx}+\left(T+\frac{\nu}{\tau}\right)u_{xx} \\ & = \lambda^{-2}(e^u-C)+J_0^2(e^{-2u}u_x)_x-2J_0\nu(e^{-u}u_{xx})_x-\frac{J_0}{\tau}(e^{-u})_x, \end{aligned} \tag{3.0.8}$$

$$\begin{aligned} V(x) & = -\left(\nu^2+\frac{\varepsilon^2}{4}\right)\left(u_{xx}+\frac{u_x^2}{2}\right)(x)+\left(T+\frac{\nu}{\tau}\right)u(x)+\frac{J_0^2}{2}e^{-2u(x)} \\ & \quad +\frac{J_0}{\tau}\int_0^x e^{-u(s)}ds+2J_0\nu e^{-u(x)}u_x(x)+2J_0\nu\int_0^x e^{-u}u_x^2ds. \end{aligned} \tag{3.0.9}$$

Equation (3.0.8) has to be solved in the interval $(0,1)$ with the boundary conditions

$$u(0)=u(1)=0,\quad u_x(0)=u_x(1)=0. \tag{3.0.10}$$

The problems (3.0.1)-(3.0.5) and (3.0.8)-(3.0.10) are equivalent for classical solutions if $n > 0$ in $(0,1)$. Indeed, we have already shown that a classical solution to (3.0.1)-(3.0.5) with $n > 0$ in $(0,1)$ provides via $u = \log n$ a classical solution to (3.0.8)-(3.0.10). Conversely, let (u, V) be a classical solution to (3.0.8)-(3.0.10). Setting $n = e^u$ gives $n > 0$ in $(0,1)$, and the equations (3.0.6) and (3.0.7) hold. Differentiating (3.0.7) twice, multiplying by n and comparing with (3.0.6) yields the Poisson equation (3.0.3). Then, differentiating (3.0.7) once and multiplying the resulting equation by n, we obtain (3.0.2). Finally, the boundary condition (3.0.5) follows from (3.0.7) using (3.0.4). Thus it is sufficient to prove the existence of solutions to (3.0.8)-(3.0.10).
Our results can be easily extended to Dirichlet boundary conditions $n(0) \neq n(1)$, following the technique used in [**44**], but we use (3.0.4) for the sake of a smoother presentation.

Our existence result is as follows.

3.1 Theorem (Existence and uniqueness). *Let $C \in L^\infty(0,1)$, $C > 0$ in $(0,1)$, $0 < \gamma < 1$, and*

$$0 < J_0 \leq \frac{\gamma}{\sqrt{2}} e^{-M(\gamma)} \sqrt{T + \frac{\varepsilon^2}{16} + \frac{\nu}{\tau}}, \tag{3.0.11}$$

where the constant $M(\gamma) > 0$ is defined in (3.1.5). Then there exists a classical solution (n, J, V) to (3.0.1)-(3.0.5) such that $n(x) \geq e^{-M(\gamma)} > 0$ for $x \in (0,1)$. Furthermore, if J_0 and $\nu^2 + \varepsilon^2$ are sufficiently small, the problem (3.0.1)-(3.0.5) has a unique solution.

The restriction (3.0.11) implies (1.2.3) since

$$\frac{J_0}{n} \leq J_0 e^{M(\gamma)} < \frac{1}{\sqrt{2}} \sqrt{T + \frac{\varepsilon^2}{16} + \frac{\nu}{\tau}}.$$

The constant γ needs to be smaller than one since $M(\gamma) \to \infty$ for $\gamma \to 1$ such that $\gamma e^{-M(\gamma)} \to 0$.
We are able to prove the semiclassical limit $\varepsilon \to 0$, the inviscid limit $\nu \to 0$ and the combined semiclassical-inviscid limit $\varepsilon \to 0$ and $\nu \to 0$. We refer to the appendix for the physical assumptions on the parameters, which correspond to such limits.

3.2 Theorem (Inviscid limit). *Let (n_ν, J_ν, V_ν) be a solution to (3.0.1)-(3.0.5) and assume that condition (3.0.11) holds for $\nu = 0$. Then, as $\nu \to 0$,* *maybe for a subsequence,*

$$\begin{aligned} n_\nu &\rightharpoonup n && \text{weakly in } H^2(0,1),\\ V_\nu &\rightharpoonup V && \text{weakly in } H^4(0,1),\\ J_\nu &\rightharpoonup J && \text{weakly in } H^1(0,1), \end{aligned}$$

and (n, J, V) is a (classical) solution of the quantum hydrodynamic equations

$$\begin{aligned} &\left(\frac{J^2}{n} + Tn\right)_x - nV_x - \frac{\varepsilon^2}{2} n \left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x = -\frac{J}{\tau},\\ &J = J_0, \quad \lambda^2 V_{xx} = n - C \quad \text{in } (0,1),\\ &n(0) = n(1) = 1, \quad n_x(0) = n_x(1) = 0, \quad V(0) = V_0. \end{aligned}$$

3.3 Theorem (Semiclassical limit). *Let $(n_\varepsilon, J_\varepsilon, V_\varepsilon)$ be a solution to (3.0.1)-(3.0.5) and assume that condition (3.0.11) holds for $\varepsilon = 0$. Then, as $\varepsilon \to 0$, maybe for a subsequence,*

$$\begin{aligned} n_\varepsilon &\rightharpoonup n && \text{weakly in } H^2(0,1),\\ V_\varepsilon &\rightharpoonup V && \text{weakly in } H^4(0,1),\\ J_\varepsilon &\rightharpoonup J && \text{weakly in } H^1(0,1), \end{aligned}$$

and (n, J, V) is a (classical) solution of

$$\begin{aligned} &\left(\frac{J^2}{n} + Tn\right)_x - nV_x = \nu J_{xx} - \frac{J}{\tau}, \quad J_x = \nu n_{xx}, \quad \lambda^2 V_{xx} = n - C \quad \text{in } (0,1),\\ &n(0) = n(1) = 1, \quad n_x(0) = n_x(1) = 0, \quad V(0) = V_0, \quad J(0) = J_0. \end{aligned}$$

3.4 Theorem (Semiclassical-inviscid limit). *Let $\delta = \nu^2 + \varepsilon^2/4$, $V_0 = J_0^2/2$, let $(n_\delta, J_\delta, V_\delta)$ be a solution to (3.0.1)-(3.0.5), and assume that condition (3.0.11) holds for $\delta = 0$. Then, as $\delta \to 0$, maybe for a subsequence (see Remark 3.11),*

$$n_\delta \rightharpoonup n \quad \text{weakly in } H^1(0,1), \tag{3.0.12}$$

$$V_\delta \rightharpoonup V \quad \text{weakly in } H^3(0,1), \tag{3.0.13}$$

$$J_\delta \rightharpoonup J \quad \text{weakly in } H^1(0,1), \tag{3.0.14}$$

and (n, J, V) is a (classical) solution of the hydrodynamic equations

$$\left(\frac{J^2}{n} + Tn\right)_x - nV_x = -\frac{J}{\tau}, \quad J = J_0, \quad \lambda^2 V_{xx} = n - C, \tag{3.0.15}$$

$$n(0) = n(1) = 1, \quad V(0) = V_0. \tag{3.0.16}$$

3.5 Remark. The convergence results for the electron density are not strong enough to conclude that the boundary condition (3.0.5) holds. However, the boundary conditions of the limit equations are sufficient to get (formally) well-posed problems.

In section (3.1) we show existence of solution to (3.0.1)-(3.0.5); the proof of theorem (3.1) is completed in section (3.2), where the uniqueness of solution is proved. Finally the inviscid and semiclassical limits (theorem (3.2), (3.3) and (3.4)) are performed in section (3.3) and the last part of the chapter concerns a sketch of the derivation of model and its scaling.

3.1 Existence of solutions

As usual, we call $u \in H_0^2(0,1)$ a *weak solution* of (3.0.8), (3.0.10) if for all $\psi \in H_0^2(0,1)$ it holds

$$\begin{aligned}(3.1.1)\qquad & -\left(\nu^2+\frac{\varepsilon^2}{4}\right)\int_0^1\left(u_{xx}+\frac{1}{2}u_x^2\right)\psi_{xx}dx-\left(T+\frac{\nu}{\tau}\right)\int_0^1 u_x\psi_x dx\\ &=2J_0\nu\int_0^1 u_{xx}e^{-u}\psi_x dx-J_0^2\int_0^1 u_x e^{-2u}\psi_x dx\\ &+\frac{J_0}{\tau}\int_0^1 e^{-u}\psi_x dx+\frac{1}{\lambda^2}\int_0^1(e^u-C)\psi dx.\end{aligned}$$

In order to prove Theorem 3.1 we consider the following truncated problem:

$$\begin{aligned}-\left(\nu^2+\frac{\varepsilon^2}{4}\right)\int_0^1\left(u_{xx}+\frac{1}{2}u_x^2\right)\psi_{xx}dx-\left(T+\frac{\nu}{\tau}\right)\int_0^1 u_x\psi_x dx&\\ =2J_0\nu\int_0^1 u_{xx}e^{-u_M}\psi_x dx-J_0^2\int_0^1 u_x e^{-2u_M}\psi_x dx&\\ +\frac{J_0}{\tau}\int_0^1 e^{-u}\psi_x dx+\frac{1}{\lambda^2}\int_0^1(e^u-C)\psi dx,&\qquad(3.1.2)\end{aligned}$$

where $M = M(\gamma) > 0$ is the constant from (3.0.11) defined in (3.1.5) below and

$$u_M=\begin{cases}u & \text{if } |u|\le M\\ M\text{sign}(u) & \text{otherwise.}\end{cases}$$

The following lemma is the key result of this part.

3.6 Lemma. **(H^2-Estimate)**. *Let $u \in H_0^2(0,1)$ be a solution of (3.1.2) and let (3.0.11) hold for some $0 < \gamma < 1$. Then*

$$(3.1.3)\qquad \left(\nu^2+\frac{\epsilon^2}{4}\right)\|u_{xx}\|_{L^2}^2+\left(T+\frac{\nu}{\tau}\right)\|u_x\|_{L^2}^2\le K(\gamma),$$

where $K(\gamma) > 0$ is independent of u, ν, and ϵ (see (3.1.7) for its definition). In particular, it follows

$$\|u\|_{L^\infty} \leq M(\gamma), \tag{3.1.4}$$

where

$$M(\gamma) = \sqrt{\frac{K(\gamma)}{T}}. \tag{3.1.5}$$

Proof. We use $\psi = u$ as a test function in the weak formulation of (3.1.2) to obtain

$$\begin{aligned} \left(\nu^2 + \frac{\varepsilon^2}{4}\right)\int_0^1 \left(u_{xx}^2 + \frac{1}{2}u_x^2 u_{xx}\right)dx + \left(T + \frac{\nu}{\tau}\right)\int_0^1 u_x^2 dx \\ = -2J_0\nu \int_0^1 u_{xx}e^{-u_M}u_x dx + J_0^2 \int_0^1 u_x^2 e^{-2u_M}dx \\ -\frac{J_0}{\tau}\int_0^1 e^{-u}u_x dx - \frac{1}{\lambda^2}\int_0^1 u(e^u - C)dx \\ = I_1 + I_2 + I_3 + I_4. \end{aligned} \tag{3.1.6}$$

We estimate the right-hand side term by term. By Young's inequality,

$$\begin{aligned} I_1 &= -2J_0\nu \int_0^1 u_{xx}e^{-u_M}u_x dx \leq 2J_0 e^M \nu \int_0^1 |u_{xx}||u_x|dx \\ &\leq (1-\eta)\nu^2 \int_0^1 u_{xx}^2 dx + \frac{J_0^2 e^{2M}}{1-\eta}\int_0^1 u_x^2 dx, \end{aligned}$$

where $0 < \eta < (1-\gamma^2)/(1-\gamma^2/2)$. Furthermore,

$$I_2 = J_0^2 \int_0^1 u_x^2 e^{-2u_M}dx \leq J_0^2 e^{2M}\int_0^1 u_x^2 dx.$$

Due to the boundary conditions (3.0.10), the third integral vanishes: $I_3 = 0$. It is not difficult to see that $1/e + \|C\log C\|_{L^\infty}$ is an upper bound for the function $u \mapsto -u(e^u - C(x))$, $u \in \mathbb{R}$, for any $x \in (0,1)$. Here we use the assumption that the concentration $C(x)$ is positive. Therefore,

$$I_4 \leq \lambda^{-2}(e^{-1} + \|C\log C\|_{L^\infty}).$$

Noticing that the integral

$$\int_0^1 u_x^2 u_{xx} dx = \frac{1}{3}(u_x^3(1) - u_x^3(0)) = 0$$

vanishes, due to the boundary conditions (3.0.10), we conclude that (3.1.6) can be estimated as

$$\left(\eta\nu^2+\frac{\varepsilon^2}{4}\right)\|u_{xx}\|_2^2+\left(T+\frac{\nu}{\tau}-\frac{2-\eta}{1-\eta}J_0^2e^{2M}\right)\|u_x\|_2^2 \le \lambda^{-2}(e^{-1}+\|C\log C\|_{L^\infty}).$$

In view of condition (3.0.11) we obtain

$$T+\frac{\nu}{\tau}-\frac{2-\eta}{1-\eta}J_0^2e^{2M} \ge \left(1-\frac{2-\eta}{1-\eta}\frac{\gamma^2}{2}\right)\left(T+\frac{\nu}{\tau}\right)-\frac{2-\eta}{1-\eta}\frac{\gamma^2}{2}\frac{\epsilon^2}{16}.$$

Using the Poincaré inequality

$$\frac{\epsilon^2}{16}\int_0^1 u_x^2dx \le \frac{\epsilon^2}{4}\int_0^1 u_{xx}^2dx,$$

this gives

$$\begin{aligned}\left[\eta\nu^2+\left(1-\frac{\gamma^2(2-\eta)}{2(1-\eta)}\right)\frac{\varepsilon^2}{4}\right]\|u_{xx}\|_{L^2}^2 &+ \left(1-\frac{\gamma^2(2-\eta)}{2(1-\eta)}\right)\left(T+\frac{\nu}{\tau}\right)\|u_x\|_{L^2}^2 \\ &\le \lambda^{-2}(e^{-1}+\|C\log C\|_{L^\infty})\end{aligned}$$

or

$$\left(\nu^2+\frac{\epsilon^2}{4}\right)\|u_{xx}\|_{L^2}^2+\left(T+\frac{\nu}{\tau}\right)\|u_x\|_{L^2}^2 \le K(\gamma),$$

where

$$K(\gamma)=\frac{1}{\lambda^2}\left(\frac{1}{e}+\|C\log C\|_{L^\infty}\right)\min\left\{\eta, 1-\frac{\gamma^2(2-\eta)}{2(1-\eta)}\right\}^{-1}. \tag{3.1.7}$$

Notice that $1-\gamma^2(2-\eta)/(2(1-\eta)) > 0$ due to the choice of η. Finally, from the Poincaré-Sobolev estimate,

$$\|u\|_{L^\infty} \le \|u_x\|_{L^2} \le M(\gamma),$$

where $M(\gamma)=\sqrt{K(\gamma)/T}$. This proves the lemma. □

3.7 Lemma. *Under the assumptions of Lemma 3.6, there exists a solution $u \in H_0^2(0,1)$ of (3.1.1).*

Proof. The existence of a solution of the problem (3.1.1) is shown by using the Leray-Schauder fixed-point theorem. For this, we consider the following linear problem for given $w \in H_0^1(0,1)$ with test functions $\psi \in H_0^2(0,1)$:

$$-a(u,\psi)=\sigma F(\psi), \tag{3.1.8}$$

where $\sigma \in [0,1]$,

$$a(u,\psi) = \left(\nu^2 + \frac{\varepsilon^2}{4}\right)\int_0^1 u_{xx}\psi_{xx}dx + \left(T + \frac{\nu}{\tau}\right)\int_0^1 u_x\psi_x dx, \tag{3.1.9}$$

and

$$\begin{aligned} F(\psi) &= -\sigma\left(\nu^2 + \frac{\varepsilon^2}{4}\right)\int_0^1 \frac{1}{2}w_x^2\psi_{xx}dx + 2J_0\sigma\nu\int_0^1 w_x(e^{-w}\psi_x)_x dx \\ &\quad + J_0^2\sigma\int_0^1 w_x e^{-2w}\psi_x dx - \frac{J_0}{\tau}\sigma\int_0^1 e^{-w}\psi_x dx - \frac{\sigma}{\lambda^2}\int_0^1 \psi(e^w - C)dx. \end{aligned} \tag{3.1.10}$$

Since the bilinear form $a(u,\psi)$ is continuous and coercive on $H_0^2(0,1) \times H_0^2(0,1)$ and the linear functional F is continuous on $H_0^2(0,1)$, we can apply the Lax-Milgram theorem to obtain the existence of a solution $u \in H_0^2(0,1)$ of (3.1.8). Thus, the operator

$$S : H_0^1(0,1) \times [0,1] \to H_0^1(0,1), \quad (w,\sigma) \mapsto u,$$

is well-defined. Moreover, it is continuous and compact since the embedding $H_0^2(0,1) \hookrightarrow H_0^1(0,1)$ is compact. Furthermore, $S(w,0) = 0$. Following the steps of the proof of Lemma 3.6, we can show that $\|u\|_{H_0^2} \le$ const. for all $(u,\sigma) \in H_1^0(0,1) \times [0,1]$ satisfying $S(u,\sigma) = u$. Therefore, the existence of a fixed point u with $S(u,1) = u$ follows from the Leray-Schauder fixed-point theorem. This fixed point is a solution of (3.1.2) and, in fact, also of (3.1.1) since $|u(x)| \le M(\gamma)$. □

3.8 Theorem. *Under the assumptions of Lemma 3.6, there exists a solution $(u,V) \in H^4(0,1) \times H^2(0,1)$ of (3.0.8)-(3.0.10).*

Proof. Let u be a weak solution of (3.1.1) or (3.0.8). Since $u \in H_0^2(0,1)$, it holds $u_x^2 \in H_0^1(0,1)$ and $(e^{-u}u_{xx})_x \in H^{-1}(0,1)$. Then, from (3.0.8), we infer $u_{xxxx} \in H^{-1}(0,1)$. Hence, there exists $w \in L^2(0,1)$ such that $w_x = u_{xxxx}$. This implies $u_{xxx} = w +$ const. $\in L^2(0,1)$ and, by (3.0.8), $u_{xxxx} \in L^2(0,1)$. This allows us to conclude that $u \in H^4(0,1)$ and from the regularity of u and from (3.0.9) follows the regularity of V. □

3.2 Uniqueness of solution

3.9 Theorem. *If the positive constants ν, ε and J_0 are sufficiently small, the problem (3.0.8)-(3.0.10) has a unique solution.*

Proof. We proceed similarly as in [**44**]. Let u, $v \in H_0^2(0,1)$ be weak solutions of (3.0.8). We observe that, in view of the boundary conditions for u_x,

$$u_x^2(x) = 2\int_0^x u_x(s)u_{xx}(s)ds \le 2\|u_x\|_{L^2}\|u_{xx}\|_{L^2}$$

and thus

$$\|u_x\|_{L^\infty} \le \frac{\alpha}{2}\|u_x\|_{L^2} + \frac{1}{2\alpha}\|u_{xx}\|_{L^2}$$

for all $\alpha > 0$. By Lemma 3.6 we obtain

$$\|u_x\|_{L^\infty} \le \left(\frac{\alpha}{2\sqrt{\nu^2+\epsilon^2/4}} + \frac{1}{2\alpha\sqrt{T+\nu/\tau}}\right)\sqrt{K(\gamma)}.$$

Choosing $\alpha = \sqrt{(T+\nu/\tau)/K(\gamma)}$ then gives

$$\|u_x\|_{L^\infty} \le \frac{\sqrt{T+\nu/\tau}}{2\sqrt{\nu^2+\epsilon^2/4}} + \frac{K(\gamma)}{T+\nu/\tau}.$$

Now we choose ν and ϵ so small that

$$\sqrt{\nu^2+\epsilon^2/4} \le \frac{(T+\nu/\tau)^{3/2}}{2K(\gamma)}.$$

As T is positive, such a choice is possible. This implies

$$\|u_x\|_{L^\infty} \le \sqrt{\frac{T+\nu/\tau}{\nu^2+\epsilon^2/4}}.$$

A similar estimate can be obtained for v_x. Therefore

$$\|(u+v)_x\|_{L^\infty} \le 2\sqrt{\frac{T+\nu/\tau}{\nu^2+\epsilon^2/4}}. \tag{3.2.1}$$

Now we start to estimate the difference $u-v$. The weak formulation of the difference of the equations satisfied by u and v, with the test function $u-v$, reads as follows:

$$\begin{aligned}
\left(\nu^2+\frac{\varepsilon^2}{4}\right)\int_0^1 (u-v)_{xx}^2 + \left(T+\frac{\nu}{\tau}\right)\int_0^1 (u-v)_x^2 dx \\
+\frac{1}{2}\left(\nu^2+\frac{\varepsilon^2}{4}\right)\int_0^1 (u_x^2-v_x^2)(u-v)_{xx}dx \\
= -2J_0\nu\int_0^1 (u_{xx}e^{-u}-v_{xx}e^{-v})(u-v)_x dx - \frac{1}{2}J_0^2\int_0^1 (e^{-2u}-e^{-2v})_x(u-v)_x dx \\
-\frac{1}{\lambda^2}\int_0^1 (e^u-e^v)(u-v)dx + \frac{J_0}{\tau}\int_0^1 (e^{-u}-e^{-v})(u-v)_x dx \\
= I_1+I_2+I_3+I_4.
\end{aligned} \tag{3.2.2}$$

The mean value theorem and the estimate (3.1.4) with $M = M(\gamma)$ yields $|e^{-u(x)} - e^{-v(x)}| \le e^M |u(x) - v(x)|$. Therefore, using Poincaré's inequality,

$$I_4 \le \frac{J_0}{\tau} e^M \|u - v\|_{L^2} \|(u - v)_x\|_{L^2} \le \frac{J_0}{\tau} e^M \|(u - v)_x\|_{L^2}^2.$$

The monotonicity of $x \mapsto e^x$ implies $I_3 \le 0$. For the estimate of the second integral we obtain similarly as above

$$I_2 = J_0^2 \int_0^1 [e^{-2u}(u-v)_x^2 + (e^{-2u} - e^{-2v}) v_x (u-v)_x] dx \le J_0^2 K_1 e^{2M} \|(u-v)_x\|_{L^2}^2,$$

where the constant $K_1 > 0$ depends on $\|v_x\|_{L^\infty}$. Finally, we write for the first integral

$$I_1 = -2J_0\nu \int_0^1 [e^{-u}(u - v)_{xx} + (e^{-u} - e^{-v}) v_{xx}](u - v)_x dx.$$

As we do not have an L^∞ bound for v_{xx}, we integrate by parts in the second addend:

$$\begin{aligned} I_1 &= -2J_0\nu \int_0^1 [e^{-u}(u - v)_{xx}(u - v)_x - e^{-u} v_x (u - v)_x^2 - (e^{-u} - e^{-v}) v_x^2 (u - v)_x \\ &\quad - (e^{-u} - e^{-v}) v_x (u - v)_{xx}] dx \\ &\le \frac{\nu^2}{2} \|(u - v)_{xx}\|_{L^2}^2 + J_0^2 e^{2M} K_2 \|(u - v)_x\|_{L^2}^2, \end{aligned}$$

and $K_2 > 0$ depends on $\|v_x\|_{L^\infty}$. In the last step we have used again the mean value theorem and Young's and Poincaré's inequalities. We conclude from (3.2.2)

$$\begin{aligned} I &:= \left(\nu^2 + \frac{\varepsilon^2}{4}\right) \int_0^1 (u - v)_{xx}^2 + \left(T + \frac{\nu}{\tau}\right) \int_0^1 (u - v)_x^2 dx \\ &\quad + \frac{1}{2}\left(\nu^2 + \frac{\varepsilon^2}{4}\right) \int_0^1 (u + v)_x (u - v)_x (u - v)_{xx} dx \qquad (3.2.3) \\ &\le \frac{\nu^2}{2} \|(u - v)_{xx}\|_{L^2}^2 + J_0 \left(\frac{e^M}{\tau} + J_0 K_1 e^{2M} + J_0 K_2 e^{2M}\right) \|(u - v)_x\|_{L^2}^2. \end{aligned}$$

The estimate of the last integral of the left-hand side of (3.2.2) is more delicate. We use the bound (3.2.1):

$$
\begin{aligned}
I \;\geq\; & \frac{1}{2}\left(\nu^2+\frac{\varepsilon^2}{4}\right)\int_0^1 (u-v)_{xx}^2+\frac{1}{2}\left(T+\frac{\nu}{\tau}\right)\int_0^1 (u-v)_x^2 dx \\
& +\frac{1}{2}\int_0^1\left(\sqrt{\nu^2+\epsilon^2/4}|(u-v)_{xx}|-\sqrt{T+\nu/\tau}|(u-v)_x|\right)^2 dx \\
& +\sqrt{\nu^2+\epsilon^2/4}\sqrt{T+\nu/\tau}\int_0^1 |(u-v)_x||(u-v)_{xx}|\left(1-\frac{1}{2}\sqrt{\frac{\nu^2+\epsilon^2/4}{T+\nu/\tau}}|(u+v)_x|\right)dx \\
\geq\; & \frac{1}{2}\left(\nu^2+\frac{\varepsilon^2}{4}\right)\int_0^1 (u-v)_{xx}^2+\frac{1}{2}\left(T+\frac{\nu}{\tau}\right)\int_0^1 (u-v)_x^2 dx.
\end{aligned}
$$

Thus putting together this estimate and (3.2.3), for sufficiently small $J_0>0$, we arrive to

$$
\frac{\varepsilon^2}{8}\int_0^1 (u-v)_{xx}^2+\frac{1}{2}\left(T+\frac{\nu}{\tau}\right)\int_0^1 (u-v)_x^2 dx \leq 0.
$$

This implies $u-v=0$ in $(0,1)$. $\square$

For the proof of Theorem 3.1 it remains to show that the solution (u,V) of (3.0.8)-(3.0.10) provides a solution (n,V) of (3.0.1)-(3.0.5). Then both formulations are equivalent and the uniqueness of solutions of (3.0.1)-(3.0.5) follows.

Let (u,V) be the unique solution of (3.0.8)-(3.0.10) and set $n=e^u$. Then we obtain (3.0.6) and (3.0.7). We differentiate (3.0.7) twice with respect to x:

$$
\begin{aligned}
V_{xx} \;=\; & -\left(2\nu^2+\frac{\varepsilon^2}{2}\right)\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_{xx}+\left(T+\frac{\nu}{\tau}\right)(\log n)_{xx}+\frac{J_0^2}{2}\left(\frac{1}{n^2}\right)_{xx} \\
& +\frac{J_0}{\tau}\left(\frac{1}{n}\right)_x+2J_0\nu\left(\frac{n_x}{n^2}\right)_{xx}+2J_0\nu\left(\frac{n_x^2}{n^3}\right)_x,
\end{aligned}
$$

and, comparing with (3.0.6), Poisson equation (3.0.3) follows. Furthermore, from (3.0.7) it holds:

$$
V(0)=-\left(2\nu^2+\frac{\varepsilon^2}{2}\right)\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)(0)+\frac{J_0^2}{2}=V_0,
$$

taking into account (3.0.5).

Now we differentiate (3.0.7) with respect to x and multiply the resulting equation with n:

$$
nV_x=-\left(2\nu^2+\frac{\varepsilon^2}{2}\right)n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x+\left(T+\frac{\nu}{\tau}\right)n_x-J_0^2\frac{n_x}{n^2}+\frac{J_0}{\tau}-2J_0\nu\left(\frac{n_x^2}{n^2}-\frac{n_{xx}}{n}\right).
$$

Introducing $J(x) := \nu n_x(x) + J_0$, equation (3.0.1) follows after differentiation. Finally, from

$$-2\nu^2 n\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)_x + \frac{\nu}{\tau} n_x - 2J_0\nu\left(\frac{n_x^2}{n^2} - \frac{n_{xx}}{n}\right) + \frac{J_0}{\tau} - J_0^2\left(\frac{n_x}{n^2}\right) = \left(\frac{J^2}{n}\right)_x - \nu J_{xx} + \frac{J}{\tau}$$

equation (3.0.2) follows.

3.3 Asymptotic limits

We only prove Theorem 3.4 as the proofs of Theorems 3.2 and 3.3 are very similar (and in fact, easier). The proof is a consequence of the key estimate (3.1.3) and the compact embedding $H^1(0,1) \hookrightarrow L^\infty(0,1)$. First we show:

3.10 Theorem. *Let (u_δ, V_δ) be a solution of (3.0.8)-(3.0.10) for $\delta = \nu^2 + \epsilon^2/4 > 0$ and let (3.0.11) hold for $\nu = 0$. Set $J_\delta = \nu \exp(u_\delta) u_{\delta,x} + J_0$. Then there exists a subsequence of $(u_\delta, J_\delta, V_\delta)$ (not relabeled) such that*

(3.3.1) $\quad u_\delta \rightharpoonup u \quad$ *weakly in H^1 and strongly in L^∞,*

(3.3.2) $\quad V_\delta \rightharpoonup V \quad$ *weakly in H^3,*

(3.3.3) $\quad J_\delta \rightharpoonup J \quad$ *weakly in H^1,*

and (u, J, V) is a solution of

$$J = J_0, \tag{3.3.4}$$

$$Tu_{xx} = \frac{e^u - C}{\lambda^2} + J_0^2(u_x e^{-2u})_x - \frac{J_0}{\tau}(e^{-u})_x, \tag{3.3.5}$$

$$V(x) = Tu(x) + \frac{1}{2}J_0^2 e^{-2u(x)} + \frac{J_0}{\tau}\int_0^x e^{-u(x)} ds, \; x \in (0,1), \tag{3.3.6}$$

with boundary conditions

$$u(0) = u(1) = 0. \tag{3.3.7}$$

Proof. From Lemma 3.6 and Poincaré's inequality we obtain a uniform H^1 bound for u_δ. Then there exists a subsequence of (u_δ) (not relabeled) such that (3.3.1) holds. The weak formulation of (3.0.8) reads, for any $\psi \in C_0^\infty(0,1)$, after integration by parts,

$$\begin{aligned}
&-\delta\int_0^1 u_\delta \psi_{xxxx} - \frac{\delta}{2}\int_0^1 u_{\delta,x}^2 \psi_{xx} dx \\
&= \left(T + \frac{\nu}{\tau}\right)\int_0^1 u_{\delta,x}\psi_x dx + 2J_0\nu\int_0^1 u_{\delta,x}^2 e^{-u_\delta}\psi_x dx - 2J_0\nu\int_0^1 u_{\delta,x}e^{-u_\delta}\psi_{xx} dx \\
&\quad - J_0^2\int_0^1 u_{\delta,x}e^{-2u_\delta}\psi_x dx + \frac{J_0}{\tau}\int_0^1 e^{-u_\delta}\psi_x dx + \frac{1}{\lambda^2}\int_0^1 (e^{u_\delta} - C)\psi dx.
\end{aligned}$$

The convergences (3.3.1) allow us to pass to the limit $\delta \to 0$ in the above equation, observing that the left-hand side vanishes in the limit:

$$-T\int_0^1 u_x\psi_x dx = -J_0^2\int_0^1 u_x e^{-2u}\psi_x dx + \frac{J_0}{\tau}\int_0^1 e^{-u}\psi_x dx + \frac{1}{\lambda^2}\int_0^1 (e^u - C)\psi dx.$$

Now we rewrite (3.0.9) as

$$\begin{aligned} V_\delta(x) = -\delta\left(u_{\delta,xx} + \frac{1}{2}u_{\delta,x}^2\right) &+ \left(T + \frac{\nu}{\tau}\right)u_\delta + 2J_0\nu e^{-u_\delta}u_{\delta,x} + 2J_0\nu\int_0^x e^{-u_\delta}u_{\delta,x}^2 ds \\ &+ \frac{1}{2}J_0^2 e^{-2u_\delta} + \frac{J_0}{\tau}\int_0^x e^{-u_\delta} ds. \end{aligned} \tag{3.3.8}$$

Differentiating this equation twice with respect to x and comparing to (3.0.8) yields

$$V_{\delta,xx} = \lambda^{-2}(e^{u_\delta} - C).$$

Thus, from (3.1.3) follows that V_δ is uniformly bounded in H^3 and (3.3.2) is proved.

Next we multiply (3.3.8) by $\phi \in C_0^\infty(0,1)$ and integrate over $(0,1)$. Integrating by parts and using (3.0.10), we find

$$\begin{aligned} \int_0^1 V_\delta\phi dx &= -\delta\int_0^1 u_\delta\phi_{xx} dx - \frac{\delta}{2}\int_0^1 u_{\delta,x}^2\phi dx + \left(T + \frac{\nu}{\tau}\right)\int_0^1 u_\delta\phi dx \\ &+ 2J_0\nu\int_0^1 e^{-u_\delta}u_{\delta,x}\phi dx + 2J_0\nu\int_0^1 \phi\int_0^x e^{-u_\delta}u_{\delta,x}^2 ds dx + \frac{1}{2}J_0^2\int_0^1 e^{-2u_\delta}\phi dx \\ &+ \frac{J_0}{\tau}\int_0^1 \phi\int_0^x e^{-u_\delta} ds dx. \end{aligned} \tag{3.3.9}$$

Using the uniform L^∞ and H^1 bounds of u_δ and the convergence (3.3.1), we can pass to the limit $\delta \to 0$ in (3.3.9):

$$\int_0^1 V\phi dx = \int_0^1 \left(Tu + \frac{1}{2}J_0^2 e^{-2u} + \frac{J_0}{\tau}\int_0^x e^{-u} ds\right)\phi dx.$$

Finally, we consider the equation

$$J_\delta = \nu e^{u_\delta}u_{\delta,x} + J_0.$$

As $\nu u_{\delta,x}$ is uniformly bounded in H^1, by Lemma 3.6, a subsequence of (J_δ) converges weakly in H^1, i.e., (3.3.3) holds. Multiplying the above equation by some $\phi \in C_0^\infty(0,1)$ and integrating over $(0,1)$ gives

$$\int_0^1 J_\delta\phi dx = -\nu\int_0^1 e^{u_\delta}\phi_x dx + J_0\int_0^1 \phi dx,$$

and the limit $\nu \to 0$ implies (3.3.4). $\square$

3.11 Remark. For sufficiently small current densities $J_0 > 0$, the quantum hydrodynamic model (3.3.4)-(3.3.7) is uniquely solvable (see, e.g., [**39, 44**]). This means that the whole sequence $(u_\delta, V_\delta, J_\delta)$ converges to (u, V, J_0) in the sense of (3.3.1)-(3.3.3).

We prove Theorem 3.4. Setting $n_\delta = e^{u_\delta}$ and $n = e^u$, where u is the solution of (3.3.5), obtained as the limit of the subsequence (u_δ), the convergence results (3.0.12)-(3.0.14) hold. We rewrite (3.3.5) in the variable n:

$$T(\log n)_{xx} = \frac{n-C}{\lambda^2} + J_0^2\left(\frac{n_x}{n^3}\right)_x - \frac{J_0}{\tau}\left(\frac{1}{n}\right)_x. \tag{3.3.10}$$

Notice that n is strictly positive since $n(x) \geq \exp(-\|u\|_{L^\infty}) \geq \exp(-M(\gamma))$, $x \in (0,1)$. Differentiating (3.3.6) twice with respect to x, we obtain

$$V_{xx}(x) = T(\log n)_{xx} + \frac{J_0^2}{2}\left(\frac{1}{n^2}\right)_{xx} + \frac{J_0}{\tau}\left(\frac{1}{n}\right)_x. \tag{3.3.11}$$

Comparing (3.3.10) and (3.3.11) gives Poisson equation (see (3.0.15)). Differentiating (3.3.6) with respect to x and multiplying by n, the resulting equation is equal to the first equation in (3.0.15). Finally, from (3.3.6) we have

$$V(0) = \frac{1}{2}J_0^2 = V_0,$$

which equals (3.0.16).

3.4 Exponential decay in time

In this section we investigate the asymptotic behaviour of solution to

$$n_t + J_x = \nu n_{xx} \tag{3.4.1}$$

$$J_t + \left(\frac{J^2}{n} + Tn\right)_x - nV_x - \frac{\varepsilon^2}{2}n\left(\frac{\sqrt{n}_{xx}}{\sqrt{n}}\right)_x = \nu J_{xx} - \frac{J}{\tau} \tag{3.4.2}$$

$$\lambda^2 V_{xx} = n - 1 \qquad x \in \Omega, \quad t > 0 \tag{3.4.3}$$

with initial conditions

$$n(\cdot,0) = n_I, \qquad J(\cdot,0) = J_I \qquad \text{in} \quad \Omega \tag{3.4.4}$$

employing the entropy dissipation method.

Let $(n, J, V) = (1, 0, 0)$ be the thermal equilibrium in $\Omega = (0,1)$; we assume that the boundary condition for (3.4.1)-(3.4.3) are the thermal equilibrium state

$$n = 1 \qquad n_x = 0 \qquad V = 0, \qquad \text{on} \quad \partial\Omega \times (0, \infty), \tag{3.4.5}$$

$$\int_{\partial\Omega} J\left[J_x\left(\frac{\epsilon^2}{4\nu} + \nu\right) - \frac{1}{2}J^2\right](\cdot, t)ds = 0, \qquad t > 0. \tag{3.4.6}$$

Boundary condition (3.4.6) can be interpreted as a generalized thermal equilibrium condition for the current density (see Remark 3.13). We prove that any strong solution of (3.4.1)-(3.4.6) converges exponentially fast to the (unique) thermal equilibrium state $(1, 0, 0)$. The rate of convergence for $n(\cdot, t)$ and $V(\cdot, t)$ depends on the viscosity constant $\nu > 0$. If $\nu = 0$, no convergence rate can be obtained.
More precisely, our main result reads as follows.

3.12 Theorem. *Let $n \in H^1(0, T^*, L^2(\Omega)) \cap L^2(0, T^*, H^3(\Omega))$, $J \in H^1(0, T^*, L^2(\Omega)) \cap L^2(0, T^*, H^2(\Omega))$, $V \in L^2(0, T^*, H^2(\Omega))$ be a solution to (3.4.1)-(3.4.3) for any $T^* > 0$ such that $n > 0$ in $\Omega \times (0, T^*)$ and let $n_I \in H^1(\Omega)$, $J_I \in L^2(\Omega)$ such that $n_I > 0$ in [0,1]. Then:*

$$\begin{aligned}
&\epsilon^2 \|n(\cdot, t) - 1\|^2_{L^\infty(\Omega)} \le 2E(0)e^{-4\nu(\epsilon^2+2T)t}, \\
&\lambda^2 \|V(\cdot, t)\|^2_{L^\infty(\Omega)} \le 2E(0)e^{-4\nu\lambda^2 t}, \\
&\left\| \frac{J(\cdot, t)}{\sqrt{n(\cdot, t)}} \right\|^2_{L^2(\Omega)} \le 2E(0)e^{-\frac{2}{\tau}t}, \qquad t > 0.
\end{aligned}$$

3.13 Remark. (1) The boundary condition (3.4.6) is needed for technical reasons. It is a consequence of the (physically reasonable, but mathematically over-determining) boundary conditions $J(0, t) = J(1, t) = 0$, $t > 0$.
(2) As expected, no convergence rate for n and V can be expected if $\nu = 0$. However, the kinetic energy $\frac{J^2(\cdot,t)}{n(\cdot,t)}$ converges to zero exponentially in the $L^1(\Omega)$ norm with a decay rate $\frac{1}{\tau}$. This is physically reasonable since τ models the momentum relaxation time.
(3) Exponential decay rates for solution of the Wigner-Fokker-Planck equation (1.0.4), (1.0.5) towards the thermal equilibrium state are obtained in [**22**]. The decay rates of [**22**] are different from ours since in our system, the electrostatic potential is given self-consistently, whereas in [**22**], the potential is a given function not depending on the particle density.

Proof of Theorem 3.12. Let $T^* > 0$ and fix $t \in (0, T^*)$. Multiply (3.4.2) by

$\frac{J}{n}$, integrate over Ω and integrate by parts:

$$\begin{aligned}\int_0^1 J_t \frac{J}{n} dx = & - \int_0^1 \left(\frac{J^2}{n}\right)_x \frac{J}{n} dx - T\int_0^1 J\frac{n_x}{n}dx \\ & + \int_0^1 V_x J dx - \frac{\epsilon^2}{2}\int_0^1 J_x\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)dx + \frac{\epsilon^2}{2}\int_{\partial\Omega} J\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)ds \\ & - \nu\int_0^1 J_x\left(\frac{J}{n}\right)_x dx + \nu\int_{\partial\Omega} J_x\left(\frac{J}{n}\right)ds - \frac{1}{\tau}\int_0^1 \frac{J^2}{n}dx = \\ & = A_1 + \ldots + A_8. \end{aligned} \tag{3.4.7}$$

Multiply (3.4.2) by the function $T\log n - \frac{J^2}{2n^2} - V - \varepsilon^2\frac{(\sqrt{n})_{xx}}{2\sqrt{n}}$, integrate over Ω and integrate by parts:

$$\begin{aligned} & \int_0^1 n_t\left(T\log n - \frac{J^2}{2n^2} - V - \varepsilon^2\frac{(\sqrt{n})_{xx}}{2\sqrt{n}}\right)dx = \\ & -\nu T\int_0^1 \frac{n_x^2}{n}dx + \nu\int_0^1 \frac{1}{2}\frac{J^2}{2n^2}n_x dx + \nu\int_0^1 V_x n_x dx - \nu\frac{\epsilon^2}{2}\int_0^1 n_{xx}\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)dx + \\ & +T\int_0^1 J(\log n)_x dx + \int_0^1 \frac{J^2 J_x}{2n^2}dx - \int_0^1 V_x J dx + \frac{\epsilon^2}{2}\int_0^1 J_x\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)dx = \\ & = B_1 + \ldots + B_8. \end{aligned} \tag{3.4.8}$$

Here, we have used that $n_x = 0$ and $V = 0$ on $\partial\Omega$.
First we consider the terms on the left-hand side of (3.4.7) and (3.4.8). Since $n_x = 0$ and $V = 0$ on $\partial\Omega$, it holds:

$$\begin{aligned} & \int_0^1 \left(\frac{JJ_t}{n} - \frac{1}{2}\frac{J^2 n_t}{n^2}\right)dx = \partial_t\int_0^1 \frac{1}{2}\frac{J^2}{n}dx, \\ & \int_0^1 n_t \log n dx = \partial_t\int_0^1 (n(\log n - 1) + 1)dx \\ & -\int_0^1 V n_t dx = -\lambda^2\int_0^1 V_{xxt} V dx = \lambda^2\int_0^1 V_{xt}V_x dx = \frac{\lambda^2}{2}\partial_t\int_0^1 V_x^2 dx, \\ & -\int_0^1 \frac{\epsilon^2}{2}n_t\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}}\right)dx = -\epsilon^2\int_0^1 \frac{n_t}{2\sqrt{n}}(\sqrt{n})_{xx}dx = \\ & -\epsilon^2\int_0^1 (\sqrt{n})_t(\sqrt{n})_{xx}dx = \frac{\epsilon^2}{2}\partial_t\int_0^1 (\sqrt{n})_x^2 dx. \end{aligned}$$

Hence, the sum of the left-hand sides of (3.4.7) and (3.4.8) is equal to $\partial_t E(t)$ where

$$E(t) = \int_0^1 \left[\frac{\epsilon^2}{2}(\sqrt{n})_x^2 + T(n(\log n - 1) + 1) + \frac{\lambda^2}{2}V_x^2 + \frac{1}{2}\frac{J^2}{n}\right](x,t)dx \geq 0.$$

Now we compute the right-hand sides of (3.4.7) and (3.4.8). Notice that $A_2 + B_5 = 0$, $A_4 + B_8 = 0$, $A_3 + B_7 = 0$. Using $n = 1$ on $\partial\Omega$, we obtain:

$$A_1 + B_6 = \int_0^1 \left(\frac{n_x J^3}{n^3} - \frac{3}{2}\frac{J^2 J_x}{n^2} \right) dx = -\frac{1}{2}\int_0^1 \left(\frac{J^3}{n^2} \right)_x dx = \frac{1}{2}J^3(0) - \frac{1}{2}J^3(1).$$

A computation gives:

$$A_6 + B_2 = \nu \int_0^1 \left(-\frac{J_x^2}{n} + \frac{2JJ_x n_x}{n^2} - \frac{J^2 n_x^2}{n^3} \right) dx = -\nu \int_0^1 \left(\frac{J_x}{\sqrt{n}} - \frac{n_x J}{n^{3/4}} \right)^2 dx.$$

By integration by parts and $n_x = 0$ on $\partial\Omega$, we obtain

$$\int_0^1 \frac{n_x^2 n_{xx}}{n^2}\, dx = \frac{2}{3}\int_0^1 \frac{n_x^4}{n^3}\, dx,$$

and therefore

$$\begin{aligned} B_4 &= -\nu\frac{\varepsilon^2}{2}\int_0^1 n_{xx}\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}} \right) dx = \varepsilon^2 \nu \int_0^1 \left(\frac{1}{8}\frac{n_x^2 n_{xx}}{n^2} - \frac{1}{4}\frac{n_{xx}^2}{n} \right) dx \\ &= -\varepsilon^2 \nu \int_0^1 \left((\sqrt{n})_{xx}^2 + \frac{1}{48}\frac{n_x^4}{n^3} \right) dx. \end{aligned}$$

Here we need that n =const on $\partial\Omega$. The above computations show that the sum of (3.4.7) and (3.4.8), integrated over (0,t), can be written as:

$$E(t) - E(0) = -\int_0^t \int_0^1 \left[\varepsilon^2\nu(\sqrt{n})_{xx}^2 + \varepsilon^2\nu\frac{1}{48}\frac{n_x^4}{n^3} + 4\nu T(\sqrt{n})_x^2 + \frac{\nu}{\lambda^2}(n-1)^2 + \right.$$
$$\left. +\nu\left(\frac{J_x}{\sqrt{n}} - \frac{n_x J}{n^{3/4}} \right)^2 + \frac{1}{\tau}\frac{J^2}{n} \right] dx d\tau + \int_0^t \int_{\partial\Omega} \left[\frac{\varepsilon^2}{2}\left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}} J \right) + \nu J J_x - \frac{1}{2}J^3 \right] ds dt.$$

The first integral on the right-hand side is the entropy dissipation rate. Since $n_x = 0$ and $n = 1$ on $\partial\Omega$, we can write the boundary integral as:

$$\int_0^t \int_{\partial\Omega} \left[\frac{\varepsilon^2}{4} n_{xx} J + \nu J J_x - \frac{1}{2}J^3 \right] ds dt.$$

The boundary condition $n(\cdot, t) = 1$ on $\partial\Omega$ implies $\nu n_{xx} - J_x(\cdot, t) = n_t(\cdot, t) = 0$ on $\partial\Omega$, and the, using (3.4.6)

$$\int_0^t \int_{\partial\Omega} \left[\frac{\varepsilon^2}{4} n_{xx} J + \nu J J_x - \frac{1}{2}J^3 \right] ds dt = \int_0^t \int_{\partial\Omega} \left[\frac{\varepsilon^2}{4\nu} J J_x + \nu J J_x - \frac{1}{2}J^3 \right] ds dt = 0.$$

We apply the Poincaré inequality:

$$\|u\|_{L^2(\Omega)} \leq \frac{1}{\sqrt{2}}\|u_x\|_{L^2(\Omega)}, \qquad \forall \quad u \in H_0^1(\Omega),$$

to $u = (\sqrt{n})_x$ to obtain:

$$\frac{\varepsilon^2}{2}\int_0^1 (\sqrt{n})_x^2(x,t)dx \leq E(t) \leq E(0) - \big(2\nu\varepsilon^2 + 4\nu T\big)\int_0^1\int_0^t (\sqrt{n})_x^2(x,t)dxdt.$$

Gronwall's lemma implies:

$$\epsilon^2\|(\sqrt{n})_x(\cdot,t)\|^2_{L^2(\Omega)} \leq 2E(0)e^{-4\nu(\epsilon^2+2T)t}, \qquad t \geq 0.$$

The Sobolev-Poincaré inequality:

$$\|u-1\|_{L^\infty(\Omega)} \leq \|u_x\|_{L^2(\Omega)}, \qquad \forall (u-1) \in H_0^1(\Omega),$$

then gives

$$\epsilon^2\|\sqrt{n}(\cdot,t) - 1\|^2_{L^\infty(\Omega)} \leq 2E(0)e^{-4\nu(\epsilon^2+2T)t}, \qquad t \geq 0.$$

Furthermore, we conclude from:

$$\frac{1}{2}\int_0^1 \frac{J^2}{n}dx \leq E(t) \leq E(0) - \frac{1}{\tau}\int_0^1\int_0^t \frac{J^2}{n}dxdt$$

the estimate

$$\left\|\frac{J(\cdot,t)}{\sqrt{n(\cdot,t)}}\right\|^2_{L^2(\Omega)} \leq 2E(0)e^{\frac{-2}{\tau}t}, \qquad t > 0.$$

Finally, from the elliptic estimate:

$$\sqrt{2}\lambda^2\|V\|_{L^2(\Omega)} \leq \|n-1\|_{L^2(\Omega)},$$

we infer:

$$\frac{\lambda^2}{2}\int_0^1\int_0^t V_x^2 dxdt \leq E(t) \leq E(0) - 2\nu\lambda^2\int_0^1\int_0^t V_x^2 dxdt,$$

and hence:

$$\lambda^2\|V(\cdot,t)\|^2_{L^\infty(\Omega)} \leq \lambda^2\|V_x(\cdot,t)\|^2_{L^2(\Omega)} \leq 2E(0)e^{-4\nu\lambda^2 t}, \quad t \geq 0.$$

This proves the theorem. $\square$

Chapter 4

A nonlinear fourth-order parabolic equation

The nonlinear fourth-order parabolic equation

$$n_t + (n(\log n)_{xx})_{xx} = 0, \quad n(\cdot, 0) = n_I \geq 0 \quad \text{in } (0,1),\ t > 0,$$

subject to the boundary conditions

$$n(0,t) = n_0, \quad n(1,t) = n_1, \quad n_x(0,t) = w_0, \quad n_x(1,t) = w_1, \quad t > 0,$$

where $n_0,\ n_1 > 0$ and $w_0,\ w_1 \in \mathbb{R}$ is analyzed. This equation has been first derived in the context of fluctuation of a stationary non equilibrium interface [**34**] and also appears in quantum semiconductor modeling; it is a zero-temperature zero-field approximation of the quantum drift-diffusion model (1.0.11). The first part of this work is devoted to the study of the existence and uniqueness of (smooth) stationary solution. The proof of this result is based on a Leray-Schauder fixed-point argument.
Then, by a time discretization, the proof of existence of weak solutions for the time dependent problem is shown.
The last part of this chapter concerns the long-time behaviour of the weak solutions and few numerical simulations are presented. The exponential decay toward the steady solution is proved by an entropy/ entropy dissipation method, using a technical assumption on this steady solution and a Cszisar-Kullback estimate provides convergence in L^1-norm.
The main results of this chapter are summarized in the following theorems

4.1 Theorem. *Let $n_0,\ n_1 > 0$ and $w_0,\ w_1 \in \mathbb{R}$. Then there exists a unique classical solution $u \in C^\infty([0,1])$ to*

$$(n(\log n)_{xx})_{xx} = 0 \quad \text{in } (0,1),$$
$$n(0) = n_0,\ n(1) = n_1,\ n_x(0) = w_0,\ n_x(1) = w_1, \tag{4.0.1}$$

satisfying $n(x) \geq m > 0$ for all $x \in [0,1]$, and the constant $m > 0$ only depends on the boundary data.

4.2 Theorem. *Let n_0, $n_1 > 0$ and w_0, $w_1 \in \mathbb{R}$. Let $n_I(x) \geq 0$ be integrable such that $\int_0^1 (n_I - \log n_I)dx < \infty$. Then there exists a weak solution n to* (1.3.1), (1.3.3) *satisfying $n(x,t) \geq 0$ in $(0,1) \times (0,\infty)$ and*

$$n \in L^{5/2}_{\mathrm{loc}}(0,\infty; W^{1,1}(0,1)) \cap W^{1,10/9}_{\mathrm{loc}}(0,\infty; H^{-2}(0,1)),\ \log n \in L^2_{\mathrm{loc}}(0,\infty; H^2(0,1)).$$

4.3 Theorem. *Let the assumptions of Theorem 4.2 hold and let $\int_0^1 n_I(\log n_I - 1)dx < \infty$. Let n be the solution to* (1.3.1), (1.3.3) *constructed in Theorem 4.2 and let n_∞ be the unique solution to* (4.0.1). *We assume that the boundary data is such that $\log n_\infty$ is concave. Then there exist constants $c, \lambda > 0$ only depending on the boundary and initial data such that for all $t > 0$,*

$$\|n(\cdot,t) - n_\infty\|_{L^1(0,1)} \leq ce^{-\lambda t}.$$

4.1 Existence and uniqueness of stationary solution

In this section we will prove Theorem 4.1. First, we perform the transformation of variables $y = \log n$ and consider the problem

$$\begin{aligned} &(e^y y_{xx})_{xx} = 0 \quad \text{in } (0,1), \\ &y(0) = y_0,\ y(1) = y_1,\ y_x(0) = \alpha,\ y_x(1) = \beta, \end{aligned} \tag{4.1.1}$$

where $y_0 = \log n_0$, $y_1 = \log n_1$, $\alpha = w_0/n_0$, and $\beta = w_1/n_1$. Clearly, any classical solution of (4.1.1) is a positive classical solution of (4.0.1). We show first some *a priori* estimates for the solution of (4.1.1).

4.4 Lemma. *Let y be a classical solution to* (4.1.1). *Then*

$$y(x) \leq M := \max\{y_0, y_1\} + |\alpha| + |\beta|. \tag{4.1.2}$$

Proof. First we observe that there exist constants a, $b \in \mathbb{R}$ such that y solves the equation $y_{xx} = (ax+b)e^{-y}$. This implies that y_{xx} can change its sign at most once. In the following we consider several cases for the sign of $y_{xx}(0)$ and $y_{xx}(1)$.

First case: Let $y_{xx}(0) \geq 0$ and $y_{xx}(1) \geq 0$. Since y_{xx} can change the sign at most once it follows that $y_{xx} \geq 0$ in $(0,1)$. We conclude that $y(x) \leq \max\{y_0, y_1\}$ for all $x \in [0,1]$.

Second case: Let $y_{xx}(0) \geq 0$ and $y_{xx}(1) < 0$. There exists $x_1 \in [0, 1)$ such that $y_{xx}(x_1) = 0$. Therefore, $ax + b \geq 0$ for all $x \in [0, x_1]$ and $ax + b \leq 0$ for all $x \in [x_1, 1]$. A Taylor expansion gives for all $x \in [x_1, 1]$

$$\begin{aligned} y(x) &= y(1) + y_x(1)(x-1) + \int_x^1 (s-x)y_{xx}(s)ds \\ &= y_1 + \beta(x-1) + \int_x^1 (s-x)(as+b)e^{-y(s)}ds \leq \max\{y_0, y_1\} + |\beta|. \end{aligned}$$

We claim that $y(x) \leq \max\{y_0, y_1\} + |\beta|$ holds for all $x \in [0, x_1]$. For this, let $x_2 \in [0, x_1]$ be such that $y(x_2) = \max\{y(x) : x \in [0, x_1]\}$. Suppose that $y(x_2) > \max\{y_0, y_1\} + |\beta|$. Then $x_2 \in (0, x_1)$ and, since $y(x)$ reaches a maximum at the interior point x_2, $y_{xx}(x_2) \leq 0$. Since $x_2 \in (0, x_1)$, we have $y_{xx}(x_2) = (ax_2 + b)e^{-y(x_2)} \geq 0$. This shows that $y_{xx}(x_2) = 0$. But then $y_{xx}(x_2) = (ax_2 + b)e^{-y(x_2)}$ implies that $ax_2 + b = 0$. Since also $ax_1 + b = 0$, it follows that $a = b = 0$ and thus $y_{xx}(x) = 0$ for all $x \in [0, 1]$; contradiction to $y_{xx}(1) < 1$. Hence, $y(x) \leq \max\{y_0, y_1\} + |\beta|$ for all $x \in [0, 1]$.

Third case: Let $y_{xx}(0) < 0$ and $y_{xx}(1) \geq 0$. By similar arguments as in the second case, it can be shown that $y(x) \leq \max\{y_0, y_1\} + |\alpha|$ for all $x \in [0, 1]$.

Fourth case: Let $y_{xx}(0) < 0$ and $y_{xx}(1) < 0$. This implies $ax + b < 0$ for all $x \in [0, 1]$ and, by a Taylor expansion,

$$y(x) = y_0 + \alpha x + \int_0^x (x-s)(as+b)e^{-y(s)}ds \leq y_0 + |\alpha|, \quad x \in [0, 1].$$

The lemma is proved. □

4.5 Lemma. *Let y be a classical solution to* (4.1.1). *Then there exists a constant $K > 0$ only depending on y_0, y_1, α, and β such that*

$$\|y\|_{H^2(0,1)} \leq K.$$

Proof. There exist constants a, $b \in \mathbb{R}$ such that y solves the equation

$$y_{xx} = (ax + b)e^{-y} \quad \text{in } (0, 1), \tag{4.1.3}$$

and $b = e^{y_0}y_{xx}(0)$, $a = e^{y_1}y_{xx}(1) - e^{y_0}y_{xx}(0)$. In order to obtain a uniform estimate for y_{xx} we have first to find uniform estimates for a and b. For this, we multiply (4.1.3) by y_x^2 and integrate over $(0, 1)$:

$$\int_0^1 (ax + b)e^{-y}y_x^2 dx = \int_0^1 y_{xx}y_x^2 dx = \frac{1}{3}\int_0^1 (y_x^3)_x dx = \frac{1}{3}(\beta^3 - \alpha^3).$$

Next we multiply (4.1.3) by y_{xx}, integrate over $(0,1)$, integrate by parts, and use the above equality:

$$\begin{aligned}\int_0^1 y_{xx}^2 dx &= \int_0^1 (ax+b)e^{-y} y_{xx} dx \\ &= \int_0^1 (ax+b)e^{-y} y_x^2 dx - a\int_0^1 e^{-y} y_x dx + [(ax+b)e^{-y(x)} y_x(x)]_0^1 \\ &= \frac{1}{3}(\beta^3-\alpha^3) + a(e^{-y_1}-e^{-y_0}) + (a+b)e^{-y_1}\beta - be^{-y_0}\alpha.\end{aligned}$$

By Young's inequality this becomes

$$\int_0^1 y_{xx}^2 dx \le C + \frac{1}{60}e^{-2M}a^2 + \frac{1}{12}e^{-2M}b^2, \tag{4.1.4}$$

where $C := (\beta^3-\alpha^3)/3 + 15e^{2M}((1+\beta)e^{-y_1}-e^{-y_0})^2 + 3e^{2M}(\beta e^{-y_1}-\alpha e^{-y_0})^2$. Taking the square of (4.1.3) and integrating over $(0,1)$ yields, by Lemma 4.4,

$$\begin{aligned}\int_0^1 y_{xx}^2 dx &= \int_0^1 (ax+b)^2 e^{-2y} dx \ge e^{-2M}\int_0^1 (ax+b)^2 dx \\ &= \frac{1}{3}e^{-2M}(a^2+3ab+3b^2) \ge \frac{1}{3}e^{-2M}\left(\frac{a^2}{10}+\frac{b^2}{2}\right),\end{aligned} \tag{4.1.5}$$

where we have used the Young inequality $3ab \ge -9a^2/10 - 5b^2/2$. Putting together (4.1.4) and (4.1.5), we obtain

$$\frac{a^2}{10}+\frac{b^2}{2} \le 3e^{2M}\int_0^1 y_{xx}^2 dx \le 3e^{2M}C + \frac{a^2}{20}+\frac{b^2}{4}. \tag{4.1.6}$$

Therefore, a and b are bounded by a constant which only depends on y_0, y_1, α, and β. By (4.1.4) this gives a uniform estimate for $\|y_{xx}\|_{L^2(0,1)}$ and, employing Poincaré inequality, also for $\|y\|_{H^2(0,1)}$. $\square$

Proof of Theorem 4.1. We wish to employ the Leray-Schauder fixed-point theorem. For this let $\sigma \in [0,1]$ and $z \in H^1(0,1)$ and let $y \in H^2(0,1)$ be the unique solution of

$$(e^z y_{xx})_{xx} = 0 \quad \text{in } (0,1), \quad y(0)=\sigma y_0,\ y(1)=\sigma y_1,\ y_x(0)=\sigma\alpha,\ y_x(1)=\sigma\beta.$$

This defined a fixed-point operator $S : H^1(0,1)\times[0,1] \to H^1(0,1)$, $S(z,\sigma) = y$. Clearly, $S(z,0) = 0$ for all z. Moreover, by standard arguments, S is continuous and compact, since the embedding $H^2(0,1) \hookrightarrow H^1(0,1)$ is compact. It remains to show that there exists a constant $K > 0$ such that for all $\sigma \in [0,1]$ and for any fixed point y of $S(\cdot,\sigma)$, the estimate $\|y\|_{H^1(0,1)} \le K$ holds. Lemma 4.5 settles the case $\sigma = 1$. For $\sigma < 1$, a similar proof as in Lemma 4.5 shows the existence of a constant $K > 0$ such that $\|y\|_{H^2(0,1)} \le K$ holds. By Leray-Schauder's theorem, this proves the existence of a solution $y \in H^2(0,1)$ to (4.1.1).

Actually, the solution y is a classical solution. Indeed, y satisfies $y_{xx} = (ax+b)e^{-y} \in H^2(0,1)$ for some $a,\ b \in \mathbb{R}$ and hence, $y \in H^4(0,1)$. By bootstrapping, $y \in H^n(0,1)$ for all $n \in \mathbb{N}$ and y is a classical solution.

In order to prove the uniqueness of solutions, we extend an idea of [**54**]. Let n_1 and n_2 be two positive classical solutions to (4.0.1). We multiply (4.0.1) for n_1 by $1-\sqrt{n_2/n_1}$ and (4.0.1) for n_2 by $\sqrt{n_1/n_2}-1$, integrate and take the difference. This yields, by integrating by parts,

$$\begin{aligned}
0 &= \int_0^1 \Big[(n_1(\log n_1)_{xx})_{xx}(1-\sqrt{n_2/n_1}) - (n_2(\log n_2)_{xx})_{xx}(\sqrt{n_1/n_2}-1)\Big]\,dx \\
&= 2\int_0^1 \left[(\sqrt{n_1})_{xxxx} - \frac{1}{\sqrt{n_1}}(\sqrt{n_1})_{xx}^2 - (\sqrt{n_2})_{xxxx} + \frac{1}{\sqrt{n_2}}(\sqrt{n_2})_{xx}^2\right](\sqrt{n_1}-\sqrt{n_2})dx \\
&= 2\int_0^1 \Big[((\sqrt{n_1})_{xx}-(\sqrt{n_2})_{xx})(\sqrt{n_1}-\sqrt{n_2})_{xx} \\
&\qquad -(\sqrt{n_1})_{xx}^2\left(1-\sqrt{\tfrac{n_2}{n_1}}\right) + (\sqrt{n_2})_{xx}^2\left(\sqrt{\tfrac{n_1}{n_2}}-1\right)\Big]dx \\
&= 2\int_0^1 \left(\sqrt[4]{\frac{n_2}{n_1}}(\sqrt{n_1})_{xx} - \sqrt[4]{\frac{n_1}{n_2}}(\sqrt{n_2})_{xx}\right)^2. \qquad (4.1.7)
\end{aligned}$$

Therefore,

$$0 = \sqrt[4]{\frac{n_2}{n_1}}(\sqrt{n_1})_{xx} - \sqrt[4]{\frac{n_1}{n_2}}(\sqrt{n_2})_{xx} \quad \text{in } (0,1).$$

Writing $n_1 = e^{y_1}$ and $n_2 = e^{y_2}$, this identity is equal to

$$\begin{aligned}
0 &= e^{(y_2-y_1)/4}(e^{y_1/2})_{xx} - e^{(y_1-y_2)/4}(e^{y_2/2})_{xx} \\
&= \frac{1}{2}e^{(y_2+y_1)/4}\left(y_{1,xx}+\frac{1}{2}y_{1,x}^2\right) - \frac{1}{2}e^{(y_1+y_2)/4}\left(y_{2,xx}+\frac{1}{2}y_{2,x}^2\right).
\end{aligned}$$

and hence

$$y_{1,xx} - y_{2,xx} = -\frac{1}{2}(y_{1,x}^2 - y_{2,x}^2) \quad \text{in } (0,1). \qquad (4.1.8)$$

We integrate this equation over $(0,x_0)$, use the boundary condition $y_{1x}(0) = y_{2x}(0)$, and take the supremum:

$$\|(y_1-y_2)_x\|_{L^\infty(0,x_0)} \le \int_0^{x_0} |(y_1+y_2)_x|\cdot|(y_1-y_2)_x|dx \le x_0 L\|(y_1-y_2)_x\|_{L^\infty(0,x_0)},$$

where $L = \|y_{1,x}\|_{L^\infty(0,1)} + \|y_{2,x}\|_{L^\infty(0,1)}$. Choosing $x_0 = 1/2L$ gives $(y_1 - y_2)_x = 0$ and hence $y_1 - y_2 = 0$ in $[0, x_0]$. In particular, $(y_1 - y_2)_x(x_0) = 0$. Therefore, integrating (4.1.8) over $(x_0, 2x_0)$ we obtain by the same arguments that $y_1 - y_2 = 0$ in $[x_0, 2x_0]$. After a finite number of steps we achieve $y_1 - y_2 = 0$ in $[0, 1]$. This proves the uniqueness of solutions. □

4.6 Remark. Equation (4.1.3) with $y(0) = y(1)$ and $y_x(0) = -y_x(1) \leq 0$ is formally related to a combustion problem. Indeed, the boundary conditions imply that y is symmetric around $x = \frac{1}{2}$ and that $y(x) \leq y(0) = y_0$ holds for any $x \in [0, 1]$. The symmetry implies further $a = e^{y_0}(y_{xx}(1) - y_{xx}(0)) = 0$ and moreover, $b = e^{y_0} y_{xx}(0) \geq 0$. Thus we can write (4.1.3) as $y_{xx} = be^{-y}$ or, introducing $z(x) = -y(x)$,

$$z_{xx} + be^z = 0 \quad \text{in } (0,1), \quad z(0) = z(1) = -y_0.$$

This is the solid fuel ignition model of [**14**]. It is well known that there exists $b^* > 0$ such that this problem has exactly two solutions if $b \in (0, b^*)$, it has exactly one solution if $b = b^*$, and no solution exists if $b > b^*$ [**14, 38**]. This relation provides a better bound for b (for the above special boundary conditions) than the estimate (4.1.6). Indeed, $a = 0$ and b is uniformly bounded by a number $b^* > 0$ *independently* of the boundary conditions (and only depending on the domain $(0, 1)$).

4.2 Existence of transient solutions

In order to prove Theorem 4.2 we again perform the exponential change of unknowns and we semi-discretize (1.3.1) in time. For this, we divide the time interval $(0, T]$ for some $T > 0$ in N subintervals $(t_{k-1}, t_k]$, with $k = 1, \ldots, N$, where $0 = t_0 < \cdots < t_N = T$. Define $\tau_k = t_k - t_{k-1} > 0$ and $\tau = \max\{\tau_k : k = 1, \ldots, N\}$. We assume that $\tau \to 0$ as $N \to \infty$.

Let $n_\infty > 0$ be the unique classical solution to (4.0.1) and set $y_\infty = \log n_\infty$. We perform the transformation $z = \log(n/n_\infty)$ and $z_0 = \log(n_I/n_\infty)$. For given $k \in \{1, \ldots, N\}$ and z_{k-1} we first solve the semi-discrete problem

$$\frac{e^{y_\infty}}{\tau_k}(e^{z_k} - e^{z_{k-1}}) = -\left(e^{z_k + y_\infty}(z_k + y_\infty)_{xx}\right)_{xx}, \quad z_k \in H_0^2(0,1). \tag{4.2.1}$$

4.7 Proposition. *For each $k = 1, \ldots, N$, there exists a unique weak solution $z_k \in H_0^2(0, 1)$ to* (4.2.1).

For the proof of this proposition we show first some *a priori* estimates.

4.8 Lemma. *Let $z_k \in H_0^2(0,1)$ be a weak solution to (4.2.1). Then there exists a constant $c > 0$ only depending on T, n_I, and n_∞ such that*

$$\|e^{z_k/2}\|_{L^2(0,1)} \leq c, \tag{4.2.2}$$

$$\sum_{i=1}^{N} \tau_i \int_0^1 e^{z_i/2} \left((z_i + y_\infty)_{xx}^2 + (z_i + y_\infty)_x^4 \right) \leq c, \tag{4.2.3}$$

$$\sum_{i=1}^{N} \tau_i \|e^{z_i}\|_{L^\infty(0,1)} \leq c. \tag{4.2.4}$$

Proof. Similarly as in the uniqueness proof of Theorem 4.1 we use the test functions $1-e^{-z_k/2} \in H_0^2(0,1)$ in the weak formulation of the semi-discretized equation (4.2.1) and $e^{z_k/2} - 1 \in H_0^2(0,1)$ in the weak formulation of the stationary equation (4.0.1) and take the sum of the corresponding equations:

$$\begin{aligned} \frac{1}{\tau_k} \int_0^1 e^{y_\infty}(e^{z_k} - e^{z_{k-1}})(1 - e^{-z_k/2})dx &= \int_0^1 e^{z_k + y_\infty}(z_k + y_\infty)_{xx}(e^{-z_k/2})_{xx}dx \\ &\quad + \int_0^1 e^{y_\infty} y_{\infty,xx}(e^{z_k/2})_{xx}dx. \end{aligned} \tag{4.2.5}$$

The right-hand side is equal to the first integral in (4.1.7) with $n_1 = e^{z_k + y_\infty}$ and $n_2 = e^{y_\infty}$. Therefore, the right-hand side is equal to the expression

$$-2 \int_0^1 \left(e^{-z_k/4}(e^{(z_k+y_\infty)/2})_{xx} - e^{z_k/4}(e^{y_\infty/2})_{xx} \right)^2 dx.$$

For the left-hand side of (4.2.5) we write

$$\begin{aligned} &\frac{1}{\tau_k} \int_0^1 e^{y_\infty}(e^{z_k} - e^{z_{k-1}})(1 - e^{-z_k/2})dx \\ &= \frac{1}{\tau_k} \int_0^1 e^{y_\infty}((e^{z_k/2} - 1)^2 - (e^{z_{k-1}/2} - 1)^2)dx + \frac{1}{\tau_k} \int_0^1 e^{y_\infty}(e^{z_k/4} - e^{z_{k-1}/2 - z_k/4})^2 dx \\ &\geq \frac{1}{\tau_k} \int_0^1 e^{y_\infty} \left((e^{z_k/2} - 1)^2 - (e^{z_{k-1}/2} - 1)^2 \right) dx. \end{aligned}$$

Therefore, we conclude from (4.2.5), for all $k = 1, \ldots, N$,

$$\begin{aligned} &\tfrac{1}{\tau_k} \textstyle\int_0^1 e^{y_\infty}(e^{z_k/2} - 1)^2 dx + 2 \int_0^1 \left(e^{-z_k/4}(e^{(z_k+y_\infty)/2})_{xx} - e^{z_k/4}(e^{y_\infty/2})_{xx} \right)^2 dx \\ &\qquad \leq \tfrac{1}{\tau_k} \textstyle\int_0^1 e^{y_\infty}(e^{z_{k-1}/2} - 1)^2 dx. \end{aligned} \tag{4.2.6}$$

This yields

$$\begin{aligned} \int_0^1 e^{y_\infty}(e^{z_k/2} - 1)^2 dx &\leq \int_0^1 e^{y_\infty}(e^{z_0/2} - 1)^2 dx \\ &= \int_0^1 (\sqrt{n_I} - \sqrt{n_\infty})^2 dx < \infty \end{aligned} \tag{4.2.7}$$

and thus (4.2.2). Moreover, after summing up (4.2.6),

$$2\sum_{i=1}^{k}\tau_i\int_0^1\left(e^{-z_i/4}(e^{(z_i+y_\infty)/2})_{xx}-e^{z_i/4}(e^{y_\infty/2})_{xx}\right)^2dx\le\int_0^1 e^{y_\infty}(e^{z_0/2}-1)^2dx.$$

Young's inequality gives

$$4\sum_{i=1}^{k}\tau_i\int_0^1 e^{-z_i/2}\left(e^{(z_i+y_\infty)/2}\right)_{xx}^2dx\le c+c\sum_{i=1}^{k}\tau_i\int_0^1 e^{z_i/2}dx,$$

where here and in the following, $c>0$ denotes a generic constant only depending on T, n_I and n_∞. In view of (4.2.7), the right-hand side is uniformly bounded. Hence

$$\begin{aligned}&\sum_{i=1}^{k}\tau_i\int_0^1 e^{-(z_i+y_\infty)/2}\left(e^{(z_i+y_\infty)/2}\right)_{xx}^2dx\\ &\le\ \|e^{y_\infty/2}\|_{L^\infty(0,1)}\sum_{i=1}^{k}\tau_i\int_0^1 e^{-z_i/2}\left(e^{(z_i+y_\infty)/2}\right)_{xx}^2dx\le c.\end{aligned}$$

Now the assertion (4.2.3) follows since, by integration by parts,

$$\int_0^1 e^{n/2}n_x^2n_{xx}dx=-\frac{1}{6}\int_0^1 e^{n/2}n_x^4+\frac{1}{3}(e^{n(1)/2}n_x(1)^3-e^{n(0)/2}n_x(0)^3)$$

for all $n\in H^2(0,1)$ and hence,

$$\begin{aligned}&\int_0^1 e^{-(z_i+y_\infty)/2}\left(e^{(z_i+y_\infty)/2}\right)_{xx}^2dx\\ &=\ \frac{1}{4}\int_0^1 e^{(z_i+y_\infty)/2}\left((z_i+y_\infty)_{xx}^2+\frac{1}{4}(z_i+y_\infty)_x^4+(z_i+y_\infty)_{xx}(z_i+y_\infty)_x^2\right)dx\\ &=\ \frac{1}{4}\int_0^1 e^{(z_i+y_\infty)/2}\left((z_i+y_\infty)_{xx}^2+\frac{1}{12}(z_i+y_\infty)_x^4\right)dx+\frac{1}{12}(e^{y_1/2}\beta^3-e^{y_0/2}\alpha^3).\end{aligned}$$

Finally, (4.2.4) is a consequence of (4.2.3) and the Poincaré-Sobolev inequality since

$$\int_0^1 e^{z_i/2}(z_i)_x^4dx=8^4\int_0^1(e^{z_i/8})_x^4\ge c\|e^{z_i/8}\|_{L^\infty(0,1)}^4.$$

This shows the lemma. □

4.9 Lemma. *Let $z_k\in H_0^2(0,1)$ be a weak solution to (4.2.1). Then there exists a constant $c>0$ only depending on T, n_I, and n_∞ such that*

$$\int_0^1(e^{z_k}-z_k)dx+\sum_{i=1}^{k}\tau_i\int_0^1(z_i+y_\infty)_{xx}^2dx\le c. \tag{4.2.8}$$

Proof. We choose the test function $e^{-y_\infty}(1-e^{-z_k}) \in H_0^2(0,1)$ in the weak formulation of (4.2.1). Then, by Young's inequality,

$$\begin{aligned}
&\int_0^1 (e^{z_k} - e^{z_{k-1}})(1-e^{-z_k})dx \\
&= -\tau_k \int_0^1 e^{z_k}(z_k+y_\infty)_{xx}(y_{\infty,x}^2 - y_{\infty,xx})dx - \tau_k \int_0^1 (z_k+y_\infty)_{xx}^2 dx \\
&\quad + \tau_k \int_0^1 (z_k+y_\infty)_x^2 (z_k+y_\infty)_{xx} dx \\
&\le \tau_k \int_0^1 e^{z_k/2}(z_k+y_\infty)_{xx}^2 dx + \tau_k \int_0^1 e^{3z_k/2}(y_{\infty,x}^2 - y_{\infty,xx})^2 dx \\
&\quad - \tau_k \int_0^1 (z_k+y_\infty)_{xx}^2 dx + \frac{\tau_k}{3}(\beta^3 - \alpha^3).
\end{aligned}$$

In view of (4.2.3) and (4.2.4), the right-hand side is uniformly bounded. The left-hand side can be estimated by

$$\int_0^1 (e^{z_k} - e^{z_{k-1}})(1-e^{-z_k})dx \ge \int_0^1 (e^{z_k} - z_k)dx - \int_0^1 (e^{z_{k-1}} - z_{k-1})dx,$$

which is a consequence of the elementary inequality $e^x - 1 \ge x$ for all $x \in \mathbb{R}$. Thus, (4.2.8) is proved. $\square$

Proof of Proposition 4.7. The existence of a solution to (4.2.1) is shown by the Leray-Schauder fixed-point theorem. For this, let $k \in \{1,\ldots,N\}$ and z_{k-1} be given. Furthermore, let $w \in H^1(0,1)$, $\sigma \in [0,1]$, and define the linear forms

$$\begin{aligned}
a(z,\phi) &= \int_0^1 e^{w+y_\infty} z_{xx}\phi_{xx} dx, \\
F(\phi) &= -\frac{1}{\tau_k}\int_0^1 e^{y_\infty}(e^w - e^{z_{k-1}})\phi dx - \int_0^1 e^{w+y_\infty} y_{\infty,xx}\phi_{xx} dx,
\end{aligned}$$

where $\phi \in H_0^2(0,1)$. Consider the linear problem

$$a(z,\phi) = \sigma F(\phi) \quad \text{for all } \phi \in H_0^2(0,1).$$

By Lax-Milgram's lemma, there exists a unique solution $z \in H_0^2(0,1)$ to this problem. This defines the fixed-point operator $S : H^1(0,1) \times [0,1] \to H^1(0,1)$, $S(w,\sigma) = z$. It is not difficult to show that S is continuous and compact, since the embedding $H_0^2(0,1) \hookrightarrow H^1(0,1)$ is compact. Moreover, $S(w,0) = 0$ for all $w \in H^1(0,1)$. It remains to prove that any fixed point of

S satisfies a uniform bound in $H^1(0,1)$. In fact, Lemma 4.9 shows that any fixed point $z \in H_0^2(0,1)$ is uniformly bounded if $\sigma = 1$. The estimate for $\sigma < 1$ is similar (and, in fact, independent of σ). This provides the wanted bound in $H^1(0,1)$, and Leray-Schauder's theorem can be applied to yield the existence of a solution to (4.2.1). □

For the proof of Theorem 4.2 we need some more uniform estimates. Let $z^{(N)}$ be defined by $z^{(N)}(x,t) = z_k(x)$ if $t \in (t_{k-1}, t_k]$, $x \in (0,1)$.

4.10 Lemma. *The following estimates hold:*

$$\|z^{(N)}\|_{L^\infty(0,T;L^1(0,1))} + \|z^{(N)}\|_{L^2(0,T;H^2(0,1))} \leq c, \tag{4.2.9}$$

$$\|z^{(N)}\|_{L^{5/2}(0,T;W^{1,\infty}(0,1))} + \|e^{z^{(N)}}\|_{L^{5/2}(0,T;W^{1,1}(0,1))} \leq c, \tag{4.2.10}$$

where $c > 0$ only depends on n_I and the boundary data.

Proof. The inequality $e^x - x \geq |x|$ for all $x \in \mathbb{R}$ and the estimate (4.2.8) imply that $z^{(N)}$ is uniformly bounded in $L^\infty(0,T;L^1(0,1))$ which, together with (4.2.8), shows (4.2.9). Then, using the Poincaré and Gagliardo-Nirenberg inequalities, we obtain from (4.2.8)

$$\begin{aligned}\|z^{(N)}\|_{L^{5/2}(0,T;W^{1,\infty}(0,1))} &\leq c\|z_x^{(N)}\|_{L^{5/2}(0,T;L^\infty(0,1))} \\ &\leq c\|z^{(N)}\|_{L^\infty(0,T;L^1(0,1))}^{1/5}\|z^{(N)}\|_{L^2(0,T;H^2(0,1))}^{4/5} \leq c.\end{aligned}$$

This estimate, (4.2.2), and the first bound in (4.2.9) imply (4.2.10) since

$$\begin{aligned}\|e^{z^{(N)}}\|_{L^{5/2}(0,T;W^{1,1}(0,1))} &\leq c\left(\|e^{z^{(N)}}\|_{L^{5/2}(0,T;L^1(0,1))} + \|(e^{z^{(N)}})_x\|_{L^{5/2}(0,T;L^1(0,1))}\right) \\ &\leq c\|e^{z^{(N)}}\|_{L^{5/2}(0,T;L^1(0,1))} \\ &\quad + c\|e^{z^{(N)}}\|_{L^\infty(0,T;L^1(0,1))}\|z_x^{(N)}\|_{L^{5/2}(0,T;L^\infty(0,1))} \\ &\leq c.\end{aligned}$$

The lemma is proved. □

We also need an estimate for the discrete time derivative. For this, introduce the shift operator $(\sigma_N(z^{(N)}))(\cdot,t) = z_{k-1}$ for $t \in (t_{k-1}, t_k]$.

4.11 Lemma. *The following estimate holds:*

$$\|e^{z^{(N)}} - e^{\sigma_N(z^{(N)})}\|_{L^{10/9}(0,T;H^{-2}(0,1))} \leq c\tau, \tag{4.2.11}$$

where $c > 0$ only depends on n_I and n_∞.

Proof. From (4.2.1) and Hölder's inequality we obtain

$$\begin{aligned}\tfrac{1}{\tau_k}\|e^{z^{(N)}} - e^{\sigma_N(z^{(N)})}\|_{L^{10/9}(0,T;H^{-2}(0,1))} &\le \|e^{z^{(N)}+y_\infty}(z^{(N)} + y_\infty)_{xx}\|_{L^{10/9}(0,T;L^2(0,1))} \\ &\le \|e^{z^{(N)}+y_\infty}\|_{L^{5/2}(0,T;L^\infty(0,1))}\|(z^{(N)} + y_\infty)_{xx}\|_{L^2(0,T;L^2(0,1))}\end{aligned}$$

and the right-hand side is uniformly bounded by (4.2.9) and (4.2.10) since $W^{1,1}(0,1) \hookrightarrow L^\infty(0,1)$. $\square$

Proof of Theorem 4.2. For any $N \in \mathbb{N}$, there exists a solution $z^{(N)} \in L^2(0,T;H_0^2(0,1))$ to the sequence of recursive equations (4.2.1) satisfying $z^{(N)}(\cdot,0) = z_0$. The uniform bounds (4.2.10) and (4.2.11) and the compact embedding $W^{1,1}(0,1) \hookrightarrow L^1(0,1)$ allow to apply Theorem 5 of [**70**] (Aubin's lemma) yielding the existence of a subsequence of $e^{z^{(N)}}$ (not relabeled) such that $e^{z^{(N)}} \to \rho$ strongly in $L^1(0,T;L^1(0,1))$ and hence also in $L^1(0,T;H^{-2}(0,1))$. The above results give, using (4.2.2) and $L^1(0,1) \hookrightarrow H^{-2}(0,1)$,

$$\begin{aligned}\|e^{z^{(N)}} - \rho\|^2_{L^2(0,T;H^{-2}(0,1))} &\le \|e^{z^{(N)}} - \rho\|_{L^\infty(0,T;H^{-2}(0,1))}\|e^{z^{(N)}} - \rho\|_{L^1(0,T;H^{-2}(0,1))} \\ &\le c\left(\|e^{z^{(N)}}\|_{L^\infty(0,T;L^1(0,1))} + \|\rho\|_{L^\infty(0,T;L^1(0,1))}\right) \\ &\qquad \times \|e^{z^{(N)}} - \rho\|_{L^1(0,T;H^{-2}(0,1))} \\ &\le c\|e^{z^{(N)}} - \rho\|_{L^1(0,T;H^{-2}(0,1))} \to 0 \quad \text{as } N \to \infty. \qquad (4.2.12)\end{aligned}$$

Moreover, the estimate (4.2.9) provides the existence of a subsequence, also denoted by $z^{(N)}$, such that

$$z^{(N)} \rightharpoonup z \quad \text{weakly in } L^2(0,T;H^2(0,1)) \text{ as } N \to \infty. \qquad (4.2.13)$$

We claim now that $e^z = \rho$. For this, let w be a smooth function. Letting $N \to \infty$ in

$$0 \le \int_0^T \langle e^{z^{(N)}} - e^w, z^{(N)} - w\rangle_{H^{-2},H_0^2} dt$$

and using the convergence results (4.2.12) and (4.2.13) yields

$$0 \le \int_0^T \int_0^1 (\rho - e^w)(w - z)dxdt.$$

The strict monotonicity of $x \mapsto e^x$ then implies that $e^z = \rho$.
Thus, $e^{z^{(N)}} \to e^z$ strongly in $L^1(0,T;L^1(0,1))$ and (maybe for a subsequence) a.e. The uniform bound (4.2.10) implies that (after extracting a subsequence) $e^{z^{(N)}} \rightharpoonup e^z$ weakly* in $L^{5/2}(0,T;L^\infty(0,1))$ since $W^{1,1}(0,1) \hookrightarrow L^\infty(0,1)$. Therefore, we conclude via Lebesgue's convergence theorem that

$$e^{z^{(N)}} \to e^z \quad \text{strongly in } L^2(0,T;L^2(0,1)). \qquad (4.2.14)$$

Finally, the uniform estimate (4.2.11) gives for a subsequence

$$\frac{1}{\tau}(e^{z^{(N)}} - e^{\sigma_N(z^{(N)})}) \rightharpoonup (e^z)_t \quad \text{weakly in } L^{10/9}(0,T;H^{-2}(0,1)). \tag{4.2.15}$$

The convergence results (4.2.13)-(4.2.15) allow to pass to the limit $N \to \infty$ in the weak formulation of (4.2.1) to obtain a weak solution $z \in L^2(0,T;H_0^2(0,1))$ to

$$e^{y_\infty}(e^z)_t = -(e^{z+y_\infty}(z+y_\infty)_{xx})_{xx} \quad \text{in } (0,1),\ t>0,$$

such that $z(\cdot,0) = z_0 = \log(n_I/n_\infty)$ in the sense of $H^{-2}(0,1)$. Transforming back to the variable $u = e^{z+y_\infty}$ gives the assertion. $\square$

4.3 Long-time behavior of the solutions

This section is devoted to the proof of Theorem 4.3. The proof is based on the entropy–entropy production method. For this we need the following lemma for lower and upper estimates for the entropy

$$E_3 = \int_0^1 e^{y_\infty}(e^z(z-1)+1)dx.$$

4.12 Lemma. *Let z, $y_\infty \in L^\infty(0,1)$. Then*

$$c_1\left(\int_0^1 e^{y_\infty}|e^z-1|dx\right)^2 \le E_3 \le c_2\|e^{z/2}-1\|^2_{L^\infty(0,1)}, \tag{4.3.1}$$

where c_1, $c_2 > 0$ depend on $\|e^{y_\infty}\|_{L^\infty(0,1)}$ and $\|e^z\|_{L^1(0,1)}$.

The lower bound for E_3 is a Csiszar-Kullback-type inequality. A similar version of this lemma is shown in [**56**].

Proof. The upper bound is proved by expanding the function $f(x) = x^2(\log x^2 - 1) + 1$ around $x = 1$:

$$\begin{aligned} f(e^{z/2}) &= f(1) + f'(1)(e^{z/2}-1) + \frac{1}{2}f''(\theta)(e^{z/2}-1)^2 \\ &= 2(\log\theta + 1)(e^{z/2}-1)^2 \le 2(e^{z/2}+1)(e^{z/2}-1)^2, \end{aligned}$$

where θ lies between $e^{z/2}$ and 1, and using the inequality $\log\theta \le \theta - 1 \le \max\{e^{z/2},1\} - 1 \le e^{z/2}$. Then

$$E_3 \le 2\int_0^1 e^{y_\infty}(e^{z/2}+1)(e^{z/2}-1)^2dx \le 2\|e^{y_\infty}\|_{L^\infty(0,1)}(\|e^z\|^{1/2}_{L^1(0,1)}+1)\|e^{z/2}-1\|^2_{L^\infty(0,1)},$$

and we set $c_2 = 2\|e^{y_\infty}\|_{L^\infty(0,1)}(\|e^z\|^{1/2}_{L^1(0,1)} + 1)$.

For the lower bound we observe that a Taylor expansion of $f(x) = x(\log x - 1) + 1$ around $x = 1$ yields

$$e^{2y_\infty}(e^z(z-1)+1) = \frac{e^{2y_\infty}}{2\theta}(e^z-1)^2,$$

and $\theta = \theta(z)$ lies between e^z and 1. Then, by the Cauchy-Schwarz inequality,

$$\begin{aligned}
\int_0^1 e^{y_\infty}|e^z-1|dx &\leq \int_{\{z<0\}} e^{y_\infty}(1-e^z)dx + \int_{\{z>0\}} e^{y_\infty}(e^z-1)dx \\
&\leq \int_{\{z<0\}} e^{y_\infty}\frac{1-e^z}{\theta(z)^{1/2}}dx + \int_{\{z>0\}} e^{y_\infty}\frac{e^z-1}{\theta(z)^{1/2}}\theta(z)^{1/2}dx \\
&\leq \text{meas}\{z<0\}^{1/2}\left(\int_{\{z<0\}} e^{2y_\infty}\frac{(1-e^z)^2}{\theta(z)}dx\right)^{1/2} \\
&\quad + \left(\int_{\{z>0\}} e^{2y_\infty}\frac{(e^z-1)^2}{\theta(z)}dx\right)^{1/2}\left(\int_{\{z>0\}}\theta(z)dx\right)^{1/2} \\
&\leq (1+\|e^z\|^{1/2}_{L^1(0,1)})\left(\int_0^1 e^{2y_\infty}\frac{(e^z-1)^2}{\theta(z)}dx\right)^{1/2} \\
&\leq \sqrt{2}\|e^{y_\infty}\|^{1/2}_{L^\infty(0,1)}(1+\|e^z\|^{1/2}_{L^1(0,1)})E_3^{1/2},
\end{aligned}$$

and the assertion follows with $c_1^{-1} = 2\|e^{y_\infty}\|_{L^\infty(0,1)}(1+\|e^z\|^{1/2}_{L^1(0,1)})^2$. $\square$

Proof of Theorem 4.3. The idea is to differentiate the entropy E_3 of the introduction with respect to time and to use the differential equation (1.3.1). Since we do not have enough regularity for the solution u to (1.3.1), we need to regularize. We set as in the proof of Theorem 4.2 $n_\infty = e^{y_\infty}$, where n_∞ is the unique solution to (4.0.1). There exist numbers a, $b \in \mathbb{R}$ such that $e^{y_\infty}y_{\infty,xx} = ax + b \leq 0$ for all $x \in (0,1)$ since $y_\infty = \log n_\infty$ is assumed to be concave. This implies that $y_\infty \geq \min\{y_\infty(0), y_\infty(1)\}$ and hence $e^{y_\infty} \geq \min\{n_0, n_1\}$ in $(0,1)$. Furthermore, let $z_k \in H^2_0(0,1)$ be a solution to (4.2.1), for given z_{k-1}. We assume for simplicity that $\tau = \tau_k$ for all $k \in \mathbb{N}$.

Using z_k as a test function in the weak formulation of (4.2.1), we obtain, after integrating by parts,

$$\begin{aligned}
\frac{1}{\tau}\int_0^1 e^{y_\infty}(e^{z_k}-e^{z_{k-1}})z_k dx &= -\int_0^1 e^{z_k+y_\infty}(z_k+y_\infty)_{xx}z_{k,xx}dx \\
&= -\int_0^1 e^{z_k+y_\infty}z^2_{k,xx}dx - \int_0^1 e^{z_k}z_{k,xx}(ax+b)dx
\end{aligned}$$

$$
\begin{aligned}
&= -\int_0^1 e^{z_k+y_\infty} z_{k,xx}^2 dx + \int_0^1 e^{z_k} z_{k,x}^2 (ax+b) dx + a\int_0^1 e^{z_k} z_{k,x} dx \\
\text{(4.3.2)}\quad &\leq -\min\{n_0, n_1\}\int_0^1 e^{z_k} z_{k,xx}^2 dx,
\end{aligned}
$$

since $ax+b \leq 0$ in $(0,1)$ and $e^{z_k(x)} = 1$ for $x = 0, 1$. The left-hand side is estimated from below by employing the elementary inequality $e^x \geq x+1$ for all $x \in \mathbb{R}$:

$$
\begin{aligned}
&\frac{1}{\tau}\int_0^1 e^{y_\infty}(e^{z_k} - e^{z_{k-1}}) z_k dx \\
&\quad = \frac{1}{\tau}\int_0^1 e^{z_k+y_\infty}(z_k - 1) dx - \frac{1}{\tau}\int_0^1 e^{z_{k-1}+y_\infty}(z_{k-1} - 1) dx \\
&\qquad + \frac{1}{\tau}\int_0^1 e^{z_{k-1}+y_\infty}(e^{z_k - z_{k-1}} + z_{k-1} - z_k - 1) dx \\
\text{(4.3.3)}\qquad &\quad \geq \frac{1}{\tau}\int_0^1 e^{z_k+y_\infty}(z_k - 1) dx - \frac{1}{\tau}\int_0^1 e^{z_{k-1}+y_\infty}(z_{k-1} - 1) dx.
\end{aligned}
$$

This shows that the sequence $E^{(k)} = \int_0^1 e^{y_\infty}(e^{z_k}(z_k - 1) + 1) dx$ is non-increasing and bounded from below by $E^{(0)} = \int_0^1 (n_I(\log(n_I/n_\infty) - 1) + 1) dx$, which is finite.

We relate the entropy production term on the right-hand side of (4.3.2) to the entropy itself. We first claim that

$$
\text{(4.3.4)}\qquad \int_0^1 e^{z_k} z_{k,xx}^2 dx \geq 4\int_0^1 (e^{z_k/2})_{xx}^2 dx.
$$

To see this we set $n = e^{z_k}$ and observe that an integration by parts yields

$$
\int_0^1 \frac{n_{xx} n_x^2}{n^2} dx = \frac{2}{3}\int_0^1 \frac{n_x^4}{n^3} dx.
$$

Then

$$
\begin{aligned}
\int_0^1 e^{z_k} z_{k,xx}^2 dx &= \int_0^1 \left(\frac{n_{xx}^2}{n} - \frac{1}{3}\frac{n_x^4}{n^3}\right) dx \geq \int_0^1 \left(\frac{n_{xx}^2}{n} - \frac{5}{12}\frac{n_x^4}{n^3}\right) dx \\
\text{(4.3.5)}\qquad &= 4\int_0^1 (\sqrt{n})_{xx}^2 dx = 4\int_0^1 (e^{z_k/2})_{xx}^2 dx.
\end{aligned}
$$

We need the Poincaré inequalities

$$
\|n\|_{L^2(0,1)} \leq \frac{1}{\pi}\|n_x\|_{L^2(0,1)}, \quad \|n\|_{L^\infty(0,1)} \leq \|n_x\|_{L^2(0,1)}
$$

for all $n \in H_0^1(0,1)$. Therefore, using Lemma 4.12, we infer

$$\begin{aligned}\int_0^1 e^{z_k} z_{k,xx}^2 dx &\geq 4\pi^2 \int_0^1 (e^{z_k/2}-1)_x^2 dx \\ &\geq 4\pi^2 \|e^{z_k/2}-1\|_{L^\infty(0,1)}^2 \geq \frac{4\pi^2}{c_2} E^{(k)}. \end{aligned} \tag{4.3.6}$$

Setting $\gamma = 4\pi^2 \min\{n_0, n_1\}/c_2$, we obtain from (4.3.2) the difference inequality

$$E^{(k)} \leq E^{(k-1)} - \gamma\tau E^{(k)},$$

from which

$$E^{(k)} \leq (1+\gamma\tau)^{-1} E^{(k-1)} \leq (1+\gamma\tau)^{-k} E^{(0)} \leq (1+\gamma\tau)^{-t/\tau} E^{(0)} \tag{4.3.7}$$

follows. The parameter γ depends on $\|e^{z_k}\|_{L^1(0,1)}$ through c_2. However, since $e^{z^{(N)}}$ is uniformly bounded in $L^\infty(0,T;L^1(0,1))$ in view of Lemma 4.9, γ is bounded uniformly in k. We have shown in the proof of Theorem 4.2 that $e^{z_k} \to e^z$ a.e. Then the uniform boundedness of e^{z_k} and z_k and Lebesgue's dominated convergence theorem imply that

$$E^{(k)} \to E_3(t) = \int_0^1 e^{y_\infty}(e^{z(\cdot,t)}(z(\cdot,t)-1)+1)dx.$$

Hence, after letting $\tau \to 0$, we conclude from (4.3.7) that $E_3(t) \leq E_3(0)e^{-\gamma t}$. The first inequality in (4.3.1) gives the assertion with $\lambda = \gamma/2$. $\square$

4.13 Remark. The decay rate λ is not optimal. For instance, we neglected the term $\int_0^1 n_x^4/12n^3 dx$ in (4.3.5) and the constants in (4.3.1) are not the best ones. For optimal constants in logarithmic Sobolev inequalities related to (1.3.1) with periodic boundary conditions, we refer to [**37**].

4.14 Remark. It is not easy to find conditions on the boundary data for which $\log n_\infty$ is concave. An example is $n_0 = n_1$ and $w_0 = -w_1 \geq 0$. Indeed, if $y = \log n_\infty$, we have $y(0) = y(1)$ and $y_x(0) = -y_x(1) \geq 0$ and therefore, y is symmetric around $x = \frac{1}{2}$. Thus (see Remark 4.6) $a = e^{y_0}(y_{xx}(1) - y_{xx}(0)) = 0$ and $b = e^{y_0} y_{xx}(0) \leq 0$. This implies $(\log n_\infty)_{xx} = y_{xx} = be^{-y} \leq 0$ in $(0,1)$.

4.15 Remark. The assumption on the concavity of $\log n_\infty$ can be slightly relaxed. Indeed, we claim that the assertion of Theorem 4.3 also holds if $((\log n_\infty)_{xx})^+$ is small enough in the sense

$$4\,\frac{\max\{n_\infty(x) : 0 \leq x \leq 1\}}{\min\{n_\infty(x) : 0 \leq x \leq 1\}} \int_0^1 ((\log n_\infty)_{xx})^+ \, dx \leq 1 - \delta \tag{4.3.8}$$

for some $\delta > 0$, where $(x)^+ = \max\{0, x\}$. We prove this result by deriving a bound on the second integral in (4.3.2) in terms of the first one, employing the weighted Poincaré inequality [**30**, Thm. 1.4]

$$\int_0^1 n_x^2 \mu(x)dx \le K \int_0^1 n_{xx}^2 dx$$

for all $n \in H^2(0,1)$ satisfying $n(0) = n(1)$ (which implies that $\int_0^1 n_x dx = 0$). The function μ is assumed to be nonnegative and measurable. The best constant $K > 0$ is not explicit but can be bounded by $K \le 4\int_0^1 \mu(x)dx$ [**30**, Rem. 1.10.4]. We choose $\mu(x) = (ax+b)^+ = (n_\infty(\log n_\infty)_{xx})^+$. Then the weighted Poincaré inequality and (4.3.4) give

$$\begin{aligned}\int_0^1 e^{z_k+y_\infty} z_{k,xx}^2 dx &\ge 4m\int_0^1 (e^{z_k/2})_{xx}^2 dx \ge \frac{4m}{K}\int_0^1 (e^{z_k/2})_x^2 \mu(x)dx \\ &= \frac{m}{K}\int_0^1 (ax+b)^+ e^{z_k} z_{k,x}^2 dx,\end{aligned}$$

where $m = \min\{n_\infty(x) : 0 \le x \le 1\}$. Inserting this inequality in (4.3.2) and using (4.3.3), we obtain

$$\begin{aligned}\frac{1}{\tau}\left(E^{(k)} - E^{(k-1)}\right) &\le -\int_0^1 e^{z_k+y_\infty} z_{k,xx}^2 dx + \int_0^1 (ax+b)^+ e^{z_k} z_{k,x}^2 dx \\ &\le \left(\frac{K}{m} - 1\right)\int_0^1 e^{z_k+y_\infty} z_{k,xx}^2 dx.\end{aligned}$$

Assumption (4.3.8) shows that $K/m \le 1-\delta$ and hence, by (4.3.6),

$$\frac{1}{\tau}\left(E^{(k)} - E^{(k-1)}\right) \le -\delta\int_0^1 e^{z_k+y_\infty} z_{k,xx}^2 dx \le -\frac{4\pi^2\delta m}{c_2}E^{(k)}.$$

Now proceed as in the proof of Theorem 4.3. The convergence rate in the L^1 norm is given by $\lambda = 2\pi^2\delta m/c_2$.

4.4 Numerical examples

In this section we show by numerical examples that the assumption of concavity of $\log n_\infty$ (or the assumption (4.3.8)), where n_∞ is the solution to (4.0.1), seems to be only technical. Equation (1.3.1) is solved numerically in the formulation

$$n_t = -n_{xxxx} + \left(\frac{n_x^2}{n}\right)_{xx} \quad \text{in } (0,1). \tag{4.4.1}$$

We use a uniform grid $(x_i, t_j) = (\triangle x \cdot i, \triangle t \cdot j)$ with spatial mesh size $\triangle x = 10^{-3}$ and time step $\triangle t = 10^{-6}$. With the approximation n_{ij} of $n(x_i, t_j)$, the fully implicit discretization reads as

$$\frac{1}{\triangle t}(n_{ij} - n_{i,j-1}) = -D^+D^-D^+D^-n_{ij} + D^+D^-\left(\frac{(D^+n_{ij})^2}{n_{ij}}\right),$$

where D^+ and D^- are the forward and backward difference operators on the spatial mesh (see [**54**]). The nonlinear equations are solved on each time level by Newton's method where the initial guess is chosen to be the solution of the previous time level.

For the first example we use the boundary conditions

$$\begin{aligned} n(0,t) &= n_0, \quad n(1,t) = n_1, \\ n_x(0,t) &= w_0 = 2\sqrt{n_0}(\sqrt{n_1} - \sqrt{n_0}), \\ n_x(1,t) &= w_1 = 2\sqrt{n_1}(\sqrt{n_1} - \sqrt{n_0}), \end{aligned} \tag{4.4.2}$$

with $n_0 \leq n_1$. The advantage of these conditions is that the stationary problem (4.0.1) has the exact solution

$$n_\infty(x) = \left((\sqrt{n_1} - \sqrt{n_0})x + \sqrt{n_0}\right)^2, \quad x \in (0,1).$$

We choose the initial condition $n_I(x) = e^{-x}\sin(3\pi x) + 3x + 1$ and the boundary values $n_0 = 1$ and $n_1 = 4$. The numerical solution at various times is displayed in Figure 4.1. The discrete solution seems to converge to the exact solution n_∞ as $t \to \infty$. Figure 4.2 shows the exponential decay of the relative entropy

$$E_3(t) = \int_0^1 n(\cdot,t)((\log(n(\cdot,t)/n_\infty) - 1) + n_\infty)dx$$

and of the L^1 deviation $\|n(\cdot,t) - n_\infty\|_{L^1(0,1)}$. As predicted by the proof of Theorem 4.3, the decay rate of the L^1 deviation is half of the rate of the relative entropy. Notice that the function $\log n_\infty$ is concave, i.e., the assumptions of Theorem 4.3 are satisfied. In the second example we show by a numerical example that the solution to (1.3.1) decays exponentially fast even if the function $\log n_\infty$ is convex. For this we choose the boundary conditions $n_0 = 1.5$, $n_1 = 0.8$, $w_0 = -4.6127$, and $w_1 = 2.0618$. The stationary solution n_∞ is computed numerically from the equation

$$n_\infty(\log n_\infty)_{xx} = ax + b, \quad x \in (0,1),$$

where $a = 1$ and $b = 3$. Then, $\log n_\infty$ is strictly convex in $(0,1)$ and the assumption (4.3.8) is not satisfied. We choose the initial function $n_I(x) = -e^{-x}\sin(2\pi x) - \frac{7}{10}x + \frac{3}{2}$. Figure 4.3 shows the discrete solution for various times. In this case, the relative entropy and the L^1 deviation are also exponentially decaying (Figure 4.4) although the condition of Theorem 4.3 is not satisfied. This suggests that the concavity hypothesis is purely technical.

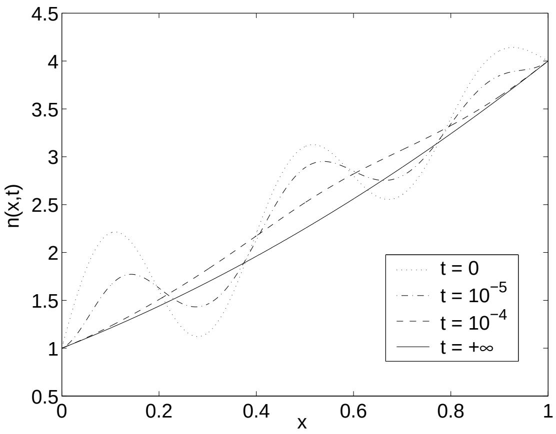


Figure 4.1: Numerical solution to (4.4.1), (4.4.2) with $n_0 = 1$, $n_1 = 4$, $w_0 = 2$, and $w_1 = 4$ at various times.

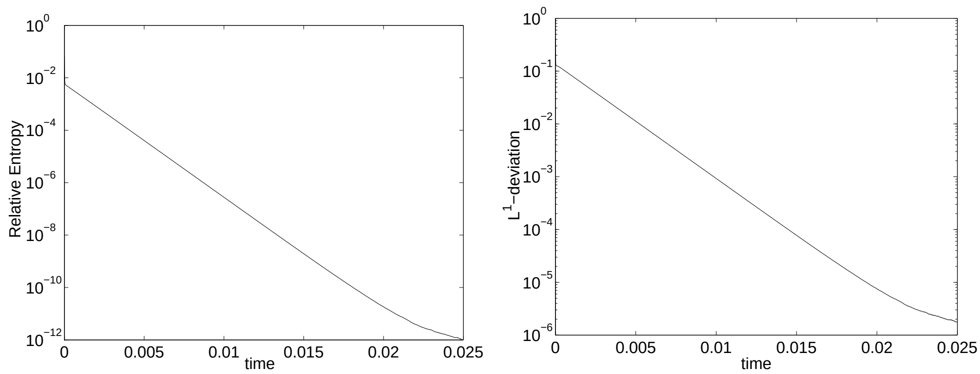


Figure 4.2: Logarithmic plot of the relative entropy $E_3(t)$ (left) and the L^1 deviation $\|n(\cdot,t) - n_\infty\|_{L^1(0,1)}$ (right) for the solution to (4.4.1), (4.4.2) with $n_0 = 1$, $n_1 = 4$.

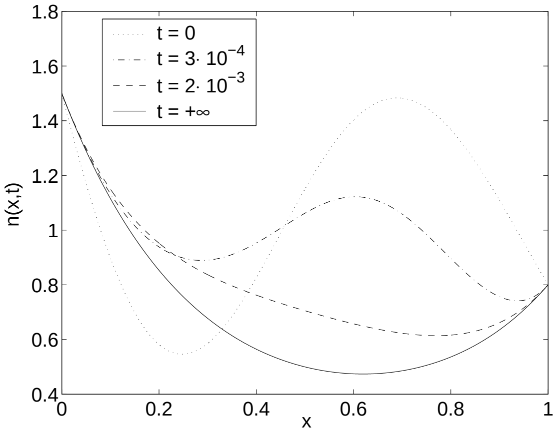
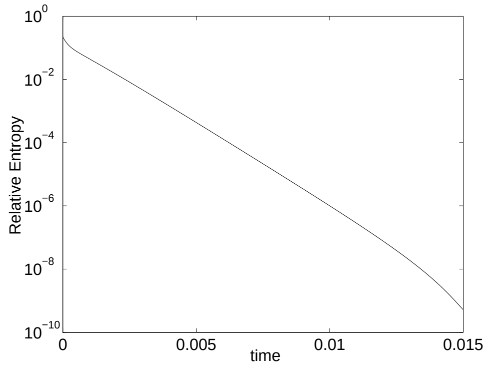


Figure 4.3: Numerical solution to (4.4.1), (1.3.3) with $n_0 = 1.5$, $n_1 = 0.8$, $w_0 = -4.6127$, and $w_1 = 2.0618$ at various times.



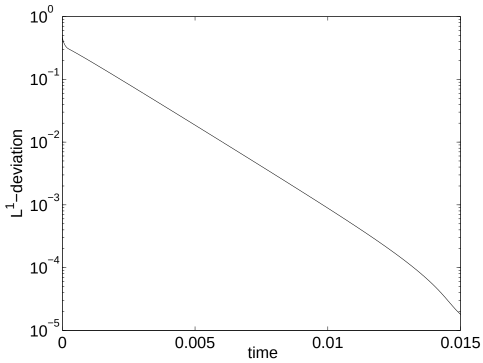


Figure 4.4: Logarithmic plot of the relative entropy $E_3(t)$ (left) and the L^1 deviation $\|n(\cdot,t) - n_\infty\|_{L^1(0,1)}$ (right) for the solution to (4.4.1), (1.3.3) with $n_0 = 1.5$, $n_1 = 0.8$, $w_0 = -4.6127$, and $w_1 = 2.0618$.

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