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DISSERTATION

Entropy analysis for nonlinear higher-order quantum diffusion equations

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Abstract

Nonlinear evolution equations of fourth- and higher-order in spatial derivatives emerge in various models of mathematical physics. This thesis is devoted to the study of nonlinear higher-order diffusion equations, which arise in the quantum modeling of semiconductor and plasma physics, and describe the evolution of densities of charged particles in a quantum fluid. These equations appear as quantum corrections to the classical models of the transport of charged particles.

Primary questions in the mathematical analysis of nonlinear higher-order equations are the existence and uniqueness of solutions, long-time behaviour and positivity of solutions, growth of the support and speed of propagation. In order to obtain the answers, many approaches rely on certain a priori estimates, called entropy production inequalities. These estimates are results of mathematical dissipation of some nonlinear functionals (entropies) along solutions of the equation under consideration, but often they also reflect the underlying physical laws, namely that of conservation of mass and energy, or the dissipation of the physical entropy. As a consequence, they provide necessary uniform bounds for solutions in corresponding Sobolev (semi-)norms.

The first part of the thesis considers an algebraic approach for proving entropy production inequalities for radially symmetric solutions to a class of higher-order diffusion equations in multiple space dimensions. The approach is an extension of the previously developed method for nonlinear evolution equations of even order in one space dimension. Key idea is to translate the problem of proving the integral inequlities into a decision problem about nonnegativity of corresponding polynomials. A benefit of this procedure is that the latter problem is always solvable in an algorithmic way. In application of the method, novel entropy production inequalities are derived for the thin-film equation, the fourth-order Derrida-Lebowitz-Speer-Spohn equation, and the sixth-order quantum diffusion equation.

In the second part, the initial-value problem for the sixth-order quantum diffusion equation with periodic boundary conditions is studied. The concept of weak nonnegative solutions for this equation is introduced and it is proved that the equation admits the global-in-time solutions in two and three space dimensions. Moreover, these solutions are smooth and classical whenever the particle density is strictly positive and particular energy functional is uniformly bounded. In addition, the long-time convergence to the spatial homogeneous equilibrium at a universal exponential rate is observed. The analysis strongly uses a special entropy production inequality, which is a direct consequence of the dissipation property of the physical entropy.

Finally, the third part is devoted to novel approximations of the fourth-order quantum diffusion equation, also known as the Derrida-Lebowitz-Speer-Spohn equation. Two different approaches are discussed, which have the common goal of preserving some qualitative properties of solutions on a (semi-)discrete level. First, the semi-discrete two-step backward difference (BDF-2) method of a reformulated equation yields the discrete entropy stability property and second-order convergence of the method in a specific case. Next, a particular variational structure of the equation is used to introduce the discrete variational derivative method in the onedimensional case. The method preserves the mass and the dissipation property of the corresponding energy (Fisher information) functional on a discrete level. Furthermore, the method is extended to the temporally more accurate multistep discrete variational derivative methods, which possess generalized discrete dissipation properties.

Chapter 1

Introduction

"I consider that I understand an equation when I can predict the properties of its solutions, without actually solving it."
– Paul A. M. Dirac

State of the art analysis of nonlinear fourth- and sixth-order evolution equations employs the so-called entropy production inequalities. They reflect the dissipation or stability property of certain nonlinear functionals (entropies) along the sought solutions, and give rise to desired a priori estimates. In this thesis, variety of such estimates have been constructed in a systematic way for radially symmetric solutions to higher-order nonlinear diffusion equations. One particular estimate, that reflects the dissipation of the physical entropy, has been exhaustively used to establish the existence result and long time behaviour of solutions to a multidimensional sixth-order quantum diffusion equation. In addition, variational structure of a fourth-order quantum diffusion equation has been employed to construct reliable numerical schemes, which preserve the original structure and its dissipation property on a discrete level.

1.1 Motivation

In the last three decades, there has been a growing interest in the analysis of fourth- and sixth-order nonlinear parabolic equations, mainly because of their increasing appearance in various models of mathematical physics. Such equations arise for example, in pattern formation models, in lubrication approximation of thin viscous fluids along solid surfaces or in thin layers, as approximations of non-local models for the transport of charged particles in quantum fluids with applications in quantum semi-conductor and cold plasma modeling, as an approximation of a nonlocal model for the Bose–Einstein condensation, etc. Below, we briefly review these specific examples and their origins in physics, assigning a special emphasis on a nonlocal quantum diffusion model and related higher-order equations for the transport of charged particles in a quantum fluid.

Rigorous results about the existence of solutions and their qualitative behavior are typically much harder to obtain than in the context of the well-studied second-order parabolic equations. One of the principal difficulties is the non-applicability of comparison principles for higher-order equations. For instance, even the fourth-order linear equation $\partial_t n + \Delta^2 n = 0$ doesn't preserve positivity of solutions. To substitute for this loss, one has to rely on suitable a priori estimates. Often, the underlying physical system conserves the energy and/or minimizes[1] the physical entropy. That provides basic a priori bounds on solutions. However, one usually needs additional a priori estimates to prove some mathematical properties of solutions. Derivation of such estimates, which depends on the equation at hand, is typically a difficult task. Having in mind the importance of good a priori estimates, leads us immediately to the first goal of the thesis — to extend the existing tools for constructiong such estimates in a systematic way.

Despite of general non-applicability of comparison principles, a particular interest has been devoted to equations that are positivity preserving. This is clearly, a core feature for equations that model for example, the evolution of particle densities. Thanks to their special nonlinear structure, such equations allow for the introduction of a suitable solution concept, which asserts that a nonnegative initial datum leads to a nonnegative global solution. Typically, sophisticated regularizations are constructed that yield smooth and strictly positive approximative solutions. The limit of vanishing regularizations, which is carried out due to certain a priori estimates and related compactness arguments, then provides a nonnegative weak solution. To perform this concisely introduced concept and general ideas for a novel multi-dimensional sixth-order quantum diffusion equation makes a further subject of the interest.

Finally, to make below listed physical models practically useful in applications and to explore their qualitative properties, it is a necessary task to develop reliable numerical schemes, which preserve as many structural properties as possible of the original model. This includes discrete conservation of mass, discrete conservation or dissipation of the energy and other discrete a priori estimates. Having such discrete properties, typically improves on the stability and convergence of schemes. Moreover, corresponding numerical solutions match the underlying physical processes better.

1.2 Model equations

Starting in the late 1970's, mainly initiated by the research on pattern formation and motion of thin viscous fluids on a solid surface, the number of nonlinear fourth- and sixth-order parabolic equations appearing in various models of mathematical physics together with the accompanying literature on the rich mathematical structure of such equations has grown rapidly.

[1] In contrast to the physical point of view, where underlying systems maximize the physical entropy.

Cahn-Hilliard equation

For historical reasons, we first mention the Cahn-Hilliard equation

$$\partial_t n + \operatorname{div}\big(\mu(n)\nabla(\Delta n - f'(n))\big) = 0\,,$$

which originates in material science describing the phase separation process in a binary mixture. The nonlinearity f is a so-called double-well potential, typically $f(n) = \gamma(n^2-1)^2$, $\gamma > 0$, and μ is the diffusional mobility, which takes a thermodynamically motivated form $\mu(n) = 1 - n^2$. The equation was first derived and studied by Cahn and Hilliard in a series of seminal papers in late 50's starting with [12]. Till date, it has been subject of hundreds of papers exploring variety of analytical, numerical and applicational aspects. Recently, a modified Cahn-Hilliard equation has also appeared as an inpainting tool in image processing [11].

Thin-film equations

Among the positivity preserving models, probably the most famous study object is the fourth-order thin-film equation

$$\partial_t n + \operatorname{div}(n^\beta \nabla\Delta n) = 0\,. \tag{1.1}$$

This equation appears in lubrication approximation of several models describing the surface tension-dominated motion of thin viscous films of height $n \geq 0$ under small slip ($\beta = 2$) or no-slip ($\beta = 3$) boundary conditions [5, 52]. Parameter $\beta = 1$ corresponds to the lubrication approximation of the Hele-Shaw flow, a Stokes flow between two parallel flat plates separated by a very small gap [17]. The one-dimensional family of equations has been first analyzed by Bernis and Friedman [4], while the multidimensional case has been studied in the work of Dal Passo et al. [18]. In both works, integral (entropy) estimates play a crucial role. On an explicit dependence on the parameter β, such estimates provide the existence and qualitative properties of solutions like, long-time behaviour [14], positivity, finite speed of propagation, growth estimates for the support [6], etc., as well as numerical schemes with respective conservation and dissipation properties [3]. The available literature on these topics is huge and steadily growing; see [3] for a collection of further references.

Other models for thin viscous films lead to sixth-order equations. One example is

$$\partial_t n + \operatorname{div}(n^\beta \nabla\Delta^2 n) = 0\,,$$

which models the spreading of a thin viscous fluid under the driving force of an elastic plate [27]. The model was first introduced in [43] in space dimension $d = 1$ with $\beta = 3$ together with a more general form of this equation arising in the isolation oxidation of silicon. Another application for such thin-film equations concerns the bonding of Silicon-Germanium films to silicon substrates [27]. Further examples of sixth-order equations can be found in [26, 37, 44].

Quantum drift-diffusion model

Recent trends in development and production of highly miniaturized devices in nanotechnology require novel models of the transport of charged particles, in which quantum effects play an important and sometimes even a dominant role. Using a moment-constrained optimization procedure, a whole hierarchy of macroscopic models with fluid-type unknowns has been derived from a many particle Schrödinger–Poisson system [34]. The models consist of balance equations for the particle density, current density and energy density. The simplest model, that of the first-order moment-constraint, is the quantum drift-diffusion model [1],

$$\begin{aligned} \partial_t n &= T\Delta n + \operatorname{div}\big(n\nabla(V_B[n] + V)\big)\,, \\ -\lambda^2 \Delta V &= n - C_{dot}\,. \end{aligned}$$

It consists of the balance equation for the particle density n, which is self-consistently coupled to the Poisson equation for the electrostatic potential V. The nonlinear term $V_B[n] = -\hbar^2\Delta\sqrt{n}/\sqrt{n}$ describes quantum effects in the model. This is the so-called Bohm potential, which also appears in the Madelung transformation of the Schrödinger equation. Other parameters of the model are the scaled temperature T, the scaled Planck constant $\hbar$, the scaled Debye length λ, and the doping profile C_{dot}, which describes the distribution of charged background ions.

Alternatively, applying a moment method to a Wigner–BGK model, Degond et al. derived in [21] a nonlocal quantum drift-diffusion model for charged particles in, for instance, semiconductors or cold plasmas. The model reads as

$$\partial_t n = \operatorname{div}(n\nabla(A - V))\,,$$

where n denotes the particle density, A is the quantum chemical potential defined implicitly as a Lagrangian multiplier of a moment-constrained minimization problem and V is a given external potential. Simplifying the model to zero external potential ($V = 0$), i.e. considering only diffusive effects, an asymptotic expansion of A in terms of the reduced Planck constant $\hbar^2$ leads to a family of parabolic equations for the particle density n. A brief note on the expansion, using pseudo-differential calculus, is attached in Appendix A. The first member of this family is the classical heat equation $\partial_t n = \Delta n$. This asserts that the semi-classical limit ($\hbar \to 0$) of the (nonlocal) quantum drift-diffusion model is the classical drift-diffusion model.

Derrida-Lebowitz-Speer-Spohn equation

The second member is the fourth-order Derrida–Lebowitz–Speer–Spohn (DLSS) equation

$$\partial_t n + \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0\,, \tag{1.2}$$

which provides another well-studied example of a fourth-order equation. Observe that, like in the original quantum drift-diffusion model, the nonlinear part contains the scaled

Bohm potential. Interestingly, the one-dimensional version of the DLSS equation, $\partial_t n + \frac{1}{2}(n(\log n)_{xx})_{xx} = 0$ arose in the context of spin systems. Derrida et al. [23] derived it in the studying of fluctuations of the interface between the regions of predominantly positive and negative particle spins in the Toom model. It has been first analyzed in [7] for local positive smooth solutions and then in [40] for global nonnegative weak solutions. The existence, non uniqueness and long-time behaviour of weak solutions to the multidimensional equation has been proven recently in [36]. Moreover, this equation possesses a particular variational structure, it constitutes the gradient flow of the Fisher information with respect to the L^2-Wasserstein metric [30].

Sixth-order quantum diffusion equation

When the non-local quantum diffusion model is expanded to order $\hbar^4$, the main part of the differential operator is of sixth order, and the corresponding equation reads as

$$\partial_t n = \operatorname{div}\left(n\nabla\left[\sum_{i,j=1}^{d}\left(\frac{1}{2}(\partial_{ij}^2 \log n)^2 + \frac{1}{n}\partial_{ij}^2(n\partial_{ij}^2 \log n)\right)\right]\right). \tag{1.3}$$

In further, we will omit the above sum and assume the Einstein's summation convention over repeated indices from 1 to d. The one-dimensional problem has recently been studied in [37]. In Chapter 3 we study in detail the initial-value problem for this equation on the d-dimensional torus $\mathbb{T}^d \cong [0,1]^d$ (imposing periodic boundary conditions) in dimensions $d = 2$ and $d = 3$.

Local model for the Bose-Einstein condensation

Our final example is related to the quantum kinetic theory for bosonic gases. Relaxation to equilibrium of spatially homogeneous and isotropic fluid of weakly interacting bosons with s-wave scattering is described by the Boltzmann-Nordheim kinetic equation [56, 58]. Assuming small energy exchange via scattering, the latter (nonlocal) equation can be approximated by the nonlinear fourth-order evolution equation [33]

$$\partial_t n = \frac{1}{\sqrt{x}}\left[x^{13/2}\left(n^4\left(\frac{1}{n}\right)_{xx} - n^2(\log n)_{xx}\right)\right]_{xx}, \quad x > 0\,,\ t > 0\,, \tag{1.4}$$

where $x > 0$ denotes the energy variable and $n(t;x)$ the energy distribution function. If the initial mass ($\|n_0\|_{L^1}$) is bigger than the prescribed critical value, an accumulation of matter appears at low energies and solutions to (1.4) eventually blow-up in finite time [33]. The finite-time singularity in solutions explains formation of the Bose-Einstein condesate.

1.3 Summary of the thesis and main results

Let n be a nonnegative solution to a nonlinear higher-order partial differential equation, and let E and Q be nonnegative functionals defined by n and its spatial derivatives. Estimates of the type

$$\frac{\mathrm{d}}{\mathrm{d}t}E[n(t)] + cQ[n(t)] \leq 0\,, \quad t > 0\,, \tag{1.5}$$

are the key tools in the mathematical analysis of such equations and make the core ingredient of this thesis. Inequalities like (1.5) provide a priori bounds for the evolution. They are a necessary first step in proofs for existence of solutions; they allow to describe the equilibration behavior of the solutions and other qualitative properties like, growth of support, speed of propagation etc. We call E an *entropy* if (1.5) holds with some suitable choice of Q and $c \geq 0$ for arbitrary solutions n of the evolution equation under consideration. Estimate (1.5) is referred to as an *entropy production inequality*, and Q is the corresponding *entropy production*. Typically, one is interested in α-functionals E_α being entropies for certain range of parameters $\alpha \in \mathbb{R}$, where

$$\begin{aligned} E_\alpha[n] &= \frac{1}{\alpha(\alpha-1)}\int_\Omega n^\alpha \mathrm{d}x\,, \quad \alpha \neq 0, 1\,, \\ E_0[n] &= \int_\Omega \big(n - \log n\big)\mathrm{d}x\,, \\ E_1[n] &= \int_\Omega \big(n\big(\log n - 1\big) + 1\big)\mathrm{d}x\,, \end{aligned} \tag{1.6}$$

and $\Omega \subset \mathbb{R}^d$ is a domain. Specially in this thesis $\Omega = B^d = \{x \in \mathbb{R}^d,\ \ |x| < 1\}$ (unit ball) or $\Omega = \mathbb{T}^d$ (d-dimensional torus). Further candidates for entropies are functionals defined by first-order derivatives

$$F_\gamma[n] = \int_\Omega |\nabla n^{\gamma/2}|^2 \mathrm{d}x\,, \quad \gamma > 0 \quad \text{and} \quad F_0[n] = \int_\Omega |\nabla \log n|^2 \mathrm{d}x\,.$$

Among them, functional F_2 often has a notion of the energy of the system, while F_1 is know as the Fisher information, since it plays an important role in the information theory. Here is more interesting as the energy of the fourth-order equation (1.2) (see Chapter 4).

The subject of the first chapter is to determine α-functionals (1.6), which are entropies along radially symmetric smooth positive solutions to the above reviewed evolution equations (1.1)–(1.3); and to prove estimates of the type (1.5) for a particular choice of entropy productions. The principal technique for proving estimates (1.5) are integration by parts formulae. In order to find as many entropies as possible, we have to employ a systematic approach, which considers all integration by parts formulae. For this purpose we adapted a systematic approach for construction of entropies proposed in [35] for a large class of nonlinear evolution equations of even order in one space variable. The main idea is to translate the procedure of integration by parts into a decision problem about the nonnegativity of certain polynomials. The latter is a well-known problem in the real algebraic geometry, which is always solvable in an algorithmic way. Briefly explained, to each evolution equation one formally associates a polynomial P in real variables ξ_j, which represent quotients $\partial_r^j n/n$. Due to explicit apperance of the radial variable r in evolution equations, additional polynomial variable η is used to represent $1/r$. For example, the fourth-order thin-film equation (1.1) for radially symmetric solutions n takes the form (see Example 2.4 (A))

$$\partial_t n + r^{-(d-1)}\partial_r \left(r^{d-1} n^{\beta+1} P\Big(\frac{1}{r}, \frac{n_r}{n}, \frac{n_{rr}}{n}, \frac{n_{rrr}}{n}\Big)\right) = 0\,,$$

where $P(\eta, \xi_1, \xi_2, \xi_3) = \xi_3 + (d-1)(\eta\xi_2 - \eta^2\xi_1)$. Assuming no-flux boundary conditions on the unit sphere in $\mathbb{R}^d$, one calculates the dissipation of the α-functionals

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t} E_\alpha[n] &= -\omega_d \int_0^1 u^{\alpha+\beta}\Big(-\frac{n_r}{n}\Big) P\Big(\frac{1}{r}, \frac{n_r}{n}, \frac{n_{rr}}{n}, \frac{n_{rrr}}{n}\Big) r^{d-1}\mathrm{d}r \\ &=: -\omega_d \int_0^1 u^{\alpha+\beta} S_0\Big(\frac{1}{r}, \frac{n_r}{n}, \frac{n_{rr}}{n}, \frac{n_{rrr}}{n}\Big) r^{d-1}\mathrm{d}r\,,\end{aligned}$$

where $S_0(\eta, \xi_1, \xi_2, \xi_3) = -\xi_1 P(\eta, \xi_1, \xi_2, \xi_3)$ and ω_d denotes the surface of the unit sphere in $\mathbb{R}^d$. Besides the no-flux condition, we also assume the homogeneous Neumann boundary condition on the sphere. Based on given boundary conditions, one finds a set of all basic integration by parts formulae with vanishing boundary terms. These are then translated into the polynomial form resulting in the so-called shift polynomials, whose linear combinations characterize all possible integration by parts formulae (see Section 2.2). Adding a linear combination of shift polynomials to S_0 then modifies polynomial S_0 into some other polynomial S, but preserves the value of the integral. If a suitable linear combination, which makes the resulting polynomial S nonnegative, can be found, then this formally gives a proof of the entropy dissipation and an estimate of the type (1.5). Further details on formulation of decision problems and finding its solutions are left for Chapter 2.

In the subsequent, let n be a radially symmetric smooth and positive solution to the respective model equations (1.1)–(1.3) on the unit ball B^d with homogeneous Neumann and no-flux boundary conditions, and the functionals E_α defined in (1.6). The following summarizes our main results of Chapter 2 (see Theorems 2.1 – 2.3).

Thin-film equation. The functionals E_α are entropies provided that $3/2 \le \alpha+\beta \le 3$. In this case, the entropy production inequality (1.5) holds with

$$c = \frac{16}{(\alpha+\beta)^4}(3-\alpha-\beta)(2(\alpha+\beta)-3) \quad \text{and} \quad Q_\alpha[n] = \int_{B^d} \big(\Delta n^{(\alpha+\beta)/2}\big)^2 \mathrm{d}x\,.$$

The obtained constant c is optimal for our method.

DLSS equation. The functionals E_α are entropies if

$$\begin{aligned} d = 1,2,3, \text{ or } 4, \text{ and } \quad & \frac{(\sqrt{d}-1)^2}{d+2} \le \alpha \le \frac{3}{2}\,, \\ d = 5,6, \text{ or } 7, \text{ and } \quad & \frac{(\sqrt{d}-1)^2}{d+2} \le \alpha \le \frac{(\sqrt{d}+1)^2}{d+2}\,, \\ d \ge 8 \text{ and } \quad & \frac{d-4}{2(d-2)} \le \alpha \le \frac{(\sqrt{d}+1)^2}{d+2}\,, \end{aligned}$$

and the entropy production inequality (1.5) holds with $Q_\alpha[n] = \int_{B^d}(\Delta n^{\alpha/2})^2 \mathrm{d}x$. The optimal choice of the constant c is given explicitly in Theorem 2.2.

Sixth-order equation. The functionals E_α, are entropies if

$$\begin{aligned} d = 1 \text{ and } \quad & 0.1927\ldots \leq \alpha \leq 1.1572\ldots, \\ d = 2 \text{ and } \quad & 0.2827\ldots \leq \alpha \leq 1.0982\ldots, \\ d = 3 \text{ and } \quad & 0.3470\ldots \leq \alpha \leq 1.0517\ldots, \\ d = 4 \text{ and } \quad & 0.3968\ldots \leq \alpha \leq 1.0123\ldots, \\ d = 5 \text{ and } \quad & 0.4380\ldots \leq \alpha \leq 0.9775\ldots. \end{aligned}$$

Moreover, in dimensions $d = 1, \ldots, 4$ and for $\alpha = 1$, the entropy production inequality (1.5) holds for some $c > 0$ if one chooses

$$Q_1[n] = \int_{B^d} \big(|\nabla\Delta\sqrt{n}|^2 + |\nabla\sqrt[6]{n}|^6\big)\mathrm{d}x\,.$$

The above results of Chapter 2 are published by the author, A. Jüngel (TU Wien) and D. Matthes (TU München) in journal *Communications in Mathematical Sciences* [10].

Chapter 3 is concerned with the analysis of the sixth-order quantum diffusion equation (1.3) whose solutions describe the evolution of the particle density in a quantum fluid. Recall that this equation has been obtained by an asymptopic expansion to the order $\hbar^4$ of the nonlocal quantum diffusion model, where $\hbar$ denotes the scaled Planck constant. A brief derivation of the equation can be found in Appendix A. We study the Cauchy problem for equation (1.3) in the d-dimensional torus $\mathbb{T}^d$ in space dimesions two and three. The aim is to prove the existence of solutions and to observe their long-time behaviour. For that purpose, two solutions concepts are compared: weak and classical. In order to prove the existence results, certain reformulations of (1.3) are necessary. First of all, the concept of weak solutions requires a form that is also well-defined for vanishing densities n, while semilinearity of new form would be most convenient for the classical approach. It turns out that the form

$$\partial_t n = \Delta^3 n + \partial^3_{ijk} F_1^{(ijk)}(n) + \partial^2_{ij} F_2^{(ij)}(n), \tag{1.7}$$

with the nonlinear operators F_1 and F_2, defined in (3.4), is appropriate to study both solution concepts. The first concept, that of weak nonnegative solutions, is an adapted generalization of the results obtained in the one-dimesional case [37]. Starting with the implicit Euler semi-discretization, additional change of variables $n = e^y$ has been employed; semi-discrete equations are regularized by an ε-elliptic term and eventually solved by means of the Leray-Schauder fixed point theorem. The key estimate of the type (1.5), which essentially provides the compactness argument to carry out the deregularization limit $\varepsilon \downarrow 0$ and later the time-continuous limit, is related to the dissipation of the physical entropy in space dimensions $d \leq 3$,

$$\frac{\mathrm{d}}{\mathrm{d}t} E_1[n] + c \int_{\mathbb{T}^d} \big(\|\nabla^3\sqrt{n}\|^2 + |\nabla\sqrt[6]{n}|^6\big)\,\mathrm{d}x \leq 0\,.$$

It has been proved by Matthes using the aforementioned entropy construction method (see Lemma 3.8). To summarize, the following two results about weak solutions are obtained (Theorems 3.1 – 3.2).

Global existence. Let $d \leq 3$ and $n_0 \in L^1(\mathbb{T}^d)$ be a nonnegative function of the finite entropy $E_1[n_0] < \infty$. Then there exists a nonnegative function n satisfying $\sqrt{n} \in L^2_{\mathrm{loc}}(0,\infty; H^3(\mathbb{T}^d))$ that is a solution to (1.7) in the following weak sense

$$\int_0^\infty \langle \partial_t n, \varphi \rangle \,\mathrm{d}t + \int_0^\infty \int_{\mathbb{T}^d} \left(\partial^3_{ijk}\varphi \, \partial^3_{ijk} n + \partial^3_{ijk}\varphi \, F_1^{(ijk)}(n) - \partial^2_{ij}\varphi \, F_2^{(ij)}(n) \right) \mathrm{d}x \,\mathrm{d}t = 0$$

for all test functions $\varphi \in L^4(0,T; H^3(\mathbb{T}^d))$.

Long-time behaviour. Let n be the weak solution to (1.7) in the previous sense. Then n converges exponentially fast to the constant steady state.

Concerning the classical solution concept, the semi-linearity of equation (1.7) allows to employ the standard theory of analytic semigroups, which yields the following (see Theorem 3.3).

Local existence. Let $n_0 \in H^2(\mathbb{T}^d)$ be strictly positive. Then there exist $T_* > 0$ and unique smooth strictly positive classical solution $n \in C^\infty((0,T_*); C^\infty(\mathbb{T}^d))$ to (1.7) with $n(t) \to n_0$ in $H^2(\mathbb{T}^d)$ as $t \downarrow 0$. Moreover, either $T_* = +\infty$, or there exists a limiting profile $n_* \in H^2(\mathbb{T}^d)$ such that $n(t) \to n_*$ in $H^2(\mathbb{T}^d)$ as $t \uparrow T_*$ and $\min_{x\in\mathbb{T}^d} n_*(x) = 0$.

Furthermore, introducing the energy functional

$$\mathcal{E}[n] = \frac{1}{2} \int_{\mathbb{T}^d} n \|\nabla^2 \log n\|^2 \,\mathrm{d}x \,,$$

one formally observes the gradient flow structure of (1.3) with respect to the L^2-Wasserstein metric

$$\partial_t n = \mathrm{div} \left(n \nabla \left(\frac{\delta \mathcal{E}[n]}{\delta n} \right) \right) \,,$$

which immediately implies the Lyapunov property of $\mathcal{E}$ along smoth positive solutions to (1.3). Assuming that the Lyapunov property holds along weak solutions, the subsequent has been proved (Theorem 3.5).

Regularity of weak solutions. Atop of the Lyapunov property of $\mathcal{E}$, assume that the weak solution n is strictly positive on some time interval. Then n equals the classical solution on that time interval.

Preprint of results presented above and discussed in Chapter 3, written by the author together with Jüngel and Matthes, has been submitted for publication at *Annales de l'Institut Henri Poincaré (C) Nonlinear Analysis* [9].

In Chapter 4, novel numerical schemes of the fourth-order quantum diffusion equation (1.2) are investigated. The goal there is to increase the temporal accuracy of approximations, but preserving some analytical properties. In particular, some estimates of the type (1.5) on a (semi-)discrete level. First we consider the two-step backward difference (BDF-2) semi-discretization. In order to accomplish that, another form of (1.2) has been employed in which the time drivative $\partial_t n$ is substituted by an α-dependent expression and the spatial operator by the standard logarithmic form,

$$\frac{2}{\alpha} n^{1-2/\alpha} \partial_t (n^{\alpha/2}) + \frac{1}{2} \partial^2_{ij} (n \partial^2_{ij} \log n) = 0 \, . \tag{1.8}$$

Above, $\alpha \geq 1$ naturally belongs to the range of real parameters establishing entropies (1.6) for equation (1.2). Equation (1.8) is discretized in time by the BDF-2 method, resulting in the sequence of elliptic problems on a time grid $\{k\tau\}_{k\geq 1}$ with a given time step $\tau > 0$. For particular admissible α, existence of weak semi-discrete solutions follows again the idea of an appropriate ε-regularization, and a uniform boundedness of the corresponding time discrete α-functional allows to perform the deregularization limit $\varepsilon \downarrow 0$ (Theorem 4.1). Unlike the implicit Euler semi-discretization, specific structure of the BDF-2 scheme infers only stability of the time discrete α-functionals ($\alpha > 1$), i.e.

$$E_\alpha[n_m] + \kappa_\alpha \tau \sum_{k=1}^{m} \int_{\mathbb{T}^d} \left(\Delta (n_k^{\alpha/2}) \right)^2 \mathrm{d}x \leq E_\alpha[n_0] \, , \quad m \geq 1 \, , \; \kappa_\alpha > 0 \, ,$$

where n_k denotes the weak solution of the BDF-2 scheme for (1.8) at the time $2\tau \leq t_k \leq T$. On the other hand, employing the G-stability of the BDF-2 method leads to novel time discrete entropies $E^G_\alpha[n_k, n_{k-1}]$, defined in (4.42), and the time discrete dissipation property

$$E^G_\alpha[n_{k+1}, n_k] + \kappa_\alpha \tau \int_{\mathbb{T}^d} \left(\Delta (n_{k+1}^{\alpha/2}) \right)^2 \mathrm{d}x \leq E^G_\alpha[n_k, n_{k-1}] \, , \quad k \geq 1 \, .$$

It is easily to see that $E^G_\alpha[n_k, n_{k-1}]$ is formally an $O(\tau)$–perturbation of $E_\alpha[n_k]$. Furthermore, assuming additional regularity of the exact solution and strict positivity of weak solutions constructed by the BDF-2, we prove for $\alpha = 1$ the second-order convergence of the method (see Theorem 4.2).

Second objective of Chapter 4 are fully discrete finite difference type approximations, which preserve the dissipation property of the Fisher information F_1 on a discrete level. The idea for the method, which explores variational structure of (1.2), has been taken from [29]. Equation (1.2) in one space dimension takes the form

$$\partial_t n = \left(n \left(\frac{\delta F_1[n]}{\delta n} \right)_x \right)_x \, , \tag{1.9}$$

where $\delta F_1[n]/\delta n = -(\sqrt{n})_{xx}/\sqrt{n}$ denotes the variational derivative of the Fisher information. Assuming periodic boundary conditions, the latter immediately implies the dissipation of F_1. Key idea of the method is to define a discrete analog $F_{1,\mathrm{d}}$ of the Fisher information and to perform a discrete variation procedure in order to define the discrete version of the variational derivative. Denoted by $\delta F_{1,\mathrm{d}}/\delta(U^{k+1},U^k)$, where $U^k \approx n(t_k)$, the discrete variational derivative makes the key ingredient of the method, which by construction dissipates $F_{1,\mathrm{d}}$ (see Theorem 4.3).

Discrete variational derivative method. Assume discrete periodic boundary conditions and an equidistant grid on the interval $(0,1)$. Numerical scheme for equation (1.9), defined by the nonlinear system

$$\frac{1}{\tau}(U_i^{k+1} - U_i^k) = \delta_i^{\langle 1\rangle}\left(U_i^{k+1}\delta_i^{\langle 1\rangle}\left(\frac{\delta F_{1,\mathrm{d}}}{\delta(U^{k+1},U^k)_i}\right)\right), \quad i = 0,\dots,N-1\,,\ k \geq 0\,,$$

where $\delta_i^{\langle 1\rangle}$ denotes the central difference approximation of the first-order derivative, conserves the mass and dissipates the energy, i.e. $F_{1,\mathrm{d}}[U^{k+1}] \leq F_{1,\mathrm{d}}[U^k]$ for all $k \geq 0$.

These properties are direct consequence of the discrete form, which resembles (1.9), and do not depend on the concrete approximation of the Fisher information and its discrete variational derivative.

Further generalization of the method, discussed in Section 4.3.2, is based on the multistep backward difference formulae and naturally increases the temporal accuracy of the enhanced scheme (see Theorem 4.7). All the aforementioned numerical schemes are implemented and tested in Matlab, using the additional NAG toolbox [53]. Results of numerical experiments, presented in the last section, confirm the analytical results. In fact, they provide even better outcomes, for instance, an obvious exponential deacy of the Fisher information and releted relative entropies. The latter naturally poses further tasks in the numerical analysis for the above schemes.

Obtained results related to Chapter 4 are under preparation for publishing in a joint paper with A. Jüngel and E. Emmrich (TU Berlin).

Chapter 2

Entropies for radially symmetric higher-order nonlinear diffusion equations

2.1 Introduction and results

In [35], Jüngel and Matthes proposed a systematic approach to the derivation of a priori estimates for certain classes of nonlinear evolution equations of even order. This procedure allows one to determine *entropies* (Lyapunov functionals) and to derive integral bounds from their dissipation, i.e. *entropy production inequalities.* The developed method has been successfully applied to several equations in one space dimension. The main idea is to translate the procedure of integration by parts — which is the core element in most derivations of a priori estimates — into an algebraic problem about the positivity of polynomials. Roughly speaking, to each evolution equation, a polynomial in the spatial derivatives of the solution is associated, and integration by parts allows one to modify the coefficients of this polynomial. If a suitable change of coefficients can be found that makes the resulting polynomial nonnegative, then this corresponds (formally) to a proof of an a priori estimate on the solutions. The key point is that such *polynomial decision problems* are well-known in real algebraic geometry, and there exist powerful methods to solve them.

The approach of [35] can, in principle, be generalized in a straightforward way to multidimensional higher-order equations by taking all partial derivatives as polynomial variables. However, this leads, even in simple situations, to huge polynomial expressions, and the corresponding algebraic problem is too complex to be solved directly, even with the aid of computer algebra systems. The method has been successfully adapted to deal with certain multidimensional equations of second order [42, 50] and fourth order [36, 51], but the systematic extension of the scheme to the general multidimensional case is still under development. In this chapter, we propose a further adaption that works generally for *radially symmetric* solutions to higher-order nonlinear equations of a certain homogeneity. And we prove its practicability by applying our scheme to the model equations (1.1)–(1.3) listed in the Introduction.

The objective of this chapter is to prove, for radially symmetric smooth positive solutions $n(t)$ to (1.1), (1.2), or (1.3) satisfying no-flux and Neumann-type boundary conditions (see below for the precise conditions), estimates of the type

$$\frac{\mathrm{d}E_\alpha}{\mathrm{d}t}[n(t)] + cQ_\alpha[n(t)] \leq 0, \tag{2.1}$$

on a specific range of parameters α, where as in (1.6),

$$\begin{aligned} E_\alpha[n] &= \frac{1}{\alpha(\alpha-1)}\int_\Omega n^\alpha \mathrm{d}x, \quad \alpha \neq 0,1, \\ E_0[n] &= \int_\Omega \big(n - \log n\big)\mathrm{d}x, \\ E_1[n] &= \int_\Omega \big(n\big(\log n - 1\big) + 1\big)\mathrm{d}x. \end{aligned} \tag{2.2}$$

Above, $\Omega = B^d = \{|x| < 1\}$ is the unit ball in $\mathbb{R}^d$, $c \geq 0$ is a constant independent of the solution n, and Q_α is a nonnegative functional containing higher-order derivatives of n.

Entropy production inequalities for the evolution equations reviewed in Introduction have been extensively studied in the literature. Concerning the thin-film equation, with no-flux and homogeneous Neumann boundary conditions, it has been shown in [6, 18] that E_α is an entropy if $3/2 \leq \alpha + \beta \leq 3$. The same result holds for periodic boundary conditions [35]. This bound turns out to be sharp, at least in the one-dimensional case [45]. Moreover, the entropy production Q_α in (2.1) can be made explicit: a valid choice is $Q_\alpha[n] = \int_\Omega |(n^{(\alpha+\beta)/2})_{xx}|^2 \mathrm{d}x$ with a suitable $c > 0$ if $3/2 < \alpha + \beta < 3$, see [35].

Let n be a smooth solution to the DLSS equation (2.6) with periodic boundary conditions. Then (2.1) holds with

$$c = \frac{2p(\alpha)}{\alpha^2(p(\alpha) - p(0))}, \tag{2.3}$$

where $p(\alpha) = -\alpha^2 + 2\alpha(d+1)/(d+2) - (d-1)^2/(d+2)^2$, and $Q_\alpha[n] = \int_\Omega (\Delta n^{\alpha/2})^2 \mathrm{d}x$ for all $0 < \alpha < 2(d+1)/(d+2)$ [36]. In the one-dimensional case, this estimate holds true for a larger range of values for α, with $c = 2/\alpha^2$ for $0 < \alpha < 4/3$ and $c = 8(3-2\alpha)/\alpha^3$ for $4/3 < \alpha < 3/2$.

Entropy estimates for the sixth-order quantum diffusion model (2.8) with periodic boundary conditions are available only in one space dimension. In fact, it has been shown in [37] that E_1 is an entropy and (2.1) holds for some $c > 0$ and with $Q_1[n] = \int_\Omega ((\sqrt{n})^2_{xxx} + (\sqrt[6]{n})^6_x)\mathrm{d}x$.

To our knowledge, no entropy production inequalities (2.1) are available for the DLSS equation with no-flux and Neumann boundary conditions[1] and for the sixth-order equation with $\alpha \neq 1$. In this chapter, we will prove such results for radially symmetric solutions.

[1] In one spatial dimension, calculations related to entropy production estimates typically carry over from one "reasonable" boundary condition to another (e.g. from periodic to no-flux or Neumann conditions). In dimensions $d \geq 2$, this is no longer true since the boundary terms resulting from integration by parts have a more complicated structure.

The advantage of considering radially symmetric solutions $n(t;x) = u(t;|x|)$ — in comparison to solutions of the full multidimensional problem — is that the reduced function $u(t;r)$ satisfies an evolution equation with only one spatial variable $r > 0$. Still, the proof of entropy production inequalities (2.1) is substantially more difficult than in the genuinely one-dimensional situation considered before [35]. The reason is that the variable r appears explicitly in the evolution equation. On the algebraic level, this adds one polynomial variable.

In the following we summarize our main results. Below, $\Omega = B^d \subset \mathbb{R}^d$ denotes the d-dimensional unit ball, and ν is the exterior unit normal vector to $\partial\Omega$.

Theorem 2.1 (Thin-film equation)**.** *Let n be a radially symmetric smooth and positive solution to the thin-film equation with homogeneous Neumann and no-flux boundary conditions:*

$$\partial_t n + \operatorname{div}(n^\beta \nabla \Delta n) = 0 \quad \textit{in } \Omega, \textit{ for } t > 0, \tag{2.4}$$

$$\nabla n \cdot \nu = n^\beta \nabla \Delta n \cdot \nu = 0 \quad \textit{on } \partial\Omega, \textit{ for } t > 0. \tag{2.5}$$

Then the functionals E_α, defined in (2.2)*, are entropies provided that $3/2 \le \alpha + \beta \le 3$. In this case, the entropy production inequality* (2.1) *holds with*

$$c = \frac{16}{(\alpha+\beta)^4}(3-\alpha-\beta)(2(\alpha+\beta)-3) \quad \textit{and} \quad Q_\alpha[n] = \int_\Omega \left(\Delta n^{(\alpha+\beta)/2}\right)^2 \mathrm{d}x.$$

The facts that E_α is a Lyapunov functional for $3/2 \le \alpha \le 3$ and that $Q_\alpha[n]$ is an entropy production, for some unspecified constant c, are well known [18]. The explicit dependence of the constant c on α and β is new. This dependence is illustrated in Figure 2.1.

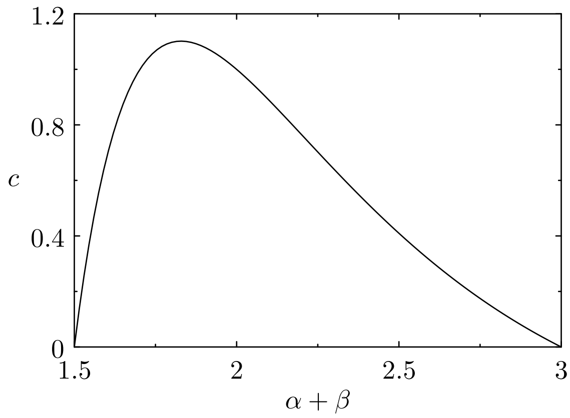


Figure 2.1: Thin-film equation: Values of c as a function of $\alpha + \beta$.

Theorem 2.2 (DLSS equation)**.** *Let n be a radially symmetric smooth positive solution to the DLSS equation with homogeneous Neumann and no-flux boundary conditions:*

$$\partial_t n + \operatorname{div}\left(n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\right) = 0 \quad \textit{in } \Omega, \textit{ for } t > 0, \tag{2.6}$$

$$\nabla n \cdot \nu = n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\cdot \nu = 0 \quad \textit{on } \partial\Omega, \textit{ for } t > 0. \tag{2.7}$$

Then the functionals E_α, defined in (2.2)*, are entropies if*

$$\begin{aligned} d = 1,2,3, \textit{ or } 4, \textit{ and } &\quad \frac{(\sqrt{d}-1)^2}{d+2} \le \alpha \le \frac{3}{2}, \\ d = 5,6, \textit{ or } 7, \textit{ and } &\quad \frac{(\sqrt{d}-1)^2}{d+2} \le \alpha \le \frac{(\sqrt{d}+1)^2}{d+2}, \\ d \ge 8 \textit{ and } &\quad \frac{d-4}{2(d-2)} \le \alpha \le \frac{(\sqrt{d}+1)^2}{d+2}, \end{aligned}$$

and the entropy production inequality (2.1) *holds with $Q_\alpha[n] = \int_\Omega (\Delta n^{\alpha/2})^2 \mathrm{d}x$ and*

$$\begin{aligned} d = 1,2,3: &\quad c = \begin{cases} \dfrac{2p(\alpha)}{\alpha^2(p(\alpha)-p(0))} & \textit{for } \dfrac{(\sqrt{d}-1)^2}{d+2} < \alpha \le \dfrac{5d+7}{3d+6}, \\ \dfrac{8(3-2\alpha)}{\alpha^3} & \textit{for } \dfrac{5d+7}{3d+6} < \alpha < \dfrac{3}{2}, \end{cases} \\ d = 4,5,6,7: &\quad c = \dfrac{2p(\alpha)}{\alpha^2(p(\alpha)-p(0))} \qquad \textit{for } \dfrac{(\sqrt{d}-1)^2}{d+2} < \alpha < \dfrac{(\sqrt{d}+1)^2}{d+2}, \\ d \ge 8: &\quad c = \begin{cases} \dfrac{16(d-2)\alpha - 8(d-4)}{d^2\alpha^3} & \textit{for } \dfrac{d-4}{2(d-2)} < \alpha \le \dfrac{d^2-5d-8}{d^2-2d-8}, \\ \dfrac{2p(\alpha)}{\alpha^2(p(\alpha)-p(0))} & \textit{for } \dfrac{d^2-5d-8}{d^2-2d-8} < \alpha < \dfrac{(\sqrt{d}+1)^2}{d+2}, \end{cases} \end{aligned}$$

where $p(\alpha) = -\alpha^2 + 2\alpha(d+1)/(d+2) - (d-1)^2/(d+2)^2$.

The dependence of c on α is illustrated in Figure 2.2 for various dimensions d. The values for c for $d = 4,5,6,7$ are the same as those derived in [36]. We are able to improve the results from [36] in the radially symmetric case for space dimensions $d = 2,3$ and $d \ge 8$, see Figure 2.3. Our main contribution is that the range of parameters α leading to entropies is larger than in [36].

It is known from [35] that the bounds $0 \le \alpha \le 3/2$ are optimal if $d = 1$. We prove in Section 2.5 that in dimension $d = 2$, no entropies exist for $\alpha \le 0$, and that the lower bound $\alpha = (d-4)/(2d-4)$ is optimal for $d \ge 8$.

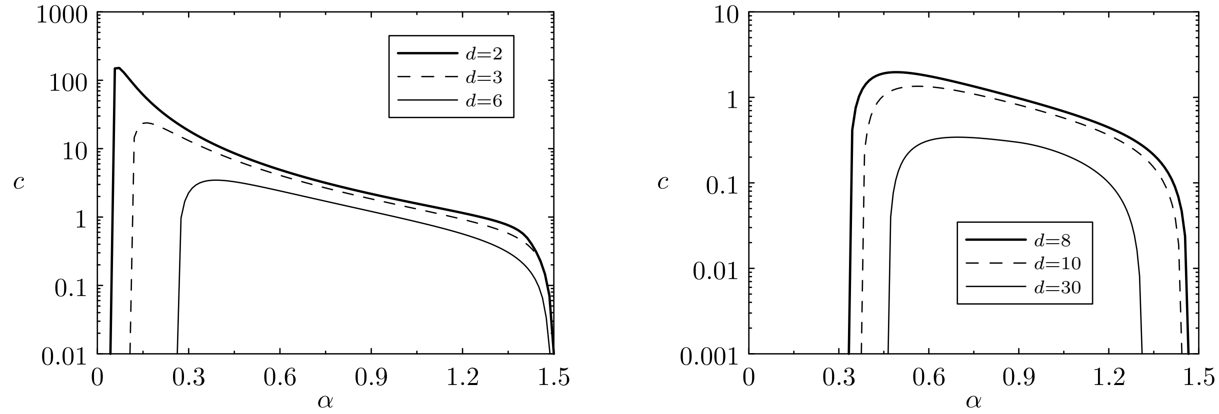


Figure 2.2: DLSS equation: Values of c as a function of d and α.

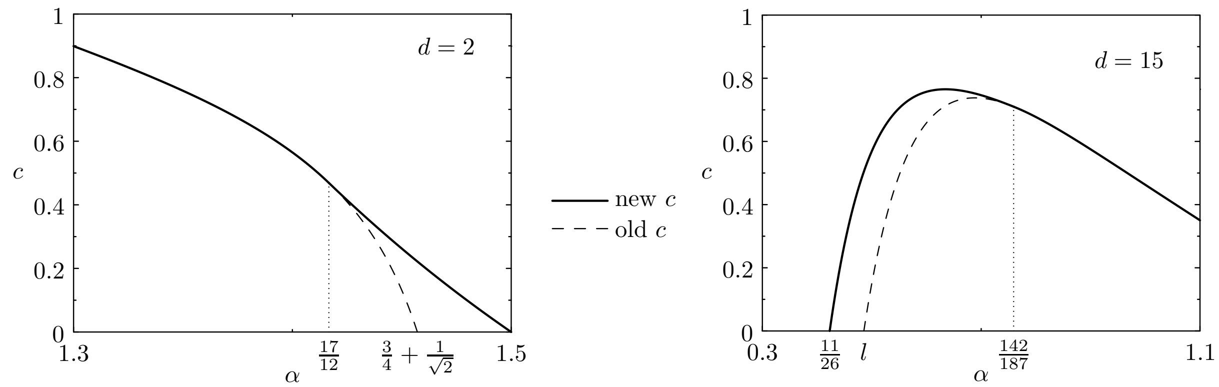


Figure 2.3: DLSS equation: Values of c as a function of α. The solid line represents the values from Theorem 2.2, the dashed line those from [36]. Here, $l = 2(8-\sqrt{15})/17$.

Theorem 2.3 (Sixth-order quantum diffusion equation)**.** *Let n be a radially symmetric smooth and positive solution to the sixth-order quantum diffusion equation:*

$$\partial_t n - \operatorname{div}\left(n\nabla\Big(\frac{1}{2}(\partial^2_{jk}\log n)^2 + \frac{1}{n}\partial^2_{jk}(n\partial^2_{jk}\log n)\Big)\right) = 0 \quad \text{in } \Omega, \text{ for } t>0, \tag{2.8}$$

$$\nabla n\cdot\nu = n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\cdot\nu = n\nabla\Big(\frac{1}{2}(\partial^2_{jk}\log n)^2 + \frac{1}{n}\partial^2_{jk}(n\partial^2_{jk}\log n)\Big)\cdot\nu = 0 \quad \text{on } \partial\Omega. \tag{2.9}$$

Then the functionals E_α, defined in (2.2)*, are entropies if*

$$\begin{aligned}
d &= 1 \ \textit{and} \quad 0.1927\ldots \le \alpha \le 1.1572\ldots,\\
d &= 2 \ \textit{and} \quad 0.2827\ldots \le \alpha \le 1.0982\ldots,\\
d &= 3 \ \textit{and} \quad 0.3470\ldots \le \alpha \le 1.0517\ldots,\\
d &= 4 \ \textit{and} \quad 0.3968\ldots \le \alpha \le 1.0123\ldots,\\
d &= 5 \ \textit{and} \quad 0.4380\ldots \le \alpha \le 0.9775\ldots.
\end{aligned}$$

Moreover, in dimensions $d = 1, \ldots, 4$ *and for* $\alpha = 1$*, the entropy production inequality* (2.1) *holds for some* $c > 0$ *if one chooses*

$$Q_1[n] = \int_\Omega \left(|\nabla\Delta\sqrt{n}|^2 + |\nabla\sqrt[6]{n}|^6\right)\mathrm{d}x. \tag{2.10}$$

The bounds for α are roots of certain polynomials and can be determined only numerically, see Figure 2.4. The Lyapunov property of E_α for $\alpha = 1$ and $d = 1$ is proved in [37]. The proof of this property for $\alpha \neq 1$ and $d > 1$ as well as the entropy production inequality are new. Interestingly, it seems that the logarithmic functional E_1 is no longer a Lyapunov functional for the sixth-order equation in (the unphysical) space dimensions higher than 4. We remark that in dimension $d = 2$, the results from Section 2.5 show that there are no entropies if $\alpha > 4/3$.

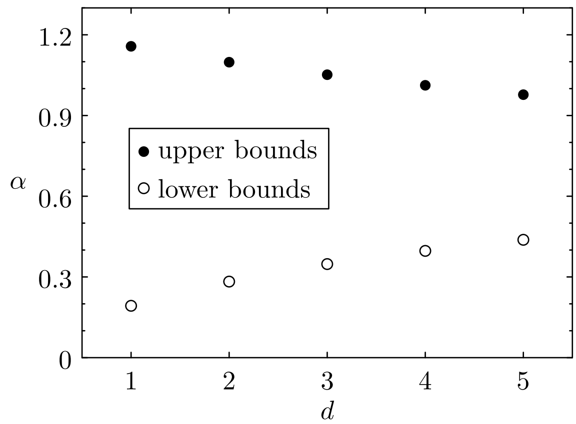


Figure 2.4: Sixth-order quantum diffusion equation: Upper and lower bounds for α depending on the dimension d.

The chapter is organized as follows. The algebraic formalism is developed in Section 2.2. Section 2.3.2 is devoted to the proof of two auxiliary results about quadratic polynomials. The proofs for Theorems 2.1 to 2.3 are given in Section 2.4. In Section 2.5, a sufficient condition is provided under which E_α is *not* an entropy.

2.2 Decision problem and shift polynomials

In this section, we establish the connection between the analytical problem of proving entropy production inequalities (2.1) and an algebraic problem about the non-negativity of certain polynomials. This correspondence — which is summarized in Lemma 2.5 below — constitutes an extension of the ideas previously developed for entropy estimates in one spatial dimension [35]; see also [45] for an alternative approach. The proof of the main theorems are then obtained by solution of the associated algebraic problems.

2.2.1 Formulation as a decision problem

To start with, let us introduce some notation. First, observe that $n : \overline{\Omega} \to \mathbb{R}_+$ is a smooth and positive radially symmetric function if and only if there exists some

$$u \in \mathcal{U} := \left\{ u \in C^\infty([0,1];\mathbb{R}_+) \;\middle|\; \partial_r^m\big|_{r=0} u(r) = 0 \text{ for all odd } m \in \mathbb{N} \right\}$$

such that $n(x) = u(r)$ with $r = |x|$ for all $x \in \Omega = B^d$. We shall refer to u as the (radial) reduction of n, and to n as the (radially symmetric) extension of u.

Throughout this article, η and ξ_1, $\xi_2, \dots$ denote real variables. For $k \in \mathbb{N}$, let Σ_k be the linear span of all monomials $\eta^s \xi_1^{p_1} \cdots \xi_k^{p_k}$ satisfying $s + 1 \cdot p_1 + \cdots + k \cdot p_k = k$. Alternatively, one can define Σ_k as the set of polynomials P in $(\eta, \xi_1, \dots, \xi_k)$ with the homogeneity property

$$P(\lambda\eta, \lambda\xi_1, \lambda^2\xi_2, \dots, \lambda^k\xi_k) = \lambda^k P(\eta, \xi_1, \xi_2, \dots, \xi_k) \tag{2.11}$$

for all $\lambda \in \mathbb{R}$. To any $P \in \Sigma_k$, we associate a non-linear differential operator D_P of order less or equal to k by

$$\mathrm{D}_P[u, r] = P\left(\frac{1}{r}, \frac{\partial_r u}{u}(r), \dots, \frac{\partial_r^k u}{u}(r)\right)$$

acting on functions $u \in \mathcal{U}$.

The key point behind this formalism is that the reductions $u(t; r)$ of radially symmetric solutions $n(t; x)$ to the evolution equations under consideration satisfy equations of the form

$$\partial_t u + r^{-(d-1)} \partial_r \big(r^{d-1} u^{\beta+1} \, \mathrm{D}_P[u, r] \big) = 0, \quad t > 0, \tag{2.12}$$

where $\beta \in \mathbb{R}$ is a parameter, $P \in \Sigma_{K-1}$ and K is order of the equation.

Example 2.4. Recall the representation of the gradient, divergence and Laplacian in radial coordinates: If $W(x) = w(r)$ is a radially symmetric function on $\Omega = B^d$, and $\mathbf{e}_r = x/r$ is the unit vector in radial direction, then

$$\nabla_x W(x) = w_r(r)\mathbf{e}_r, \quad \mathrm{div}_x(W(x)\mathbf{e}_r) = w_r(r) + \frac{d-1}{r} w(r) = r^{-(d-1)} \partial_r \big(r^{d-1} w(r) \big),$$

and, in combination,

$$\Delta_x W(x) = w_{rr}(r) + \frac{d-1}{r} w_r(r) =: \Delta_r w(r).$$

For our examples, this leads to the following:

(A) A radially symmetric solution $n(t; x) = u(t; r)$ to the thin-film equation (2.4) satisfies:

$$\partial_t n = -\,\mathrm{div}_x(n^\beta \nabla_x \Delta_x n) = -\,\mathrm{div}_x \left[u^{\beta+1} \left(\frac{u_{rrr}}{u} + \frac{d-1}{r} \Big(\frac{u_{rr}}{u} - \frac{u_r}{ru} \Big) \right) \mathbf{e}_r \right].$$

This equation is of the form (2.12), with

$$P(\eta, \xi) = \xi_3 + (d-1)\big(\eta\xi_2 - \eta^2 \xi_1 \big).$$

(B) A radially symmetric solution to the DLSS equation (2.6) satisfies:

$$\begin{aligned}\partial_t n &= -\operatorname{div}_x\left[n\nabla_x\left(\frac{\Delta_x\sqrt{n}}{\sqrt{n}}\right)\right] = -\operatorname{div}_x\left[u\,\partial_r\left(\frac{(\sqrt{u})_{rr}}{\sqrt{u}} + \frac{d-1}{r}\frac{(\sqrt{u})_r}{\sqrt{u}}\right)\mathbf{e}_r\right]\\ &= -\operatorname{div}_x\left[u\left(\frac{1}{2}\frac{u_{rrr}}{u} - \frac{u_{rr}}{u}\frac{u_r}{u} + \frac{1}{2}\frac{u_r^3}{u^3} + \frac{d-1}{2r}\left(\frac{u_{rr}}{u} - \frac{u_r^2}{u^2} - \frac{u_r}{ru}\right)\right)\mathbf{e}_r\right].\end{aligned}$$

Also this equation is of the form (2.12), with $\beta = 0$ and

$$P(\eta,\xi) = \frac{1}{2}\big(\xi_3 - 2\xi_2\xi_1 + \xi_1^3 + (d-1)(\eta\xi_2 - \eta\xi_1^2 - \eta^2\xi_1)\big).$$

(C) If $n(t;x) = u(t;r)$ is a radially symmetric solution to the sixth order equation (2.8), then tedious but straightforward computations show that $\partial_t n = \operatorname{div}_x(u\,G(u)\mathbf{e}_r)$, where

$$\begin{aligned}G(u) = &-6\frac{u_r^5}{u^5} + 18\frac{u_r^3}{u^3}\frac{u_{rr}}{u} - 11\frac{u_r}{u}\frac{u_{rr}^2}{u^2} - 8\frac{u_r^2}{u}\frac{u_{rrr}}{u} + 3\frac{u_r}{u}\frac{u_{rrrr}}{u} + 5\frac{u_{rr}}{u}\frac{u_{rrr}}{u} - \frac{u_{rrrrr}}{u}\\ &-(d-1)\frac{1}{r}\left(-6\frac{u_r^4}{u^4} + (2d-7)\frac{1}{r}\frac{u_r^3}{u^3} + 14\frac{u_r^2}{u^2}\frac{u_{rr}}{u} + (3d-8)\frac{1}{r^2}\frac{u_r^2}{u^2} - 4\frac{u_{rr}^2}{u^2}\right.\\ &-3(d-4)\frac{1}{r}\frac{u_r}{u}\frac{u_{rr}}{u} - 6\frac{u_r}{u}\frac{u_{rrr}}{u} + 3(d-3)\frac{1}{r^3}\frac{u_r}{u} - 3(d-3)\frac{1}{r^2}\frac{u_{rr}}{u}\\ &\left.+(d-5)\frac{1}{r}\frac{u_{rrr}}{u} + 2\frac{u_{rrrr}}{u}\right).\end{aligned}$$

In principle, one can easily deduce the correct choice of P from here.

Equation (2.12) is supplemented by initial conditions at $t = 0$,

$$u(0,r) = u_0(r). \tag{2.13}$$

For the fourth order equations ($K = 4$), homogeneous Neumann and no-flux boundary conditions are assumed,

$$u_r(r) = 0, \quad r^{d-1}\,\mathrm{D}_P[u,r] = 0 \qquad \text{at } r = 0 \text{ and } r = 1. \tag{2.14}$$

An additional boundary conditions will be specified for the sixth-order equation (2.8), when $K = 6$.

Notice that the Neumann condition at $r = 0$ is already implied by $u \in \mathcal{U}$. On the other hand, the no-flux condition at $r = 0$ is in general *not* trivially satisfied since $\mathrm{D}_P[u,r]$ might contain terms with negative powers of r. More precisely, the condition is that

$$\lim_{r\downarrow 0}\big(r^{d-1}\,\mathrm{D}_P[u,r]\big) = 0.$$

In terms of the radially symmetric extension $n(t;x) = u(t;r)$, the homogeneous Neumann and no-flux boundary conditions (2.14) for an equation of the form $\partial_t n = \mathrm{div}_x(n^{\beta+1}G(n))$ correspond to

$$\nu \cdot \nabla n(t;x) = 0, \quad \nu \cdot n^{\beta+1}G(n) = 0 \qquad \text{for all } x \in \partial\Omega \text{ and } t > 0,$$

with $\nu = \mathbf{e}_r$ denoting the outer normal vector at the boundary of the unit sphere.

For radially symmetric solutions $n(t;x) = u(t;r)$, the entropy functionals in (2.2) become

$$E_\alpha[n(t)] = \frac{\omega_d}{\alpha(\alpha-1)} \int_0^1 u(t;r)^\alpha r^{d-1} \mathrm{d}r,$$

where ω_d is the surface of the unit sphere in $\mathbb{R}^d$. For the time derivative along (2.12), one calculates

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} E_\alpha[n(t)] &= \frac{\omega_d}{\alpha-1} \int_0^1 u(t;r)^{\alpha-1} \partial_t u(t;r) r^{d-1} dr \\ &= -\omega_d \int_0^1 u^{\alpha+\beta} \left(-\frac{\partial_r u}{u}\right) P\left(\frac{1}{r}, \frac{\partial_r u}{u}, \dots, \frac{\partial_r^{K-1} u}{u}\right) r^{d-1} \mathrm{d}r, \end{aligned} \tag{2.15}$$

where the no-flux boundary conditions in (2.14) have been taken into account. The integrand in (2.15) is again of polynomial structure: defining $S_0 \in \Sigma_K$ by

$$S_0(\eta, \xi) = -\xi_1 P(\eta, \xi_1, \dots, \xi_{K-1}),$$

one can write

$$\frac{\mathrm{d}}{\mathrm{d}t} E_\alpha[n(t)] = -\omega_d I_0[u(t)] \quad \text{with} \quad I_0[u(t)] := \int_0^1 u(t;r)^{\alpha+\beta}\, \mathrm{D}_{S_0}[u(t), r] r^{d-1} \mathrm{d}r. \tag{2.16}$$

Following [35], we call S_0 the *canonical symbol* that characterizes the dissipation of E_α by (2.12).

Recall that the primary goal is to identify — for a given equation of the form (2.12) — those entropies E_α which are monotone in time along all smooth radially symmetric solutions. Thus, we wish to determine values $\alpha \in \mathbb{R}$ such that the corresponding functional I_0 in (2.16) is nonnegative on $\mathcal{U}$. To prove nonnegativity, we apply integration by parts to the integral expression for I_0 in a systematic way that we explain now.

Let $\gamma \in \mathbb{R}$ and a polynomial $R \in \Sigma_{K-1}$ be given. Introduce the *divergence* $T = \delta_\gamma R$ as the unique element $T \in \Sigma_K$ which satisfies

$$\partial_r\big(r^{d-1} u(r)^\gamma\, \mathrm{D}_R[u,r]\big) = r^{d-1} u(r)^\gamma\, \mathrm{D}_T[u,r]$$

for all $u \in \mathcal{U}$. Formally, $\delta_\gamma : \Sigma_{K-1} \to \Sigma_K$ is a linear map that acts on monomials $R(\eta,\xi) = \eta^s \xi_1^{p_1} \cdots \xi_{K-1}^{p_{K-1}}$ as follows,

$$\delta_\gamma R(\eta,\xi) = \Big[(d-1-s)\eta + (\gamma - p_1 - \dots - p_{K-1})\xi_1 + p_1 \frac{\xi_2}{\xi_1} + \dots + p_{K-1} \frac{\xi_K}{\xi_{K-1}}\Big] R(\eta,\xi). \tag{2.17}$$

For $S = S_0 + T$ with $T = \delta_\gamma R$, where $\gamma = \alpha + \beta$ and $R \in \Sigma_{K-1}$, it follows by the fundamental theorem of calculus that

$$I[u] := \int_0^1 u(r)^{\alpha+\beta}\,\mathrm{D}_S[u,r]r^{d-1}\mathrm{d}r = \int_0^1 u(r)^{\alpha+\beta}\big(\mathrm{D}_{S_0}[u,r] + \mathrm{D}_T[u,r]\big)r^{d-1}\mathrm{d}r$$
$$= I_0[u] + \Big[u(r)^{\alpha+\beta}\,\mathrm{D}_R[u,r]r^{d-1}\Big]_{r=0}^{r=1}.$$

Assuming that u satisfies boundary conditions which imply in particular that

$$r^{d-1}\,\mathrm{D}_R[u,r] = 0 \quad \text{at } r = 1 \text{ and for } r \downarrow 0, \tag{2.18}$$

then $I[u] = I_0[u]$, i.e., the replacement $S_0 \mapsto S = S_0 + T$ modifies the integrand but does *not* change the value of the integral. Hence, if there exists an $R \in \Sigma_{K-1}$ for which $S = S_0 + \delta_{\alpha+\beta}R$ is a nonnegative polynomial, then it follows that $I_0[u] = I[u]$ is nonnegative for all $u \in \mathcal{U}$ that satisfy (2.18). Consequently, if the boundary conditions (2.14) for (2.12) imply (2.18), then $E_\alpha[n(t)]$ is monotone in time for all smooth radially symmetric solutions.

In practice, it is more convenient to work directly with the polynomials $T = \delta_\gamma R \in \Sigma_K$ rather than with their pre-images $R \in \Sigma_{K-1}$. Let R_1 to R_m be a collection of linearly independent polynomials in Σ_{K-1} for which (2.18) holds; we refer to Section 2.2.2 below for details on how to select appropriate R's. Denote by $T_1 = \delta_\gamma R_1$ to $T_m = \delta_\gamma R_m$ their respective divergences, which can be explicitly calculated using the rule (2.17) above. In analogy to [35], we call them *shift polynomials*. In conclusion of our discussion, the following is now obvious.

Lemma 2.5. *If the algebraic decision problem*

$$\exists c_1, \dots, c_m \in \mathbb{R} : \forall (\eta, \xi) \in \mathbb{R}^{K+1} : \big(S_0 + c_1T_1 + \cdots + c_mT_m\big)(\eta,\xi) \geq 0 \tag{2.19}$$

can be solved affirmatively, then E_α is a Lyapunov functional for (2.12).

Algebraic decision problems of the type (2.19) are solvable in an algorithmic way; this is discussed in Section 2.3 below. We remark that it would suffice to prove (2.19) for all $\xi \in \mathbb{R}^K$ and *positive* $\eta \in \mathbb{R}$ only, since $\eta = 1/r > 0$. However, since both S_0 and the T_j satisfy the homogeneity property (2.11) with an *even* K, their values at (η,ξ) and $(-\eta,-\xi)$ agree; thus, (2.19) is true under the restriction $\eta > 0$ if and only if it is true without this restriction. We prefer to work directly with (2.19).

2.2.2 Determination of the shift polynomials

The next goal is the following. For the boundary conditions at $\partial\Omega$ as prescribed in Theorems 2.1 to 2.3, we shall compose a list of linearly independent shift polynomials $T \in \Sigma_K$. Recall that shift polynomials are divergencies $T = \delta_\gamma R$ of polynomials $R \in \Sigma_{K-1}$ satisfying the relations (2.18). Consequently, the key is to characterize these R in a systematic way and select among all of them those, which satisfy (2.18) in *all* dimensions $d \geq 1$ and give rise to "useful" (in a specific sense explained below) shift polynomials.

To begin with, we discuss the case $K = 4$ of the DLSS and the thin-film equation. First, we use that fact that $u \in \mathcal{U}$ satisfies *homogeneous Neumann boundary conditions*,

$$u_r(0) = u_r(1) = 0. \tag{2.20}$$

We wish to find all polynomials $R \in \Sigma_{K-1} = \Sigma_3$ for which (2.18) holds. To this end, observe that

$$\big(r^{d-1}\,\mathrm{D}_R[u,r]\big)\big|_{r=1} = R\Big(1, 0, \frac{u_{rr}(1)}{u(1)}, \dots\Big).$$

Observe further that $R(1, 0, \xi_2, \xi_3) = 0$ for arbitrary ξ_2 and ξ_3 if and only if R can be factored in the form $R(\eta, \xi_1, \xi_2, \xi_3) = \xi_1 Q(\eta, \xi_1, \xi_2)$ with some $Q \in \Sigma_2$. Among polynomials R of this type, it remains to single out those for which also

$$\lim_{r\downarrow 0}\big(r^{d-1}\,\mathrm{D}_R[u,r]\big) = 0. \tag{2.21}$$

Since Σ_2 is spanned by ξ_2, ξ_1^2, $\eta\xi_1$, and η^2, we need to investigate (2.21) for $R_1 = \xi_1\xi_2$, $R_2 = \xi_1^3$, $R_3 = \eta\xi_1^2$, and $R_4 = \eta^2\xi_1$, respectively. Since R_1 and R_2 are independent of η, both satisfy (2.21). Further, by l'Hospital's rule, and since $u_r(0) = 0$ and $d \geq 1$,

$$\lim_{r\downarrow 0}\big(r^{d-1}\,\mathrm{D}_{R_3}[u,r]\big) = \lim_{r\downarrow 0}\Big(\frac{u_r(r)}{r}\frac{r^{d-1}u_r(r)}{u(r)^2}\Big) = \frac{u_r(0)u_{rr}(0)}{u(0)^2}\lim_{r\downarrow 0} r^{d-1} = 0,$$
$$\lim_{r\downarrow 0}\big(r^{d-1}\,\mathrm{D}_{R_4}[u,r]\big) = \lim_{r\downarrow 0}\Big(\frac{u_r(r)}{r}\frac{r^{d-2}}{u(r)^2}\Big) = \frac{u_{rr}(0)}{u(0)}\lim_{r\downarrow 0} r^{d-2}.$$

The second limit does not vanish in dimensions $d = 1$ and $d = 2$. Therefore, we shall not use R_4 for further computations.

According to (2.17), the corresponding shift polynomials are

$$T_1(\eta,\xi) = \delta_{\alpha+\beta}R_1(\eta,\xi) = (\alpha+\beta-2)\xi_1^2\xi_2 + \xi_1\xi_3 + \xi_2^2 + (d-1)\eta\xi_1\xi_2, \tag{2.22}$$
$$T_2(\eta,\xi) = \delta_{\alpha+\beta}R_2(\eta,\xi) = (\alpha+\beta-3)\xi_1^4 + 3\xi_1^2\xi_2 + (d-1)\eta\xi_1^3, \tag{2.23}$$
$$T_3(\eta,\xi) = \delta_{\alpha+\beta}R_3(\eta,\xi) = (\alpha+\beta-2)\eta\xi_1^3 + (d-2)\eta^2\xi_1^2 + 2\eta\xi_1\xi_2. \tag{2.24}$$

This finishes the discussion of the homogeneous Neumann boundary conditions (2.20) for equations of order $K = 4$.

Next, we continue to assume $K = 4$, and we recall that $u \in \mathcal{U}$ also satisfies *no-flux boundary conditions*, i.e.,

$$r^{d-1}\,\mathrm{D}_P[u,r] = 0 \qquad \text{at } r = 0 \text{ and } r = 1$$

with the corresponding polynomials $P \in \Sigma_3$ given in Example 2.4 (A) and (B). Thus, trivially, P itself satisfies (2.18), giving rise to the shift polynomial $T_4 = \delta_{\alpha+\beta}P$. However, it is easily seen that T_4 is of no use for our calculations: The coefficient of ξ_3 in the polynomial P is positive, so the coefficient of ξ_4 in T_4 is positive as well. Recalling that $S_0 = -\xi_1 P$ does not contain ξ_4 at all, it follows that $S = S_0 + c_4 T_4$ diverges to $-\infty$ as $\xi_4 \to \pm\infty$ if $c_4 \lessgtr 0$ (keeping η, ξ_1, ξ_2 and ξ_3 fixed). Hence, for $S = S_0 + c_4 T_4$ to have a definite sign, it is required that $c_4 = 0$. Consequently, we omit T_4 in the following.

Remark 2.6. The argument is not completely conclusive, since there could be another shift polynomial $T_5 \in \Sigma_4$ for which $T_4 + T_5$ is non-trivial and does not contain ξ_4. In fact, this cannot happen in the context of radially symmetric solutions, but cancellations of this type do occur when dealing with general multi-dimensional solutions.

We turn to the sixth-order equation (2.8) and start again with the discussion of homogeneous Neumann boundary conditions (2.20). Arguing as for $K = 4$ above, it suffices to consider polynomials R of the form $R_i(\xi, \eta) = \xi_1 Q(\xi, \eta)$ with $Q \in \Sigma_{K-2} = \Sigma_4$, There are 12 such polynomials, listed in Table 2.1 below.

Remark 2.7. Observe that the 5-tuples $(p_1, \ldots, p_5)$ in the table represent precisely the integer partitions of $5 - s$ with $p_1 \geq 1$. Generally, for a differential operator of order K, one would find $(K-1)$-tuples of integer partitions. This indicates the rapid growth of the number of shift polynomials with K.

#	s	p_1	p_2	p_3	p_4	p_5
1	0	5	0	0	0	0
2	0	3	1	0	0	0
3	0	1	2	0	0	0
4	0	2	0	1	0	0
5	0	1	0	0	1	0
6	1	4	0	0	0	0
7	1	2	1	0	0	0
8	1	1	0	1	0	0
9	2	3	0	0	0	0
10	2	1	1	0	0	0
11	3	2	0	0	0	0
12	4	1	0	0	0	0

Table 2.1: Exponents of the monomials $\eta^s \xi_1^{p_1} \cdots \xi_5^{p_5}$ satisfying $s + p_1 + 2p_2 + \cdots + 5 \cdot p_5 = 5$ and $p_1 \geq 1$.

We investigate the limits (2.21) corresponding to these R_i. For $R_8 = \eta\xi_1\xi_3$, $R_9 = \eta^2\xi_1^3$, $R_{10} = \eta^2\xi_1\xi_2$, $R_{11} = \eta^3\xi_1^2$, and $R_{12} = \eta^4\xi_1$, respectively, one obtains by l'Hospital's rule (using that $u_r(0) = u_{rrr}(0) = 0$ for all $u \in \mathcal{U}$) that

$$\lim_{r\downarrow 0} \left(r^{d-1}\, \mathrm{D}_{R_8}[u,r] \right) = \lim_{r\downarrow 0} \left(\frac{u_r(r)}{r} \frac{r^{d-1} u_{rrr}(r)}{u(r)^2} \right) = \frac{u_{rr}(0) u_{rrrr}(0)}{u(0)^2} \lim_{r\downarrow 0} r^d = 0,$$

$$\lim_{r\downarrow 0} \left(r^{d-1}\, \mathrm{D}_{R_9}[u,r] \right) = \lim_{r\downarrow 0} \left(\frac{u_r(r)^3}{r^3} \frac{r^d}{u(r)^3} \right) = \left(\frac{u_{rr}(0)}{u(0)} \right)^3 \lim_{r\downarrow 0} r^d = 0,$$

$$\lim_{r\downarrow 0} \left(r^{d-1}\, \mathrm{D}_{R_{10}}[u,r] \right) = \lim_{r\downarrow 0} \left(\frac{u_r(r)}{r} \frac{r^{d-2} u_{rr}(r)}{u(r)^2} \right) = \left(\frac{u_{rr}(0)}{u(0)} \right)^2 \lim_{r\downarrow 0} r^{d-2},$$

$$\lim_{r\downarrow 0}\left(r^{d-1}\,\mathrm{D}_{R_{11}}[u,r]\right) = \lim_{r\downarrow 0}\left(\frac{u_r(r)^2}{r^2}\frac{r^{d-2}}{u(r)^2}\right) = \left(\frac{u_{rr}(0)}{u(0)}\right)^2 \lim_{r\downarrow 0} r^{d-2},$$
$$\lim_{r\downarrow 0}\left(r^{d-1}\,\mathrm{D}_{R_{12}}[u,r]\right) = \lim_{r\downarrow 0}\left(\frac{u_r(r)}{r}\frac{r^{d-4}}{u(r)}\right) = \frac{u_{rr}(0)}{u(0)} \lim_{r\downarrow 0} r^{d-4}.$$

The limits corresponding to R_{10}, R_{11} and R_{12} do not vanish in general in dimensions $d = 1$ or $d = 2$; we thus shall not use these mononomials directly for the derivation of shift polynomials; however, we will employ a suitable linear combination of them below. Omitting the analogous calculation, we remark that (2.21) is also satisfied for $R_6 = \eta\xi_1^4$ and $R_7 = \eta\xi_1^2\xi_2$ in $d \geq 1$. For all the remaining monomials R_1 to R_5, property (2.21) holds trivially since these R_i are independent of η.

Since equation (2.8) is of sixth order, additional boundary conditions can be imposed. We choose

$$\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\cdot\nu = 0 \quad \text{on } \partial\Omega.$$

In terms of the reduction u, this means that we assume

$$\frac{u_{rrr}(r)}{u(r)} + (d-1)\frac{u_{rr}(r)}{ru(r)} = 0 \quad \text{at } r = 1. \tag{2.25}$$

There are polynomials $R \in \Sigma_5$ for which $r^{d-1}\,\mathrm{D}_R[u,r]$ vanishes for $r \downarrow 0$ and at $r = 1$ because of (2.25), and *not* on grounds of the homogeneous Neumann conditions alone. In analogy to the case of Neumann boundary data, these polynomials can be written in the form $R(\eta,\xi) = (\xi_3 + (d-1)\xi_2\eta)Q(\eta,\xi)$ with an appropriate $Q \in \Sigma_2$. There is no need to consider $Q = \xi_1^2$, since then R contains ξ_1 as a factor, and this has already been investigated above. It is easily seen that the choice $R = (\xi_3 + (d-1)\eta\xi_2)\eta^2$ does not satisfy (2.18) in dimension $d = 1$. On the other hand, $R_* = (\xi_3 + (d-1)\eta\xi_2)\xi_2$ gives

$$\begin{aligned}\lim_{r\downarrow 0}\left(r^{d-1}\,\mathrm{D}_{R_*}[u,r]\right) &= \lim_{r\downarrow 0}\frac{r^{d-1}u_{rr}(r)u_{rrr}(r)}{u(r)^2} + \left(\frac{u_{rr}(0)}{u(0)}\right)^2 \lim_{r\downarrow 0} r^{d-2} \\ &= \frac{u_{rr}(0)u_{rrrr}(0)}{u(0)^2}\lim_{r\downarrow 0} r^d + \left(\frac{u_{rr}(0)}{u(0)}\right)^2 \lim_{r\downarrow 0} r^{d-2}.\end{aligned}$$

While the first term vanishes in all dimensions $d \geq 1$, the second diverges for $d = 1$ or is finite but generally nonzero for $d = 2$. However, it can be annihilated by a suitable linear combination of R_{10} and R_{11}. Indeed, replacing R_{10} by

$$R'_{10}(\eta,\xi) := (d-1)\eta^2\xi_1\xi_2 - 2(d-1)\eta^3\xi_1^2 + (\xi_3 + (d-1)\eta\xi_2)\xi_2,$$

it is now easily verfied that R'_{10} has the property (2.18). Finally, the shift polynomial arising from the no-flux boundary condition is neglected for the same reason as in the case $K = 4$ above.

In summary, we shall use the following expressions for the definition of the shift polynomials:

$$\begin{aligned}
&R_1 = \xi_1^5, \quad R_2 = \xi_1^3\xi_2, \quad R_3 = \xi_1\xi_2^2, \quad R_4 = \xi_1^2\xi_3, \quad R_5 = \xi_1\xi_4,\\
&R_6 = \eta\xi_1^4, \quad R_7 = \eta\xi_1^2\xi_2, \quad R_8 = \eta\xi_1\xi_3, \quad R_9 = \eta^2\xi_1^3,\\
&R'_{10} = \xi_2\xi_3 + (d-1)(\eta^2\xi_1\xi_2 - 2\eta^3\xi_1^2 + \eta\xi_2^2).
\end{aligned}$$

The corresponding shift polynomials read as follows:

$$T_1(\eta,\xi) = (\alpha+\beta-5)\xi_1^6 + 5\xi_1^4\xi_2 + (d-1)\eta\xi_1^5, \tag{2.26}$$
$$T_2(\eta,\xi) = (\alpha+\beta-4)\xi_1^4\xi_2 + 3\xi_1^2\xi_2^2 + \xi_1^3\xi_3 + (d-1)\eta\xi_1^3\xi_2, \tag{2.27}$$
$$T_3(\eta,\xi) = (\alpha+\beta-3)\xi_1^2\xi_2^2 + \xi_2^3 + 2\xi_1\xi_2\xi_3 + (d-1)\eta\xi_1\xi_2^2, \tag{2.28}$$
$$T_4(\eta,\xi) = (\alpha+\beta-3)\xi_1^3\xi_3 + 2\xi_1\xi_2\xi_3 + \xi_1^2\xi_4 + (d-1)\eta\xi_1^2\xi_3, \tag{2.29}$$
$$T_5(\eta,\xi) = (\alpha+\beta-2)\xi_1^2\xi_4 + \xi_1\xi_5 + \xi_2\xi_4 + (d-1)\eta\xi_1\xi_4, \tag{2.30}$$
$$T_6(\eta,\xi) = (\alpha+\beta-4)\eta\xi_1^5 + 4\eta\xi_1^3\xi_2 + (d-2)\eta^2\xi_1^4, \tag{2.31}$$
$$T_7(\eta,\xi) = (\alpha+\beta-3)\eta\xi_1^3\xi_2 + 2\eta\xi_1\xi_2^2 + \eta\xi_1^2\xi_3 + (d-2)\eta^2\xi_1^2\xi_2, \tag{2.32}$$
$$T_8(\eta,\xi) = (\alpha+\beta-2)\eta\xi_1^2\xi_3 + \eta\xi_2\xi_3 + \eta\xi_1\xi_4 + (d-2)\eta^2\xi_1\xi_3, \tag{2.33}$$
$$T_9(\eta,\xi) = (\alpha+\beta-3)\eta^2\xi_1^4 + 3\eta^2\xi_1^2\xi_2 + (d-3)\eta^3\xi_1^3, \tag{2.34}$$
$$\begin{aligned}
T_{10}(\eta,\xi) = {}& \xi_2\xi_4 + \xi_3^2 + (\alpha+\beta-2)\xi_1\xi_2\xi_3 + (d-1)(\alpha+\beta-2)\eta\xi_1\xi_2^2\\
&+ 3(d-1)\eta\xi_2\xi_3 + (d-1)\eta^2\xi_1\xi_3 + (d-1)^2\eta^2\xi_2^2 + (d-1)(\alpha+\beta-2)\eta^2\xi_1^2\xi_2\\
&+ (d-1)(d-7)\eta^3\xi_1\xi_2 - 2(d-1)(\alpha+\beta-2)\eta^3\xi_1^3 - 2(d-1)(d-4)\eta^4\xi_1^2.
\end{aligned} \tag{2.35}$$

2.3 Solution of the algebraic problem

We discuss the solution of the algebraic problem derived in the previous section and we solve two easy quantifier elimination problems.

2.3.1 Quantifier elimination and sum of squares

The algebraic problem stated in Lemma 2.5 is of quantifier elimination type: one is given a statement about a polynomial inequality with quantifiers over certain polynomial variables, and one wishes to find an equivalent formula in which all quantified variables are eliminated. Specifically, in (2.19), all variables *except* α are quantified, and one wants to derive a statement that involves α *only*. The latter statement provides the range of parameter value α such that E_α is an entropy.

Problems of this kind have been studied extensively in (real) algebraic geometry. In his pioneering work [59], Tarski has proven that a quantified formula for polynomial inequalities can be reduced to a quantifier free formula (for another set of polynomial inequalities) in an algorithmic way. He even proposed such an algorithm, which, however, is rather impractical. Nowadays, a variety of computer algebra tools are available that perform quantifier elimination efficiently. Most of them are based on *cylindrical algebraic decomposition (CAD)*, which was originally introduced by Collins [16] and has since then been improved by various authors. Quantifier elimination performed by a computer with such an algorithm is equivalent to a genuine proof (to the extend to which one is willing to accept computer-aided proofs at all).

For the solution of the problems arising in the proofs of Theorems 2.1 to 2.3, we have made use of the command `Reduce` provided by the computer algebra software `Mathematica`, which uses an implementation of CAD. For Theorems 2.1 and 2.2, it has *a posteriori* — i.e., knowing from the `Mathematica`'s result what the solution should be — been possible to write down an explicit proof, choosing suitable values for the variables c_i and applying Lemma 2.8 and 2.9 below. For Theorem 2.3, the effort of giving an explicit proof would have been too large, so instead, the output of `Mathematica` is presented in Appendix B.

A remark on the (im)possible extension of our method to more complicated equations is in order here. The main problem with the CAD-based algorithms is that their complexity grows doubly exponentially in the number of polynomial variables (novel algorithms with single exponential complexity, see e.g. [2], are not yet implemented). This limits the type of problems that can be dealt with in practice. The calculations involved in the computer-aided proof of Theorem 2.3 appear to be already at the edge of feasability. In fact, the solution with `Mathematica` was only possible after performing *a priori* simplifications of the problem. Entropy calculations for PDEs of order $K = 8$ are currently out of reach.

An alternative — more efficient but less rigorous — approach to the solution of the specific decision problem (2.19) is provided by sum-of-squares (SOS) decompositions. Instead of verifying the existence of decision variables c_1 to c_m for which the polynomial $S_c := S_0 + c_1T_1 + \cdots + c_mT_m$ is non-negative for all $(\eta, \xi) \in \mathbb{R}^{K+1}$, one tries to determine specific values of the c_i such that S_c can be written as the sum of squares of polynomials in (η, ξ). The existence of such an SOS decomposition for S_c clearly implies its non-negativity, but it is in general far from being equivalent. The reformulation of (2.19) as an SOS problem allows for its approximate solution by application of efficient numerical optimization tools, also in situations where the complexity for CAD would be by far too high.

In contrast to the quantifier elimination algorithms discussed before, the numerical SOS method never delivers a proof of the statement, and its results will in general be suboptimal due to the non-equivalence of positivity and the existence of a SOS decomposition. However, the SOS approach often reveals invaluable information about the suitable choice of the decision variables c_i, and this information can later be used for the simplification in the (rigorous) quantifier elimination. For *a priori* simplifications in the proof of Theorem 2.3, we have employed the MATLAB tool `yalmip` [48], see Remark 2.10.

2.3.2 Two auxiliary lemmas

In this section, we solve two easy quantifier elimination problems by elementary means. These results will be useful later to perform the proofs for Theorems 2.1 and 2.2 completely explicitly, and to reduce the computational effort for proving Theorem 2.3 with computer aid.

Lemma 2.8. *Let*

$$P(\eta, \xi_1, \xi_2) = a_1\xi_1^4 + a_2\xi_1^2\xi_2 + a_3\xi_2^2 + a_4\eta\xi_1^3 + a_5\eta^2\xi_1^2 + a_6\eta\xi_1\xi_2$$

be a polynomial with real coefficients. Then the quantified formula

$$\forall(\eta, \xi_1, \xi_2) \in \mathbb{R}^3 : \; P(\eta, \xi_1, \xi_2) \geq 0 \tag{2.36}$$

is equivalent to the quantifier free formula

$$\begin{aligned} &\textit{either } a_3 > 0 \textit{ and} \\ &\quad \big[(4a_3a_5 - a_6^2 > 0 \textit{ and } 4a_1a_3a_5 - a_3a_4^2 - a_2^2a_5 - a_1a_6^2 + a_2a_4a_6 \geq 0) \textit{ or} \\ &\quad (4a_3a_5 - a_6^2 = 2a_4a_3 - a_2a_6 = 0 \textit{ and } 4a_3a_1 - a_2^2 \geq 0)\big] \\ &\textit{or } a_3 = 0 \textit{ and } a_2 = a_6 = 0 \textit{ and} \\ &\quad \big[(a_5 > 0 \textit{ and } 4a_5a_1 - a_4^2 \geq 0) \textit{ or } (a_4 = a_5 = 0 \textit{ and } a_1 \geq 0)\big]. \end{aligned} \tag{2.37}$$

Proof. The polynomial P is nonnegative on the hyperplane $\xi_1 = 0$ if and only if $a_3 \geq 0$. For $\xi_1 \neq 0$, formula (2.36) is equivalent to the statement that the quadratic polynomial

$$p(x_1, x_2) = a_1 + a_2x_2 + a_3x_2^2 + a_4x_1 + a_5x_1^2 + a_6x_1x_2$$

is nonnegative for all real values $x_1 = \eta/\xi_1$ and $x_2 = \xi_2/\xi_1^2$. For fixed $x_1^* \in \mathbb{R}$, the quadratic polynomial in x_2,

$$p(x_1^*, x_2) = (a_1 + a_4x_1^* + a_5(x_1^*)^2) + (a_2 + a_6x_1^*)x_2 + a_3x_2^2,$$

is nonnegative if and only if

$$\begin{aligned} &\text{either } a_3 > 0 \text{ and } q_1(x_1^*) := 4a_3(a_1 + a_4x_1^* + a_5(x_1^*)^2) - (a_2 + a_6x_1^*)^2 \geq 0 \\ &\text{or } a_3 = 0 \text{ and } q_2(x_1^*) := a_2 + a_6x_1^* = 0 \text{ and } q_3(x_1^*) := a_1 + a_4x_1^* + a_5(x_1^*)^2 \geq 0. \end{aligned} \tag{2.38}$$

Therefore, $p(x_1, x_2)$ is nonnegative if and only if $q_1(x_1) \geq 0$ or if $q_2(x_1) = 0$ and $q_3(x_1) \geq 0$ for all $x_1 \in \mathbb{R}$. The polynomial

$$q_1(x_1) = 4a_3a_1 - a_2^2 + 2(2a_3a_4 - a_2a_6)x_1 + (4a_3a_5 - a_6^2)x_1^2$$

is nonnegative if and only if

$$\begin{aligned} &\text{either } 4a_3a_5 - a_6^2 > 0 \text{ and } (4a_3a_5 - a_6^2)(4a_3a_1 - a_2^2) - (2a_3a_4 - a_2a_6)^2 \geq 0 \\ &\text{or } 4a_3a_5 - a_6^2 = 2a_4a_3 - a_2a_6 = 0 \text{ and } 4a_3a_1 - a_2^2 \geq 0. \end{aligned}$$

The polynomial q_2 vanishes on $\mathbb{R}$ if and only if $a_2 = a_6 = 0$, and $q_3(x_1) = a_1 + a_4x_1 + a_5x_1^2$ is nonnegative if and only if

$$\begin{aligned} &\text{either } a_5 > 0 \text{ and } 4a_5a_1 - a_4^2 \geq 0 \\ &\text{or } a_4 = a_5 = 0 \text{ and } a_1 \geq 0. \end{aligned}$$

Inserting these statements into (2.38) yields (2.37). □

Lemma 2.9. *Let the polynomial* $P(x) = b_0 + b_1x + b_2x^2$ *with* $b_2 \geq 0$ *and real numbers* $z_1 < z_2$ *be given. Then the quantified formula*

$$\exists x \in (z_1, z_2) : \;\; P(x) \leq 0 \tag{2.39}$$

is equivalent to the quantifier free expression

$$\begin{aligned} &\textit{either } b_2 > 0 \textit{ and } \big[b_0 + b_1z_1 + b_2z_1^2 < 0 \textit{ or } (4b_0b_2 - b_1^2 \leq 0 \textit{ and } 2b_2z_1 + b_1 < 0)\big] \\ &\quad \textit{and } \big[b_0 + b_1z_2 + b_2z_2^2 < 0 \textit{ or } (4b_0b_2 - b_1^2 \leq 0 \textit{ and } 2b_2z_2 + b_1 > 0)\big] \\ &\textit{or } b_2 = 0 \textit{ and } \big[(b_1 > 0 \textit{ and } b_0 + b_1z_1 < 0) \textit{ or } (b_1 < 0 \textit{ and } b_0 + b_1z_2 < 0) \\ &\quad \textit{or } (b_1 = 0 \textit{ and } b_0 \leq 0)\big]. \end{aligned} \tag{2.40}$$

Proof. First assume that $b_2 > 0$. Then the quadratic polynomial P is nonpositive in some interval if and only if $4b_0b_2 - b_1^2 \leq 0$ and exactly for those x which lie in between the two real roots $x_\pm = (\pm\sqrt{b_1^2 - 4b_0b_2} - b_1)/2b_2$. The statement (2.39) is then equivalent to $z_1 < x_+$ and $z_2 > x_-$, which can be rephrased as the first two lines of (2.40). Indeed, if $z_1 + b_1/2b_2 < 0$ then $z_1 < x_+$ is always satisfied, and if $z_1 + b_1/2b_2 \geq 0$ then $z_1 < x_+$ is equivalent to $b_0+b_1z_1+b_2z_1^2 < 0$. Notice that this inequality is satisfied only if $4b_0b_2-b_1^2 \leq 0$.

If $b_2 = 0$, then P is linear. If additionally $b_1 = 0$, (2.39) is equivalent to $b_0 \leq 0$. Therefore, let $b_1 \neq 0$. Then P vanishes at $x_0 = -b_0/b_1$, and (2.39) is equivalent to $z_1 < x_0$ (if $b_1 > 0$) or $z_2 > x_0$ (if $b_1 < 0$). This leads to the last two lines of (2.40). □

2.4 Proofs of the theorems

2.4.1 Proof of Theorem 2.1

By Example 2.4 (A) and (2.16), the canonical symbol of (2.4) reads as follows:

$$S_0(\eta, \xi) = -\xi_1\xi_3 - (d-1)\eta\xi_1\xi_2 + (d-1)\eta^2\xi_1^2.$$

We have to solve the decision problem

$$\exists c_1, c_2, c_3 \in \mathbb{R} : \forall(\eta, \xi_1, \xi_2, \xi_3) \in \mathbb{R}^4 : S(\eta, \xi) = (S_0 + c_1T_1 + c_2T_2 + c_3T_3)(\eta, \xi) \geq 0, \tag{2.41}$$

where the shift polynomials T_1, T_2, and T_3 are given by (2.22)-(2.24).

This problem can be simplified. Indeed, the variable ξ_3 appears in S only in the term $\xi_1\xi_3$, and its coefficient $-1+c_1$ has to vanish; otherwise, $S(\eta, \xi)$ would become negative for $\xi_1 \equiv 1$ and $\xi_3 \to \pm\infty$ if $c_1 \lesseqgtr 1$. Thus, $c_1 = 1$, and the decision problem reduces to finding c_2, $c_3 \in \mathbb{R}$ such that for all $(\eta, \xi) = (\eta, \xi_1, \xi_2) \in \mathbb{R}^3$,

$$\begin{aligned} S(\eta, \xi) &= (S_0 + T_1 + c_2T_2 + c_3T_3)(\eta, \xi) \\ &= a_1\xi_1^4 + a_2\xi_1^2\xi_2 + a_3\xi_2^2 + a_4\eta\xi_1^3 + a_5\eta^2\xi_1^2 + a_6\eta\xi_1\xi_2 \geq 0, \end{aligned}$$

where, setting $\gamma = \alpha + \beta$,

$$a_1 = (\gamma - 3)c_2, \qquad a_2 = \gamma - 2 + 3c_2, \qquad a_3 = 1,$$
$$a_4 = (\gamma - 2)c_3 + (d-1)c_2, \qquad a_5 = (d-2)c_3 + d - 1, \qquad a_6 = 2c_3.$$

In this proof, we perform the quantifier elimination explicitly, without computer aid. By Lemma 2.8, this decision problem is equivalent to either

$$0 < 4a_3a_5 - a_6^2 = -4(c_3+1)(c_3-d+1) =: -4C, \tag{2.42}$$
$$\begin{aligned} 0 \le q(c_2,c_3) &:= 4a_1a_3a_5 - a_3a_4^2 - a_2^2a_5 - a_1a_6^2 + a_2a_4a_6 \\ &= \big(9C - (d-3c_3-1)^2\big)c_2^2 + 2C\gamma c_2 + (\gamma-2)^2C \end{aligned} \tag{2.43}$$

or

$$0 = 4a_3a_5 - a_6^2 = -4(c_3+1)(c_3-d+1), \tag{2.44}$$
$$0 = 2a_3a_4 - a_2a_6 = 2c_2(d-3c_3-1), \tag{2.45}$$
$$\begin{aligned} 0 &\le 4a_1a_3 - a_2^2 = 4(\gamma-3)c_2 - (3c_2+\gamma-2)^2 \\ &= -9\left(c_2 + \frac{\gamma}{9}\right)^2 + \frac{8}{9}(3-\gamma)\left(\gamma - \frac{3}{2}\right). \end{aligned} \tag{2.46}$$

First, we solve (2.44)-(2.46). Equation (2.45) yields $c_2 = 0$ or $c_3 = (d-1)/3$. Because of (2.44), the latter case is only possible if $d = 1$. Let $c_2 = 0$. Then (2.46) is fulfilled if and only if $\gamma = 2$. On the other hand, if $c_3 = (d-1)/3$ (and hence, $d = 1$), the largest range for γ fulfilling (2.46) is obtained by choosing the maximizing value $c_2 = -\gamma/9$. With this choice, (2.46) is fulfilled if and only if $3/2 \le \gamma \le 3$. This shows that (2.44)-(2.46) holds for some c_2, $c_3 \in \mathbb{R}$ if and only if $d = 1$ and $3/2 \le \gamma \le 3$ or if $d > 1$ and $\gamma = 2$.

Next, we solve (2.42)-(2.43). The first inequality implies that $-1 < c_3 < d-1$. For any fixed c_3, the polynomial $q(c_2,c_3)$ is quadratic in c_2 with a strictly negative leading coefficient (since $C < 0$ by (2.42)). Thus, there exists $c_2 \in \mathbb{R}$ such that $q(c_2,c_3) \le 0$ if and only if the discriminant of $q(\cdot,c_3)$ is nonnegative:

$$0 \le \big(2C\gamma\big)^2 - 4\big(9C - (d-3c_3-1)^2\big)(\gamma-2)^2C = 4C\Delta(c_3),$$

where

$$\Delta(c_3) = \gamma^2c_3^2 + 3(\gamma-2)^2(d-4-\gamma^2d)c_3 + (\gamma-2)^2(d-1)(d+8) + \gamma^2 - \gamma^2d.$$

Since $C < 0$, the discriminant is nonnegative if and only if the quadratic polynomial $\Delta(c_3)$ is nonpositive for some $-1 < c_3 < d-1$. By Lemma 2.9, this is the case if either $d = 1$ and $3/2 < \gamma < 3$ or $d > 1$ and $3/2 \le \gamma \le 3$. Thus, there exist $c_2 \in \mathbb{R}$, $c_3 \in (-1, d-1)$ such that (2.42)-(2.43) holds if and only if $3/2 \le \gamma \le 3$. This shows that E_α are entropies for all $3/2 \le \alpha + \beta \le 3$.

We wish to quantify the constant $c > 0$ in the entropy production inequality (2.1) for the choice

$$Q_\alpha[n] = \int_\Omega \big(\Delta n^{\gamma/2}\big)^2 \mathrm{d}x = \omega_d \int_0^1 u^\gamma \,\mathrm{D}_W[u,r] r^{d-1}\mathrm{d}r.$$

The symbol W that characterizes Q_α is

$$\begin{aligned}W(\eta,\xi) &= \left(\frac{\gamma}{2}\right)^2\left(\frac{\gamma}{2}-1\right)^2\xi_1^4 + 2\left(\frac{\gamma}{2}\right)^2\left(\frac{\gamma}{2}-1\right)\xi_1^2\xi_2 + \left(\frac{\gamma}{2}\right)^2\xi_2^2\\ &\quad + 2(d-1)\left(\frac{\gamma}{2}\right)^2\left(\frac{\gamma}{2}-1\right)\eta\xi_1^3 + (d-1)^2\left(\frac{\gamma}{2}\right)^2\eta^2\xi_1^2 + 2(d-1)\left(\frac{\gamma}{2}\right)^2\eta\xi_1\xi_2.\end{aligned}$$

We wish to find the largest $c>0$ for which there exist c_2, $c_3\in\mathbb{R}$ such that for all $(\eta,\xi)=(\eta,\xi_1,\xi_2)\in\mathbb{R}^3$ it holds

$$S_c(\eta,\xi) = (S-cW)(\eta,\xi) = a_1\xi_1^4 + a_2\xi_1^2\xi_2 + a_3\xi_2^2 + a_4\eta\xi_1^3 + a_5\eta^2\xi_1^2 + a_6\eta\xi_1\xi_2 \geq 0,$$

where

$$\begin{aligned}a_1 &= (\gamma-3)c_2 - c\left(\frac{\gamma}{2}\right)^2\left(\frac{\gamma}{2}-1\right)^2,\\ a_2 &= \gamma-2+3c_2-2c\left(\frac{\gamma}{2}\right)^2\left(\frac{\gamma}{2}-1\right),\\ a_3 &= 1-c\left(\frac{\gamma}{2}\right)^2,\\ a_4 &= (\gamma-2)c_3+(d-1)c_2-2c(d-1)\left(\frac{\gamma}{2}\right)^2\left(\frac{\gamma}{2}-1\right),\\ a_5 &= (d-2)c_3+d-1-c(d-1)^2\left(\frac{\gamma}{2}\right)^2,\\ a_6 &= 2c_3-2c(d-1)\left(\frac{\gamma}{2}\right)^2.\end{aligned}$$

We consider the cases $a_3>0$ and $a_3=0$ separately. First, let $a_3=0$, which is equivalent to $c=4/\gamma^2$. By Lemma 2.8, we find that $a_2=a_6=0$, which gives $c_2=0$ and $c_3=d-1$. Furthermore, we obtain $a_5=0$. Hence, by the same lemma, $a_4=0$ and $a_1=-(\gamma/2-1)^2\geq 0$, implying that $\gamma=2$. Next, let $a_3>0$. By Lemma 2.8, the nonnegativity of S_c for certain values c, c_2, and c_3 is equivalent to either

$$0 < 4a_3a_5-a_6^2 = -(c_3-d+1)(4c_3-\gamma^2dc+4) =: -E, \tag{2.47}$$

$$\begin{aligned}0 &\leq q(c_2,c_3,c) := 4a_1a_3a_5 - a_3a_4^2 - a_2^2a_5 - a_1a_6^2 + a_2a_4a_6 \\ &= \frac{1}{4-\gamma^2c}\big(9E-(2d-2-6c_3+\gamma^2(d-1))^2c\big)c_2^2 + \frac{E}{2}\gamma c_2 + \frac{E}{4}(\gamma-2)^2\end{aligned} \tag{2.48}$$

or

$$0 = 4a_3a_5-a_6^2 = -(c_3-d+1)(4c_3-\gamma^2cd+4), \tag{2.49}$$

$$0 = 2a_3a_4-a_2a_6 = c_2\big(2d-2-6c_3+\gamma^2c(d-1)\big), \tag{2.50}$$

$$\begin{aligned}0 &\leq 4a_1a_3-a_2^2 = -9c_2^2+\frac{\gamma}{2}(\gamma^2c-4)+\frac{1}{2}(\gamma-2)^2(\gamma^2c-4)\\ &= -9\left(c_2-\frac{\gamma}{36}(\gamma^2c-4)\right)^2+\frac{1}{144}(\gamma^2c-4)\big(\gamma^4c+32\gamma^2+144(1-\gamma)\big).\end{aligned} \tag{2.51}$$

First, we solve (2.49)-(2.51). We obtain a maximal value for c by choosing $c_2 = \gamma(\gamma^2 c - 4)/36$. Since $a_3 = 1 - \gamma^2 c/4 > 0$ by assumption, we have $c_2 < 0$. With this choice of c_2, condition (2.51) implies that $c \le 16(2\gamma - 3)(3 - \gamma)/\gamma^4$. Furthermore, by (2.50), $c_3 = (d-1)(\gamma^2 c + 2)/6$. Condition (2.49) can be satisfied only if $d = 1$.

Next, we consider (2.47)-(2.48). The polynomial $q(\cdot, c_3, c)$ is quadratic in c_2 with a negative leading coefficient (since $a_3 > 0$). Hence, there exists $c_2 \in \mathbb{R}$ such that $q(c_2, c_3, c)$ is nonnegative if and only if its discriminant $D(c_3, c) = E\Delta_0(c_3, c)/4$ is nonnegative, where $E < 0$ (by (2.47)) and

$$\begin{aligned}\Delta_0(c_3, c) = {} & 4\gamma^2 c_3^2 + \big(8\gamma^2 + 12(\gamma-2)^2(d-4) - 4\gamma^2 d - \gamma^4 cd\big)c_3 \\ & + 4(\gamma-2)^2(d-1)(d+8) - 4\gamma^2 d + 4\gamma^2 - 4\gamma^2 c(\gamma-2)^2(d-1)^2 - \gamma^4 cd + \gamma^4 cd^2\end{aligned}$$

is a quadratic polynomial in c_3. Applying Lemma 2.9, we find that

$$\begin{aligned}&\text{if } d = 1 \text{ and } \gamma \in \left(\frac{3}{2}, 3\right): && c < \frac{16}{\gamma^4}(2\gamma-3)(3-\gamma); \\ &\text{if } d > 1 \text{ and } \gamma \in \left(\frac{3}{2}, 3\right)\setminus\{2\}: && c \le \frac{16}{\gamma^4}(2\gamma-3)(3-\gamma).\end{aligned}$$

The case $a_3 = 0$ provides the choice $\gamma = 2$ with $c = 16/\gamma^4 = 1$. This proves the theorem.

2.4.2 Proof of Theorem 2.2

By Example 2.4 (B), the canonical symbol S_0 for entropy dissipation along the DLSS equation (2.6) is given by

$$S_0(\eta, \xi) = -\frac{1}{2}\xi_1\xi_3 + \xi_2\xi_1^2 - \frac{1}{2}\xi_1^4 - \frac{1}{2}(d-1)\eta\xi_1(\xi_2 - \xi_1^2 - \eta\xi_1).$$

Again, we have to solve the decision problem (2.41). The same argument as in the previous subsection shows that $c_1 = 1$. Thus, we wish to find c_2, $c_3 \in \mathbb{R}$ such that for all $(\eta, \xi) = (\eta, \xi_1, \xi_2) \in \mathbb{R}^3$,

$$2S(\eta, \xi) = a_1\xi_1^4 + a_2\xi_1^2\xi_2 + a_3\xi_2^2 + a_4\eta\xi_1^3 + a_5\eta^2\xi_1^2 + a_6\eta\xi_1\xi_2 \ge 0,$$

where

$$\begin{aligned}&a_1 = (\alpha-3)c_2 - 1, && a_2 = \alpha + 3c_2, && a_3 = 1, \\ &a_4 = (\alpha-2)c_3 + (d-1)(c_2+1), && a_5 = (d-2)c_3 + d - 1, && a_6 = 2c_3.\end{aligned}$$

According to Lemma 2.8, the above decision problem is equivalent to either

$$0 < 4a_3a_5 - a_6^2 = -4(c_3+1)(c_3-d+1) =: -4C, \tag{2.52}$$

$$\begin{aligned}0 \le q(c_2, c_3) &:= 4a_1a_3a_5 - a_3a_4^2 - a_2^2a_5 - a_1a_6^2 + a_2a_4a_6 \\ &= \big(9C - (d-3c_3-1)^2\big)c_2^2 - 2\big(d^2 + 4d + (d-7)c_3 - 5 - \alpha C\big)c_2 \\ &\quad + \alpha^2 C - d^2 - 2d + 4c_3 + 3\end{aligned} \tag{2.53}$$

or

$$0 = 4a_3a_5 - a_6^2 = -4(c_3+1)(c_3-d+1), \tag{2.54}$$
$$0 = 2a_3a_4 - a_2a_6 = -2(c_2+2c_3+3c_2c_3+1) + 2(c_2+1)d, \tag{2.55}$$
$$0 \le 4a_1a_3 - a_2^2 = -4 - \alpha^2 - 12c_2 - 2\alpha c_2 - 9c_2^2. \tag{2.56}$$

First, we solve (2.54)-(2.56). Condition (2.54) implies that either $c_3 = -1$ or $c_3 = d-1$. In the former case, (2.55) gives $c_2 = -(d+1)/(d+2)$. Then (2.56) is equivalent to

$$\alpha^2 - \frac{2(d+1)}{d+2}\alpha + \frac{(d-1)^2}{2(d+2)^2} \le 0,$$

which is satisfied if and only if

$$\frac{(\sqrt{d}-1)^2}{d+2} \le \alpha \le \frac{(\sqrt{d}+1)^2}{d+2}. \tag{2.57}$$

In the latter case $c_3 = d-1$, (2.55) is satisfied if $d=1$ or if $d>1$ and $c_2 = -1/2$. If $d=1$, we choose the maximizing value $c_2 = -(\alpha+6)/9$ for (2.56). Then, this inequality is satisfied if and only if $0 \le \alpha \le 3/2$. On the other hand, if $d>1$, (2.56) can be written as $\alpha^2 - \alpha + 1/4 \le 0$, which is satisfied if and only if $\alpha = 1/2$. We have shown that the decision problem is solvable if $d=1$ and $0 \le \alpha \le 3/2$ or if $d>1$ and (2.57) hold.

Next, we solve (2.52)-(2.53). The discriminant $D(c_3)$ of the quadratic polynomial $q(\cdot, c_3)$ factorizes as $D(c_3) = 4C\Delta(c_3)$, where

$$\begin{aligned}\Delta(c_3) = {} & \alpha^2c_3^2 + 2(\alpha^2(d-5) - \alpha(d-7))c_3 + (d^2+6d-7)\alpha^2 \\ & - 2\alpha(d^2+4d-5) + (d-1)^2.\end{aligned}$$

Notice that $C<0$ by (2.52). An application of Lemma 2.9 shows that $D(c_3)$ is nonnegative if $d=1$ and $0<\alpha<3/2$, or $d \in \{2,3\}$ and $(\sqrt{d}-1)^2/(d+2) < \alpha \le 3/2$, or $d \in \{4,5,6,7\}$ and $(\sqrt{d}-1)^2/(d+2) < \alpha < (\sqrt{d}+1)^2/(d+2)$, or $d \ge 8$ and $(d-4)/(2d-4) \le \alpha < (\sqrt{d}+1)^2/(d+2)$. This proves that $dE_\alpha/dt \le 0$ if these conditions are satisfied.

The estimates for the entropy production term $\omega_d \int (\Delta_r u^{\alpha/2})^2 r^{d-1} \mathrm{d}r$ are obtained by similar arguments as in the previous subsection. Therefore, we omit the lengthy proof here.

2.4.3 Proof of Theorem 2.3

The canonical symbol associated to the sixth-order equation (2.8) can be read off from the representation of its radially symmetric solutions as given in Example 2.4 (C). One finds

$$\begin{aligned}S_0(\eta,\xi) = {} & 6\xi_1^6 - 18\xi_1^4\xi_2 + 11\xi_1^2\xi_2^2 + 8\xi_1^3\xi_3 - 3\xi_1^2\xi_4 - 5\xi_1\xi_2\xi_3 + \xi_1\xi_5 \\ & + (d-1)\big[-6\eta\xi_1^5 + (2d-7)\eta^2\xi_1^4 + 14\eta\xi_1^3\xi_2 + (3d-8)\eta^3\xi_1^3 - 4\eta\xi_1\xi_2^2 \\ & - 3(d-4)\eta^2\xi_1^2\xi_2 - 6\eta\xi_1^2\xi_3 + 3(d-3)\eta^4\xi_1^2 - 3(d-3)\eta^3\xi_1\xi_2 + (d-5)\eta^2\xi_1\xi_3 \\ & + 2\eta\xi_1\xi_4\big].\end{aligned}$$

We have to solve the decision problem

$$\exists c_1, \ldots, c_{10} \in \mathbb{R} : \forall (\eta, \xi) : S(\eta, \xi) = (S_0 + c_1 T_1 + \cdots + c_{10} T_{10})(\eta, \xi) \geq 0,$$

where the shift polynomials T_i are given by (2.26)-(2.35) with $\beta = 0$. Again, we can simplify this problem by eliminating the terms whose sign cannot be controlled. We choose $c_3 = 0$ to eliminate ξ_2^3, $c_5 = -1$ to eliminate $\xi_1\xi_5$, $c_8 = -(d-1)$ to eliminate $\eta\xi_1\xi_4$, $c_4 = \alpha - 2$ to eliminate $\xi_1^2\xi_4$, and $c_{10} = 1$ to eliminate the product $\xi_2\xi_4$ introduced by T_5. With these choices,

$$\begin{aligned}
S(\eta, \xi) &= \big(c_1 T_1 + c_2 T_2 + 0 \cdot T_3 + (\alpha - 2) T_4 + (-1) \cdot T_5 + c_6 T_6 + c_7 T_7 - (d-1) T_8 \\
&\quad + c_9 T_9 + 1 \cdot T_{10}\big)(\eta, \xi) \\
&= \big((\alpha - 5)c_1 + 6\big)\xi_1^6 + \big(5c_1 + (\alpha - 4)c_2 - 18\big)\xi_1^4\xi_2 + (3c_2 + 11)\xi_1^2\xi_2^2 \\
&\quad + \big(c_2 + (\alpha + 1)(\alpha - 3) + 8\big)\xi_1^3\xi_3 + (3\alpha - 5)\xi_1\xi_2\xi_3 \\
&\quad + \big((\alpha - 4)c_6 + (d-1)(c_1 - 6)\big)\eta\xi_1^5 \\
&\quad + \big((\alpha - 3)c_9 + (d-2)c_6 + (d-1)(2d-7)\big)\eta^2\xi_1^4 \\
&\quad + \big((\alpha - 3)c_7 + 4c_6 + (d-1)(c_2 + 14)\big)\eta\xi_1^3\xi_2 \\
&\quad + \big((d-3)c_9 - 2(\alpha - 2)(d-1) + (d-1)(3d-8)\big)\eta^3\xi_1^3 \\
&\quad + \big(2c_7 + (\alpha - 6)(d-1)\big)\eta\xi_1\xi_2^2 \\
&\quad + \big((\alpha - 2)(d-1) + 3c_9 + (d-2)c_7 - 3(d-1)(d-4)\big)\eta^2\xi_1^2\xi_2 \\
&\quad + \big(c_7 - 3(d-1)\big)\eta\xi_1^2\xi_3 + (d-1)^2\eta^4\xi_1^2 - 2(d-1)^2\eta^3\xi_1\xi_2 \\
&\quad - 2(d-1)\eta^2\xi_1\xi_3 + 2(d-1)\eta\xi_2\xi_3 + (d-1)^2\eta^2\xi_2^2 + \xi_3^2.
\end{aligned}$$

The corresponding decision problem contains the four variables η, $\xi_1, \ldots, \xi_3$ and the five coefficients c_1, c_2, c_6, c_7 and c_9. For further simplification, we make a change of variables. Let

$$\zeta_1 = \frac{\eta}{\xi_1}, \quad \zeta_2 = \frac{\xi_2}{\xi_1^2} - \frac{\eta}{\xi_1}, \quad \zeta_3 = \frac{\xi_3}{\xi_1^3} - 3\frac{\eta}{\xi_1}\left(\frac{\xi_2}{\xi_1^2} - \frac{\eta}{\xi_1}\right). \tag{2.58}$$

These definitions are motivated by the observation that for any radially symmetric function $n(x) = u(r)$, the tensors $\nabla_x n$, $\nabla_x^2 n$ and $\nabla_x^3 n$ of the first, second and third total derivatives take the form

$$\begin{aligned}
\nabla_x n(x) &= u\xi_1 \mathbf{e}_r, \\
\nabla_x^2 n(x) &= u\xi_1^2\big(\zeta_2 \mathbf{e}_r \otimes \mathbf{e}_r + \zeta_1 \mathbf{1}\big), \\
\nabla_x^3 n(x) &= u\xi_1^3\big(\zeta_3 \mathbf{e}_r \otimes \mathbf{e}_r \otimes \mathbf{e}_r + \zeta_1\zeta_2 \mathbf{e}_r \otimes_s \mathbf{1}\big),
\end{aligned}$$

where $(\mathbf{e}_r \otimes_s \mathbf{1})_{ijk} = \delta_{ij}x_k + \delta_{jk}x_i + \delta_{ik}x_j$. It turns out that S can be expressed in terms of $\zeta = (\zeta_1, \zeta_2, \zeta_3)$ only. Furthermore, choosing $c_7 = -c_9 = (\alpha + 1/2)(d-1)$ — see Remark 2.10 below — some higher-order terms cancel, and we end up with $S_1(\zeta) = \xi_1^6 S(\eta, \xi)$, which is defined in Appendix B in input line 6 of the `Mathematica` notebook. For any fixed ζ_1

and ζ_2, the polynomial $S_1(\zeta)$ is quadratic in ζ_3, with leading coefficient equal to one. This quadratic polynomial is nonnegative if and only if its discriminant

$$D(\zeta_1, \zeta_2) = \big(\partial_{\zeta_3} S_1(\zeta_1, \zeta_2, 0)\big)^2 - 4S_1(\zeta_1, \zeta_2, 0)$$

is nonpositive. Thus, the nonnegativity of S_0 for some coefficients c_i is reduced to the following decision problem:

$$\exists c_1, c_2, c_6 \in \mathbb{R} : \forall \zeta_1, \zeta_2 \in \mathbb{R} : -D(\zeta_1, \zeta_2) \geq 0.$$

The discriminant $D(\zeta_1, \zeta_2)$ is again of quadratic type, now in terms of ζ_1 and ζ_2. Thus Lemma 2.8 is applicable and yields several conditions on c_1, c_2 and c_6 for the nonpositivity of D. This nonlinear system of equations and inequalities is solved by the computer algebra system `Mathematica` (see Appendix B for more details). As a result, we obtain, for given dimension $d \geq 1$, conditions on the admissible values of α. More precisely, α has to be in between the numbers $\alpha_0(d)$ and $\alpha_1(d)$, and $\alpha_i(d)$ are the positive roots of certain higher-order polynomials which are explicit. Their roots, however, can be calculated only numerically and are given in the statement of the theorem.

The entropy production

$$\omega_d \int_0^1 \big((\Delta_r \sqrt{u})_r^2 + (\sqrt[6]{u})_r^6\big) r^{d-1} \mathrm{d}r$$

is represented by the symbol

$$\begin{aligned} W(\eta, \xi) &= \frac{1}{4}\Big(\xi_3 - \frac{3}{2}\xi_2\xi_1 + \frac{3}{4}\xi_1^3 + (d-1)(\eta\xi_2 - \frac{1}{2}\eta\xi_1^2 - \eta^2\xi_1)\Big)^2 + \frac{1}{46656}\xi_1^6 \\ &= \frac{\xi_1^6}{64}\big(4\zeta_3 + (2\zeta_2 - 1)((2d+4)\zeta_1 - 3)\big)^2 + \frac{\xi_1^6}{46656} =: \xi_1^6 W_1(\zeta). \end{aligned}$$

Setting $\alpha = 1$ in the definition of $S_1(\zeta)$, we obtain the decision problem

$$\exists c_1, c_2, c_6 \in \mathbb{R}, c > 0 : \forall \zeta = (\zeta_1, \zeta_2, \zeta_3) \in \mathbb{R}^3 : S_1(\zeta) - cW_1(\zeta) \geq 0.$$

Our solution strategy is the same as before. We observe that $S_1 - cW_1$ is a quadratic polynomial in ζ_3, and we calculate the respective discriminant. The latter turns out to be quadratic in the remaining variables ζ_1 and ζ_2. Omitting the details, we remark that the reduced decision problem for the discriminant is again solvable with the aid of Lemma 2.8 and `Mathematica`. This results in numerical values for $c > 0$ such that (2.1) holds.

Remark 2.10. The *ad hoc* choice of the coefficients c_7 and c_9 in the proof was originally motivated by the numerical result for the SOS decomposition of S_1 obtained with `yalmip` [48]. There are several reasons to believe that this choice is indeed optimal: First, $c_9 = -c_7$ cancels the coefficient of the indefinite term ζ_1^3, which is obtained after rewriting S_1 in terms of $(\zeta_1, \zeta_2, \zeta_3)$. Second, with $c_7 = (\alpha + 1/2)(d-1)$, the coefficient of the term $\zeta_1\zeta_2^2$ in the discriminant $D(\zeta_1, \zeta_2)$ vanishes, such that the remaining polynomial becomes quadratic in ζ_1 and ζ_2.

2.5 Absence of entropies

Similarly as in [35, 45], it is possible to prove that certain functionals E_α *cannot* be entropies. Below, we generalize Theorem 19 in [35] to the multidimensional, radially symmetric situation. Specifically, let $\gamma \in \mathbb{R}$ and $S \in \Sigma_K$ be given, and define

$$\mathbb{I}[u] = \int_0^1 u(r)^\gamma \, \mathrm{D}_S[u,r] r^{d-1} \mathrm{d}r.$$

Further, define the components of a vector $\bar{\xi} \in \mathbb{R}^K$ by

$$\bar{\xi}_1 = \sigma, \quad \bar{\xi}_2 = \sigma(\sigma-1), \ldots, \quad \bar{\xi}_K = \sigma(\sigma-1)\cdots(\sigma-K+1),$$

where $\sigma = (K-d)/\gamma$. By inserting $(\eta, \xi) = (1, \bar{\xi})$ into formula (2.17), one easily verifies that all shift polynomials T_k vanish at this particular point. Therefore, the values of any two characteristic symbols S and S' coincide at $(1, \bar{\xi})$. Hence, if the given S is negative at $(1, \bar{\xi})$, so is *any* affine combination $S + c_1 T_1 + \cdots + c_m T_m$. In this case, $\mathbb{I}[u]$ cannot be written as an integral over a pointwise nonnegative expression by the method developed before. This statement can be strengthened as follows.

Theorem 2.11. *Assume that $S(1, \bar{\xi}) < 0$. Then there exists a family of functions $u_\varepsilon \in \mathcal{U}$ with $u_\varepsilon(r) = 1$ for $r \in [2/3, 1]$ satisfying* $\lim_{\varepsilon \downarrow 0} \mathbb{I}[u_\varepsilon] = -\infty$.

The set $\mathcal{U}$ is defined on page 19. We remark that, since the functions u_ε are equal to a positive constant for $r > 2/3$, they satisfy any homogeneous boundary condition that involves derivatives at $r = 1$.

The principal idea for our definition of u_ε in (2.59) is borrowed from Laugesen's construction of a "trial function" in one space dimension [45]. Our definition and also the proof of $\mathbb{I}[u_\varepsilon] \to -\infty$ are more straight-forward, since we work under the assumption of strict homogeneity (2.11); the proof in [45] has been designed for a slightly more general situation. The functions u_ε are chosen as suitable ε-regularizations of the radially symmetric power function $\tilde{u}(x) = r^\sigma$. A purely formal calculation gives $D_S[r, \tilde{u}] = r^{\gamma\sigma - K} S(1, \bar{\xi})$ and, even more formally, $\mathbb{I}[\tilde{u}] = S(1, \bar{\xi}) \int_0^1 r^{-1} dr = -\infty$. The rigorous calculations below heavily exploit the marginal singularity of the r^{-1}-integral for the estimation of the additional terms that originate from the regularization $\tilde{u} \to u_\epsilon$; the argument would not work for $\sigma \neq (K-d)/\gamma$.

Proof. Let a cut-off function $\phi \in C^\infty(\mathbb{R})$ with $0 \leq \phi \leq 1$ be given that satisfies

$$\phi(r) = 1 \quad \text{for } r \leq 1/3 \text{ and } \quad \phi(r) = 0 \quad \text{for } r \geq 2/3.$$

Choose $\varepsilon \in (0, 1/2)$ arbitrary and define u_ε by

$$u_\varepsilon(r) = \phi(r/\varepsilon)\, \varepsilon^\sigma + [1 - \phi(r/\varepsilon)]\phi(r)\, r^\sigma + 1 - \phi(r). \tag{2.59}$$

Clearly, u_ε is positive and of class C^∞. Moreover, notice that $u_\varepsilon(r) = 1$ for $2/3 \le r \le 1$ as stated in the theorem. We need to evaluate the integral

$$\mathbb{I}[u_\varepsilon] = \int_0^1 u_\varepsilon(r)^\gamma \, \mathrm{D}_P[u_\varepsilon, r] r^{d-1} \mathrm{d}r.$$

This is done by splitting the domain $[0,1]$ into three intervals. To start with, let $r \in [0, 2\varepsilon/3]$. Then $u_\varepsilon(r) = \varepsilon^\sigma \psi(r/\varepsilon)$, where $\psi(\rho) = \phi(\rho) + [1 - \phi(\rho)]\rho^\sigma$, and consequently

$$\frac{\partial_r^k u_\varepsilon(r)}{u_\varepsilon(r)} = \varepsilon^{-k} \frac{\partial_\rho^k \psi(\rho)}{\psi(\rho)},$$

with $\rho = r/\varepsilon$. The homogeneity (2.11) of $S \in \Sigma_K$ now implies

$$\mathrm{D}_S[u_\varepsilon, r] = \varepsilon^{-K} \, \mathrm{D}_S[\psi, \rho].$$

Substitution of $r = \varepsilon\rho$ under the integral leads to

$$I_1 := \int_0^{2\varepsilon/3} u_\varepsilon(r)^\gamma \, \mathrm{D}_P[u_\varepsilon, r] r^{d-1} \mathrm{d}r = \varepsilon^{\sigma\gamma - K + d} \int_0^{2/3} \psi(\rho)^\gamma \, \mathrm{D}_P[\psi, \rho] \rho^{d-1} \mathrm{d}\rho.$$

Since ψ is positive and smooth, and all of its derivatives vanish at $\rho = 0$, the last integral is well-defined and finite. In fact, the value of I_1 is independent of ε, since $\sigma\gamma = K - d$ by definition of σ.

Next, let $r \in [2\varepsilon/3, 1/3]$ and notice that $u_\varepsilon(r) = r^\sigma$. It follows that

$$\partial_r^k u_\varepsilon(r) = \sigma(\sigma - 1) \cdots (\sigma - k + 1) r^{\sigma - k} = r^{-k} \bar{\xi}_k u_\varepsilon(r).$$

Using the homogeneity (2.11) once again, we obtain $\mathrm{D}_S[u_\varepsilon, r] = r^{-K} S(1, \bar{\xi}_1, \ldots, \bar{\xi}_K)$, and thus

$$\begin{aligned} I_2 : &= \int_{2\varepsilon/3}^{1/3} u_\varepsilon(r)^\gamma \, \mathrm{D}_S[u_\varepsilon, r] r^{d-1} \mathrm{d}r = S(1, \bar{\xi}_1, \ldots, \bar{\xi}_K) \int_{2\varepsilon/3}^{1/3} r^{\gamma\sigma + d - K} \frac{\mathrm{d}r}{r} \\ &= S(1, \bar{\xi}_1, \ldots, \bar{\xi}_K) \ln[1/(2\varepsilon)]. \end{aligned}$$

Finally, for $r \in [1/3, 1]$, the function $u_\varepsilon(r)$ is smooth and positive, and does not depend on $\varepsilon > 0$. In other words,

$$I_3 := \int_{1/3}^1 u_\varepsilon(r)^\gamma \, \mathrm{D}_S[u_\varepsilon, r] r^{d-1} \mathrm{d}r$$

is a finite, ε-independent value. In summary, there is some constant $C > 0$ for which

$$\mathbb{I}[u_\varepsilon] = I_1 + I_2 + I_3 = C + S(1, \bar{\xi}_1, \ldots, \bar{\xi}_K) \ln[1/(2\varepsilon)].$$

This sum converges to $-\infty$ as $\varepsilon \downarrow 0$ since $S(1, \bar{\xi}_1, \ldots, \bar{\xi}_K) < 0$ by assumption. $\square$

As a corollary, we obtain that E_α cannot be an entropy for the evolution equation (2.12) if the associated canonical symbol S_0 has the property that

$$S_0\big(1, \sigma, \sigma(\sigma-1), \ldots, \sigma(\sigma-1)\cdots(\sigma-K+1)\big) < 0$$

for $\sigma = (K-d)/(\alpha+\beta)$. Indeed, we may use the corresponding function u_ε constructed in the proof of Theorem 2.11 above as an initial condition u_0 in (2.13). The functions u_ε are positive and smooth, and they satisfy the boundary conditions since u_ε is constant close to the boundary. By classical parabolic theory, there exists a corresponding solution $u_\varepsilon(t)$, at least locally in time, i.e. for $t \in [0, \tau]$, and this solution and its spatial derivatives depend continuously on $t \in [0, \tau]$. Hence,

$$E_\alpha[u_\varepsilon(\tau)] - E_\alpha[u_\varepsilon] = -\omega_d \int_0^\tau \int_0^1 u_\varepsilon(t;r)^\gamma \, \mathrm{D}_{S_0}[u_\varepsilon(t), r] r^{d-1} \mathrm{d}r \, \mathrm{d}t.$$

Choosing ε and τ sufficiently small, the double integral on the right-hand side is negative, and one concludes that $E_\alpha[u_\varepsilon(\tau)] > E_\alpha[u_\varepsilon]$.

We apply this result to the fourth- and sixth-order equations introduced in the introduction. It turns out that for the thin-film equation (2.4), we have $S_0(1, \bar{\xi}) < 0$ if and only if $\alpha + \beta \notin [3/2, 3]$ for $d = 1$, $\alpha + \beta \in (-\infty, 1)$ for $d = 2$, $\alpha + \beta \in (-1, 1/2)$ for $d = 3$, and $\alpha + \beta \in (-(d-4)/2, (d-4/(d+2))$ for $d > 4$. (Our method does not give any statement for $d = 4$.) In one space dimension, we achieve the optimal bounds for $\alpha + \beta$, being in the interval $[3/2, 3]$ (as in [45, 35]). However, we obtain much less information for $d > 1$.

For the DLSS equation (2.6), $S_0(1, \bar{\xi}) < 0$ holds if and only if $\alpha \notin [0, 3/2]$ for $d = 1$, $\alpha \in (-\infty, 0)$ for $d = 2$, $\alpha \in (-1/2, 0)$ for $d = 3$, and $\alpha \in (0, (d-4)/(2d-4))$ for $d \geq 4$. We recover the optimal range in the one-dimensional case. Moreover, we see that the lower bound for $d \geq 8$ is optimal, at least for nonnegative values for α.

Finally, for the sixth-order equation (2.8), we have $S_0(1, \bar{\xi}) < 0$ if and only if $\alpha \in (5/4, 10/3)$ for $d = 1$, $\alpha \in (4/3, \infty)$ for $d = 2$, $\alpha \notin [-3(1-\sqrt{33})/8, -3(1+\sqrt{33})/8]$ for $d = 3$, and $\alpha \in (-\infty, -1)$ for $d = 4$. For higher space dimensions, $S_0(1, \bar{\xi}) \geq 0$ holds for all $\alpha \in \mathbb{R}$, and we do not obtain any information. In the two-dimensional case, there are no entropies for $\alpha > 4/3$, which is not far from the upper bound $\alpha = 1.0982\ldots$ obtained in Theorem 2.3.

Chapter 3

Nonlinear sixth-order quantum diffusion equation

3.1 Introduction and results

This chapter is concerned with the sixth-order quantum diffusion equation obtained from an expansion to order $\hbar^4$ of the nonlocal quantum diffusion model. Employing Einstein's summation convention, equation (1.3) reads as

$$\partial_t n = \operatorname{div}\Big(n\nabla\Big(\frac{1}{2}(\partial^2_{ij}\log n)^2 + \frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n)\Big)\Big). \tag{3.1}$$

We study the initial-value problem for (3.1) in the d-dimensional torus $\mathbb{T}^d \cong [0,1]^d$ in dimensions $d = 2$ and $d = 3$.

Specifically, we compare two solution concepts for (3.1). The first concept is concerned with adapted weak nonnegative solutions. In this framework we generalize the global existence result from [37] to the *multidimensional* situation. The second concept is that of positive classical solutions. In analogy to the results obtained by Bleher et al. for the fourth-order DLSS equation [7]

$$\partial_t n + \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0\,, \tag{3.2}$$

we are able to establish the existence of such regular solutions for (3.1) locally in time. Naturally, a classical solution is also a weak solution on the time interval of its existence. Vice versa, from a given weak solution, one obtains classical solutions on all time subintervals where the weak solution is a strictly positive and energetic (see Definition 3.4 below) density function. Since we are not able to rule out the loss of strict positivity due to the evolution, it thus might happen that the classical solution concept breaks down on certain, possibly even infinite time intervals along the globally well-defined weak solution.

We shall provide further motivations to study (3.1) in Section 3.2 below. At this point, we simply want to put equation (3.1) into the general context of higher-order parabolic equations.

In the existence analysis for equations like (3.2), one of the main difficulties is to establish non-negativity of the solutions. Typically, sophisticated regularizations are constructed that lead to smooth and *strictly positive* approximative solutions. The limit of vanishing regularizations then provides a nonnegative weak solution.

For our equation (3.1), the situation is more delicate since the nonlinearity in the equation is not well-defined when n vanishes. This is a problem: Although nonnegativity of the solution is expected on physical grounds, the possibility that a vacuum (localized in time and space) is created from an initially strictly positive density cannot be ruled out. Thus, atop of constructing strictly positive approximations, we need to define a solution concept that works also for merely nonnegative densities, so that the passage to the limit of vanishing regularizations is sensible.

The key idea here is to rewrite the nonlinearity in (3.1) in a way that substitutes the logarithm by an expression that is still well-defined for $n = 0$. It turns out that the following equivalent representation of equation (3.1),

$$\partial_t n = \Delta^3 n + \partial^3_{ijk} F_1^{(ijk)}(n) + \partial^2_{ij} F_2^{(ij)}(n), \tag{3.3}$$

with the nonlinear operators

$$\begin{aligned} F_1^{(ijk)}(n) &= 4\partial_i\sqrt{n}\big(4\partial_j\sqrt[4]{n}\partial_k\sqrt[4]{n} - 3\partial^2_{jk}\sqrt{n}\big), \\ F_2^{(ij)}(n) &= 8\sum_{k=1}^{d}\big(\partial^2_{ik}\sqrt{n} - 4\partial_i\sqrt[4]{n}\partial_k\sqrt[4]{n}\big)\big(\partial^2_{jk}\sqrt{n} - 4\partial_j\sqrt[4]{n}\partial_k\sqrt[4]{n}\big) \end{aligned} \tag{3.4}$$

is appropriate to study both concepts of solutions: weak and classical. Here and in the following, we employ the notations $\partial_i = \partial/\partial x_i$, $\partial^2_{ij} = \partial^2/\partial x_i \partial x_j$, etc. and the summation convention over repeated indices from 1 to d.

The construction of strictly positive approximative solutions uses yet another transformation of the nonlinearity. First, (3.1) is discretized in time with the implicit Euler scheme. The semi-discrete equation is regularized by an additional term of the form $\varepsilon(-\Delta)^3 \log n$. Each time step then requires the solution of a *strictly* elliptic problem in terms of $y = \log n$. Classical elliptic theory provides L^∞-bounds on y and thus strict positivity of $n = \exp(y)$.

The required compactness to perform the deregularization limit $\varepsilon \downarrow 0$ and later the passage to the time-continuous limit is obtained from the dissipation of a distinguished Lyapunov functional: The physical entropy[1]

$$\mathcal{H}[u] = \int_{\mathbb{T}^d} \big(u(\log u - 1) + 1\big)\,\mathrm{d}x \tag{3.5}$$

is nonincreasing along the solutions. In fact, using the entropy construction method of [35], which is based on systematic integration by parts, we are able to prove that the entropy

[1]The same functional is in the context of α-functionals denoted by E_1. In this chapter we use $\mathcal{H}$, which is Boltzmann's notation for the entropy.

dissipation $-\,\mathrm{d}\mathcal{H}/\,\mathrm{d}t$ controls certain spatial derivatives,

$$-\frac{\mathrm{d}\mathcal{H}[n]}{\mathrm{d}t} \geq \kappa \int_{\mathbb{T}^d} \left(\|\nabla^3 \sqrt{n}\|^2 + |\nabla \sqrt[6]{n}|^6 \right) \mathrm{d}x, \tag{3.6}$$

where ∇^k denotes the tensor of all partial derivatives of order k. The resulting estimates are sufficient to pass to the limit.

Our main results about weak solutions are the following two theorems.

Theorem 3.1 (Global existence of weak solutions). *Let $n_0 \in L^1(\mathbb{T}^d)$ be a nonnegative function with finite entropy $\mathcal{H}[n_0] < \infty$. Then there exists a nonnegative function $n \in W^{1,4/3}_{\mathrm{loc}}(0,\infty;\ H^{-3}(\mathbb{T}^d))$, satisfying $\sqrt{n} \in L^2_{\mathrm{loc}}(0,\infty; H^3(\mathbb{T}^d))$ and $n(0) = n_0$, that is a solution to* (3.3) *in the following weak sense:*

$$\int_0^\infty \langle \partial_t n, \varphi \rangle \,\mathrm{d}t + \int_0^\infty \int_{\mathbb{T}^d} \left(\partial^3_{ijk}\varphi\, \partial^3_{ijk} n + \partial^3_{ijk}\varphi\, F_1^{(ijk)}(n) - \partial^2_{ij}\varphi\, F_2^{(ij)}(n) \right) \mathrm{d}x\,\mathrm{d}t = 0 \tag{3.7}$$

for all test functions $\varphi \in L^4(0,T; H^3(\mathbb{T}^d))$ and given terminal time $T > 0$.

It is not trivial at all to see that all integrals on the right-hand side of (3.7) are well-defined for functions n of the stated regularity. At this point, we just mention that under these hypotheses, $\sqrt[4]{n}$ is a well-defined Sobolev function; see Lemma C.4 in Appendix C as well as [47] and [30, Section 3] for a discussion about the regularity of square and fourth roots of nonnegative functions. The relevant estimates on the pairings inside the integrals are established in the cause of the proof; see, e.g., Lemma 3.11 below. Since dimension-dependent Sobolev embeddings are involved, this particular concept of weak solution does not carry over to space dimensions $d \geq 4$.

Theorem 3.2 (Exponential time decay). *Let $n_0 \in L^1(\mathbb{T}^d)$ be a nonnegative function of finite entropy $\mathcal{H}[n_0] < \infty$ and unit mass $\int_{\mathbb{T}^d} n_0 dx = 1$. Let n be the weak solution to* (3.3) *constructed in Theorem 3.1. Then there exists a constant $\lambda > 0$, depending on d, such that for all $t > 0$,*

$$\|n(t;\cdot) - 1\|_{L^1(\mathbb{T}^d)} \leq \sqrt{2\mathcal{H}[n_0]}e^{-\lambda t}.$$

Since equation (3.3) is semi-linear parabolic, it is accessible by methods from the theory of analytic semigroups. This approach leads to the following result on classical solutions.

Theorem 3.3 (Existence and uniqueness of a classical solution). *Let $n_0 \in H^2(\mathbb{T}^d)$ be strictly positive. Then there exist $T_* > 0$ and precisely one smooth and strictly positive classical solution $n \in C^\infty((0,T_*); C^\infty(\mathbb{T}^d))$ to* (3.3) *with $n(t) \to n_0$ in $H^2(\mathbb{T}^d)$ as $t \downarrow 0$. Moreover, either $T_* = +\infty$, or there exists a limiting profile $n_* \in H^2(\mathbb{T}^d)$ such that $n(t) \to n_*$ in $H^2(\mathbb{T}^d)$ as $t \uparrow T_*$ and $\min_{x\in\mathbb{T}^d} n_*(x) = 0$.*

In other words, the only possibility for a classical solution to break down is the loss of strict positivity. This result parallels the one of [7] for the fourth-order DLSS equation in space dimension $d = 1$. Since stronger Sobolev embeddings are available for the sixth-order equation (3.3), our result holds in dimensions $d = 2$ and $d = 3$ as well. It is an open problem if loss of positivity can occur at $t > 0$ or not.

Naturally, we shall establish a connection between the concept of weak solutions, defined in (3.7), and classical solutions. To do so, we need to introduce the *energy*: For a positive and smooth function $u \in C^\infty(\mathbb{T}^d)$, define

$$\mathcal{E}[u] = \frac{1}{2} \int_{\mathbb{T}^d} u \|\nabla^2 \log u\|^2 \, \mathrm{d}x. \tag{3.8}$$

This functional is equivalent to the L^2-norm of $\nabla^2 \sqrt{u}$ in the sense that

$$c \big\| \nabla^2 \sqrt{u} \big\|_{L^2}^2 \leq \mathcal{E}[u] \leq C \big\| \nabla^2 \sqrt{u} \big\|_{L^2}^2 \tag{3.9}$$

for some constants $0 < c \leq C$ [30, 36]. For smooth and positive solutions to (3.3), one easily proves that $\mathcal{E}$ is a Lyapunov functional, see Lemma 3.7 below. The functional $\mathcal{E}[u]$ extends in a weakly lower semi-continuous manner to all nonnegative functions u with $\sqrt{u} \in H^2(\mathbb{T}^d)$; see [30, Section 3] for details. Hence, if n is a weak solution in the sense of Theorem 3.1, then $\mathcal{E}[n(t)]$ is well-defined for almost every $t > 0$.

We expect that $\mathcal{E}$ is a Lyapunov functional also for weak solutions, but currently we are not able to prove this conjecture, mainly because $\mathcal{E}$ is not a convex functional. Therefore we *assume* the Lyapunov property.

Definition 3.4. Let $n \in C^0((0,\infty); H^{-3}(\mathbb{T}^d))$ be the t-continuous representative of a weak solution in the sense of (3.7). We call n *energetic on the interval* $(T_1, T_2) \subset \mathbb{R}_+$ if $\mathcal{E}[n(t)]$ is uniformly bounded for all $t \in (T_1, T_2)$.

Notice that a weak solution is energetic on (T_1, T_2) if and only if $\sqrt{n} \in L^\infty(T_1, T_2; H^2(\mathbb{T}^d))$.

Theorem 3.5 (Regularity of weak solutions)**.** *Assume that the weak solution n from Theorem 3.1 is energetic on (T_1, T_2) and strictly positive at some time $t_0 \in [T_1, T_2)$; here $T_1 = 0$ and/or $T_2 = +\infty$ are admissible. Then there exists $T_* \in (T_1, T_2]$ such that n equals the classical solution from Theorem 3.3 on (t_0, T_*). Moreover, either $T_* = T_2$ or $n(t)$ loses strict positivity as $t \uparrow T_*$ in the sense of Theorem 3.3.*

In summary, an energetic weak solution is classical on each time interval on which it is strictly positive, and the loss of positivity occurs in an H^2-continuous way.

The chapter is organized as follows. Section 3.2 provides some background information on the derivation and properties of (3.1). In Section 3.3, we derive the alternative formulation (3.3) of (3.1) and we prove the entropy inequality (3.6). Sections 3.4, 3.5, 3.6, and 3.7 are devoted to the proofs of Theorems 3.1, 3.2, 3.3, and 3.5, respectively. Some technical lemmas and known results which are used in the existence analysis are collected in Appendix C.

3.2 Derivation and motivation

In this section, we indicate several motivations to study equation (3.1) by reviewing its derivation from the nonlocal quantum model, putting it in the context of gradient flows, and establishing connections to the heat and DLSS equations.

3.2.1 On the derivation from the nonlocal quantum model

Degond et al. derived in [21] the nonlocal and nonlinear quantum diffusion model

$$\partial_t n = \operatorname{div}(n\nabla A) \quad \text{in } \mathbb{R}^d,\ t > 0, \tag{3.10}$$

where the potential A is defined implicitly as the unique solution to

$$n(t;x) = \int_{\mathbb{R}^d} \operatorname{Exp}\Big(A(t;x) - \frac{|p|^2}{2}\Big)\,\mathrm{d}p.$$

The so-called quantum exponential Exp is defined as the Wigner transformed operator exponential: Denoting by W the Wigner transformation and by W^{-1} the corresponding Weyl quantization, then $\operatorname{Exp}(f) = W^{-1} \circ \exp \circ W(f)$; see [21] for details.

In the semi-classical limit $\hbar \downarrow 0$, the expression $\operatorname{Exp}(A - |p|^2/2)$ converges to e^A, so that $A = \log n$, and we recover from (3.10) the classical heat equation. For $\hbar > 0$, however, the quantum exponential is a complicated, genuinely nonlocal operator. An asymptotic expansion in terms of $\hbar$ has been performed in Appendix A, leading to the following local approximation of A in terms of n:

$$A = A_0 + \frac{\hbar^2}{24}A_1 + \frac{\hbar^4}{360}A_2 + O(\hbar^6) \tag{3.11}$$

with the local expressions

$$A_0 = \log n, \quad A_1 = -4\frac{\Delta\sqrt{n}}{\sqrt{n}}, \quad A_2 = \frac{1}{2}(\partial^2_{ij}\log n)^2 + \frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n).$$

Replacing A in (3.10) by A_0, A_1, or A_2 yields, respectively, the heat equation, the DLSS equation (3.2), or the sixth-order equation (3.1). In this sense, (3.2) and (3.1) constitute, respectively, the primary and secondary quantum corrections to the classical diffusion equation.

3.2.2 Gradient-flow structure

Equation (3.1) possesses—at least on a formal level—a variational structure. The divergence form implies that solutions n formally conserve the total mass, i.e., the integral $m = \int_{\mathbb{T}^d} n(t;x)\,\mathrm{d}x$ is independent of t. By homogeneity, we can assume $m = 1$ without loss of generality. Thus, any solution to (3.1) defines a curve $t \mapsto n(t)$ in the space of probability measures on $\mathbb{T}^d$. Provided that n is regular enough, this curve realizes a steepest descent in the energy landscape of the energy functional $\mathcal{E}$ from (3.8) with respect to the L^2-Wasserstein metric. Indeed, by a formal calculation, we obtain the gradient-flow representation

$$\partial_t n = \operatorname{div}\left(n\nabla\frac{\delta\mathcal{E}[n]}{\delta n}\right)$$

from (3.10) with $A \equiv A_2$, where $A_2 = \delta\mathcal{E}[n]/\delta n$ is the variational derivative of $\mathcal{E}$.

This variational structure is a remarkable property by itself. Atop of that, it establishes yet another connection to the heat and DLSS equations. It is well known since the seminal paper [32] that the heat equation is the gradient flow of the entropy functional $\mathcal{H}$ from (3.5) with respect to the L^2-Wasserstein distance. The dissipation of $\mathcal{H}$ along its own gradient flow amounts to the *Fisher information*,

$$\mathcal{F}[n] = -\frac{1}{2}\frac{\mathrm{d}\mathcal{H}[n]}{\mathrm{d}t} = \frac{1}{2}\int_{\mathbb{T}^d} n|\nabla\log n|^2\,\mathrm{d}x,$$

while the second-order time derivative produces the energy from (3.8),

$$\mathcal{E}[n] = \frac{1}{4}\frac{\mathrm{d}^2\mathcal{H}[n]}{\mathrm{d}t^2} = \frac{1}{2}\int_{\mathbb{T}^d} n\|\nabla^2\log n\|^2\,\mathrm{d}x.$$

The Fisher information, in turn, has been proven to generate the DLSS equation (3.2) as a gradient flow with respect to the L^2-Wasserstein distance [30]. It is readily checked that $\mathcal{E}$ also equals the first-order time derivative of the entropy along solutions of the DLSS equation. In this sense, the sixth-order equation (3.1) is related to the fourth-order equation (3.2) in the same way as (3.2) itself is related to the heat equation.

We mention this point because the intimate relation between the heat and the DLSS equations (and, more generally, between second-order porous medium and fourth-order diffusion equations) has been the key tool in obtaining optimal rates for the intermediate asymptotics of solutions to (3.2) in [51]. It would be interesting to derive estimates on the long-time behavior of solutions to (3.1) by similar means.

3.3 Alternative formulations and functional inequalities

In this section, we derive two alternative formulations of the sixth-order equation (3.1) and prove an energy-dissipation formula and an entropy-dissipation estimate. First, we show that (3.1) can be written as the sum of a symmetric sixth-order term and a fourth-order remainder, and as the sum of a linear sixth-order part and a fifth-order remainder.

Lemma 3.6. *Equation* (3.1) *can be written for smooth positive solutions equivalently as*

$$\partial_t n = \partial^3_{ijk}\big(n\,\partial^3_{ijk}\log n\big) + 2\partial^2_{ij}\big(n\,\partial^2_{ik}\log n\,\partial^2_{jk}\log n\big) \quad \textit{in } \mathbb{T}^d,\ t>0, \tag{3.12}$$

and also equivalently as

$$\partial_t n = \Delta^3 n + \partial^3_{ijk} F_1^{(ijk)}(n) + \partial^2_{ij} F_2^{(ij)}(n) \quad \text{in } \mathbb{T}^d,\ t > 0, \tag{3.13}$$

where the nonlinear operators $F_1^{(ijk)}$ *and* $F_2^{(ij)}$ *are defined in* (3.4).

We recall that we have employed the summation convention in the above formulas.

Proof. For the following formal calculations, we introduce the shorthand notations $y = \log n$, $y_i = \partial_i \log n$, $y_{ij} = \partial^2_{ij} \log n$ etc. Observing that $\partial_k n = n y_k$, $n\partial_k(1/n) = -(\partial_k n)/n = -y_k$, we calculate

$$\frac{1}{2} n\partial_k(\partial^2_{ij} \log n)^2 = n\partial^2_{ij} y \partial^2_{ij} y_k,$$

and

$$\begin{aligned} n\partial_k\Big(\frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n)\Big) &= \partial^3_{ijk}(ny_{ij}) - y_k\partial^2_{ij}(ny_{ij}) \\ &= \partial^2_{ij}\big(y_k(ny_{ij}) + ny_{ijk}\big) - y_k\partial^2_{ij}(ny_{ij}) \\ &= \partial_i\big(y_k\partial_j(ny_{ij}) + y_{jk}(ny_{ij})\big) - y_k\partial^2_{ij}(ny_{ij}) + \partial^2_{ij}(ny_{ijk}) \\ &= y_{ik}\partial_j(ny_{ij}) + y_{ijk}(ny_{ij}) + y_{jk}\partial_i(ny_{ij}) + \partial^2_{ij}(n\partial^2_{ij}y_k) \\ &= 2y_{ik}\partial_j(ny_{ij}) + n\partial^2_{ij}y\partial^2_{ij}y_k + \partial^2_{ij}(n\partial^2_{ij}y_k) \\ &= 2\partial_j(ny_{ij}y_{ik}) - n\partial^2_{ij}y\partial^2_{ij}y_k + \partial^2_{ij}(n\partial^2_{ij}y_k). \end{aligned}$$

Summing these results, we obtain

$$\frac{1}{2}n\partial_k(\partial^2_{ij}\log n)^2 + n\partial_k\Big(\frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n)\Big) = \partial^2_{ij}(n\partial^2_{ij}y_k) + 2\partial_j(ny_{ij}y_{ik}).$$

Differentiation with respect to x_k yields

$$\partial_k\Big(\frac{1}{2}n\partial_k(\partial^2_{ij}\log n)^2 + n\partial_k\Big(\frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n)\Big)\Big) = \partial^3_{ijk}(n\partial^3_{ijk}y) + 2\partial^2_{jk}(ny_{ij}y_{ik}),$$

which shows (3.12).

Similarly, introducing $u = \sqrt[4]{n}$, $u_i = \partial_i u$, $u_{ij} = \partial^2_{ij}u$, etc. and observing that $\partial_k n = 4u^3 u_k$, $\partial^2_{ij} n = 12u^2 u_i u_j + 4u^3 u_{ij}$, and $uu_{ij} = \partial^2_{ij}(u^2)/2 - u_i u_j$, we calculate

$$\begin{aligned} n\partial^3_{ijk}y &= \partial^3_{ijk}n - \frac{3}{n}\partial^2_{ij}n\partial_k n + \frac{2}{n^2}\partial_i n\partial_j n\partial_k n \\ &= \partial^3_{ijk}n - 48u^2 u_{ij}u_k - 16uu_iu_ju_k \\ &= \partial^3_{ijk}n - 12\partial^2_{ij}(u^2)\partial_k(u^2) + 16u_iu_j\partial_k(u^2) \\ &= \partial^3_{ijk}n + 4\partial_k\sqrt{n}\big(4\partial_i\sqrt[4]{n}\partial_j\sqrt[4]{n} - 3\partial^2_{ij}\sqrt{n}\big) \\ &= \partial^3_{ijk}n + F_1^{(ijk)}(n), \end{aligned} \tag{3.14}$$

$$\begin{aligned} 2ny_{ik}y_{jk} &= 32u^4\Big(\frac{u_{ik}}{u} - \frac{u_iu_k}{u^2}\Big)\Big(\frac{u_{jk}}{u} - \frac{u_ju_k}{u^2}\Big) \\ &= 8\big(\partial^2_{ik}(u^2) - 4u_iu_k\big)\big(\partial^2_{jk}(u^2) - 4u_ju_k\big) \\ &= 8\big(\partial^2_{ik}\sqrt{n} - 4\partial_i\sqrt[4]{n}\partial_k\sqrt[4]{n}\big)\big(\partial^2_{jk}\sqrt{n} - 4\partial_j\sqrt[4]{n}\partial_k\sqrt[4]{n}\big) \\ &= F_2^{(ij)}(n). \end{aligned}$$

Differentiating both equations and summing them leads to

$$\partial^3_{ijk}(n\partial^3_{ijk}y) + 2\partial^2_{ij}(ny_{ik}y_{jk}) = \Delta^3 n + \partial^3_{ijk}F_1^{(ijk)} + \partial^2_{ij}F_2^{(ij)}, \tag{3.15}$$

which gives (3.13). □

In the next lemma, we make our claim about the Lyapunov property of the energy $\mathcal{E}$, defined in (3.8), more precise.

Lemma 3.7. *If $n \in C^\infty((t_1,t_2);C^\infty(\mathbb{T}^d))$ is a positive and classical solution to* (3.1)*, then the energy $\mathcal{E}[n(t)]$ is a smooth and nonincreasing function on the inverval (t_1,t_2). In fact, the energy is dissipated according to*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}[n(t)] = -\int_{\mathbb{T}^d} n\Big|\nabla\Big(\frac{1}{2}\big(\partial^2_{ij}\log n\big)^2 + \frac{1}{n}\partial^2_{ij}\big(n\partial^2_{ij}\log n\big)\Big)\Big|^2\,\mathrm{d}x, \quad t>0. \tag{3.16}$$

Proof. The smoothness of $\mathcal{E}[n(t)]$ follows since on the set of positive functions $u \in C^\infty(\mathbb{T}^d)$, the operation $u \mapsto \log u$ is a smooth map from $C^\infty(\mathbb{T}^d)$ to itself. Dissipation formula (3.16) follows by using formulation (3.1) and integration by parts:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}[n] &= \int_{\mathbb{T}^d}\left(\frac{1}{2}\partial_t n(\partial^2_{ij}\log n)^2 + n\partial^2_{ij}(\log n)\partial^2_{ij}\Big(\frac{\partial_t n}{n}\Big)\right)\mathrm{d}x \\ &= \int_{\mathbb{T}^d}\partial_t n\left(\frac{1}{2}(\partial^2_{ij}\log n)^2 + \frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n)\right)\mathrm{d}x \\ &= -\int_{\mathbb{T}^d} n\Big|\nabla\Big(\frac{1}{2}(\partial^2_{ij}\log n)^2 + \frac{1}{n}\partial^2_{ij}(n\partial^2_{ij}\log n)\Big)\Big|^2\,\mathrm{d}x,\end{aligned}$$

which shows the claim. □

Finally, we prove the entropy production inequality (3.6).

Lemma 3.8 (D. Matthes)**.** *Let $d \le 3$ and let $u \in H^3(\mathbb{T}^d)$ be strictly positive on $\mathbb{T}^d$. Then there exists $\kappa > 0$, only depending on d, such that*

$$\begin{aligned}&\int_{\mathbb{T}^d}\big(\partial^3_{ijk}(\log u)\partial^3_{ijk}u + \partial^3_{ijk}(\log u)F_1^{(ijk)}(u) - \partial^2_{ij}(\log u)F_2^{(ij)}(u)\big)\,\mathrm{d}x \\ &\qquad \ge \kappa\int_{\mathbb{T}^d}\big(|\nabla^3\sqrt{u}|^2 + |\nabla\sqrt[6]{u}|^6\big)\,\mathrm{d}x.\end{aligned} \tag{3.17}$$

Proof. The proof is based on an extension of the entropy construction method developed in [35] for one-dimensional equations. A proof for $d=1$ is given in [37]. Therefore, we restrict ourselves to the cases $d=2$ and $d=3$. By (3.15), (3.17) is equivalent to, up to a factor,

$$\int_{\mathbb{T}^d} u\big((\partial^3_{ijk}\log u)^2 - 2\partial^2_{ij}\log u(\partial^2_{ik}\log u\partial^2_{jk}\log u)\big)\,\mathrm{d}x \ge \frac{\kappa}{12}\int_{\mathbb{T}^d}\big(2^6|\nabla^3\sqrt{u}|^2 + 6^6|\nabla\sqrt[6]{u}|^6\big)\,\mathrm{d}x. \tag{3.18}$$

Setting $y = \log n$, $y_i = \partial_i \log n$, $y_{ij} = \partial^2_{ij} \log n$, etc., a tedious computation shows that (3.18) is equivalent to

$$\int_{\mathbb{T}^d} u\big(12S[u] - \kappa R[u]\big)\,\mathrm{d}x \geq 0, \tag{3.19}$$

where $S[u] = y_{ijk}^2 - 2y_{ij}y_{jk}y_{ki}$ and

$$R[u] = 2y_i^2y_j^2y_k^2 + 12y_i^2y_jy_{jk}y_k + 8y_iy_jy_ky_{ijk} + 24y_iy_{ij}y_{jk}y_k + 12y_i^2y_{jk}^2 + 48y_iy_{ijk}y_{jk} + 16y_{ijk}^2.$$

The idea of the entropy construction method is to find the "right" integrations by parts which are necessary to write the integrand of (3.19) as a sum of squares. To this end, we define the vector field $v = (v_1, \ldots, v_d)^\top : \mathbb{T}^d \to \mathbb{R}^d$ by

$$\begin{aligned} v_k &= (2y_i^2y_j^2 + y_{ii}y_j^2 + 5y_{ij}y_iy_j + 5y_{iij}y_j)y_k \\ &\quad + (3y_i^2y_j + 11y_{iij} + 24y_iy_{ij})y_{jk} - (5y_iy_j + 11y_{ij})y_{ijk}. \end{aligned}$$

A tedious but straight-forward computation shows that the weighted divergence

$$T[u] = \frac{1}{u}\,\mathrm{div}(uv) = e^{-y}\partial_k(e^yv_k)$$

can be written as

$$\begin{aligned} T[u] &= 2y_i^2y_j^2y_k^2 + 3y_i^2y_j^2y_{kk} + 16y_i^2y_jy_{jk}y_k + 9y_i^2y_jy_{jkk} + y_i^2y_{jj}y_{kk} + 7y_{ii}y_jy_{jk}y_k \\ &\quad + 40y_iy_{ij}y_{jk}y_k + 3y_i^2y_{jk}^2 + 5y_iy_{ijj}y_{kk} + 40y_iy_{ij}y_{jkk} + 3y_iy_{ijk}y_{jk} + 11y_{ijj}y_{ikk} \\ &\quad - 11y_{ijk}^2 + 24y_{ij}y_{jk}y_{ki}. \end{aligned}$$

By the divergence theorem, we have

$$\int_{\mathbb{T}^d} uT[u]\,\mathrm{d}x = 0.$$

Hence, (3.19) is equivalent to

$$\int_{\mathbb{T}^d} u\big(12S[u] - \kappa R[u] + T[u]\big)\,\mathrm{d}x \geq 0. \tag{3.20}$$

We prove that there exists $\kappa > 0$ such that the integrand is nonnegative. The expression $T[u]$ turns out to be the "right" integration-by parts formula allowing us to prove the nonnegativity of the above integral. At this point, we need to distinguish the space dimension.

First, consider $d = 2$. Let $x \in \mathbb{T}^d$ be fixed. Without loss of generality, we may assume that $\nabla u(x)$ points into the first coordinate direction, i.e. $y_2 = 0$ at x. Then we compute

$$\begin{aligned}12S[u] - \varepsilon R[u] + T[u] &= (2-2\varepsilon)y_1^6 + 3y_1^4(y_{11}+y_{22}) + 4(4-3\varepsilon)y_1^4 y_{11} + 9y_1^3(y_{111}+y_{122}) \\ &\quad - 8\varepsilon y_1^3 y_{111} + y_1^2(y_{11}+y_{22})^2 + 7y_1^2 y_{11}(y_{11}+y_{22}) + 8(5-3\varepsilon)y_1^2(y_{11}^2+y_{12}^2) \\ &\quad + 3(1-4\varepsilon)y_1^2(y_{11}^2 + 2y_{12}^2 + y_{22}^2) + 5y_1(y_{111}+y_{122})(y_{11}+y_{22}) \\ &\quad + 40y_1\big(y_{11}(y_{111}+y_{122}) + y_{12}(y_{122}+y_{222})\big) \\ &\quad + 3(1-16\varepsilon)y_1\big(y_{11}y_{111} + 2y_{12}y_{112} + y_{22}y_{122}\big) \\ &\quad + 11\big((y_{111}+y_{122})^2 + (y_{112}+y_{222})^2\big) + (1-16\varepsilon)\big(y_{111}^2 + 3y_{112}^2 + 3y_{122}^2 + y_{222}^2\big) \\ &= \xi^\top A_\varepsilon \xi + \eta^\top B_\varepsilon \eta,\end{aligned}$$

where ξ and η are the vectors

$$\xi = (y_1^3, y_1y_{11}, y_1y_{22}, y_{111}, y_{122})^\top, \quad \eta = (y_1y_{12}, y_{112}, y_{222})^\top,$$

and the symmetric matrices A_ε and B_ε are defined by

$$A_\varepsilon = \frac{1}{2}\begin{pmatrix} 4-4\varepsilon & 19-12\varepsilon & 3 & 9-8\varepsilon & 9 \\ 19-12\varepsilon & 102-72\varepsilon & 9 & 48-48\varepsilon & 45 \\ 3 & 9 & 8-24\varepsilon & 5 & 8-48\varepsilon \\ 9-8\varepsilon & 48-48\varepsilon & 5 & 24-32\varepsilon & 22 \\ 9 & 45 & 8-48\varepsilon & 22 & 28-96\varepsilon \end{pmatrix},$$

$$B_\varepsilon = \begin{pmatrix} 46-48\varepsilon & 23-48\varepsilon & 20 \\ 23-48\varepsilon & 14-48\varepsilon & 11 \\ 20 & 11 & 12-16\varepsilon \end{pmatrix}.$$

Sylvester's criterion shows that the unperturbed matrices A_0 and B_0 are positive definite. Indeed, the principal minors fo A_0 are 2, 47/4, 20, 13, and 149/4, and the principal minors of B_0 are 46, 115, and 334. Since the set of (strictly) positive definite matrices is open in the set of all real symmetric matrices, there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, the matrices A_ε and B_ε are positive definite, too. This shows that $12S[u] - \varepsilon R[u] + T[u] \geq 0$ for $0 < \varepsilon < \varepsilon_0$, which implies (3.20).

Next, let $d = 3$. This case is similar to the previous one, but technically more involved. Again, we fix some $x \in \mathbb{T}^d$ and assume that $\nabla u(x)$ is parallel to the first coordinate direction, i.e. $y_2 = y_3 = 0$. For easier presentation, we introduce the abbreviations

$$\begin{aligned} &p_+ = y_{22} + y_{33}, \quad p_- = y_{22} - y_{33}, \\ &q_{j+} = y_{j22} + y_{j33}, \quad q_{j-} = y_{j22} - y_{j33}, \quad j = 1,2,3. \end{aligned}$$

Observe that

$$\begin{aligned} 2(y_{22}^2 + y_{33}^2) &= p_+^2 + p_-^2, \\ 2(y_{j22}^2 + y_{j33}^2) &= q_{j+}^2 + q_{j-}^2, \\ 2(y_{22}y_{j22} + y_{33}y_{j33}) &= p_+q_{j+} + p_-q_{j-}. \end{aligned}$$

With these notations, we find that

$$\begin{aligned}
12S[u] - \varepsilon R[u] + T[u] &= (2-2\varepsilon)y_1^6 + 3y_1^4(y_{11}+p_+) + 4(4-3\varepsilon)y_1^4 y_{11} + 9y_1^3(y_{111}+q_{1+}) \\
&\quad - 8\varepsilon y_1^3 y_{111} + y_1^2(y_{11}+p_+)^2 + 7y_1^2 y_{11}(y_{11}+p_+) + 8(5-3\varepsilon)y_1^2(y_{11}^2+y_{12}^2+y_{13}^2) \\
&\quad + 3(1-4\varepsilon)y_1^2\big(y_{11}^2 + \tfrac{1}{2}(p_-^2+p_+^2) + 2(y_{12}^2+y_{13}^2+y_{23}^2)\big) + 5y_1(y_{111}+q_{1+})(y_{11}+p_+) \\
&\quad + 40y_1\big(y_{11}(y_{111}+q_{1+}) + y_{12}(y_{112}+q_{2+}) + y_{13}(y_{113}+q_{3+})\big) \\
&\quad + 3(1-16\varepsilon)y_1\big(y_{111}y_{11} + \tfrac{1}{2}(q_{1+}p_+ + q_{1-}p_-) + 2(y_{112}y_{12}+y_{113}y_{13}+y_{123}y_{23})\big) \\
&\quad + 11\big((y_{111}+q_{1+})^2 + (y_{112}+q_{2+})^2 + (y_{113}+q_{3+})^2\big) \\
&\quad + (1-16\varepsilon)\big(y_{111}^2 + 3(y_{112}^2+y_{113}^2) + \tfrac{3}{2}(q_{1+}^2+q_{1-}^2+q_{2+}^2+q_{2-}^2+q_{3+}^2+q_{-3}^2) + 6y_{123}^2\big) \\
&= \xi^\top A_\varepsilon \xi + \sum_{j=2}^3 \eta_j^\top B_\varepsilon \eta_j + \zeta^\top C_\varepsilon \zeta + 2\nu^\top C_\varepsilon \nu + \frac{1}{4}(1-16\varepsilon)(q_{2+}^2+q_{2-}^2),
\end{aligned}$$

where

$$\begin{aligned}
&\xi = (y_1^3, y_1y_{11}, y_1p_+, y_{111}, q_{1+})^\top, \quad \eta_j = (y_1y_{1j}, y_{11j}, q_{j+})^\top, \\
&\zeta = (y_1p_-, q_{1-})^\top, \quad \nu = (y_1y_{23}, y_{123})^\top.
\end{aligned}$$

The matrices A_ε and B_ε are almost identical to those given above, with minor modifications in the third and fifth rows and columns:

$$A_\varepsilon = \frac{1}{2}\begin{pmatrix} 4-4\varepsilon & 19-12\varepsilon & 3 & 9-8\varepsilon & 9 \\ 19-12\varepsilon & 102-72\varepsilon & 9 & 48-48\varepsilon & 45 \\ 3 & 9 & 5-12\varepsilon & 5 & 13/2-24\varepsilon \\ 9-8\varepsilon & 48-48\varepsilon & 5 & 24-32\varepsilon & 22 \\ 9 & 45 & 13/2-24\varepsilon & 22 & 25-48\varepsilon \end{pmatrix},$$

$$B_\varepsilon = \begin{pmatrix} 46-48\varepsilon & 23-48\varepsilon & 20 \\ 23-48\varepsilon & 14-48\varepsilon & 11 \\ 20 & 11 & 47/4-12\varepsilon \end{pmatrix}.$$

Furthermore, the matrix C_ε is given by

$$C_\varepsilon = \begin{pmatrix} 3-12\varepsilon & 3/2-24\varepsilon \\ 3/2-24\varepsilon & 3-48\varepsilon \end{pmatrix}.$$

Again, the Sylvester criterion shows that A_0, B_0, and C_0 are positive definite. The principal minors of A_0 are 2, 47/4, 19/8, 5/8, and 453/64, while those of B_0 are 46, 115, and 1221/4, and those of C_0 are 3 and 27/4. Thus, there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, also A_ε, B_ε, and C_ε are positive definite. □

3.4 Existence of weak solutions

The proof of Theorem 3.1 is divided into several steps.

3.4.1 Solution of the semi-discretized problem

Let $T > 0$ and $\tau > 0$ be given. We wish to solve, for a given initial datum $n_0 \in L^1(\mathbb{T}^d)$, the semi-discrete problem

$$\frac{1}{\tau}(n - n_0) = \Delta^3 n + \partial^3_{ijk} F_1^{(ijk)}(n) + \partial^2_{ij} F_2^{(ij)}(n) \quad \text{in } \mathbb{T}^d,$$

where $F_1^{(ijk)}$ and $F_2^{(ij)}$ are defined in (3.4).

Proposition 3.9. *For a nonnegative function $n_0 \in L^1(\mathbb{T}^d)$ of unit mass, $\|n_0\|_{L^1} = 1$, and of finite entropy, $\mathcal{H}[n_0] < \infty$, there exists a sequence of solutions $n_1^\tau, n_2^\tau, \ldots$ in $H^3(\mathbb{T}^d)$ to the elliptic problems*

$$\frac{1}{\tau}\int_{\mathbb{T}^d} \big(n_k^\tau - n_{k-1}^\tau\big)\phi \,\mathrm{d}x + \int_{\mathbb{T}^d} \big(\partial^3_{ijk}\phi \partial^3_{ijk} n_k^\tau + \partial^3_{ijk}\phi F_1^{(ijk)}(n_k^\tau) - \partial^2_{ij}\phi F_2^{(ij)}(n_k^\tau)\big) \,\mathrm{d}x = 0, \tag{3.21}$$

holding for all test functions $\phi \in H^3(\mathbb{T}^d)$, with the initial solution $n_0^\tau = n_0$. These solutions are of unit mass, and the entropy estimate

$$\mathcal{H}[n_k^\tau] + \kappa\tau \int_{\mathbb{T}^d} \Big(\big\|\nabla^3 \sqrt{n_k^\tau}\big\|^2 + \big|\nabla \sqrt[6]{n_k^\tau}\big|^6\Big) \,\mathrm{d}x \le \mathcal{H}[n_{k-1}^\tau], \quad k \ge 1, \tag{3.22}$$

holds with $\kappa > 0$ given in Lemma 3.8.

Proof. For simplicity, we only give the argument for the construction of $n = n_1^\tau$ from n_0. The passage from n_k^τ to n_{k+1}^τ works precisely in the same way since finiteness of the entropy is inherited from one step to the next.

Regularized problem. In a first step, we are going to construct strictly positive solutions $n_\varepsilon \in H^3(\mathbb{T}^d)$ to the regularized problem

$$\frac{1}{\tau}(n - n_0) = \Delta^3 n + \partial^3_{ijk} F_1^{(ijk)}(n) + \partial^2_{ij} F_2^{(ij)}(n) + \varepsilon\big(\Delta^3 \log n - \log n\big). \tag{3.23}$$

Writing $n = e^y$, it follows from (3.14) that

$$\Delta^3 n = \partial^3_{ijk}(n\partial^3_{ijk} y) - \partial^3_{ijk} F_1^{(ijk)}(n).$$

Thus, assuming strict positivity and H^3-regularity of n, we can reformulate (3.23) as

$$\frac{1}{\tau}(n - n_0) = \partial^3_{ijk}\big((n + \varepsilon)\partial^3_{ijk} y\big) - \varepsilon y + \partial^2_{ij} F_2^{(ij)}(n), \tag{3.24}$$

which is an equation in $H^{-3}(\mathbb{T}^d)$.

Fixed point operator. We define the continuous map $S_\varepsilon : X \times [0,1] \to W^{2,4}(\mathbb{T}^d)$ on the set

$$X = \Big\{ u \in W^{2,4}(\mathbb{T}^d) : \min_{x\in\mathbb{T}^d} u(x) > 0 \Big\}$$

as follows. For given $n \in X$ and $\sigma \in [0,1]$, introduce

$$a(y,z) = \int_{\mathbb{T}^d} \big((\sigma n + \varepsilon)\partial^3_{ijk} y\, \partial^3_{ijk} z + \varepsilon y z\big)\,\mathrm{d}x$$
$$f(z) = -\frac{\sigma}{\tau}\int_{\mathbb{T}^d} (n - n_0) z\,\mathrm{d}x + \sigma \int_{\mathbb{T}^d} F_2^{(ij)}(n)\partial^2_{ij} z\,\mathrm{d}x$$

for all $y, z \in H^3(\mathbb{T}^d)$. Observe that a is a bounded and coercive bilinear form on $H^3(\mathbb{T}^d)$,

$$a(z,z) \geq \varepsilon \int_{\mathbb{T}^d} \big(|\nabla z|^2 + z^2\big)\,\mathrm{d}x \geq c\varepsilon \|z\|^2_{H^3}$$

for some constant $c > 0$, and a varies continuously with $(n,\sigma) \in X \times [0,1]$, since the embedding $W^{2,4}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ is continuous.

Next, we claim that f is a linear form on $H^3(\mathbb{T}^d)$. Indeed, due to the continuity of the Sobolev embedding $W^{2,4}(\mathbb{T}^d) \hookrightarrow W^{1,8}(\mathbb{T}^d)$ in dimensions $d \leq 3$ and the strict positivity and continuity of functions in $W^{2,4}(\mathbb{T}^d)$, the mapping $F_2^{(ij)}$ allows for the representation

$$F_2^{(ij)}(n) = 2\frac{\partial^2_{ik} n \partial^2_{kj} n}{n} - 4\frac{\partial^2_{ik} n \partial_k n \partial_j n}{n^2} + 2\frac{(\partial_k n)^2 \partial_i n \partial_j n}{n^3},$$

from which $F_2^{(ij)}(n) \in L^2(\mathbb{T}^d)$ follows for all $n \in W^{2,4}(\mathbb{T}^d)$. In fact, f varies continuously with $(n,\sigma) \in X \times [0,1]$.

The Lax-Milgram Lemma provides the existence and uniqueness of a solution $y \in H^3(\mathbb{T}^d)$ to the elliptic equation

$$a(y,z) = f(z) \quad \text{for all } z \in H^3(\mathbb{T}^d).$$

This solution depends H^3-continuously on $(n,\sigma) \in X \times [0,1]$. In particular, $y \equiv 0$ if $\sigma = 0$, and y solves (3.24) if $\sigma = 1$.

The definition of the fixed point operator S_ε is now completed by setting

$$S_\varepsilon(n,\sigma) = e^y.$$

Since $y \in H^3(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$, it is clear that $S_\varepsilon(n,\sigma) \in H^3(\mathbb{T}^d)$ is a strictly positive and bounded function. In view of the compactness of the embedding $H^3(\mathbb{T}^d) \hookrightarrow W^{2,4}(\mathbb{T}^d)$, S_ε maps bounded subsets of $X \times [0,1]$ into precompact sets in $W^{2,4}(\mathbb{T}^d)$. Finally, notice that $S_\varepsilon(n,0) \equiv 1$ for all $n \in X$ and $S_\varepsilon(n_*,1) = n_*$ for some $n_* \in X$ if and only if n_* is a solution to (3.23). To verify the last statement, observe that $n_* = S_\varepsilon(n_*,1)$ implies the H^3-regularity of n_*, which justifies the passage from (3.24) to (3.23), and in particular it allows us to define $\Delta^3 \log n_*$ as an element of $H^{-3}(\mathbb{T}^d)$.

A priori bound. Our goal is to obtain a fixed point of $S_\varepsilon(\cdot,1)$ by means of the Leray–Schauder theorem. Having already verified the continuity and relative compactness of S_ε as well as the condition $S_\varepsilon(\cdot,0) = 1$, it remains to find a suitable closed, bounded, convex subset $B \subset X$ such that all solutions $n_* \in X$ of $S_\varepsilon(n_*, \sigma) = n_*$ for some $\sigma \in [0,1]$ lie in the interior of B. We shall choose

$$B = \big\{ u \in W^{2,4}(\mathbb{T}^d) : \min u \geq \delta,\ \|u\|_{W^{2,4}} \leq \delta^{-1} \big\} \tag{3.25}$$

with a suitable $\delta > 0$ determined below.

Let $n_* \in W^{2,4}(\mathbb{T}^d)$ be a fixed point of $S(\cdot, \sigma)$ for some $\sigma \in [0,1]$. By construction, we have $n_* = e^{y_*} \in H^3(\mathbb{T}^d)$ for $y_* \in H^3(\mathbb{T}^d)$, and n_* is strictly positive. The convexity of $h(s) = s(\log s - 1) + 1$ implies that

$$\begin{aligned}
\frac{1}{\tau}(\mathcal{H}[n_*] - \mathcal{H}[n_0]) &= \frac{1}{\tau}\int_{\mathbb{T}^d} (h(n_*) - h(n_0))\,\mathrm{d}x \\
&\leq \frac{1}{\tau}\int_{\mathbb{T}^d} (n_* - n_0)h'(n_*)\,\mathrm{d}x = \frac{1}{\tau}\int_{\mathbb{T}^d} (n_* - n_0)\log n_*\,\mathrm{d}x \\
&= -\int_{\mathbb{T}^d} \big(\partial^3_{ijk} y_*\, \partial^3_{ijk} n_* + \partial^3_{ijk} y_* F_1^{(ijk)}(n_*) - \partial^2_{ij} y_* F_2^{(ij)}(n_*)\big)\,\mathrm{d}x \\
&\quad - \frac{\varepsilon}{\sigma}\int_{\mathbb{T}^d} \big(\|\nabla^3 y_*\|^2 + y_*^2\big)\,\mathrm{d}x \\
&\leq -\kappa \int_{\mathbb{T}^d} \big(\|\nabla^3 \sqrt{n_*}\|^2 + |\nabla \sqrt[6]{n_*}|^6\big)\,\mathrm{d}x - \frac{\varepsilon}{\sigma}\int_{\mathbb{T}^d} \big(\|\nabla^3 y_*\|^2 + y_*^2\big)\,\mathrm{d}x.
\end{aligned}$$

For the last estimate, the functional inequality (3.17) has been used. Thus, we have proven

$$\mathcal{H}[n_*] + \tau\kappa \int_{\mathbb{T}^d} \big(\|\nabla^3 \sqrt{n_*}\|^2 + |\nabla \sqrt[6]{n_*}|^6\big)\,\mathrm{d}x + \frac{\tau\varepsilon}{\sigma}\int_{\mathbb{T}^d} \big(\|\nabla^3 y_*\|^2 + y_*^2\big)\,\mathrm{d}x \leq \mathcal{H}[n_0]. \tag{3.26}$$

A consequence of this inequality is that y_* is bounded in $H^3(\mathbb{T}^d)$,

$$\|y_*\|_{H^3} \leq C \int_{\mathbb{T}^d} \big(\|\nabla^3 y_*\|^2 + y_*^2\big)\,\mathrm{d}x \leq \frac{C\mathcal{H}[n_0]}{\tau\varepsilon}$$

for some constant $C > 0$ depending on τ and ε (which are fixed positive numbers at this point), but not on $\sigma \in [0,1]$. The continuity of the embedding $H^3(\mathbb{T}^d) \hookrightarrow W^{2,4}(\mathbb{T}^d)$ yields the σ-independent bound

$$\|n_*\|_{W^{2,4}} \leq \frac{C\mathcal{H}[n_0]}{\tau\varepsilon}, \tag{3.27}$$

maybe for another constant $C > 0$. Furthermore, the continuity of the embedding $H^3(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ provides the estimate

$$\min n_* \geq \min \exp\big(-\|y_*\|_{L^\infty}\big) \geq \exp\left(-\frac{C\mathcal{H}[n_0]}{\tau\varepsilon}\right) > 0. \tag{3.28}$$

From (3.27) and (3.28) follows that there exists a set B of the form (3.25) which contains all potential fixed points n_*. The Leray–Schauder fixed point theorem in the version of

[55] (see Theorem C.7) applies to our situation and yields the existence of a solution n_ε to $n = S_\varepsilon(n, 1)$.

Deregularization. From the entropy estimate, it follows that $\sqrt{n_\varepsilon}$ is ε-uniformly bounded in $H^3(\mathbb{T}^d)$, and $\sqrt[6]{n_\varepsilon}$ is ε-uniformly bounded in $W^{1,6}(\mathbb{T}^d)$. Hence, there exists a limit function $n \in H^3(\mathbb{T}^d)$, such that, as $\varepsilon \downarrow 0$, up to subsequences,

$$\sqrt{n_\varepsilon} \rightharpoonup \sqrt{n} \quad \text{in } H^3(\mathbb{T}^d), \tag{3.29}$$

$$\sqrt{n_\varepsilon} \to \sqrt{n} \quad \text{in } W^{2,4}(\mathbb{T}^d) \text{ and in } W^{1,\infty}(\mathbb{T}^d), \tag{3.30}$$

$$\sqrt[4]{n_\varepsilon} \to \sqrt[4]{n} \quad \text{in } W^{1,4}(\mathbb{T}^d), \tag{3.31}$$

$$\sqrt[4]{n_\varepsilon} \rightharpoonup \sqrt[4]{n} \quad \text{in } W^{1,12}(\mathbb{T}^d). \tag{3.32}$$

Here we take (3.29) for the definition of n; then (3.30) follows from the compactness of the embedding $H^3(\mathbb{T}^d) \hookrightarrow W^{2,4}(\mathbb{T}^d)$. The strong convergence in (3.31) is a direct consequence of Proposition C.6, since $\sqrt[4]{n_\varepsilon}$ is "sandwiched" between $\sqrt{n_\varepsilon}$ and $\sqrt[6]{n_\varepsilon}$. Concerning (3.32), observe that $H^3(\mathbb{T}^d)$ embeds continuously into $W^{2,6}(\mathbb{T}^d)$, so that $\sqrt[4]{n_\varepsilon}$ is bounded in $W^{1,12}(\mathbb{T}^d)$ by Lemma C.4. In particular, $\sqrt[4]{n_\varepsilon}$ converges weakly to some limit in that space—which necessarily agrees with the strong $W^{1,4}(\mathbb{T}^d)$-limit obtained in (3.31).

For the various terms in (3.23), this implies the following. The sequence

$$\partial^3_{ijk} n_\varepsilon = 2\sqrt{n_\varepsilon}\partial^3_{ijk}\sqrt{n_\varepsilon} + 6\partial_i\sqrt{n_\varepsilon}\partial^2_{jk}\sqrt{n_\varepsilon}$$

converges weakly in $L^2(\mathbb{T}^d)$ to $\partial^3_{ijk} n$, since $\sqrt{n_\varepsilon}$ converges strongly in $L^\infty(\mathbb{T}^d)$ and $\partial^3_{ijk}\sqrt{n_\varepsilon}$ converges weakly in $L^2(\mathbb{T}^d)$, while $\partial_i\sqrt{n_\varepsilon}$ and $\partial^2_{jk}\sqrt{n_\varepsilon}$ both converge strongly in $L^4(\mathbb{T}^d)$. Further, the sequence

$$F_1^{(ijk)}(n_\varepsilon) = 4\partial_i\sqrt{n_\varepsilon}\big(4\partial_j\sqrt[4]{n_\varepsilon}\partial_k\sqrt[4]{n_\varepsilon} - 3\partial^2_{jk}\sqrt{n_\varepsilon}\big)$$

converges strongly in $L^2(\mathbb{T}^d)$, since $\partial_i\sqrt{n_\varepsilon}$ converges strongly in $L^\infty(\mathbb{T}^d)$, $\partial^2_{jk}\sqrt{n_\varepsilon}$ converges strongly in $L^2(\mathbb{T}^d)$, and $\partial_j\sqrt[4]{n_\varepsilon}$ and $\partial_k\sqrt[4]{n_\varepsilon}$ both converge strongly in $L^4(\mathbb{T}^d)$. Finally, we consider

$$\begin{aligned} F_2^{(ij)}(n_\varepsilon) = 8\big(&\partial_{ik}\sqrt{n_\varepsilon}\partial_{jk}\sqrt{n_\varepsilon} - 4\partial^2_{jk}\sqrt{n_\varepsilon}\partial_k\sqrt[4]{n_\varepsilon}\partial_i\sqrt[4]{n_\varepsilon} \\ &- 4\partial^2_{ik}\sqrt{n_\varepsilon}\partial_k\sqrt[4]{n_\varepsilon}\partial_j\sqrt[4]{n_\varepsilon} + 16\partial_i\sqrt[4]{n_\varepsilon}\partial_j\sqrt[4]{n_\varepsilon}(\partial_k\sqrt[4]{n_\varepsilon})^2\big). \end{aligned}$$

The first term converges strongly in $L^2(\mathbb{T}^d)$ since it is the product of two second-order derivatives of $\sqrt{n_\varepsilon}$ which converge strongly in $L^4(\mathbb{T}^d)$. The second and third expressions converge strongly in $L^{4/3}(\mathbb{T}^d)$ since each of them is the product of three strongly L^4-convergent terms. To obtain weak $L^{6/5}$-convergence of the last product, we use the strong L^4-convergence of $\partial_i\sqrt[4]{n_\varepsilon}$ to conclude strong convergence of $\partial_j\sqrt[4]{n_\varepsilon}(\partial_k\sqrt[4]{n_\varepsilon})^2$ in $L^{4/3}(\mathbb{T}^d)$, and combine this with the weak convergence of $\partial_i\sqrt[4]{n_\varepsilon}$ in $L^{12}(\mathbb{T}^d)$. Notice that weak convergence in $L^{6/5}(\mathbb{T}^d)$ suffices, since $F_2^{(ij)}(n_\varepsilon)$ is tested in (3.21) against $\phi \in H^3(\mathbb{T}^d)$ and hence, $\partial^2_{ij}\phi \in L^6(\mathbb{T}^d)$.

Finally, the entropy estimate (3.26) shows that $(\sqrt{\varepsilon}y_\varepsilon)$ is bounded in $H^3(\mathbb{T}^d)$ and hence,

$$\varepsilon y_\varepsilon \to 0 \quad \text{strongly in } H^3(\mathbb{T}^d).$$

The above convergence results allow us to perform the limit $\varepsilon \to 0$ in (3.23), i.e., both sides converge in $H^{-3}(\mathbb{T}^d)$. Hence, n is a nonnegative solution to (3.21).

Proof of auxiliary properties. It remains to verify that n has unit mass and that the dissipation inequality (3.22) holds. Conservation of mass follows directly from (3.21) by using $\phi = 1$ as a test function. The entropy estimate (3.26) shows that n_ε satisfies

$$\mathcal{H}[n_\varepsilon] + \tau\kappa \int_{\mathbb{T}^d} \left(\|\nabla^3 \sqrt{n_\varepsilon}\|^2 + |\nabla \sqrt[6]{n_\varepsilon}|^6 \right) \mathrm{d}x \le \mathcal{H}[n_0].$$

Since $\nabla^3 \sqrt{n_\varepsilon} \rightharpoonup \nabla^3 \sqrt{n}$ weakly in $L^2(\mathbb{T}^d)$
and $\nabla \sqrt[6]{n_\varepsilon} \rightharpoonup \nabla \sqrt[6]{n_\varepsilon}$ weakly in $L^6(\mathbb{T}^d)$, we conclude by lower semi-continuity that

$$\begin{aligned}\mathcal{H}[n] + \tau\kappa \int_{\mathbb{T}^d} &\left(\|\nabla^3 \sqrt{n}\|^2 + |\nabla \sqrt[6]{n}|^6 \right) \mathrm{d}x \\ &\le \lim_{\varepsilon\to 0} \mathcal{H}[n_\varepsilon] + \tau\kappa \liminf_{\varepsilon \to 0} \int_{\mathbb{T}^d} \left(\|\nabla^3 \sqrt{n_\varepsilon}\|^2 + |\nabla \sqrt[6]{n_\varepsilon}|^6 \right) \mathrm{d}x \le \mathcal{H}[n_0].\end{aligned}$$

This finishes the proof. □

3.4.2 Passage to the continuous limit

Proposition 3.9 guarantees the existence of a solution sequence $(n_0^\tau, n_1^\tau, n_2^\tau, \ldots)$ to the semi-discrete implicit Euler scheme (3.21). Define accordingly the piecewise constant interpolants $\overline{n^\tau} \in L^\infty(0,\infty; H^3(\mathbb{T}^d))$ by

$$\overline{n^\tau}(t) = n_k^\tau \quad \text{for } (k-1)\tau < t \le k\tau,\ k \in \mathbb{N}, \quad \overline{n^\tau}(0) = n_0^\tau,$$

and introduce the discrete time derivative

$$\delta_\tau \overline{n^\tau}(t) = \frac{1}{\tau}\left(n_k^\tau - n_{k-1}^\tau \right) \quad \text{for } (k-1)\tau < t \le k\tau,\ k \in \mathbb{N}.$$

Corollary 3.10. *The interpolated function $\overline{n^\tau}$ satisfies*

$$\int_0^T \int_{\mathbb{T}^d} \delta_\tau \overline{n^\tau} \varphi \,\mathrm{d}x\,\mathrm{d}t + \int_0^T \int_{\mathbb{T}^d} \left(\partial^3_{ijk}\varphi\, \partial^3_{ijk} \overline{n^\tau} + \partial^3_{ijk}\varphi F_1^{(ijk)}(\overline{n^\tau}) - \partial^2_{ij}\varphi F_2^{(ij)}(\overline{n^\tau}) \right) \mathrm{d}x\,\mathrm{d}t = 0 \tag{3.33}$$

for all test functions $\varphi \in L^4(0,T; H^3(\mathbb{T}^d))$.

Proof. Equation (3.33) is a direct consequence of (3.21), and the definitions of $\overline{n^\tau}$ and $\delta_\tau \overline{n^\tau}$. Simply choose $\phi = \varphi(t) \in H^3(\mathbb{T}^d)$ as a test function in (3.21) for $(k-1)\tau < t \le k\tau$ and integrate with respect to $t \in (0,T)$. Notice that at this point, the L^4-regularity of φ with respect to time is not of importance. In fact, we could replace L^4 by L^1. □

The following lemma summarizes various consequences of the discrete entropy estimate (3.22). Recall that we are working in spatial dimensions $d \le 3$.

Lemma 3.11. *For any finite $T > 0$,*

$$(\overline{n^\tau}) \quad \text{is bounded in } L^{4/3}(0,T;H^3(\mathbb{T}^d)), \tag{3.34}$$

$$(\nabla\sqrt{\overline{n^\tau}}) \quad \text{is bounded in } L^{12/5}(0,T;L^\infty(\mathbb{T}^d)), \tag{3.35}$$

$$(\nabla^2\sqrt{\overline{n^\tau}}) \quad \text{is bounded in } L^3(0,T;L^2(\mathbb{T}^d)) \text{ and in } L^{8/3}(0,T;L^{12/5}(\mathbb{T}^d)), \tag{3.36}$$

$$(\nabla\sqrt[4]{\overline{n^\tau}}) \quad \text{is bounded in } L^6(0,T;L^4(\mathbb{T}^d)) \text{ and in } L^{16/3}(0,T;L^{24/5}(\mathbb{T}^d)), \tag{3.37}$$

$$(\nabla\sqrt[6]{\overline{n^\tau}}) \quad \text{is bounded in } L^6(0,T;L^6(\mathbb{T}^d)), \tag{3.38}$$

uniformly with respect to $\tau > 0$.

Proof. First notice that the boundedness of $\sqrt{\overline{n^\tau}}$ in $L^2(0,T;H^3(\mathbb{T}^d))$ follows from the entropy estimate (3.22). Indeed, by Lemma C.1 and the conservation of mass, we find that

$$\|\sqrt{\overline{n^\tau}}(t)\|_{H^3} \le C\big(\|\nabla^3\sqrt{\overline{n^\tau}}(t)\|_{L^2} + \|\sqrt{\overline{n^\tau}}(t)\|_{L^2}\big) = C\big(\|\nabla^3\sqrt{\overline{n^\tau}}(t)\|_{L^2} + 1\big),$$

where $C > 0$ does not depend on τ. Therefore,

$$\|\sqrt{\overline{n^\tau}}\|_{L^2(0,T;H^3)} \le C\big(\|\nabla^3\sqrt{\overline{n^\tau}}\|_{L^2(0,T;H^3)} + T^{1/2}\big) \le C(\mathcal{H}[n_0] + T^{1/2}).$$

Estimate (3.38) follows also from the entropy estimate (3.22).

To prove the remaining estimates, first notice that, by the Gagliardo-Nirenberg inequality (see Lemma C.3), for some constants $B_i > 0$,

$$\begin{aligned}
\|\sqrt{\overline{n^\tau}}(t)\|_{L^\infty} &\le B_1\|\sqrt{\overline{n^\tau}}(t)\|_{H^3}^{d/6}\|\sqrt{\overline{n^\tau}}(t)\|_{L^2}^{1-d/6}, \\
\|\nabla\sqrt{\overline{n^\tau}}(t)\|_{L^\infty} &\le B_2\|\sqrt{\overline{n^\tau}}(t)\|_{H^3}^{1/3+d/6}\|\sqrt{\overline{n^\tau}}(t)\|_{L^2}^{2/3-d/6}, \\
\|\nabla^2\sqrt{\overline{n^\tau}}(t)\|_{L^2} &\le B_3\|\sqrt{\overline{n^\tau}}(t)\|_{H^3}^{2/3}\|\sqrt{\overline{n^\tau}}(t)\|_{L^2}^{1/3}.
\end{aligned}$$

Integrating over $(0,T)$, we infer that

$$\|\sqrt{\overline{n^\tau}}\|_{L^{12/d}(0,T;L^\infty)} \le B_1\|\sqrt{\overline{n^\tau}}\|_{L^2(0,T;H^3)}^{d/6}\|\sqrt{\overline{n^\tau}}\|_{L^\infty(0,T;L^2)}^{1-d/6} \le C, \tag{3.39}$$

$$\|\nabla\sqrt{\overline{n^\tau}}\|_{L^{12/(d+2)}(0,T;L^\infty)} \le B_2\|\sqrt{\overline{n^\tau}}\|_{L^2(0,T;H^3)}^{(2+d)/6}\|\sqrt{\overline{n^\tau}}\|_{L^\infty(0,T;L^2)}^{(4-d)/6} \le C, \tag{3.40}$$

$$\|\nabla^2\sqrt{\overline{n^\tau}}\|_{L^3(0,T;L^2)} \le B_3\|\sqrt{\overline{n^\tau}}\|_{L^2(0,T;H^3)}^{2/3}\|\sqrt{\overline{n^\tau}}\|_{L^\infty(0,T;L^2)}^{1/3} \le C, \tag{3.41}$$

where $C > 0$ does not depend on τ. Estimate (3.40) implies the bound (3.35) since $12/(d+2) \ge 12/5$ for $d \le 3$. Taking into account

$$\begin{aligned}
\partial^3_{ijk}\overline{n^\tau} &= \partial^3_{ijk}(\sqrt{\overline{n^\tau}})^2 \\
&= 2\sqrt{\overline{n^\tau}}\partial^3_{ijk}\sqrt{\overline{n^\tau}} + 2\big(\partial_i\sqrt{\overline{n^\tau}}\,\partial^2_{jk}\sqrt{\overline{n^\tau}} + \partial_j\sqrt{\overline{n^\tau}}\,\partial^2_{ik}\sqrt{\overline{n^\tau}} + \partial_k\sqrt{\overline{n^\tau}}\,\partial^2_{ij}\sqrt{\overline{n^\tau}}\big),
\end{aligned}$$

Hölder's inequality and estimates (3.39)-(3.41) give

$$\begin{aligned}
\|\nabla^3\overline{n^\tau}\|_{L^{4/3}(0,T;L^2)}^{4/3} &\le C\int_0^T \big(\|\sqrt{\overline{n^\tau}}\|_{L^\infty}^{4/3}\|\nabla^3\sqrt{\overline{n^\tau}}\|_{L^2}^{4/3} + \|\nabla\sqrt{\overline{n^\tau}}\|_{L^\infty}^{4/3}\|\nabla^2\sqrt{\overline{n^\tau}}\|_{L^2}^{4/3}\big)\,\mathrm{d}t \\
&\le C\|\sqrt{\overline{n^\tau}}\|_{L^4(0,T;L^\infty)}^{4/3}\|\nabla^3\sqrt{\overline{n^\tau}}\|_{L^2(0,T;L^2)}^{4/3} \\
&\quad + C\|\nabla\sqrt{\overline{n^\tau}}\|_{L^{12/5}(0,T;L^\infty)}^{4/3}\|\nabla^2\sqrt{\overline{n^\tau}}\|_{L^3(0,T;L^2)}^{4/3} \le C,
\end{aligned}$$

since $12/d \geq 4$ for $d \leq 3$. This proves (3.34). The first bound in (3.36) follows from (3.40), while

$$\int_0^T \|\nabla^2\sqrt{\overline{n^\tau}}(t)\|_{L^{12/5}}^{8/3}\,\mathrm{d}t \leq B_4 \int_0^T \|\sqrt{\overline{n^\tau}}(t)\|_{H^3}^{2(24+d)/27}\|\sqrt{\overline{n^\tau}}(t)\|_{L^2}^{2(12-d)/27}\,\mathrm{d}t,$$

yields the second bound, since $2(24+d)/27 \leq 2$. Finally, (3.37) is a consequence of (3.36) in combination with the Lions-Villani estimate [47] on square roots (see Lemma C.4). □

Lemma 3.12. *For any finite $T > 0$, the sequence*

$$(\delta_\tau\overline{n^\tau}) \quad \text{is bounded in } L^{4/3}(0,T;H^{-3}(\mathbb{T}^d)), \tag{3.42}$$

uniformly in $\tau > 0$.

Proof. We need to show that there exists a constant $M > 0$ such that

$$\left|\int_0^T \int_{\mathbb{T}^d} \delta_\tau\overline{n^\tau}(t;x)\varphi(t;x)\,\mathrm{d}x\,\mathrm{d}t\right| \leq M\|\varphi\|_{L^4(0,T;H^3)}$$

holds for every test function $\varphi \in L^4(0,T;H^3(\mathbb{T}^d))$, independently of $\tau > 0$. Since, according to (3.33), the discrete time derivative can be decomposed as

$$\delta_\tau\overline{n^\tau} = \Delta^3\overline{n^\tau} + \partial^3_{ijk}F_1^{(ijk)}(\overline{n^\tau}) + \partial^2_{ij}F_2^{(ij)}(\overline{n^\tau})$$

in the sense of $L^{4/3}(0,T;H^{-3}(\mathbb{T}^d))$, it suffices to discuss the three terms on the right-hand side separately. For $\Delta^3\overline{n^\tau}$, using Hölder inequality, it follows that

$$\begin{aligned}\left|\int_0^T \int_{\mathbb{T}^d} \partial^3_{ijk}\varphi(t;x)\partial^3_{ijk}\overline{n^\tau}(t;x)\,\mathrm{d}x\,\mathrm{d}t\right| &\leq \int_0^T \|\varphi(t)\|_{H^3}\|\overline{n^\tau}(t)\|_{H^3}\,\mathrm{d}t \\ &\leq \|\varphi\|_{L^4(0,T;H^3)}\|\overline{n^\tau}\|_{L^{4/3}(0,T;H^3)},\end{aligned}$$

and the last expression is uniformly bounded with respect to τ in view of (3.34). Concerning $\partial^3_{ijk}F_1^{(ijk)}$, we find that

$$\begin{aligned}&\left|\int_0^T \int_{\mathbb{T}^d} \partial^3_{ijk}\varphi(t;x)F_1^{(ijk)}(\overline{n^\tau}(t;x))\,\mathrm{d}x\,\mathrm{d}t\right| \\ &\quad\leq 4\int_0^T \|\varphi(t)\|_{H^3}\|\nabla\sqrt{\overline{n^\tau}}(t)\|_{L^\infty}\big(3\|\nabla^2\sqrt{\overline{n^\tau}}(t)\|_{L^2} + 4\|\nabla\sqrt[4]{\overline{n^\tau}}(t)\|_{L^4}^2\big)\,\mathrm{d}t \\ &\quad\leq 4\|\varphi\|_{L^4(0,T;H^3)}\|\nabla\sqrt{\overline{n^\tau}}\|_{L^{12/5}(0,T;L^\infty)}\big(3\|\nabla^2\sqrt{\overline{n^\tau}}\|_{L^3(0,T;L^2)} + 4\|\nabla\sqrt[4]{\overline{n^\tau}}\|_{L^6(0,T;L^4)}^2\big),\end{aligned}$$

which is bounded, in view of (3.35), (3.36), and (3.37). Finally,

$$\begin{aligned}\left|\int_0^T \int_{\mathbb{T}^d} \partial^2_{ij}\varphi(t;x)F_2^{(ij)}(\overline{n^\tau}(t;x))\,\mathrm{d}x\,\mathrm{d}t\right| &\leq \int_0^T \|\nabla^2\varphi(t)\|_{L^6}\big\|F_2(\overline{n^\tau}(t))\big\|_{L^{6/5}}\,\mathrm{d}t \\ &\leq C\int_0^T \|\varphi(t)\|_{H^3}\big(\big\|\nabla^2\sqrt{\overline{n^\tau}}(t)\big\|_{L^{12/5}} + 8\big\|\nabla\sqrt[4]{\overline{n^\tau}}(t)\big\|_{L^{24/5}}^2\big)^2\,\mathrm{d}t \\ &\leq 2C\|\varphi\|_{L^4(0,T;H^3)}\big(\big\|\nabla^2\sqrt{\overline{n^\tau}}\big\|_{L^{8/3}(0,T;L^{12/5})}^2 + 16\big\|\nabla\sqrt[4]{\overline{n^\tau}}\big\|_{L^{16/3}(0,T;L^{24/5})}^4\big)\end{aligned}$$

shows that also $\partial^2_{ij}F_2^{(ij)}$ is uniformly bounded with respect to τ in $L^{4/3}(0,T;H^{-3}(\mathbb{T}^d))$, see (3.36) and (3.37). □

Lemma 3.13. *There exists a nonnegative function $n \in L^{4/3}(0,T;H^3(\mathbb{T}^d))$ such that along a suitable sequence $\tau \downarrow 0$,*

$$\overline{n^\tau} \rightharpoonup n \quad \text{in } L^{4/3}(0,T;H^3(\mathbb{T}^d)), \tag{3.43}$$

$$\delta_\tau \overline{n^\tau} \rightharpoonup \partial_t n \quad \text{in } L^{4/3}(0,T;H^{-3}(\mathbb{T}^d)), \tag{3.44}$$

$$\sqrt{\overline{n^\tau}} \to \sqrt{n} \quad \text{in } L^2(0,T;H^2(\mathbb{T}^d)), \tag{3.45}$$

$$\sqrt[4]{\overline{n^\tau}} \to \sqrt[4]{n} \quad \text{in } L^4(0,T;W^{1,4}(\mathbb{T}^d)). \tag{3.46}$$

Proof. Estimate (3.34) immediately implies (3.43), i.e., (a subsequence of) $\overline{n^\tau}$ converges weakly to some limit n in $L^{4/3}(0,T;H^3(\mathbb{T}^d))$. This convergence is even stronger: The τ-uniform bound (3.42) on $\delta_\tau\overline{n^\tau}$ allows us to apply Aubin's compactness lemma [57] to $\overline{n^\tau}$ (using Lemma A.2 of [15]). It follows that $\overline{n^\tau}$ converges strongly to the same limit n in $L^{4/3}(0,T;H^2(\mathbb{T}^d))$ and that $\delta_\tau\overline{n^\tau}$ converges to $\partial_t n$ weakly in $L^{4/3}(0,T;H^{-3}(\mathbb{T}^d))$, proving (3.44).

Of course, $\overline{n^\tau}$ also converges strongly to n in $L^1(0,T;L^1(\mathbb{T}^d))$. Therefore,

$$\int_0^T\int_{\mathbb{T}^d}\left|\sqrt{\overline{n^\tau}}(t;x)-\sqrt{n}(t;x)\right|^2 \mathrm{d}x\,\mathrm{d}t \le \int_0^T\int_{\mathbb{T}^d}\left|\overline{n^\tau}(t;x)-n(t;x)\right|\mathrm{d}x\,\mathrm{d}t \to 0,$$

since $|\sqrt{a}-\sqrt{b}|^2 \le |a-b|$ for a, $b \ge 0$. It follows that $\sqrt{\overline{n^\tau}}$ converges strongly to $\sqrt{n}$ in $L^2(0,T;L^2(\mathbb{T}^d))$. Invoking the Gagliardo-Nirenberg inequality, we obtain

$$\begin{aligned}\int_0^T \|\nabla^2\sqrt{\overline{n^\tau}}(t)-\nabla^2\sqrt{n}(t)\|_{L^2}^2\,\mathrm{d}t &\le B\int_0^T \|\sqrt{\overline{n^\tau}}(t)-\sqrt{n}(t)\|_{H^3}^{4/3}\|\sqrt{\overline{n^\tau}}(t)-\sqrt{n}(t)\|_{L^2}^{2/3}\,\mathrm{d}t\\ &\le B\left(\int_0^T\left(\|\sqrt{\overline{n^\tau}}(t)\|_{H^3}^2+\|\sqrt{n}(t)\|_{H^3}^2\right)\mathrm{d}t\right)^{2/3}\left(\int_0^T\|\sqrt{\overline{n^\tau}}(t)-\sqrt{n}(t)\|_{L^2}^2\,\mathrm{d}t\right)^{2/3},\end{aligned}$$

which tends to zero since $\sqrt{\overline{n^\tau}}$ is uniformly bounded with respect to τ in $L^2(0,T;H^3(\mathbb{T}^d))$, by (3.34), and it converges strongly to $\sqrt{n}$ in $L^2(0,T;L^2(\mathbb{T}^d))$. This proves (3.45).

Finally, (3.46) is a consequence of Proposition C.6, applied with $\alpha = 1/2$, $\beta = 1/6$, $\gamma = 1/4$, and $p = 2$, $q = 6$, $r = 4$. Indeed, simply combine the strong convergence of $\sqrt{\overline{n^\tau}}$ in $L^2(0,T;H^2(\mathbb{T}^d))$ with the boundedness of $(\sqrt[6]{\overline{n^\tau}})$ in $L^6(0,T;W^{1,6}(\mathbb{T}^d))$ (see (3.38)), which gives the conclusion. □

Proof of Theorem 3.1. It remains to prove that the limit function $n \in L^{4/3}(0,T;H^3(\mathbb{T}^d))$ from Lemma 3.13 is the sought weak solution for (3.7). In other words, we need to identify the limit $\partial_t n$ with the right-hand side of (3.3). We recall that, by the weak convergence of $\delta_\tau\overline{n^\tau}$ to $\partial_t n$ in $L^{4/3}(0,T;H^{-3}(\mathbb{T}^d))$,

$$\int_0^T\langle\partial_t n,\varphi\rangle\,\mathrm{d}t = \lim_{\tau\downarrow 0}\int_0^T\langle\delta_\tau\overline{n^\tau},\varphi\rangle\,\mathrm{d}t$$

holds for all $\varphi \in L^4(0,T;H^3(\mathbb{T}^d))$. In view of (3.33), the goal is thus to prove that

$$\lim_{\tau\downarrow 0}\int_0^T\int_{\mathbb{T}^d}\big(\partial^3_{ijk}\varphi\partial^3_{ijk}\overline{n^\tau}+\partial^3_{ijk}\varphi F_1^{(ijk)}(\overline{n^\tau})-\partial^2_{ij}\varphi F_2^{(ij)}(\overline{n^\tau})\big)\,\mathrm{d}x\,\mathrm{d}t$$
$$=\int_0^T\int_{\mathbb{T}^d}\big(\partial^3_{ijk}\varphi\partial^3_{ijk}n+\partial^3_{ijk}\varphi F_1^{(ijk)}(n)-\partial^2_{ij}\varphi F_2^{(ij)}(n)\big)\,\mathrm{d}x\,\mathrm{d}t$$

for all test functions φ from some dense set of $L^4(0,T;H^3(\mathbb{T}^d))$. Since the C^∞ functions are dense in that set, it suffices to prove the weak convergence of $\partial^3_{ijk}\overline{n^\tau}$, $F_1^{(ijk)}(\overline{n^\tau})$, and $F_2^{(ij)}(\overline{n^\tau})$ to their respective limits $\partial^3_{ijk}n$, $F_1^{(ijk)}(n)$, and $F_2^{(ij)}(n)$ in $L^1(0,T;L^1(\mathbb{T}^d))$.

First term of the integrand. From (3.43), it follows in particular that $\partial^3_{ijk}\overline{n^\tau}$ converges weakly to $\partial^3_{ijk}n$ in $L^{4/3}(0,T;L^2(\mathbb{T}^d))$ for any combination of the indices i, j, and k, and thus, as $\tau\downarrow 0$,

$$\int_0^T\int_{\mathbb{T}^d}\partial^3_{ijk}\varphi\partial^3_{ijk}\overline{n^\tau}\,\mathrm{d}x\,\mathrm{d}t\to\int_0^T\int_{\mathbb{T}^d}\partial^3_{ijk}\varphi\partial^3_{ijk}n\,\mathrm{d}x\,\mathrm{d}t.$$

Second term of the integrand. We recall the definition of $F_1^{(ij)}$ from (3.4). As a consequence of (3.46), the first-order derivatives $\partial_j\sqrt[4]{\overline{n^\tau}}$ converge strongly to $\partial_j\sqrt[4]{n}$ in $L^4(0,T;L^4(\mathbb{T}^d))$ for all j. As a product of strongly convergent sequences, each $\partial_j\sqrt[4]{\overline{n^\tau}}\,\partial_k\sqrt[4]{\overline{n^\tau}}$ converges strongly in $L^2(0,T;L^2(\mathbb{T}^d))$ to the respective product $\partial_j\sqrt[4]{n}\,\partial_k\sqrt[4]{n}$. Clearly, all second-order derivatives $\partial^2_{jk}\sqrt{\overline{n^\tau}}$ tend strongly to their respective limits $\partial^2_{jk}\sqrt{n}$ in $L^2(0,T;L^2(\mathbb{T}^d))$ as well, taking into account (3.45). In combination with the strong convergence of $\partial_i\sqrt{\overline{n^\tau}}$ to $\partial_i\sqrt{n}$ in $L^2(0,T;L^2(\mathbb{T}^d))$, by (3.45), it follows that each $F_1^{(ijk)}(\overline{n^\tau})$ is the sum of products of two strongly convergent sequences in $L^2(0,T;L^2(\mathbb{T}^d))$ and consequently, the product converges strongly in $L^1(0,T;L^1(\mathbb{T}^d))$ to the product of the limits:

$$\int_0^T\int_{\mathbb{T}^d}\partial^3_{ijk}\varphi F_1^{(ijk)}(\overline{n^\tau})\,\mathrm{d}x\,\mathrm{d}t\to\int_0^T\int_{\mathbb{T}^d}\partial^3_{ijk}\varphi F_1^{(ijk)}(n)\,\mathrm{d}x\,\mathrm{d}t.$$

Third term of the integrand. Arguing as above, it follows from (3.45) and (3.46) that both summands in $F_2^{(ij)}(\overline{n^\tau})$ converge strongly in $L^2(0,T;L^2(\mathbb{T}^d))$ to their respective limits, and so the sequence of the product converges strongly in $L^1(0,T;L^1(\mathbb{T}^d))$ to the product of the limit. This means that

$$\int_0^T\int_{\mathbb{T}^d}\partial^2_{ij}\varphi F_2^{(ij)}(\overline{n^\tau})\,\mathrm{d}x\,\mathrm{d}t\to\int_0^T\int_{\mathbb{T}^d}\partial^2_{ij}\varphi F_2^{(ij)}(n)\,\mathrm{d}x\,\mathrm{d}t.$$

finishing the proof. □

3.5 Exponential time decay of weak solutions

Proof of Theorem 3.2. Let $\tau>0$ and let n_1^τ, n_2^τ, … be the sequence of solutions to the semi-discretized problem constructed in Proposition 3.9. The discrete entropy estimate

(3.22) implies that

$$\mathcal{H}[n_k^\tau] + \tau\kappa \int_{\mathbb{T}^d} |\nabla^3 \sqrt{n_k^\tau}|^2 \, \mathrm{d}x \leq \mathcal{H}[n_{k-1}^\tau], \quad k \in \mathbb{N}.$$

with a positive constant $\kappa > 0$ independent of k and τ. Employing the generalized logarithmic Sobolev inequality,

$$\int_{\mathbb{T}^d} n_k^\tau \log\Big(\frac{n_k^\tau}{\|n_k^\tau\|_{L^1(\mathbb{T}^d)}}\Big) \, \mathrm{d}x \leq \frac{1}{32\pi^6} \int_{\mathbb{T}^d} \|\nabla^3 \sqrt{n_k^\tau}\|^2 \, \mathrm{d}x,$$

which is proven as in [36], and observing that $\|n_k^\tau\|_{L^1(\mathbb{T}^d)} = \|n_0\|_{L^1(\mathbb{T}^d)} = 1$, we infer that

$$\mathcal{H}[n_k^\tau] \leq \frac{1}{32\pi^6} \int_{\mathbb{T}^d} \|\nabla^3 \sqrt{n_k^\tau}\|^2 \, \mathrm{d}x.$$

Then the above entropy inequality yields

$$\mathcal{H}[n_k^\tau] + 32\pi^6\tau\kappa\mathcal{H}[n_k^\tau] \leq \mathcal{H}[n_{k-1}^\tau], \quad k \in \mathbb{N},$$

which in turn implies for all $t \in ((k-1)\tau, k\tau]$ that

$$\mathcal{H}[\overline{n^\tau}(t)] \leq \big(1 + 32\pi^6\tau\kappa\big)^{-t/\tau}\mathcal{H}[n_0],$$

since $k \geq t/\tau$. Recall that $\overline{n^\tau}(t)$ converges a.e. to $n(t)$ as $\tau \to 0$, and observe that $(1 + 32\pi^6\tau\kappa)^{-t/\tau}$ converges to $\exp(-32\pi^6\kappa t)$. Thus the limit $\tau \to 0$ gives

$$\mathcal{H}[n(t)] \leq \mathcal{H}[n_0]e^{-32\pi^6\kappa t}, \quad t \geq 0.$$

An application of the Csiszár-Kullback-Pinsker inequality (see, e.g., [60, Section 2]) concludes the proof. □

3.6 Existence and uniqueness of classical solutions

In this section, we invoke the machinery of analytic semigroups to prove Theorem 3.3. Our approach follows closely the strategy developed in [7] by Bleher at al. for the fourth-order DLSS equation. However, the more complicated structure of the nonlinearities in our sixth-order equation induces a variety of additional technical difficulties.

3.6.1 Definitions

We collect some standard results on the operator Δ^3. By abuse of notation, we use the symbol Δ^3 for the $L^1(\mathbb{T}^d)$-closure of the operator $\Delta^3\varphi = \sum_{i,j,k=1}^d \partial_i^2\partial_j^2\partial_k^2\varphi$, defined for $\varphi \in C^\infty(\mathbb{T}^d)$. Define the auxiliary function $H \in C^\infty(\mathbb{R}^d)$ by

$$H(z) = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{-|\zeta|^6} e^{i\zeta\cdot z} \, \mathrm{d}\zeta,$$

and introduce for each $t > 0$ the so-called solution kernel $G(t) \in C^\infty(\mathbb{T}^d)$ by

$$G(t;y) = t^{-d/6} \sum_{\Lambda \in \mathbb{Z}^d} H\big(t^{-1/6}(y+\Lambda)\big).$$

The series converges since $H(z)$ decays exponentially for $|z| \to \infty$. Classical parabolic theory provides the following result.

Lemma 3.14. *Let $m \in \mathbb{N}_0$, $p \in [1,\infty)$, and $\alpha \in (0,1)$. If $u \in W^{m,p}(\mathbb{T}^d)$, then the convolution $U(t) = G(t) \star u$ defines a smooth curve, satisfying*

$$U \in C^\infty((0,\infty); C^\infty(\mathbb{T}^d)) \cap C^0([0,\infty); W^{m,p}(\mathbb{T}^d)), \quad \frac{\mathrm{d}}{\mathrm{d}t}U(t) = \Delta^3 U(t),\ U(0) = u. \tag{3.47}$$

If $w \in C^\alpha([t_1,t_2]; W^{m,p}(\mathbb{T}^d))$ is a Hölder continuous curve on $[t_1,t_2]$, then the function

$$W(t) = \int_{t_1}^{t} G(t-s) \star w(s)\,\mathrm{d}s$$

defines a Hölder continuously differentiable curve, satisfying

$$W \in C^{1,\alpha}([t_1,t_2]; W^{m+6,p}(\mathbb{T}^d)), \quad \frac{\mathrm{d}}{\mathrm{d}t}W(t) = \Delta^3 W(t) + w(t),\ W(t_1) = 0. \tag{3.48}$$

Proof. The proof of (3.47) and (3.48) is technical but standard. One possible approach, which would be most similar to [7], is to observe that $-\Delta^3$ is the generator of the analytic semigroup defined by $t \mapsto G(t) \star f$ for all $f \in L^1(\mathbb{T}^d)$. We refer to [31, Chapter 3] or to [54, Chapter 4] for further details on the semigroup approach. □

Apart from Lemma 3.14, we shall not need classical results on parabolic equations. Instead, we derive our core estimates with the help of the following lemma.

Lemma 3.15. *For given $\alpha \in \mathbb{N}_0^d$, $p \geq 1$, and $t > 0$, the kernel G satisfies the estimate*

$$\big\| \mathrm{D}^\alpha G(t) \big\|_{L^p} \leq \Gamma t^{-(|\alpha|+d(1-1/p))/6}, \tag{3.49}$$

where $\Gamma > 0$ is independent of $t > 0$.

Here and in the following, D^α denotes a partial derivative of order $|\alpha|$.

Proof. For $t > 0$, define the half-open cube $Q(t) = [0, t^{-1/6})^d \subset \mathbb{R}^d$. Using the change of variables $z(t) = t^{-1/6}y$, we obtain

$$\begin{aligned}
\| \mathrm{D}^\alpha G(t) \|_{L^p(\mathbb{T}^d)} &= t^{-d/6} \left(\int_{[0,1)^d} \sum_{\Lambda \in \mathbb{Z}^d} \big| \mathrm{D}_y^\alpha H\big(t^{-1/6}(y+\Lambda)\big)\big|^p \,\mathrm{d}y \right)^{1/p} \\
&\leq t^{-d/6} \sum_{\Lambda \in \mathbb{Z}^d} \left(\int_{Q(t)} \big| t^{-|\alpha|/6}\, \mathrm{D}_z^\alpha H(z + t^{-1/6}\Lambda)\big|^p t^{d/6}\,\mathrm{d}z \right)^{1/p} \\
&= t^{-(d+|\alpha|-d/p)/6} \left(\int_{\mathbb{R}^d} \big| \mathrm{D}_z^\alpha H(z) \big|^p \,\mathrm{d}z \right)^{1/p}.
\end{aligned}$$

Here we used the Minkowski inequality and the fact that, for each $t > 0$, the space $\mathbb{R}^d$ is the disjoint union of the cubes $Q(t) + t^{-1/6}\Lambda$, where $\Lambda \in \mathbb{Z}^d$. So $\Gamma = \|\mathrm{D}^\alpha H\|_{L^p(\mathbb{R}^d)}$ is the required constant. □

3.6.2 Existence and uniqueness of a mild solution

Our main result of this subsection is contained in the following proposition.

Proposition 3.16. *Let $n_0 \in H^2(\mathbb{T}^d)$ be strictly positive. Then there exist $T > 0$ and precisely one continuous curve $n : [0,T] \to H^2(\mathbb{T}^d)$ with $n(0) = n_0$ that satisfies the following "very mild" formulation of* (3.3)*:*

$$n(t) = G(t) \star n_0 + \partial^3_{ijk} \int_0^t G(t-s) \star F_1^{(ijk)}(n(s))\,\mathrm{d}s + \partial^2_{ij} \int_0^t G(t-s) \star F_2^{(ij)}(n(s))\,\mathrm{d}s \tag{3.50}$$

for every $t \in (0,T)$. This solution is differentiable with respect to $t \in (0,T)$ with a Hölder continuous derivative, i.e. $n \in C^{1,1/12}([\tau,T]; H^2(\mathbb{T}^d))$ for every $\tau \in (0,T)$.

To prove Proposition 3.16, we adapt the proof of Theorem 4.2 (a) in [7] to the situation at hand. That means, we are going to obtain the solution n to (3.50) as the unique fixed point of the map $u \mapsto \Phi[u]$, defined by

$$\Phi[u](t) = G(t) \star n_0 + \Psi[u](t) \tag{3.51}$$

on a suitable set $V_T \subset C^0([0,T]; H^2(\mathbb{T}^d))$, where $\Psi = \partial^3_{ijk}\psi_1^{(ijk)} + \partial^2_{ij}\psi_2^{(ij)}$ and

$$\psi_1^{(ijk)}[u](t) = \int_0^t G(s) \star F_1^{(ijk)}(u(t-s))\,\mathrm{d}s, \quad \psi_2^{(ij)}[u](t) = \int_0^t G(s) \star F_2^{(ij)}(u(t-s))\,\mathrm{d}s. \tag{3.52}$$

The core ingredient of the proof of Proposition 3.16 is the following Lipschitz estimate on the nonlinearities $F_1^{(ijk)}$ and $F_2^{(ij)}$.

Lemma 3.17. *For any $0 < \delta < 1$, $F_1^{(ijk)}$ and $F_2^{(ij)}$ are Lipschitz continuous as mappings from any bounded subset of*

$$U_\delta = \left\{ u \in H^2(\mathbb{T}^d) : \min_x u(x) \geq \delta,\ \|u\|_{H^2} \leq \delta^{-1} \right\} \tag{3.53}$$

into $L^{3/2}(\mathbb{T}^d)$ and into $L^1(\mathbb{T}^d)$, respectively, satisfying

$$\|F_1^{(ijk)}(u)\|_{L^{3/2}} \leq M_1\delta^{-5}, \quad \|F_1^{(ijk)}(u_1) - F_1^{(ijk)}(u_2)\|_{L^{3/2}} \leq M_1\delta^{-4}\|u_1 - u_2\|_{H^2}, \tag{3.54}$$

$$\|F_2^{(ij)}(u)\|_{L^1} \leq M_2\delta^{-7}, \quad \|F_2^{(ij)}(u_1) - F_2^{(ij)}(u_2)\|_{L^1} \leq M_2\delta^{-6}\|u_1 - u_2\|_{H^2}, \tag{3.55}$$

for all $u, u_1, u_2 \in U_\delta$*, where* M_1 *and* M_2 *are universal constants. Moreover,* $F_1^{(ijk)}$ *and* $F_2^{(ij)}$ *map*

$$U'_\delta = \left\{ u \in U_\delta \cap W^{3,3/2}(\mathbb{T}^d) : \|u\|_{W^{3,3/2}} \leq \delta^{-1} \right\}$$

into $L^2(\mathbb{T}^d)$ *and* $L^{3/2}(\mathbb{T}^d)$*, respectively, satisfying*

$$\|F_1^{(ijk)}(u)\|_{L^2} \leq M'_1 \delta^{-5}, \quad \|F_1^{(ijk)}(u_1) - F_1^{(ijk)}(u_2)\|_{L^2} \leq M'_1 \delta^{-4} \|u_1 - u_2\|_{H^2}, \tag{3.56}$$

$$\|F_2^{(ij)}(u)\|_{L^{3/2}} \leq M'_2 \delta^{-7}, \quad \|F_2^{(ij)}(u_1) - F_2^{(ij)}(u_2)\|_{L^{3/2}} \leq M'_2 \delta^{-6} \|u_1 - u_2\|_{H^2}, \tag{3.57}$$

for all $u, u_1, u_2 \in U'_\delta$*, where* M'_1 *and* M'_2 *are universal constants.*

Proof. Since we are working in dimensions $d \leq 3$, every $u \in U_\delta$ is a strictly positive and continuous function on $\mathbb{T}^d$, with $\partial^2_{ij} u \in L^2(\mathbb{T}^d)$ and $\partial_i u \in L^6(\mathbb{T}^d)$. It follows that we can write

$$F_1^{(ijk)}(u) = 2\frac{\partial_i u \partial_j u \partial_k u}{u^2} - 3\frac{\partial_i u \partial^2_{jk} u}{u}, \tag{3.58}$$

$$F_2^{(ij)}(u) = 2\frac{\partial^2_{ik} u \partial^2_{kj} u}{u} - 4\frac{\partial^2_{ik} u \partial_k u \partial_j u}{u^2} + 2\frac{(\partial_k u)^2 \partial_i u \partial_j u}{u^3}. \tag{3.59}$$

Thus, $F_1^{(ijk)}$ and $F_2^{(ij)}$ are sums of products of derivatives (of order one or two) of u, divided by a power of u. By application of Hölder's inequality and the continuity of the Sobolev embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,6}(\mathbb{T}^d)$, one readily verifies the first inequalities in (3.54) and (3.55). The Lipschitz continuity is straightforward to verify from the representations (3.58) and (3.59) by repeated application of the triangle inequality. For proving (3.56) and (3.57), we use additionally the continuous embedding $W^{3,3/2}(\mathbb{T}^d) \hookrightarrow W^{2,3}(\mathbb{T}^d)$. □

A consequence of the above lemma is that Ψ maps bounded curves u into Hölder continuous curves.

Lemma 3.18. *Assume that there exists a* $\delta > 0$ *such that* $u \in C([0,T); H^2(\mathbb{T}^d))$ *satisfies*

1. either $u(t) \geq \delta$ *and* $\|u(t)\|_{H^2} \leq \delta^{-1}$*,*
2. or $u(t) > 0$ *and* $\mathcal{E}[u(t)] \leq \delta^{-1}$

for all $0 \leq t \leq T$*. Then* $\Psi[u] \in C^{1/12}([0,T]; H^2(\mathbb{T}^d))$*, i.e.,*

$$\|\Psi[u](t') - \Psi[u](t)\|_{H^2} \leq L|t' - t|^{1/12} \quad \textit{for all } t, t' \in [0,T], \tag{3.60}$$

where $L > 0$ *depends on* δ*, but not on* u*.*

Proof. To begin with, we remark that

$$\|F_1^{(ijk)}(u(t))\|_{L^{3/2}} \leq Z_1 \quad \text{and} \quad \|F_2^{(ij)}(u(t))\|_{L^1} \leq Z_2 \tag{3.61}$$

holds for all $t \in [0,T]$, where the positive constants Z_1 and Z_2 depend on $\delta > 0$ only. Indeed, if the first set of assumptions on u is satisfied, then (3.61) is an immediate consequence of Lemma 3.17. If instead the second set of assumptions is satisfied, then Hölder's inequality implies

$$\begin{aligned}\|F_1^{(ijk)}(u(t))\|_{L^{3/2}} &\leq 4\|\nabla\sqrt{u(t)}\|_{L^6}\big(4\|\nabla\sqrt[4]{u(t)}\|_{L^4}^2 + 3\|\nabla^2\sqrt{u(t)}\|_{L^2}\big),\\ \|F_2^{(ij)}(u(t))\|_{L^1} &\leq 8\big(\|\nabla^2\sqrt{u(t)}\|_{L^2} + 4\|\nabla\sqrt[4]{u(t)}\|_{L^4}^2\big)^2.\end{aligned}$$

In view of (3.9) and Lemma C.4, these right-hand sides are controlled in terms of $\mathcal{E}[u(t)] \leq \delta^{-1}$ only.

Now, let t, $t' \in [0,T]$ be given with $\tau = t' - t > 0$. For a given $\alpha \in \mathbb{N}_0^d$ with $|\alpha| = 2$, introduce

$$\Theta^\alpha(t;\tau) = \big\| \mathrm{D}^\alpha \left(\Psi[u](t+\tau) - \Psi[u](t)\right)\big\|_{L^2}.$$

By definition of Ψ and a change of variables under the integrals, we find that

$$\begin{aligned}\Theta^\alpha(t;\tau) \leq \int_0^t &\Big(\big\| \mathrm{D}^\alpha\, \partial^3_{ijk}(G(s+\tau) - G(s)) \star F_1^{(ijk)}(u(t-s))\big\|_{L^2}\\ &+ \big\| \mathrm{D}^\alpha\, \partial^2_{ij}(G(s+\tau) - G(s)) \star F_2^{(ij)}(u(t-s))\big\|_{L^2}\Big)\,\mathrm{d}s\\ &+ \int_0^\tau \Big(\big\| \mathrm{D}^\alpha\, \partial^3_{ijk}G(s) \star F_1^{(ijk)}(u(t+\tau-s))\big\|_{L^2}\\ &+ \big\| \mathrm{D}^\alpha\, \partial^2_{ij}G(s) \star F_2^{(ij)}(u(t+\tau-s))\big\|_{L^2}\Big)\,\mathrm{d}s.\end{aligned}$$

Using (3.61) and Young's inequality for convolutions,

$$\|\phi \star \psi\|_{L^p} \leq \Upsilon\|\phi\|_{L^q}\|\psi\|_{L^r},$$

for $\phi \in L^p(\mathbb{R}^d)$, $\psi \in L^r(\mathbb{R}^d)$, and $1 + 1/p = 1/q + 1/r$, where $\Upsilon > 0$, the term under the last integral above can be estimated for $0 < s < \tau$ as follows:

$$\begin{aligned}\big\| \mathrm{D}^\alpha\, \partial^3_{ijk}G(s) \star F_1^{(ijk)}(u(t+\tau-s))\big\|_{L^2} &\leq \Upsilon_1\|\nabla^5 G(s)\|_{L^{6/5}}\|F_1(u(t+\tau-s))\|_{L^{3/2}}\\ &\leq \frac{\Upsilon_1 Z_1 \Gamma_1}{s^{\vartheta_1}},\\ \big\| \mathrm{D}^\alpha\, \partial^2_{ij}G(s) \star F_2^{(ij)}(u(t+\tau-s))\big\|_{L^2} &\leq \Upsilon_2\|\nabla^4 G(s)\|_{L^2}\|F_2(u(t+\tau-s))\|_{L^1}\\ &\leq \frac{\Upsilon_2 Z_2 \Gamma_2}{s^{\vartheta_2}},\end{aligned}$$

where, according to (3.49), the exponents are given by

$$\vartheta_1 = (5 + d/6)/6 < 1 \quad \text{and} \quad \vartheta_2 = (4 + d/2)/6 < 1.$$

We apply the analogous estimate to the expression under the first integral, and estimate further by employing relation (3.47). For $0 < s < t$, we have

$$\begin{aligned}&\big\|\nabla^5(G(\tau+s) - G(s))\big\|_{L^{6/5}} \leq \left\|\nabla^5\int_s^{s+\tau}\Delta^3 G(\sigma)\,\mathrm{d}\sigma\right\|_{L^{6/5}}\\ &\leq \int_s^{s+\tau}\big\|\nabla^5(\Delta^3 G(\sigma))\big\|_{L^{6/5}}\,\mathrm{d}\sigma \leq \Gamma_1'\int_s^{s+\tau}\frac{\mathrm{d}\sigma}{\sigma^{1+\vartheta_1}} = \frac{\Gamma_1'}{\vartheta_1}\big(s^{-\vartheta_1} - (s+\tau)^{-\vartheta_1}\big).\end{aligned}$$

In a similar fashion, we obtain

$$\left\|\nabla^4(G(s+\tau)-G(s))\right\|_{L^2} \le \frac{\Gamma_2'}{\vartheta_2}\big(s^{-\vartheta_2}-(s+\tau)^{-\vartheta_2}\big).$$

In summary, this leads to

$$\begin{aligned}\Theta^\alpha(t;\tau) &\le \frac{\Upsilon_1 Z_1\Gamma_1'}{\vartheta_1}\int_0^t \big(s^{-\vartheta_1}-(s+\tau)^{-\vartheta_1}\big)\,\mathrm{d}s + \frac{\Upsilon_2 Z_2\Gamma_2'}{\vartheta_2}\int_0^t \big(s^{-\vartheta_2}-(s+\tau)^{-\vartheta_2}\big)\,\mathrm{d}s \\ &\quad + \Upsilon_1 Z_1\Gamma_1\int_0^\tau s^{-\vartheta_1}\,\mathrm{d}s + \Upsilon_2 Z_2\Gamma_2\int_0^\tau s^{-\vartheta_2}\,\mathrm{d}s \\ &\le \frac{\Upsilon_1 Z_1\Gamma_1'}{(1-\vartheta_1)\vartheta_1}\big((t+\tau)^{1-\vartheta_1}-t^{1-\vartheta_1}\big) + \frac{\Upsilon_2 Z_2\Gamma_2'}{(1-\vartheta_2)\vartheta_2}\big((t+\tau)^{1-\vartheta_2}-t^{1-\vartheta_2}\big) \\ &\quad + \frac{\Upsilon_1 Z_1\Gamma_1}{1-\vartheta_1}\tau^{1-\vartheta_1} + \frac{\Upsilon_2 Z_2\Gamma_2}{1-\vartheta_2}\tau^{1-\vartheta_2}.\end{aligned}$$

To finish the proof, we observe that, since $0<\vartheta_i<1$, we have $(t+\tau)^{1-\vartheta_i}\le t^{1-\vartheta_i}+\tau^{1-\vartheta_i}$, and $\vartheta_i\le 11/12$ in dimensions $d\le 3$. This proves the Hölder continuity of $\Theta^\alpha(t;\tau)$ with exponent $1/12$ for $|\alpha|=2$. The cases $|\alpha|=1$ and $\alpha=0$ are similar. □

Proof of Proposition 3.16. As indicated above, we are going to show that Φ, given by (3.51), is a well-defined contraction on a suitable subset $V_T\subset C([0,T];H^2(\mathbb{T}^d))$ for some sufficiently small $T>0$.

Recall the definition of U_δ from (3.53). Since $n_0\in H^2(\mathbb{T}^d)$ is strictly positive by assumption, we can choose $\delta>0$ such that $n_0\in U_{2\delta}$. Accordingly, for a given $T>0$, define

$$V_T=\big\{u\in C^0([0,T];H^2(\mathbb{T}^d)) : u(t)\in U_\delta \text{ for all } t\in[0,T]\big\}.$$

Fix a curve $u\in V_T$. In view of Lemma 3.17, $F_1^{(ijk)}(u)$ and $F_2^{(ij)}(u)$ are continuous curves on $[0,T]$ with values in $L^{3/2}(\mathbb{T}^d)$ and $L^1(\mathbb{T}^d)$, respectively.

Since $\Phi[u](0)=n_0$ for every $u\in V_T$, the H^2-distance of $\Phi[u](t)$ to n_0 becomes small as $t\downarrow 0$, uniformly in $u\in V_T$. Moreover, since the infimum of $\Phi[u](t)$ is controlled in terms of this distance, one may choose $T>0$ sufficiently small to achieve $\Phi[u](t)\in U_\delta$ for all $t\in[0,T]$ and $u\in V_T$. Hence, $\Phi:V_T\to V_T$ is well-defined.

Next, we verify the contraction property of Φ. The calculations follow the same pattern as above, now using the Lipschitz estimates in (3.54) and (3.55). Let $u_1,u_2\in V_T$ be given.

Then, for $|\alpha| = 2$,

$$
\begin{aligned}
\big\| \mathrm{D}^\alpha \big(\Phi[u_1](t) - \Phi[u_2](t)\big) \big\|_{L^2} &\le \int_0^t \Big(\big\| \nabla^5 G(t-s) \star (F_1^{(ijk)}(u_1(s)) - F_1^{(ijk)}(u_2(s))) \big\|_{L^2} \\
&\qquad + \big\| \nabla^4 G(t-s) \star (F_2^{(ij)}(u_1(s)) - F_2^{(ij)}(u_2(s))) \big\|_{L^2} \Big) \,\mathrm{d}s \\
&\le \Upsilon_1 M_1 \delta^{-4} \int_0^t (t-s)^{-\vartheta_1} \|u_1(s) - u_2(s)\|_{H^2} \,\mathrm{d}s \\
&\qquad + \Upsilon_2 M_2 \delta^{-6} \int_0^t (t-s)^{-\vartheta_2} \|u_1(s) - u_2(s)\|_{H^2} \,\mathrm{d}s \\
&\le \left(\frac{\Upsilon_1 M_1}{\delta^4 (1-\vartheta_1)} + \frac{\Upsilon_2 M_2}{\delta^6 (1-\vartheta_2)} \right) T^{1/12} \\
&\qquad \times \sup_{0 \le s' \le T} \|u_1(s') - u_2(s')\|_{H^2}.
\end{aligned}
$$

Similar estimates are obtained for $|\alpha| \le 1$. Diminishing T further if necessary, it follows that Φ is contractive on V_T. The claim about the Hölder continuity is a consequence of (3.60) in combination with (3.47). □

3.6.3 Bootstrapping

We prove that the very mild solution to (3.3) is actually smooth for $t > 0$. To this end, we need the following lemma.

Lemma 3.19. *Let $\delta > 0$ be given. For each $m \ge 1$, there exist continuous and increasing functions $Q_1^{(m)}, Q_2^{(m)} : \mathbb{R}_+ \to \mathbb{R}_+$ such that*

$$\|F_1^{(ijk)}(u_1) - F_1^{(ijk)}(u_2)\|_{H^m} \le Q_1^{(m)}\big(\|u_1\|_{H^{m+1}} + \|u_2\|_{H^{m+1}}\big) \|u_1 - u_2\|_{H^{m+2}}, \tag{3.62}$$

$$\|F_2^{(ij)}(u_1) - F_2^{(ij)}(u_2)\|_{W^{m,3/2}} \le Q_2^{(m)}\big(\|u_1\|_{H^{m+1}} + \|u_2\|_{H^{m+1}}\big) \|u_1 - u_2\|_{H^{m+2}} \tag{3.63}$$

holds (componentwise) for all $u \in U_\delta \cap H^{m+2}(\mathbb{T}^d)$.

Observe that this lemma does not apply for $m = 0$, in which case one has to resort to the estimates provided in Lemma 3.17.

Proof. Basically, we follow the ideas of the proof of Lemma 3.17, namely we apply several times the triangle inequality, the Hölder inequality, and continuous Sobolev embeddings. However, due to the higher-order derivatives, the proof is technically more involved. Representations (3.58) and (3.59) show that $F_1^{(ijk)}$ and $F_2^{(ij)}$ are sums of products of derivatives of u divided by a power of u, i.e. sums of monomials of the form

$$\frac{\mathrm{D}^{\alpha^1} u \ldots \mathrm{D}^{\alpha^k} u}{u^{k-1}}, \tag{3.64}$$

where $\alpha^\ell \in \mathbb{N}_0^d$, $\ell = 1,\dots,k$, $1 \le |\alpha^\ell| \le 2$, and $\sum_{\ell=1}^k |\alpha^l| = K$ equals 3 or 4 for $F_1^{(ijk)}$ or $F_2^{(ij)}$, respectively. A partial derivative of such a monomial is again a sum of monomials of the form (3.64):

$$\mathrm{D}^\alpha \left(\frac{\mathrm{D}^{\alpha^1} u \dots \mathrm{D}^{\alpha^k} u}{u^{k-1}} \right) = \sum \frac{\mathrm{D}^{\beta^1} u \; \mathrm{D}^{\beta^2} u \dots \mathrm{D}^{\beta^r} u}{u^{r-1}},$$

for $\alpha \in \mathbb{N}_0^d$, $|\alpha| \le m$, $1 \le |\beta^\ell| \le m+2$, $k \le r \le k+|\alpha|$, and $\sum_{\ell=1}^r |\beta^\ell| = K+|\alpha|$. In view of the continuous Sobolev embeddings $H^{m+2}(\mathbb{T}^d) \hookrightarrow W^{m+1,6}(\mathbb{T}^d)$ and $H^{m+2}(\mathbb{T}^d) \hookrightarrow C^m(\mathbb{T}^d)$, it follows from the above representation of $\mathrm{D}^\alpha F_1^{(ijk)}(u)$ and $\mathrm{D}^\alpha F_2^{(ij)}(u)$ that for every $u \in H^{m+2}(\mathbb{T}^d)$, it holds $\mathrm{D}^\alpha F_1^{(ijk)}(u) \in L^2(\mathbb{T}^d)$ and $\mathrm{D}^\alpha F_2^{(ij)}(u) \in L^{3/2}(\mathbb{T}^d)$ for each $|\alpha| \le m$ and $m \ge 1$. Then, by the repeated application of the triangle and Hölder inequalities, we obtain functions $Q_1^{(m)}$ and $Q_2^{(m)}$ as well as the estimates (3.62) and (3.63). □

Proposition 3.20. *The very mild solution from Proposition 3.16 is a continuously differentiable curve from* $(0,T]$ *to* $C^\infty(\mathbb{T}^d)$.

Proof. Let $\tau \in (0,T)$ be fixed. We are going to prove, inductively on m, that

$$n \in C^{1,1/12}([\tau,T]; H^{m+2}(\mathbb{T}^d)) \tag{3.65}$$

for every integer $m \in \mathbb{N}_0$. For $m = 0$, the claim (3.65) is part of the conclusion of Proposition 3.16 above. The compositions of the Hölder continuous curve n with the locally Lipschitz continuous nonlinearities $F_1^{(ijk)}$ and $F_2^{(ij)}$ (see Lemma 3.17) are Hölder continuous with the same exponent, $F_1^{(ijk)}(n) \in C^{1/12}([\tau,T]; L^{3/2}(\mathbb{T}^d))$ and $F_2^{(ij)}(n) \in C^{1/12}([\tau,T]; L^1(\mathbb{T}^d))$. For $\psi_1^{(ijk)}$ and $\psi_2^{(ij)}$, defined in (3.52), the second part of Lemma 3.14 implies that $\psi_1^{(ijk)}[n] \in C^{1,1/12}([\tau,T]; W^{6,3/2}(\mathbb{T}^d))$ and $\psi_2^{(ij)}[n] \in C^{1,1/12}([\tau,T]; W^{6,1}(\mathbb{T}^d))$. In combination with (3.47), it thus follows directly from (3.50) that $n \in C^{1,1/12}([\tau,T]; W^{3,3/2}(\mathbb{T}^d))$. An iteration leads, via (3.56), to the improved regularity $F_1^{(ijk)}(n) \in C^{1/12}([\tau,T]; L^2(\mathbb{T}^d))$, and thus to $\psi_1^{(ijk)}[n] \in C^{1,1/12}([\tau,T]; H^6(\mathbb{T}^d))$. Furthermore, by (3.57), we infer that $F_2^{(ij)}(n) \in C^{1/12}([\tau,T]; L^{3/2}(\mathbb{T}^d))$ and hence, $\psi_2^{(ij)}[n] \in C^{1,1/12}([\tau,T]; W^{6,3/2}(\mathbb{T}^d))$. By the continuity of the embedding $W^{6,3/2}(\mathbb{T}^d) \hookrightarrow H^5(\mathbb{T}^d)$, it follows that $\psi_2^{(ij)}[n] \in C^{1,1/12}([\tau,T]; H^5(\mathbb{T}^d))$. Then the representation (3.50) proves (3.65) with $m = 1$.

Assuming (3.65) for some $m \ge 1$, it follows from Lemma 3.19 that $F_1^{(ijk)}(n) \in C^{1/12}([\tau,T];\, H^m(\mathbb{T}^d))$ and $F_2^{(ij)}(n) \in C^{1/12}([\tau,T]; W^{m,3/2}(\mathbb{T}^d))$. By property (3.48) of the kernel G and since the Sobolev embedding $W^{m+6,3/2}(\mathbb{T}^d) \hookrightarrow H^{m+5}(\mathbb{T}^d)$ is continuous, we infer that $\psi_1^{(ijk)} \in C^{1,1/12}([\tau,T]; H^{m+6}(\mathbb{T}^d))$ and $\psi_2^{(ij)} \in C^{1/12}([\tau,T]; H^{m+5}(\mathbb{T}^d))$. Using this inside the representation (3.50) and combining it with the smoothness property (3.47), we arrive at $n \in C^{1,1/12}([\tau,T]; H^{m+3}(\mathbb{T}^d))$, which implies (3.65) with m replaced by $m+1$. □

Proof of Theorem 3.3. First, we extend the local solution $n \in C([0,T]; H^2(\mathbb{T}^d))$ obtained from Proposition 3.16 to the respective *maximal* solution $n_{\max}$ by the usual procedure: Provided that $n(T) \in H^2(\mathbb{T}^d)$ is strictly positive, we can invoke Proposition 3.16 with the new initial datum $\tilde{n}_0 := n(T)$, thus obtaining another "very mild" solution $\tilde{n} : [0, \tilde{T}] \to H^2(\mathbb{T}^d)$ to (3.3). Using the semigroup property $G(\tau) \star G(\sigma) = G(\tau + \sigma)$ for arbitrary σ, $\tau > 0$, it can be easily checked that the concatenation $n_+ : [0, T + \tilde{T}] \to H^2(\mathbb{T}^d)$, given by

$$n_+(t) = \begin{cases} n(t) & \text{for } 0 \leq t \leq T, \\ \tilde{n}(t - T) & \text{for } T \leq t \leq T + \tilde{T} \end{cases},$$

is another continuous curve satisfying (3.50).

The maximal solution $n_{\max} : [0, T_*) \to H^2(\mathbb{T}^d)$ is the uniquely determined curve that satisfies (3.50) on every subinterval $[0, T] \subset [0, T_*)$, but it cannot be extended to a solution on $[0, T_*]$. In view of our solution concept, this means that

1. *either* $T_* = +\infty$, i.e., the solution is global,
2. *or* $n_{\max}(t) \to n_*$ in $H^2(\mathbb{T}^d)$ as $t \uparrow T_*$, but the limiting profile n_* is *not* strictly positive,
3. *or* $n_{\max}(t)$ does not converge in $H^2(\mathbb{T}^d)$ as $t \uparrow T_*$.

We are going to exclude the last option. First notice that Proposition 3.20 guarantees that n is a classical and positive solution on every subinterval $(0, T] \subset (0, T_*)$, so $n_{\max} \in C^\infty((0, T_*); C^\infty(\mathbb{T}^d))$, as desired. This means that, in turn, the formal calculation (3.16) is rigorous. Combining this with the continuity of $n_{\max}(t)$ in $H^2(\mathbb{T}^d)$ at $t = 0$, it follows that $\mathcal{E}[n_{\max}(t)] \leq \mathcal{E}[n_0] < \infty$ is uniformly bounded on $[0, T_*)$. If $T_* < \infty$, then $n_{\max}$ satisfies hypothesis (2) of Lemma 3.18. Since $n_{\max}(t) = G(t) \star n_0 + \Psi[n_{\max}](t)$ by definition, it is a Hölder continuous curve with exponent $1/12$ in $H^2(\mathbb{T}^d)$ on, say, $[T_*/2, T_*)$ with a *uniform* Hölder constant L. This implies, in particular, that $n_{\max}(t)$ converges in $H^2(\mathbb{T}^d)$ to a limit n_*. □

3.7 From weak to classical solutions

In this brief last section, we prove Theorem 3.5 about the passage from energetic weak to classical solutions. In preparation of the proof of Theorem 3.5, we first show that any weak solution satisfies the very mild formulation (3.50), but in a weaker sense.

Lemma 3.21. *Any weak solution n in the sense of Theorem 3.1 is a Hölder continuous curve in $H^{-3}(\mathbb{T}^d)$, satisfying, for $t > 0$,*

$$n(t) = G(t) \star n_0 + \partial^3_{ijk} \int_0^t G(t - s) \star F_1^{(ijk)}(n(s))\,\mathrm{d}s + \partial^2_{ij} \int_0^t G(t - s) \star F_2^{(ij)}(n(s))\,\mathrm{d}s. \tag{3.66}$$

Proof. By our definition of a weak solution, n lies in $W^{1,4/3}_{\mathrm{loc}}(0, \infty; H^{-3}(\mathbb{T}^d))$. As a consequence, n is a Hölder continuous curve with exponent $1/3$ in $H^{-3}(\mathbb{T}^d)$ and, in particular, n is absolutely continuous in $H^{-3}(\mathbb{T}^d)$. Hence, its time derivative $\partial_t n(t)$ is defined in $H^{-3}(\mathbb{T}^d)$

for almost every $t > 0$. Moreover, $n \in L^{4/3}_{\mathrm{loc}}(0,\infty;H^3(\mathbb{T}^d))$, thus, $n(t) \in H^3(\mathbb{T}^d)$ for almost every $t > 0$ and $\Delta^3 n \in L^{4/3}_{\mathrm{loc}}(0,\infty;H^{-3}(\mathbb{T}^d))$. It follows that

$$g := \partial_t n - \Delta^3 n \in L^{4/3}_{\mathrm{loc}}(0,\infty;H^{-3}(\mathbb{T}^d)).$$

For fixed $t > 0$, consider the continuous curve $u : (0,t) \to C^\infty(\mathbb{T}^d)$, defined by $u(s) = G(t-s) \star n(s)$. Recalling (3.47), it follows for arbitrary $0 < s < t$ that

$$\begin{aligned} \partial_s u(s) &= -\Delta^3 G(t-s) \star n(s) + G(t-s) \star \partial_s n(s) \\ &= G(t-s) \star (\partial_s n(s) - \Delta^3 n(s)) = G(t-s) \star g(s). \end{aligned}$$

Therefore, $u \in W^{1,4/3}_{\mathrm{loc}}(0,\infty;H^{-3}(\mathbb{T}^d))$, and

$$\lim_{t'\uparrow t} u(t') = u(0) + \int_0^t G(t-s) \star g(s)\,\mathrm{d}s.$$

Since $u(0) = G(t) \star n_0$ and $u(t') \to n(t)$ in $H^{-3}(\mathbb{T}^d)$ as $t' \uparrow t$, formula (3.66) follows. □

Lemma 3.22. *Let n be the energetic weak solution to* (3.50)*. Then $F_1^{(ijk)}(n(t))$ is bounded in $L^{3/2}(\mathbb{T}^d)$ and $F_2^{(ij)}(n(t))$ is bounded in $L^1(\mathbb{T}^d)$, uniformly in (T_1,T_2).*

Proof. By the Hölder and the Sobolev inequalities and Lemma C.4, it follows that

$$\begin{aligned} \|F_1^{(ijk)}(n(t))\|_{L^{3/2}} &\le 4\|\nabla\sqrt{n(t)}\|_{L^6}\big(4\|\nabla\sqrt[4]{n(t)}\|_{L^4}^2 + 3\|\nabla^2\sqrt{n(t)}\|_{L^2}\big) \\ &\le 4C\|\sqrt{n(t)}\|_{H^2}(4C_{\mathrm{LV}}^2\|\sqrt{n(t)}\|_{H^2} + 3)\|\sqrt{n(t)}\|_{H^2}, \\ \|F_2^{(ij)}(n(t))\|_{L^1} &\le 8\big(\|\nabla^2\sqrt{n(t)}\|_{L^2} + 4\|\nabla\sqrt[4]{n(t)}\|_{L^4}^2\big)^2 \\ &\le 8\big(1 + 4C_{\mathrm{LV}}^2\|\sqrt{n(t)}\|_{H^2}\big)^2\|\sqrt{n(t)}\|_{H^2}^2. \end{aligned}$$

The last terms are uniformly controlled in terms of $\mathcal{E}[n(t)]$ which concludes the proof. □

In the following, let n be a weak solution satisfying the hypotheses of Theorem 3.5. Without loss of generality we may take $t_0 = 0$. Then $n_0 \in H^2(\mathbb{T}^d)$ and $\min n_0(x) > 0$. Since we are working with an energetic solution, it is a priori clear that $n(t)$ is bounded in $H^2(\mathbb{T}^d)$. Actually, more is true.

Lemma 3.23. *The energetic solution n is a Hölder continuous curve in $H^2(\mathbb{T}^d)$.*

Proof. Let $t > 0$ and $\tau > 0$ be fixed. Since $G(t-s) \in C^\infty(\mathbb{T}^d)$ and $f(n(s)) = \partial^3_{ijk}F_1^{(ijk)}(n(s)) + \partial^2_{ij}F_2^{(ij)}(n(s)) \in H^{-3}(\mathbb{T}^d)$ for all $s \in (0,t)$, we have $G(t-s) \star f(n(s)) \in C^\infty(\mathbb{T}^d)$. It follows that

$$\nabla^2 G(t-s) \star f(n(s)) = \nabla^2\partial^3_{ijk}G(t-s) \star F_1^{(ijk)}(n(s)) + \nabla^2\partial^2_{ij}G(t-s) \star F_2^{(ij)}(n(s)).$$

By Young's inequality, it follows further that

$$\begin{aligned}\|\nabla^2 G(t-s)\star f(n(s))\|_{L^2} &\le C\big(\|\nabla^5 G(t-s)\|_{L^{6/5}}\|F_1^{(ijk)}(n(s))\|_{L^{3/2}}\\ &\quad + \|\nabla^4 G(t-s)\|_{L^2}\|F_2^{(ij)}(n(s))\|_{L^1}\big)\\ &\le C\big((t-s)^{-(5+d/6)/6}+(t-s)^{-(4+d/2)/6}\big)\\ &\le C(t-s)^{-11/12},\end{aligned}$$

where $C>0$ is a generic constant and recalling that $d\le 3$. This implies that, for all $t\in(0,T)$ and $\tau>0$,

$$\left\|\nabla^2\int_t^{t+\tau} G(t+\tau-s)\star f(n(s))\,\mathrm{d}s\right\|_{L^2} \le C\big((t+\tau)^{1/12}-t^{1/12}\big)\le C\tau^{1/12}.$$

Similarly, we find that

$$\begin{aligned}&\big\|\nabla^2\big(G(t+\tau-s)-G(t-s)\star f(n(s))\big)\big\|_{L^2}\\ &\quad\le C\big(\big\|\nabla^5(G(t+\tau-s)-G(t-s))\|_{L^{6/5}}\|F_1^{(ijk)}(n(s))\|_{L^{3/2}}\\ &\qquad+\big\|\nabla^4\big(G(t+\tau-s)-G(t-s)\big)\|_{L^2}\|F_2^{(ij)}(n(s))\|_{L^1}\big).\end{aligned}$$

By relation (3.47), for $m=4,5$,

$$\begin{aligned}\big\|\nabla^m\big(G(t+\tau-s)-G(t-s)\big)\|_{L^p} &\le \left\|\nabla^m\int_{t-s}^{t+\tau-s}\frac{\mathrm{d}G}{\mathrm{d}\theta}G(\vartheta)\,\mathrm{d}\vartheta\right\|_{L^p}\\ &\le \int_{t-s}^{t+\tau-s}\|\nabla^m\Delta^3 G(\vartheta)\|_{L^p}\,\mathrm{d}\vartheta \le \Gamma\int_{t-s}^{t+\tau-s}\vartheta^{-1-(m+d(1-1/p))/6}\,\mathrm{d}\vartheta.\end{aligned}$$

As in the proof of Lemma 3.18, this proves the continuity with the Hölder exponent 1/12. □

The above results, together with Theorem 3.3, provide the proof of Theorem 3.5.

Chapter 4

Entropy stable and energy dissipative approximations of the fourth-order quantum diffusion equation

4.1 Introduction and results

This chapter is devoted to the study of several approximations of the fourth-order equation appearing as the second member in the local expansion of the quantum diffusion model,

$$\partial_t n + \operatorname{div}\left(n\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)\right) = 0\,. \tag{4.1}$$

It can be easily seen that for smooth positive solutions equation (4.1) admits a symmetric logarithmic form

$$\partial_t n + \frac{1}{2}\partial^2_{ij}(n\partial^2_{ij}\log n) = 0\,, \tag{4.2}$$

which is exactly the multidimensional form of the originally onedimensional Derrida-Lebowitz-Speer-Spohn (DLSS for short) equation [23]. Again we employed the summation convention over repeated indices. Throughout this chapter we assume that periodic boundary conditions are imposed and an initial data is given by a nonnegative measurable function n_0.

The existence theory for the DLSS equation was subject of many papers and it is by now resonably well understood. The very first result can be found in paper by Bleher et. al [7], in which they used classical semigroup approach to prove the existence and uniqueness of a local in time positive solution. In [36] Jüngel and Matthes proved the existence of global in time weak nonnegative solutions and observed their convergence to the homogeneous steady state. Results in there rely on entropy dissipation techniques and low-dimensional Sobolev embeddings. It has been shown that α-functionals, defined in (1.6) with $\Omega = \mathbb{T}^d$, are Lyapunov functionals for the DLSS equation for all $(\sqrt{d}-1)^2/(d+2) \leq \alpha \leq (\sqrt{d}+1)^2/(d+2)$. Moreover, if α lies strictly between these bounds, entropy production inequality

$$\frac{\mathrm{d}}{\mathrm{d}t}E_\alpha[n(t)] + \kappa_\alpha \int_{\mathbb{T}^d} \left(\Delta n^{\alpha/2}\right)^2 \mathrm{d}x \le 0 \tag{4.3}$$

holds, where $\kappa_\alpha > 0$ can be computed explicitly (see Lemma C.5). Gianazza et. al [30] were the first who explored the variational structure of the equation. They proved that equation (4.1) constitutes the gradient flow of the Fisher information

$$\mathcal{F}[n] = \int_\Omega |\nabla\sqrt{n}|^2 \mathrm{d}x$$

with respect to the L^2-Wasserstein metric. The variational derivative of the Fisher information equals $\delta\mathcal{F}[n]/\delta n = -\Delta\sqrt{n}/\sqrt{n}$ and equation (4.1) then — under appropriate boundary conditions — directly implies the dissipation of the Fisher information along its solutions,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[n(t)] + \int_\Omega n \left|\nabla\left(\frac{\delta\mathcal{F}[n]}{\delta n}\right)\right|^2 \mathrm{d}x = 0\,. \tag{4.4}$$

Estimates (4.3) and (4.4) play a crucial role in the analysis of the DLSS equation. As we already pointed out in the introduction chapter, such inequalities are essential for the existence theory, long time behaviour of solutions and other qualitative properties of solutions. Furthermore, estimate (4.3) for $\alpha = 1$ and (4.4) have a physical meaning of the entropy and the energy dissipation, respectively. It is therefore a desirable and challenging task to propose (semi-)discrete approximations and eventually develop numerical schemes, which preserve these structural properties on a (semi-)discrete level. Several numerical schemes have been proposed in the literature to solve equation (4.1) or (4.2). Most of them are based on finite differences in one space dimension and preserve positivity of solutions [13, 38]. Instead of a direct approximation of the equation itself, a novel approach has been introduced recently in [24]. It employs the variational structure of equation (4.1) on a fully discrete level and respective numerical solutions are obtained by introducing the discrete minimizing movement scheme. This approach directly implies global decay of the discrete Fisher information and nonnegativity of solutions.

If we replace the time derivative by the backward difference formula and discretize equation (4.2) by the standard implicit Euler scheme,

$$\frac{1}{\tau}(n_{k+1} - n_k) + \frac{1}{2}\partial^2_{ij}(n_{k+1}\partial^2_{ij}\log n_{k+1}) = 0\,, \quad k \ge 0\,, \tag{4.5}$$

where $\tau > 0$ is the time step and n_k approximates $n(t_k, \cdot)$ with $t_k = \tau k$, then an entropy dissipation on the time discrete level holds ([36, Lemma 4.1]),

$$E_\alpha[n_{k+1}] + \tau\kappa_\alpha \int_{\mathbb{T}^d} \left(\Delta n_{k+1}^{\alpha/2}\right)^2 \mathrm{d}x \le E_\alpha[n_k] \quad \text{for all } k \ge 0\,. \tag{4.6}$$

This is the key estimate for the existence result in [36], and moreover, it says that the implicit Euler scheme *dissipates the entropy* i.e. *it preserves the entropy dissipation structure* on the time discrete level. Since the Euler scheme (4.5) is only of the first order in time, our aim is to consider possibly higher-order schemes, which are entropy dissipative or at least entropy stable, i.e. $E_\alpha[n_k] \le C$ for all $k \ge 1$ with $C > 0$ independent of k. There are numerous numerical schemes developed for ordinary differential equations which exhibit higher-order accuracy and all of them could formally be incorporated for our DLSS equation. However, due to complexity of the nonlinear term, we will restrict our attention to the well-known multi-step backward difference methods. An even more important feature of these methods are remarkable stability properties (up to order 6) for stiff systems, which also include parabolic equations.

For a given ordinary differential equation

$$y'(t) = f(t, y)\,,$$

the q-step backward difference method takes the form

$$\sum_{j=0}^{q} \beta_j y_{k+1-j} = \tau f(t_{k+1}, y_{k+1})\,, \quad k \ge q-1\,,$$

where coefficients β_j are uniquely determined by interpolating points (t_{k+1-q}, y_{k+1-q}), ..., (t_{k+1}, y_{k+1}) with the q-th degree Lagrange interpolation polynomial L_y and requiring the collocation condition $L'_y(t_{k+1}) = f(t_{k+1}, y_{k+1})$. Table 4.1 below brings coefficients of the first three BDF-q schemes, in particular those which will be considered here. Using any

	β_0	β_1	β_2	β_3
BDF-1	1	-1	–	–
BDF-2	3/2	-2	1/2	–
BDF-3	11/6	-3	3/2	1/3

Table 4.1: Coefficients in backward differentiation methods.

q-step method, the first $q-1$ values must be initialized somehow; usually, by a one-step or some other methods, but keeping in mind the desired accuracy of the method in total.

In order to prove the existence result for the two-step backward difference method, we employ yet another form of the DLSS equation, so-called *α-entropic* form

$$\frac{2}{\alpha} n^{1-\alpha/2} \partial_t (n^{\alpha/2}) + \frac{1}{2} \partial^2_{ij} (n \partial^2_{ij} \log n) = 0\,, \tag{4.7}$$

which has been already introduced in [41]. From practical reasons $\alpha \ge 1$ belongs to the range of real parameters determining Lyapunov functionals E_α to the equation. Note that equation (4.7) is for smooth and positive solutions equivalent to the orginal equation. Further details in favor to the new form are discussed in Section 4.2. We will analyze its BDF-2 time approximation

$$\frac{2}{\alpha\tau} v_{k+1}^{2/\alpha-1} \Big(\frac{3}{2} v_{k+1} - 2 v_k + \frac{1}{2} v_{k-1} \Big) + \frac{1}{2} \partial^2_{ij} (n_{k+1} \partial^2_{ij} \log n_{k+1}) = 0 \quad \text{in } \mathbb{T}^d\,,\ k \ge 1\,, \tag{4.8}$$

where $v_k = n_k^{\alpha/2}$. Assume that $v_0 = n_0^{\alpha/2}$ is given initial datum and v_1 is constructed from v_0 by the implicit Euler scheme

$$\frac{2}{\alpha\tau} v_1^{2/\alpha-1}\big(v_1 - v_0\big) + \frac{1}{2}\partial_{ij}^2(n_1\partial_{ij}^2 \log n_1) = 0 \quad \text{in } \mathbb{T}^d . \tag{4.9}$$

Using additional change of variables $n = e^y$ and employing the standard ε-regularization strategy as in [36] and in Section 3.4, a sequence of strictly positive approximative solutions is constructed by use of the Leray-Schauder fixed point theorem. In particular, the integral inequality related to the BDF-2 scheme (for $\alpha > 1$),

$$\begin{aligned}\frac{3}{2\alpha(\alpha-1)}\int_{\mathbb{T}^d} v_{k+1}^2 \mathrm{d}x + \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}(v_{k+1}-v_k)^2\mathrm{d}x + \kappa_\alpha\tau\int_{\mathbb{T}^d}(\Delta v_{k+1})^2\mathrm{d}x \\ \le \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\Big(2v_k^2 - \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x + \int_{\mathbb{T}^d}(v_k - v_{k-1})^2\mathrm{d}x\,, \quad k \ge 1\,,\end{aligned}$$

provides the required a priori bounds and compactness arguments to perform the deregularization limit $\varepsilon \downarrow 0$. That gives us the existence of weak nonnegative solutions to (4.8). If we fix $\alpha = 1$ and assume in addition that our weak solutions remain strictly positive and bounded from below with a positve constant, then such solutions are smooth and we can prove the second-order convergence of the scheme.

The following two theorems summarize our main results for the two-step backward difference method.

Theorem 4.1 (Existence of semi-discrete solutions). *Let $1 \le \alpha < (\sqrt{d}+1)^2/(d+2)$ and let $n_0 \in L^1(\mathbb{T}^d)$ be nonnegative measurable function such that $E_\alpha[n_0] < \infty$. Let $v_1 = n_1^{\alpha/2}$ be a weak solution of the implicit Euler scheme (4.9). Then there exists a sequence $(v_k) = (n_k^{\alpha/2})$ of weak nonnegative solutions to (4.8) satisfying*

$$v_k \ge 0 \ \textit{a.e.}, \quad v_k \in H^2(\mathbb{T}^d)$$

and for all $\phi \in W^{2,\infty}(\mathbb{T}^d)$

$$\begin{aligned}\frac{1}{\alpha\tau}\int_{\mathbb{T}^d} v_{k+1}^{2/\alpha-1}\Big(\frac{3}{2}v_{k+1} - 2v_k + \frac{1}{2}v_{k-1}\Big)\phi\mathrm{d}x \\ + \int_{\mathbb{T}^d}\Big(\frac{1}{2\alpha}v_{k+1}^{2/\alpha-1}\partial_{ij}^2 v_{k+1} - \frac{\alpha}{2}\partial_i(v_{k+1}^{1/\alpha})\partial_j(v_{k+1}^{1/\alpha})\Big)\partial_{ij}^2\phi\mathrm{d}x = 0.\end{aligned} \tag{4.10}$$

If $\alpha > 1$, the scheme (4.8) is entropy stable and moreover, the a priori estimate

$$E_\alpha[n_m] + \kappa_\alpha\tau\sum_{k=1}^{m}\int_{\mathbb{T}^d}\big(\Delta(n_k^{\alpha/2})\big)^2\mathrm{d}x \le E_\alpha[n_0]\,, \quad m \ge 1\,, \tag{4.11}$$

holds.

Remarks.

(i) If n is a positive solution to the DLSS equation, then Lemma C.5 (Appendix C) yields an H^2-bound on $v = n^{\alpha/2}$ for the given range of α's. This motivates to rewrite the nonlinear term into formally equivalent forms:

$$\frac{1}{2} n \partial_{ij}^2 \log n = \frac{1}{\alpha} n^{1-\alpha/2} \partial_{ij}^2 (n^{\alpha/2}) - \alpha \partial_i \sqrt{n} \partial_j \sqrt{n} = \frac{1}{\alpha} v^{2/\alpha - 1} \partial_{ij}^2 v - \alpha \partial_i (v^{1/\alpha}) \partial_j (v^{1/\alpha}) , \tag{4.12}$$

which are then used to obtain weak solutions.

(ii) Existence of weak solution $v_1 = n_1^{\alpha/2}$ to the implicit Euler scheme (4.9) follows the same steps as in [36, Section 4.1] and moreover, the discrete entropy dissipation $E_\alpha[n_1] \leq E_\alpha[n_0]$ holds. Construction of v_1 can also be recovered from the procedure of constructing v_k, $k \geq 2$ in the BDF-2 scheme. Therefore, we omit this step here.

(iii) Due to restrictions of Sobolev embeddings in higher-dimensions, Theorem 4.1 is valid only in phisically relevant space dimensions $1 \leq d \leq 3$.

Theorem 4.2 (Second-order convergence)**.** *Let the assumptions of Theorem 4.1 hold, let $\alpha = 1$ and (v_k) sequance of smooth positive solutions to* (4.8)*, with v_1 being solution to* (4.9)*. Let n be smooth and positive solution to equation* (4.2)*, such that $(\sqrt{n})_{ttt} \in L^2(\mathbb{T}^d \times (0,T))$ and $(\sqrt{n})_{tt} \in L^\infty(\mathbb{T}^d \times (0,T))$. Then for $k \geq 2$*

$$\|v_k - \sqrt{n(t_k)}\|_{L^2(\mathbb{T}^d)} \leq C\tau^2 ,$$

where $C > 0$ does not depend on τ.

Unlike the semi-discrete BDF-2 method, which approximates equation (4.7) and paves the attention on the stability of entropies, the following fully discrete finite difference type method approximates the original equation equation (4.1) and preserves its energy dissipation property (4.4) on a discrete time-space grid. For the ease of presentation we restrict our consideration to the spatially onedimensional case. Let $\mathbb{T}_N = \{x_0, \ldots, x_N\}$ denote an equidistant grid on $\mathbb{T}$ consisiting of N points, such that $0 = x_0 \simeq x_{N+1} = 1$ and let $U_i^k \approx n(t_k, x_i)$. According to [29], the key idea for this method is to define a discrete version of the Fisher information (energy) $\mathcal{F}_\mathrm{d}$ and to derive the discrete variational derivative $\delta\mathcal{F}_\mathrm{d}/\delta(U^{k+1}, U^k)$ so that the discrete chain rule holds,

$$\mathcal{F}_\mathrm{d}[U^{k+1}] - \mathcal{F}_\mathrm{d}[U^k] = \sum_{i=0}^{N-1} \frac{\delta\mathcal{F}_\mathrm{d}}{\delta(U^{k+1}, U^k)_i} (U_i^{k+1} - U_i^k) h . \tag{4.13}$$

Discrete variational derivative method is then defined by a sparsely coupled system of nonlinear equations

$$\frac{1}{\tau}(U_i^{k+1} - U_i^k) = \delta_i^{\langle 1 \rangle} \left(U_i^{k+1} \delta_i^{\langle 1 \rangle} \left(\frac{\delta\mathcal{F}_\mathrm{d}}{\delta(U^{k+1}, U^k)_i} \right) \right) , \quad i = 0, \ldots, N-1 , \; k \geq 0 , \tag{4.14}$$

where $\delta_i^{\langle 1\rangle}$ denotes the central difference approximation of the derivative at points $x_i \in \mathbb{T}_N$. In particular, the following choice of discrete Fisher information

$$\mathcal{F}_{\mathrm{d}}[U] = \frac{1}{2}\sum_{i=0}^{N-1}\big((\delta_i^+ V_i)^2 + (\delta_i^- V_i)^2\big)h\,,$$

yields, according to (4.13) and periodic boundary conditions,

$$\frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1},U^k)_i} = -\frac{\delta_i^{\langle 2\rangle}(V_i^{k+1}+V_i^k)}{V_i^{k+1}+V_i^k}\,,\quad i=0,\ldots,N-1\,,\ k\geq 0.$$

Obviously by construction (assuming the existence of nonnegative solutions), numerical scheme (4.14), like its continuous version (4.1), directly implies the discrete dissipation property analogous to (4.4),

$$\frac{1}{\tau}\big(\mathcal{F}_{\mathrm{d}}[U^{k+1}] - \mathcal{F}_{\mathrm{d}}[U^k]\big) + \sum_{i=0}^{N-1} U_i^{k+1}\left(\delta_i^{\langle 1\rangle}\left(\frac{\delta\mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1},U^k)_i}\right)\right)^2 h = 0\,.$$

Main properties of the scheme are given by

Theorem 4.3. *Numerical scheme* (4.14) *is consistent of order* $(1,2)$ *with respect to the time-space discretization, i.e. the local discretization error is of order* $O(\tau,h^2)$*. Let* $N\in\mathbb{N}$ *and* $U^0\in\mathbb{R}^N$*,* $U_i^0\geq 0$ *for all* $i=0,\ldots,N-1$*, such that* $\sum_{i=0}^{N-1}U_i^0 h = 1$ *and* $\mathcal{F}_{\mathrm{d}}[U^0]<\infty$*. Let* $(U^k)\subset(\mathbb{R}^N)^{\mathbb{N}}$ *be sequence of solutions to scheme* (4.14)*. Then* $(U^k)\in l^\infty(\mathbb{R}^N)$*,* $\sum_{i=0}^{N-1}U_i^k h = 1$ *for all* $k\geq 1$ *and the discrete Fisher information is monotonically decreasing,* $\mathcal{F}_{\mathrm{d}}[U^{k+1}]\leq\mathcal{F}_{\mathrm{d}}[U^k]$ *for all* $k\geq 0$*.*

Generalization of the method on the d-dimensional torus $\mathbb{T}^d$ is straightforward if we assume rectangular grids. Further adaptation of the idea to the Galerkin framework in case of nonrectangular grids is also possible, but we don't open this subject here. We do, however, try to increase the temporal accuracy of the method. This is subjet of Section 4.3.2. Finally, to conclude this chapter, in Section 4.4 we give a few numerical illustrations, which show in favor of the aforementiond numerical schemes.

4.2 Two-step backward difference (BDF-2) time approximation

Before we start with the BDF-2 method, let us briefly recall the implicit Euler and the dissipation structure therein. Multiplying equation (4.5) by the test function $\tau\phi'_\alpha(n_{k+1})$, where $\phi_\alpha(s) = s^\alpha/(\alpha(\alpha-1))$, $\alpha\neq 1$, and $\phi_1(s) = s(\log s - 1)+1$ and integrating over $\mathbb{T}^d$, integration by parts formulae yield

$$\int_{\mathbb{T}^d}(n_{k+1}-n_k)\phi'_\alpha(n_{k+1})\mathrm{d}x + \frac{\tau}{2}\int_{\mathbb{T}^d} n_{k+1}\partial_{ij}^2\log n_{k+1}\partial_{ij}^2\phi'_\alpha(n_{k+1})\mathrm{d}x = 0\,.$$

Convexity of function ϕ_α gives the control from below on the first term

$$\int_{\mathbb{T}^d} (n_{k+1} - n_k)\phi'_\alpha(n_{k+1})\mathrm{d}x \geq \int_{\mathbb{T}^d} \phi_\alpha(n_{k+1})\mathrm{d}x - \int_{\mathbb{T}^d} \phi_\alpha(n_k)\mathrm{d}x \,,$$

while Lemma C.5 gives

$$\frac{\tau}{2}\int_{\mathbb{T}^d} n_{k+1}\partial^2_{ij}\log n_{k+1}\partial^2_{ij}\phi'_\alpha(n_{k+1})\mathrm{d}x \geq \tau\kappa_\alpha \int_{\mathbb{T}^d} \left(\Delta n_{k+1}^{\alpha/2}\right)^2\mathrm{d}x.$$

The last two inequalities now obviously imply the time discrete dissipation property (4.6). Of course, the above arguments are only formal and work in general for smooth positive solutions, but everything can be justyfied also in an appropriate setting of weak solutions as precisely described in [36].

Now discretizing equation (4.2) by the two-step backward difference formula (BDF-2) in time we get a sequence of equations for time approximated solutions n_k:

$$\frac{1}{\tau}\Big(\frac{3}{2}n_{k+1} - 2n_k + \frac{1}{2}n_{k-1}\Big) + \frac{1}{2}\partial^2_{ij}(n_{k+1}\partial^2_{ij}\log n_{k+1}) = 0 \quad \text{in } \mathbb{T}^d,\ k \geq 1\,. \tag{4.15}$$

Following the idea presented for the implicit Euler — multiply equation (4.15) by the test function $\tau\phi'_\alpha(n_{k+1})$ and integrate over $\mathbb{T}^d$ — convexity of function ϕ_α this time gives

$$\begin{aligned}\int_{\mathbb{T}^d}\Big(\frac{3}{2}n_{k+1} - 2n_k + \frac{1}{2}n_{k-1}\Big)\phi'_\alpha(n_{k+1})\mathrm{d}x \geq \frac{3}{2}\int_{\mathbb{T}^d}\phi_\alpha(n_{k+1})\mathrm{d}x - 2\int_{\mathbb{T}^d}\phi_\alpha(n_k)\mathrm{d}x \\ +\frac{1}{2}\int_{\mathbb{T}^d}\phi_\alpha(n_{k-1})\mathrm{d}x + \int_{\mathbb{T}^d}\frac{\phi''_\alpha(\bar{n})}{2}(n_{k-1} - n_k)(n_{k+1} - n_{k-1})\mathrm{d}x,\end{aligned}$$

where $\bar{n}$ comes from the Lagrange mean value theorem for ϕ'_α. Since the last term on the right hand side is a priori indefinite, we cannot conclude the "BDF-2 dissipation" of the entropy analogous to the implicit Euler case (4.6). Due to the lack of convexity argument, we are forced to reformulate the original equation (4.2) in a form which is more appropriate for algebraic manipulations and in fact appreciates the G-stability (see Definition 4.4 below) of the BDF-2 method. This motivates the α*–entropic* form (4.7) and its BDF-2 approximation (4.8) is eventually analyzed throughout this section.

Definition 4.4. A q-step method is G-stable if and only if there exists a positive definite matrix G, such that

$$\|\mathbf{v}_{k+1} - \mathbf{w}_{k+1}\|_G \leq \|\mathbf{v}_k - \mathbf{w}_k\|_G \quad \text{for all} \ \ k \geq q-1\,,$$

where $\mathbf{v}_{k+1} = (v_{k+1}, v_k, \ldots, v_{k-q+2})$ and $\mathbf{w}_{k+1} = (w_{k+1}, v_k, \ldots, w_{k-q+2})$ are two solutions of the method with initial values $\mathbf{v}_{q-1}$ and $\mathbf{w}_{q-1}$, respectively, and the norm is defined by $\|\mathbf{v}\|^2_G = \mathbf{v}^T G\mathbf{v}$.

It can be proved that $\|\cdot\|_G$ is a Lyapunov functional for the method (see [19]).

The following algebraic inequalities imply the G-stability of the BDF-2 method and are essential for our existence proof, the entropy stability property and the convergence result.

Lemma 4.5. *For all $a, b, c \in \mathbb{R}$ it holds*

$$2\Big(\frac{3}{2}a - 2b + \frac{1}{2}c\Big)a \geq \frac{3}{2}a^2 - 2b^2 + \frac{1}{2}c^2 + (a-b)^2 - (b-c)^2\,, \tag{4.16}$$

$$2\Big(\frac{3}{2}a - 2b + \frac{1}{2}c\Big)a \geq \frac{1}{2}\big(a^2 + (2a-b)^2 - b^2 - (2b-c)^2\big)\,. \tag{4.17}$$

Proofs are easily obtained by elementary algebraic identities.

Let us comment at this point that we were not able to obtain similar inequalities for the BDF-q methods when $q \geq 3$. Hence, no entropy stability neither improved convergence results could be achieved with this approach. The reason for that might be the fact that the only G-stable BDF methods are the implicit Euler (BDF-1) and the BDF-2 (see [20]).

4.2.1 Existence of solutions, entropy stability – proof of Theorem 4.1

In the following part we provide the proof of Theorem 4.1, which is devided into several steps. Concept of the proof is, first to regularize the scheme by adding an ε-elliptic term, which asserts the existence of a strictly positive solution in the sense of the Leray-Schauder fixed point theorem. Then, based on an a priori estimate, which we derive below, and continuity and compactness of Sobolev embeddings, we are able to perform the limit $\varepsilon \downarrow 0$ and finally obtain the existance of weak nonnegative solution in the sense of (4.10).

Proof of Theorem 4.1. Regularized problem. Writing $n = e^y = v^{2/\alpha}$, equation (4.7) becomes

$$\frac{2}{\alpha} e^{(1-\alpha/2)y}\partial_t v + \frac{1}{2}\partial^2_{ij}(e^y \partial^2_{ij} y) = 0.$$

For the sake of brevity, let us denote $y_{k+1} \approx y(t_{k+1}, \cdot)$ simply by y, hence $v_{k+1} = e^{\alpha y/2}$. Also, assume we have solved first $k \geq 1$ equations, i.e. values v_0, $v_1, \ldots, v_k$ are known and the last $k-1$ values are solutions to (4.10) in the sense of Theorem 4.1. We discretize the above equation by the BDF-2 method and regularize it by adding a strongly elliptic operator

$$\frac{2}{\alpha\tau} e^{(1-\alpha/2)y}\Big(\frac{3}{2}e^{\alpha y/2} - 2v_k + \frac{1}{2}v_{k-1}\Big) + \frac{1}{2}\partial^2_{ij}(e^y\partial^2_{ij}y) + \varepsilon L_\alpha(y) = 0, \quad k \geq 1,\ \varepsilon > 0\,, \tag{4.18}$$

where

$$L_\alpha(y) = \Delta(e^{-(\alpha-1)y}\Delta y) - (\alpha-1)\,\mathrm{div}(e^{-(\alpha-1)y}|\nabla y|^2\nabla y) + e^{-(\alpha-1)y}y, \quad \alpha \geq 1.$$

Solution of the regularized problem – fixed point operator. Let $\varepsilon > 0$ be given, we want to find weak solution for equation (4.18) by means of the Lerray-Schauder fixed-point theorem (Theorem C.7). Let $\sigma \in [0,1]$ and $z \in X$, where

$$X = \{z \in H^2(\mathbb{T}^d)\ :\ \|z\|_{W^{1,4}} \leq M\} \subset W^{1,4}(\mathbb{T}^d),$$

for a given constant $M > 0$ that will be specified later. X is closed and convex subset of $W^{1,4}(\mathbb{T}^d)$. For $y, \phi \in H^2(\mathbb{T}^d)$ define bilinear form and linear functional on $H^2(\mathbb{T}^d)$:

$$\begin{aligned} a_\alpha(y,\phi) &= \frac{\sigma}{2}\int_{\mathbb{T}^d} e^z \partial^2_{ij} y \partial^2_{ij}\phi \mathrm{d}x + \varepsilon \int_{\mathbb{T}^d} e^{-(\alpha-1)z}(\Delta y \Delta\phi + (\alpha-1)|\nabla z|^2 \nabla y\cdot\nabla\phi + y\phi)\mathrm{d}x\,, \\ f_\alpha(\phi) &= \frac{2\sigma}{\alpha\tau}\int_{\mathbb{T}^d} e^{(1-\alpha/2)z}\Big(\frac{3}{2}e^{\alpha z/2} - 2v_k + \frac{1}{2}v_{k-1}\Big)\phi \mathrm{d}x\,. \end{aligned}$$

Since $W^{1,4}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ in space dimensions $d \le 3$, it follows $\|z\|_{L^\infty} \le C\|z\|_{W^{1,4}} \le CM$ and $e^{-(\alpha-1)z} \ge e^{-(\alpha-1)\|z\|_{L^\infty}} \ge e^{-(\alpha-1)CM} =: \mu$. Therefore is a_α continuous and coercive

$$a_\alpha(y,y) \ge \varepsilon c_\alpha \int_{\mathbb{T}^d}\big((\Delta y)^2 + y^2\big)\mathrm{d}x \ge C_\alpha \varepsilon \|y\|^2_{H^2}\,,$$

with $c_\alpha = \mu$ for $\alpha > 1$ and $c_\alpha = 1$ if $\alpha = 1$. Continuous embedding $W^{1,4}(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$ also yields continuity of the linear functional f_α. Consequently, Lax-Milgram's lemma asserts the existence of a unique solution $y \in H^2(\mathbb{T}^d)$ to the problem

$$a_\alpha(y,\phi) = -f_\alpha(\phi) \quad \text{for all } \phi \in H^2(\mathbb{T}^d)\,.$$

Now define the fixed-point operator $S_\varepsilon : X \times [0,1] \to W^{1,4}(\mathbb{T}^d)$ by $S_\varepsilon(z,\sigma) := y$. The solution depends H^2-continously on $z \in X$. Particularly, $y = 0$ if $\sigma = 0$ and $S_\varepsilon(y,1) = y$ is equivalent to (4.18). Due to compactness of embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$, operator S_ε is also compact.

A priori bound. It remains to obtain a uniform bound for all fixed points of $S_\varepsilon(\cdot,\sigma)$. First consider the case $\alpha > 1$. Let $y \in H^2(\mathbb{T}^d)$ be a fixed point of $S_\varepsilon(\cdot,\sigma)$ for some $\sigma \in [0,1]$. Take the test function $\phi = \big(e^{(\alpha-1)y} - 1\big)/(\alpha-1) \in H^2(\mathbb{T}^d)$, then $\Delta\phi = e^{(\alpha-1)y}\big(\Delta y + (\alpha-1)|\nabla y|^2\big)$, $\nabla\phi = e^{(\alpha-1)y}\nabla y$ and the weak form of (4.18) reads as

$$\begin{aligned} \frac{2\sigma}{\alpha(\alpha-1)\tau}&\int_{\mathbb{T}^d} e^{(1-\alpha/2)y}\Big(\frac{3}{2}e^{\alpha y/2} - 2v_k + \frac{1}{2}v_{k-1}\Big)\big(e^{(\alpha-1)y} - 1\big)\mathrm{d}x \\ &+ \frac{\sigma}{2(\alpha-1)}\int_{\mathbb{T}^d} e^y \partial^2_{ij} y \partial^2_{ij}(e^{(\alpha-1)y})\mathrm{d}x \\ &+ \varepsilon\int_{\mathbb{T}^d}\big((\Delta y)^2 + (\alpha-1)(\Delta y|\nabla y|^2 + |\nabla y|^4)\big)\mathrm{d}x \\ &+ \frac{\varepsilon}{\alpha-1}\int_{\mathbb{T}^d} y(1 - e^{-(\alpha-1)y})\mathrm{d}x = 0\,. \end{aligned} \tag{4.19}$$

Using algebraic inequality (4.16), and Young's inequality, the first term in the above weak form can be controled from below

$$\begin{aligned}
&\frac{2\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\Big(\frac{3}{2}e^{\alpha y/2}-2v_k+\frac{1}{2}v_{k-1}\Big)\big(e^{\alpha y/2}-e^{(1-\alpha/2)y}\big)\mathrm{d}x\\
&\qquad\geq\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\Big(\frac{3}{2}e^{\alpha y}-2v_k^2+\frac{1}{2}v_{k-1}^2-(v_k-v_{k-1})^2\Big)\mathrm{d}x\\
&\qquad\quad-\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\Big(3e^{y}+\frac{1}{2}v_{k-1}^2+\frac{1}{2}e^{(2-\alpha)y}\Big)\mathrm{d}x\\
&\qquad=\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\Big(\frac{3}{2}e^{\alpha y}-3e^{y}-\frac{1}{2}e^{(2-\alpha)y}\Big)\mathrm{d}x\\
&\qquad\quad-\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\big(2v_k^2+(v_k-v_{k-1})^2\big)\mathrm{d}x\,.
\end{aligned}$$

Since term $(\alpha(\alpha-1))^{-1}\big(e^{\alpha y}/2-3e^{y}-e^{(2-\alpha)y}/2\big)\geq -c_\alpha$, for some $c_\alpha>0$, is bounded from below uniformly in y, application of the Young's inequality in further yields

$$\begin{aligned}
&\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\Big(\frac{3}{2}e^{\alpha y}-3e^{y}-\frac{1}{2}e^{(2-\alpha)y}\Big)\mathrm{d}x-\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\big(2v_k^2+(v_k-v_{k-1})^2\big)\mathrm{d}x\\
&\qquad\geq\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}e^{\alpha y}\mathrm{d}x-\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}(4v_k^2+2v_{k-1}^2)\mathrm{d}x-\frac{\sigma}{\tau}c_\alpha\,.
\end{aligned}\tag{4.20}$$

The second term in (4.19) is bounded from below by inequality (C.7),

$$\frac{\sigma}{2(\alpha-1)}\int_{\mathbb{T}^d}e^{y}\partial_{ij}^2 y\,\partial_{ij}^2(e^{(\alpha-1)y})\mathrm{d}x\geq\sigma\kappa_\alpha\int_{\mathbb{T}^d}\big(\Delta e^{\alpha y/2}\big)^2\mathrm{d}x\,,\tag{4.21}$$

with $\kappa_\alpha>0$ explicitly computed (C.9). Also the regularizing terms can be easily estimated. First, by the Cauchy-Schwartz inequality we find

$$\varepsilon\int_{\mathbb{T}^d}\big((\Delta y)^2+(\alpha-1)(\Delta y|\nabla y|^2+|\nabla y|^4)\big)\mathrm{d}x\geq\varepsilon\int_{\mathbb{T}^d}\Big(\frac{3-\alpha}{2}(\Delta y)^2+\frac{\alpha-1}{2}|\nabla y|^4\Big)\mathrm{d}x\,,\tag{4.22}$$

and an elementary calculus showes

$$\frac{\varepsilon}{\alpha-1}\int_{\mathbb{T}^d}y(1-e^{-(\alpha-1)y})\mathrm{d}x\geq\frac{\sigma\varepsilon}{\alpha-1}\int_{\mathbb{T}^d}|y|\mathrm{d}x-\frac{\sigma\varepsilon}{(\alpha-1)^2}\,.\tag{4.23}$$

Now summing up the obtained inequalities (4.20)–(4.23) gives us an a priory bound:

$$\begin{aligned}
&\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}e^{\alpha y}\mathrm{d}x+\sigma\kappa_\alpha\int_{\mathbb{T}^d}\big(\Delta e^{\alpha y/2}\big)^2\mathrm{d}x\\
&\qquad+\varepsilon\int_{\mathbb{T}^d}\Big(\frac{3-\alpha}{2}(\Delta y)^2+\frac{\alpha-1}{2}|\nabla y|^4\Big)\mathrm{d}x+\frac{\sigma\varepsilon}{\alpha-1}\int_{\mathbb{T}^d}|y|\mathrm{d}x\\
&\qquad\leq\frac{\sigma}{\alpha(\alpha-1)\tau}\int_{\mathbb{T}^d}\big(4v_k^2+2v_{k-1}^2\big)\mathrm{d}x+\frac{\sigma}{\tau}c_\alpha+\frac{\sigma\varepsilon}{(\alpha-1)^2}\,.
\end{aligned}$$

Hence, we proved

$$E_\alpha[n] + \tau\kappa_\alpha \int_{\mathbb{T}^d} \big(\Delta e^{\alpha y/2}\big)^2 \mathrm{d}x + \frac{\tau\varepsilon}{\sigma}\int_{\mathbb{T}^d}\Big(\frac{3-\alpha}{2}(\Delta y)^2 + \frac{\alpha-1}{2}|\nabla y|^4\Big)\mathrm{d}x \\ + \frac{\tau\varepsilon}{\alpha-1}\int_{\mathbb{T}^d}|y|\mathrm{d}x \le 4E_\alpha[n_k] + 2E_\alpha[n_{k-1}] + c_\alpha + \frac{\tau\varepsilon}{(\alpha-1)^2}\,. \tag{4.24}$$

This inequality together with the Poincaré inequality implies that y is uniformly bounded in $H^2(\mathbb{T}^d)$,

$$\|y\|_{H^2}^2 \le C\int_{\mathbb{T}^d}\big((\Delta y)^2 + y^2\big)\mathrm{d}x \le C_\alpha\,,$$

where constant $C_\alpha = C(\alpha, v_k, v_{k-1}, \varepsilon, \tau) > 0$ does not depend on σ. Continuity of the embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$ then yields uniform (σ-independent) bound on y in $W^{1,4}(\mathbb{T}^d)$,

$$\|y\|_{W^{1,4}} \le C_\alpha\,, \tag{4.25}$$

where $C_\alpha > 0$ may now change. Taking $M \ge C_\alpha$, we have obtained a uniform bound on the set of all potential fixed points of $S_\varepsilon(\cdot,\sigma)$. Leray-Schauder fixed-point theorem then provides existence of a solution y_ε to $S_\varepsilon(y,1) = y$.

Next, we consider the case $\alpha = 1$. Again, let $y \in H^2(\mathbb{T}^d)$ be a fixed point of $S_\varepsilon(\cdot,\sigma)$ for some $\sigma \in [0,1]$. In this case take the test function $\phi = y$, since the formal pointwise limit

$$\lim_{\alpha\searrow 1}\frac{1}{\alpha-1}\big(e^{(\alpha-1)y} - 1\big) = y\,.$$

Then we get from the weak form

$$\frac{2\sigma}{\tau}\int_{\mathbb{T}^d} e^{y/2}\Big(\frac{3}{2}e^{y/2} - 2v_k + \frac{1}{2}v_{k-1}\Big)y\mathrm{d}x \\ + \frac{\sigma}{2}\int_{\mathbb{T}^d} e^y(\partial_{ij}^2 y)^2\mathrm{d}x + \varepsilon\int_{\mathbb{T}^d}\big((\Delta y)^2 + y^2\big)\mathrm{d}x = 0\,. \tag{4.26}$$

In order to estimate the first term in the weak form, we separate the domain of integration into two parts $\{y<0\}$ and $\{y\ge 0\}$ and apply Young's inequality:

$$\begin{aligned}\frac{2\sigma}{\tau}\int_{\mathbb{T}^d} e^{y/2}\Big(\frac{3}{2}e^{y/2} - 2v_k + \frac{1}{2}v_{k-1}\Big)y\mathrm{d}x &= \frac{\sigma}{\tau}\int_{\{y<0\}}\big(3e^y y - 4e^{y/2}v_k y + e^{y/2}v_{k-1}y\big)\mathrm{d}x \\ &\quad + \frac{\sigma}{\tau}\int_{\{y\ge 0\}}\big(3e^y y - 4e^{y/2}v_k y + e^{y/2}v_{k-1}y\big)\mathrm{d}x \\ &\ge \frac{\sigma}{\tau}\int_{\{y<0\}}\Big(3e^y y - \frac{5}{2}e^y y^2 - 2v_k^2 - \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x \\ &\quad + \frac{\sigma}{\tau}\int_{\{y\ge 0\}}\Big(3e^y y - \frac{5}{2}e^y - \frac{5}{4}y^4 - v_k^4 - \frac{1}{4}v_{k-1}^4\Big)\mathrm{d}x\,.\end{aligned}$$

Thus,

$$\begin{aligned}\frac{2\sigma}{\tau}\int_{\mathbb{T}^d} e^{y/2}\Big(\frac{3}{2}e^{y/2} - 2v_k + \frac{1}{2}v_{k-1}\Big)y\mathrm{d}x \\ \geq \frac{\sigma}{\tau}\int_{\{y<0\}}\Big(e^y(y-1) + \Big(1+2y-\frac{5}{2}y^2\Big)e^y - 2v_k^2 - \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x \\ + \frac{\sigma}{\tau}\int_{\{y\geq 0\}}\Big(e^y(y-1) + 2e^y y - \frac{3}{2}e^y - \frac{5}{4}y^4 - v_k^4 - \frac{1}{4}v_{k-1}^4\Big)\mathrm{d}x\,.\end{aligned}$$

Next, since $(1+2y-5y^2/2)e^y \geq -c_{y<0}$ and $2e^y y - 3e^y/2 - 5y^4/4 > -c_{y\geq 0}$, where $c_{y<0}, c_{y\geq 0}$ are positive constants independent of $y<0$ and $y>0$, respectively, we obtain an estimate

$$\begin{aligned}\frac{\sigma}{\tau}\int_{\{y<0\}}\Big(e^y(y-1) + \Big(1+2y-\frac{5}{2}y^2\Big)e^y - 2v_k^2 - \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x \\ + \frac{\sigma}{\tau}\int_{\{y\geq 0\}}\Big(e^y(y-1) + 2e^y y - \frac{3}{2}e^y - \frac{5}{4}y^4 - v_k^4 - \frac{1}{4}v_{k-1}^4\Big)\mathrm{d}x \\ \geq \frac{\sigma}{\tau}\int_{\mathbb{T}^d} e^y(y-1)\mathrm{d}x - \frac{\sigma}{\tau}\int_{\mathbb{T}^d}\Big(2v_k^2 + v_k^4 + \frac{1}{2}v_{k-1}^2 + \frac{1}{4}v_{k-1}^4\Big)\mathrm{d}x - \frac{\sigma}{\tau}c_1\,,\end{aligned} \tag{4.27}$$

with $c_1 = c_{y<0} + c_{y\geq 0} > 0$. For the second term we use inequality (C.8),

$$\sigma\int_{\mathbb{T}^d} e^y(\partial_{ij}^2 y)^2\mathrm{d}x \geq \sigma\kappa_1\int_{\mathbb{T}^d}\big(\Delta e^{y/2}\big)^2\mathrm{d}x\,, \tag{4.28}$$

where $\kappa_1 > 0$ is explicitly given. Bringing together the last two inequalities one obtains

$$\begin{aligned}\frac{\sigma}{\tau}\int_{\mathbb{T}^d} e^y(y-1)\mathrm{d}x + \sigma\kappa_1\int_{\mathbb{T}^d}\big(\Delta e^{y/2}\big)^2\mathrm{d}x + \varepsilon\int_{\mathbb{T}^d}\big((\Delta y)^2 + y^2\big)\mathrm{d}x \\ \leq \frac{\sigma}{\tau}\int_{\mathbb{T}^d}\Big(2v_k^2 + v_k^4 + \frac{1}{2}v_{k-1}^2 + \frac{1}{4}v_{k-1}^4\Big)\mathrm{d}x + \frac{\sigma}{\tau}c_1\,.\end{aligned} \tag{4.29}$$

Thus,

$$\begin{aligned}E_1(u) + \tau\kappa_1\int_{\mathbb{T}^d}\big(\Delta e^{y/2}\big)^2\mathrm{d}x + \frac{\varepsilon\tau}{\sigma}\int_{\mathbb{T}^d}\big((\Delta y)^2 + y^2\big)\mathrm{d}x \\ \leq \int_{\mathbb{T}^d}\Big(2v_k^2 + v_k^4 + \frac{1}{2}v_{k-1}^2 + \frac{1}{4}v_{k-1}^4\Big)\mathrm{d}x + c_1\,.\end{aligned} \tag{4.30}$$

The right hand side gives a uniform bound, since our solutions $v_{k-1}, v_k \in W^{1,4}(\mathbb{T}^d)$. The last inequality together with Poincaré inequality implies that y is uniformly bounded in $H^2(\mathbb{T}^d)$,

$$\|y\|_{H^2}^2 \leq C\int_{\mathbb{T}^d}\big((\Delta y)^2 + y^2\big)\mathrm{d}x \leq C_1\,,$$

where $C_1 > 0$ does not depend on σ, but on $\varepsilon, \tau, v_{k-1}$ and v_k, only. In the same way as in the case before, continuity of the embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$ then yields uniform (σ-independent) bound on y in $W^{1,4}(\mathbb{T}^d)$,

$$\|y\|_{W^{1,4}} \leq C_1 \,, \tag{4.31}$$

where C_1 has may changed. Taking now $M \geq C_1$, we have obtained a uniform bound on the set of all potential fixed points of $S_\varepsilon(\cdot, \sigma)$. Leray-Schauder fixed-point theorem again provides the existence of a solution y_ε to $S_\varepsilon(y, 1) = y$.

Deregularization. By construction we have $v_\varepsilon = n_\varepsilon^{\alpha/2} = e^{\alpha y_\varepsilon/2} \geq \mu_\varepsilon > 0$, since $y_\varepsilon \in L^\infty(\mathbb{T}^d) \hookrightarrow H^2(\mathbb{T}^d)$. A priori estimates (4.24) and (4.30) imply that (v_ε) is uniformly bounded in $H^2(\mathbb{T}^d)$. Therefore, there exists a limit function $v \in H^2(\mathbb{T}^d)$, such that, up to a subsequence, as $\varepsilon \to 0$

$$v_\varepsilon \rightharpoonup v \quad \text{weakly in } H^2(\mathbb{T}^d) \,, \tag{4.32}$$

and due to compact embeddings $H^2(\mathbb{T}^d) \hookrightarrow W^{1,4}(\mathbb{T}^d)$ and $H^2(\mathbb{T}^d) \hookrightarrow L^\infty(\mathbb{T}^d)$

$$v_\varepsilon \to v \quad \text{strongly in } W^{1,4}(\mathbb{T}^d) \text{ and } L^\infty(\mathbb{T}^d) \,. \tag{4.33}$$

All together,

$$v_\varepsilon \partial_{ij}^2 v_\varepsilon \rightharpoonup v \partial_{ij}^2 v \quad \text{weakly in } L^2(\mathbb{T}^d) \quad \text{for all } i, j = 1, \ldots, d \,. \tag{4.34}$$

Recall that $1 \leq \alpha < (\sqrt{d} + 1)^2/(d + 2)$. First, let us assume $\alpha > 1$. According to the Lions-Villani result on the regularity of the square root of Sobolev functions (Lemma C.4),

$$\|\sqrt{v_\varepsilon}\|_{W^{1,4}}^2 \leq C \|v_\varepsilon\|_{H^2} \,.$$

Hence, $(\sqrt{v_\varepsilon})$ is uniformly bounded in $W^{1,4}(\mathbb{T}^d)$. Since $1/2 < 1/\alpha < 1$ for $d \leq 3$, Proposition C.6 then yields

$$v_\varepsilon^{1/\alpha} \to v^{1/\alpha} \quad \text{strongly in } W^{1,2\alpha}(\mathbb{T}^d) \,,$$

which implies

$$(\nabla v_\varepsilon^{1/\alpha})^2 \to (\nabla v^{1/\alpha})^2 \quad \text{strongly in } L^\alpha(\mathbb{T}^d) \text{ (componentwise).} \tag{4.35}$$

If $\alpha = 1$ then obviously from (4.33)

$$(\nabla v_\varepsilon)^2 \to (\nabla v)^2 \quad \text{strongly in } L^2(\mathbb{T}^d) \text{ (componentwise).} \tag{4.36}$$

Inequalities (4.24), (4.30) and coercivity of the bilinear form a_α also imply

$$\|y_\varepsilon\|_{H^2} \leq C_\alpha \varepsilon^{-1/2} \quad \text{and} \quad \|\nabla y_\varepsilon\|_{L^4} \leq C_\alpha \varepsilon^{-1/4} \,,$$

with $C_\alpha > 0$ now independent of $\varepsilon > 0$. Thus,

$$\varepsilon L_\alpha(y_\varepsilon) \rightharpoonup 0 \quad \text{weakly in } H^{-2}(\mathbb{T}^d) \,. \tag{4.37}$$

Defining $v_{k+1} := v$ and testing equation (4.18) by the test functions $\phi \in W^{2,\infty}(\mathbb{T}^d)$ and applying convergence results (4.33)–(4.37) we are able to pass to the limit in (4.18) as $\varepsilon \to 0$ and finally obtain weak form (4.10). Note that if $\alpha = 1$, one can use test functions $\phi \in H^2(\mathbb{T}^d)$ in (4.10), and if $\alpha > 1$, one can take test functions from the space $W^{1,\frac{\alpha}{\alpha-1}}(\mathbb{T}^d)$. Since v_{k+1} is obviously nonnegative a.e., we are able to define $n_{k+1} := v_{k+1}^{2/\alpha}$ and convergence results in (4.33) show that $n_\varepsilon \to n_{k+1}$ strongly in $W^{1,4}(\mathbb{T}^d)$.

Entropy stability. Let $\alpha > 1$ and $k \geq 1$. Assume we have constructed solutions $v_0, v_1, \ldots, v_{k-1}$. For the implicit Euler scheme we have the following stability condition

$$\frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d} v_1^2 \mathrm{d}x - \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d} v_0^2 \mathrm{d}x + \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}(v_1 - v_0)^2 \mathrm{d}x + \tau\kappa_\alpha \int_{\mathbb{T}^d}(\Delta v_1)^2 \mathrm{d}x \leq 0\,. \tag{4.38}$$

Let us reconsider construction of v_{k+1}. Using $\tau e^{(\alpha-1)y_\varepsilon}/(\alpha-1) \in H^2(\mathbb{T}^d)$ as a test function in (4.18) and applying algebraic inequality (4.16) we estimate the first term from below:

$$\begin{aligned}\frac{2}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\Big(\frac{3}{2}v_\varepsilon - 2v_k + \frac{1}{2}v_{k-1}\Big)v_\varepsilon \mathrm{d}x \geq & \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\Big(\frac{3}{2}v_\varepsilon^2 - 2v_k^2 + \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x \\ & + \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\big((v_\varepsilon - v_k)^2 - (v_k - v_{k-1})^2\big)\mathrm{d}x\,.\end{aligned}$$

The nonlinear term is again estimated according to Lemma C.5,

$$\frac{\tau}{2(\alpha-1)}\int_{\mathbb{T}^d} e^{y_\varepsilon}\partial_{ij}^2 y_\varepsilon \partial_{ij}^2 e^{(\alpha-1)y_\varepsilon}\mathrm{d}x \geq \kappa_\alpha\tau\int_{\mathbb{T}^d}\big(\Delta e^{\alpha y_\varepsilon/2}\big)^2 \mathrm{d}x = \kappa_\alpha\tau\int_{\mathbb{T}^d}(\Delta v_\varepsilon)^2\mathrm{d}x\,.$$

Thus we obtain

$$\begin{aligned}\frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\Big(\frac{3}{2}v_\varepsilon^2 - 2v_k^2 + \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x + \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\big((v_\varepsilon - v_k)^2 - (v_k - v_{k-1})^2\big)\mathrm{d}x \\ + \kappa_\alpha\tau\int_{\mathbb{T}^d}(\Delta v_\varepsilon)^2\mathrm{d}x + \frac{\varepsilon\tau}{\alpha-1}\int_{\mathbb{T}^d} L_\alpha(y_\varepsilon)e^{(\alpha-1)y_\varepsilon}\mathrm{d}x \leq 0\,.\end{aligned}$$

Convergence results (4.20), (4.33), (4.37) and lower semicontinuity of the functional $\int_{\mathbb{T}^d}(\Delta w)^2\mathrm{d}x$ imply an apriori bound for the limit function v_{k+1}

$$\begin{aligned}\frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\Big(\frac{3}{2}v_{k+1}^2 - 2v_k^2 + \frac{1}{2}v_{k-1}^2\Big)\mathrm{d}x + \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\big((v_{k+1} - v_k)^2 - (v_k - v_{k-1})^2\big)\mathrm{d}x \\ + \kappa_\alpha\tau\int_{\mathbb{T}^d}(\Delta v_{k+1})^2\mathrm{d}x \leq 0\,.\end{aligned} \tag{4.39}$$

Summing (4.38) and in (4.39) over $k = 1, \ldots, m-1$ many terms cancel out and we get

$$\frac{3}{2\alpha(\alpha-1)}\int_{\mathbb{T}^d} v_m^2\mathrm{d}x + \kappa_\alpha\tau\sum_{k=0}^{m-1}\int_{\mathbb{T}^d}(\Delta v_{k+1})^2\mathrm{d}x \leq \frac{1}{2\alpha(\alpha-1)}\int_{\mathbb{T}^d}\big(v_{m-1}^2 + v_1^2 + v_0^2\big)\mathrm{d}x\,.$$

Using the time discrete entropy dissipation of the implicit Euler scheme and applying the induction principle for this recursive inequality, we find

$$\frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d} v_m^2 \mathrm{d}x + \kappa_\alpha \tau \sum_{k=1}^{m}\int_{\mathbb{T}^d}(\Delta v_k)^2 \mathrm{d}x \le \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d} v_0^2 \mathrm{d}x$$

and therefore,

$$E_\alpha[n_m] + \kappa_\alpha \tau \sum_{k=1}^{m}\int_{\mathbb{T}^d}\big(\Delta n_k^{\alpha/2}\big)^2 \mathrm{d}x \le E_\alpha[n_0]\,,$$

which is the desired a priori estimate and implies entropy stability of the scheme. This finishes the proof. □

Introducing the relative entropy $E_\alpha^{rel}[n_k] := E_\alpha[n_k] - E_\alpha[\int_{\mathbb{T}^d} n_k]$ and applying generalized convex Sobolev inequality [36, Lemma 2.5, (2.8)] to the above a priori estimate, one obtains an a priori bound for the relative entropy

$$E_\alpha^{rel}[n_m] + 8\pi^4\alpha^2\kappa_\alpha\tau\sum_{k=1}^{m} E_\alpha^{rel}[n_k] \le E_\alpha[n_0]\,. \tag{4.40}$$

Recall that the BDF-2 method is G-stable and if we apply inequality (4.17) instead of (4.16), then at the place of (4.39) we obtain

$$\frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\frac{1}{2}\big(v_{k+1}^2 + (2v_{k+1}-v_k)^2\big)\mathrm{d}x - \frac{1}{\alpha(\alpha-1)}\int_{\mathbb{T}^d}\frac{1}{2}\big(v_k^2 + (2v_k - v_{k-1})^2\big)\mathrm{d}x$$
$$+ \kappa_\alpha\tau\int_{\mathbb{T}^d}(\Delta v_{k+1})^2\mathrm{d}x \le 0\,. \tag{4.41}$$

Defining the discrete quantity

$$E_\alpha^G[n_k, n_{k-1}] := \frac{1}{2\alpha(\alpha-1)}\int_{\mathbb{T}^d}\big(n_k^\alpha + (2n_k^{\alpha/2} - n_{k-1}^{\alpha/2})^2\big)\mathrm{d}x\,, \quad k \ge 1\,, \tag{4.42}$$

and rewriting inequality (4.41) in terms of E_α^G,

$$E_\alpha^G[n_{k+1}, n_k] + \kappa_\alpha\tau\int_{\mathbb{T}^d}\big(\Delta n_{k+1}^{\alpha/2}\big)^2\mathrm{d}x \le E_\alpha^G[n_k, n_{k-1}]\,, \quad k \ge 1\,,$$

E_α^G is to be interpreted as a Lyapunov functional for the BDF-2 scheme, since $E_\alpha^G[n_{k+1}, n_k] \le E_\alpha^G[n_k, n_{k-1}]$ for all $k \ge 1$. By the usual Taylor expansion procedure one formally observes aproximation relation $E_\alpha^G[n_k, n_{k-1}] = E_\alpha[n_k] + O(\tau)$ for $k \ge 2$.

Remark 4.6. At this point we don't discuss in which sense (in which parabolic spaces) sequence (v_k) converges to a solution of the contionous DLSS equation, but we rather emphasize only on the order of convergence.

4.2.2 Regularity of weak semi-discrete solutions

In the following we consider particular case $\alpha = 1$. Let us assume in addition that weak solutions solutions $v_k \in H^2(\mathbb{T}^d)$ from Theorem 4.1 are bounded from below with a positive constant μ_k, i.e. $v_k \geq \mu_k > 0$ a.e. in $\mathbb{T}^d$ for all $k \geq 1$. The weak form (4.10) reads as

$$\frac{1}{\tau}\int_{\mathbb{T}^d} v_{k+1}\Big(\frac{3}{2}v_{k+1} - 2v_k + \frac{1}{2}v_{k-1}\Big)\phi \mathrm{d}x + \frac{1}{2}\int_{\mathbb{T}^d}\big(v_{k+1}\partial^2_{ij}v_{k+1} - \partial_i v_{k+1}\partial_j v_{k+1}\big)\partial^2_{ij}\phi \mathrm{d}x = 0\,.$$

Sobolev embeddings and uniform bound from below give $u_{k+1} = v_{k+1}^2 \in H^2(\mathbb{T}^d)$ and $\log n_{k+1} \in H^2(\mathbb{T}^d)$, while integration by parts in the above weak form together with (4.12) yield

$$\frac{1}{\tau}v_{k+1}\Big(\frac{3}{2}v_{k+1} - 2v_k + \frac{1}{2}v_{k-1}\Big) + \frac{1}{4}\partial^2_{ij}(n_{k+1}\partial^2_{ij}\log n_{k+1}) = 0 \quad \text{in } H^{-2}(\mathbb{T}^d)\,. \tag{4.43}$$

Since, formally (for smooth and positive w)

$$\partial^2_{ij}(w\partial^2_{ij}\log w) = \Delta^2 w - \operatorname{div}\Big(2\frac{\partial^2_{ij}w\partial_j w}{w} - \frac{(\partial_j w)^2\partial_i w}{w^2}\Big)\,,$$

equation (4.43) is in the H^{-2}-sense equivalent to

$$\Delta^2 n_{k+1} = \operatorname{div}\Big(2\frac{\partial^2_{ij}n_{k+1}\partial_j n_{k+1}}{n_{k+1}} - \frac{(\partial_j n_{k+1})^2\partial_i n_{k+1}}{n_{k+1}^2}\Big) - \frac{4}{\tau}v_{k+1}\Big(\frac{3}{2}v_{k+1} - 2v_k + \frac{1}{2}v_{k-1}\Big)\,. \tag{4.44}$$

Second term on the right hand side of (4.44) possesses H^2-regularity. Continuity of the Sobolev embedding $H^2(\mathbb{T}^d) \hookrightarrow W^{1,6}(\mathbb{T}^d)$ implies $(\partial_j n_{k+1})^2\partial_i n_{k+1}/n_{k+1}^2 \in L^2(\mathbb{T}^d)$ for all $i = 1,\dots,d$. Moreover, we have $\partial^2_{ij}n_{k+1}\partial_j n_{k+1}/n_{k+1} \in L^{3/2}(\mathbb{T}^d) \hookrightarrow H^{-1/2}(\mathbb{T}^d)$. Hence, the right hand side of (4.44) lies in $H^{-3/2}(\mathbb{T}^d)$, i.e.

$$\Delta^2 n_{k+1} \in H^{-3/2}(\mathbb{T}^d)\,.$$

The standard regularity theory for elliptic operators, using Fourier transform on the torus, yields $n_{k+1} \in H^{5/2}(\mathbb{T}^d)$. The latter embeddes continuously into $W^{2,3}(\mathbb{T}^d)$, in space dimensions $d \leq 3$. Taking into account the improved regularity for n_{k+1} and applying variety of Sobolev embeddings in a procedure like above, we conclude in the next step

$$\Delta^2 n_{k+1} \in H^{-1}(\mathbb{T}^d)\,.$$

The last conclusion again improves on the regularity of n_{k+1}, namely we conclude like before $n_{k+1} \in H^3(\mathbb{T}^d)$. By this bootstrapping procedure we obtain H^m-regularity for n_{k+1} of arbitrary order $m \in \mathbb{N}$. Therefore we conclude that positive, bounded from below, solutions of the BDF-2 scheme are smooth.

4.2.3 Convergence of the BDF-2 scheme

Through this subsection we again assume $\alpha = 1$ and weak solutions from Theorem 4.1 remain positive and bounded from below with a positive constant. We have shown that these solutions are smooth. Next, we want to consider convergence of the method under these assumptions and prove Theorem 4.2.

Since $\phi/v_{k+1} \in H^2(\mathbb{T}^d)$ for all $\phi \in H^2(\mathbb{T}^d)$, using ϕ/v_{k+1} as a test function in (4.10) we obtain

$$\frac{1}{\tau}\Big(\frac{3}{2}v_{k+1} - 2v_k + \frac{1}{2}v_{k-1}\Big) + \frac{1}{2v_{k+1}}\partial^2_{ij}(v^2_{k+1}\partial^2_{ij}\log v_{k+1}) = 0 \quad \text{in } H^{-2}(\mathbb{T}^d)\,. \tag{4.45}$$

Proof of Theorem 4.2. Let $(v_k) = (\sqrt{n_k})$ be sequence of smooth positive solutions to (4.10) and n be a solution to (4.2) satisfying $(\sqrt{n})_{ttt} \in L^2(\mathbb{T}^d \times (0,T))$ and $(\sqrt{n})_{tt} \in L^\infty(\mathbb{T}^d \times (0,T))$. Taylor expansion shows that

$$v_t(t_{k+1}) = \frac{1}{\tau}\Big(\frac{3}{2}v(t_{k+1}) - 2v(t_k) + \frac{1}{2}v(t_{k-1})\Big) + \frac{f_k}{\tau}, \quad k \geq 1,$$

where f_k is given by the remainder terms and it is to be interpreted as the local truncation error

$$f_k = -\int_{t_k}^{t_{k+1}} v_{ttt}(s)(t_k - s)^2 ds + \frac{1}{4}\int_{t_{k-1}}^{t_{k+1}} v_{ttt}(s)(t_{k-1} - s)^2 ds.$$

Estimating f_k we find

$$\sum_{k=1}^{m-1} \|f_k\|^2_{L^2(\mathbb{T}^d)} \leq C_R \|v_{ttt}\|^2_{L^2(\mathbb{T}^d\times(0,T))}\tau^5, \tag{4.46}$$

where $C_R > 0$ does not depend on τ and $m \in \mathbb{N}$. Similarly, with the same assumptions on solutions of the implicit Euler scheme we get

$$v_t(t_1) = \frac{1}{\tau}(v(t_1) - v(t_0)) + \frac{f_0}{\tau},$$

where f_0 is the local truncation error of the scheme

$$f_0 = \int_0^\tau v_{tt}(s) s ds,$$

and under assumed regularities on the exact solution, we are able to estimate it as

$$\|f_0\|^2_{L^2(\mathbb{T}^d)} \leq \frac{1}{3}\|v_{tt}\|^2_{L^2(\mathbb{T}^d\times(0,\tau))}\tau^3 \leq \frac{1}{3}\|v_{tt}\|^2_{L^\infty(\mathbb{T}^d\times(0,T))}\tau^4. \tag{4.47}$$

Thus, $v = u^{\alpha/2}$ solves

$$v(t_1) - v(t_0) + \frac{\tau}{2v(t_1)}\partial^2_{ij}\big(v(t_1)^2\partial^2_{ij}\log v(t_1)\big) = -f_0\,, \quad k = 0\,,$$

$$\frac{3}{2}v(t_{k+1}) - 2v(t_k) + \frac{1}{2}v(t_{k-1}) + \frac{\tau}{2v(t_{k+1})}\partial^2_{ij}\big(v(t_{k+1})^2\partial^2_{ij}\log v(t_{k+1})\big) = -f_k\,, \quad k \geq 1\,.$$

Taking the difference of these equations with (4.9) and (4.45), respectively, we obtain error equations for $e_k = v_k - v(t_k)$,

$$e_1 - e_0 + \tau\big(A(v_1) - A(v(t_1))\big) = f_0\,, \quad k = 0\,,$$
$$\frac{3}{2}e_{k+1} - 2e_k + \frac{1}{2}e_{k-1} + \tau\big(A(v_{k+1}) - A(v(t_{k+1}))\big) = f_k\,, \quad k \geq 1\,,$$

where we introduced the operator $A : H^2(\mathbb{T}^d) \to H^{-2}(\mathbb{T}^d)$ defined for positive functions by

$$A(v) = \frac{1}{2v}\partial^2_{ij}(v^2\partial^2_{ij}\log v)\,.$$

Multiplying the error equations by e_{k+1} for $k \geq 0$, respectively, integrating over $\mathbb{T}^d$ and finally summing over $k = 0, \ldots, m-1$ one finds

$$\int_{\mathbb{T}^d}(e_1 - e_0)e_1 \mathrm{d}x + \sum_{k=1}^{m-1}\int_{\mathbb{T}^d}\Big(\frac{3}{2}e_{k+1} - 2e_k + \frac{1}{2}e_{k-1}\Big)e_{k+1}\mathrm{d}x \tag{4.48}$$
$$+ \tau\sum_{k=0}^{m-1}\int_{\mathbb{T}^d}\big(A(v_{k+1}) - A(v(t_{k+1}))\big)(v_{k+1} - v(t_{k+1}))\mathrm{d}x = \sum_{k=0}^{m-1}\int_{\mathbb{T}^d} f_k e_{k+1}\mathrm{d}x\,.$$

According to algebraic inequality (4.16), we obtain

$$\begin{aligned} e_1^2 &+ \sum_{k=1}^{m-1}\Big(\frac{3}{2}e_{k+1} - 2e_k + \frac{1}{2}e_{k-1}\Big)e_{k+1} \\ &\geq e_1^2 + \sum_{k=1}^{m-1}\Big(\frac{3}{4}e_{k+1}^2 - e_k^2 + \frac{1}{4}e_{k-1}^2 + \frac{1}{2}\big((e_{k+1} - e_k)^2 - (e_k - e_{k-1})^2\big)\Big) \\ &= e_1^2 + \frac{3}{4}e_m^2 - \frac{1}{4}e_{m-1}^2 + \frac{1}{2}(e_m - e_{m-1})^2 - \frac{3}{4}e_1^2 + \frac{1}{4}e_0^2 - \frac{1}{2}(e_1 - e_0)^2 \\ &\geq \frac{3}{4}e_n^2 - \frac{1}{4}e_{n-1}^2 - \frac{1}{4}e_1^2. \end{aligned}$$

In the last inequality we also used the fact that $e_0 = 0$. Next, we use monotonicity of the operator A. It has been proved in [39, Formula (3.3)] that for positive functions $w_1, w_2 \in H^4(\mathbb{T}^d)$ it holds

$$\int_{\mathbb{T}^d}\big(A(w_1) - A(w_2)\big)(w_1 - w_2)\mathrm{d}x = \int_{\mathbb{T}^d}\frac{1}{w_1 w_2}\Big|\operatorname{div}\Big(w_1^2\nabla\Big(\frac{w_1 - w_2}{w_1}\Big)\Big)\Big|^2\mathrm{d}x \geq 0\,.$$

The right hand side in (4.48) can be estimated applying Young's inequality:

$$\int_{\mathbb{T}^d} f_0 e_1 \mathrm{d}x \leq 2\|f_0\|^2_{L^2} + \frac{1}{8}\|e_1\|^2_{L^2} \quad \text{for } k = 0\,,$$
$$\int_{\mathbb{T}^d} f_k e_{k+1}\mathrm{d}x \leq \frac{1}{2\tau}\|f_k\|^2_{L^2} + \frac{\tau}{2}\|e_{k+1}\|^2_{L^2} \quad \text{for } k \geq 1\,.$$

Bringing together the above considerations and the bounds (4.46), (4.47) for f_k, we get

$$\begin{aligned}\frac{3}{4}\|e_m\|_{L^2}^2 &\le \frac{1}{4}\|e_{m-1}\|_{L^2}^2 + \frac{1}{4}\|e_1\|_{L^2}^2 + 2\|f_0\|_{L^2}^2 + \frac{1}{8}\|e_1\|_{L^2}^2 + \frac{1}{2\tau}\sum_{k=1}^{m-1}\|f_k\|_{L^2}^2 + \frac{\tau}{2}\sum_{k=1}^{m-1}\|e_{k+1}\|_{L^2}^2 \\ &\le \frac{1}{4}\|e_{m-1}\|_{L^2}^2 + \frac{3}{8}\|e_1\|_{L^2}^2 + 2C_0\tau^4 + \frac{1}{2}C_R\tau^4 + \frac{\tau}{2}\sum_{k=2}^{m}\|e_k\|_{L^2}^2\,,\end{aligned}$$

where $C_0, C_R > 0$ now also depend on v, but not on τ. Taking the maximum over $m = 1,\ldots,M$, gives

$$\frac{3}{4}\max_{m=1\ldots,M}\|e_m\|_{L^2}^2 \le \frac{5}{8}\max_{m=1\ldots,M}\|e_{m-1}\|_{L^2}^2 + C\tau^4 + \frac{\tau}{2}\sum_{k=2}^{M}\|e_k\|_{L^2}^2\,,$$

where $C = 2C_0 + C_R/2$. The first term on the right-hand side is controlled by the term on the left-hand side. Thus,

$$\|e_M\|_{L^2}^2 \le \max_{m=1\ldots,M}\|e_m\|_{L^2}^2 \le 8C\tau^4 + 8\tau\sum_{k=2}^{M}\|e_k\|_{L^2}^2\,.$$

We separate the last summand in the sum

$$(1-8\tau)\|e_M\|_{L^2}^2 \le 8C\tau^4 + 8\tau\sum_{k=2}^{M-1}\|e_k\|_{L^2}^2\,,$$

and apply the discrete Gronwall lemma, see e.g., [61, Theorem 4]

$$\|e_M\|_{L^2}^2 \le \frac{8C\tau^4}{1-8\tau}\Big(1+\frac{8\tau}{1-8\tau}\Big)^{M-2} = 8C\tau^4(1-8\tau)^{-M+1}\,.$$

Since

$$(1-8\tau)^{-M+1} = (1-8\tau)^{-t_{M-1}/\tau} \le \exp\Big(\frac{8t_{M-1}}{1-8\tau}\Big)\,,$$

the result follows, for $\tau < 1/16$, with the konstant $\sqrt{8C}\exp(8T)$, where $T > 0$ is some terminal time. □

4.3 Fully discrete structure preserving finite difference approximations

Recall again that the DLSS equation shares a particular variational structure, which is the gradient flow of the Fisher information with respect to the L^2-Wasserstein metric. Special form of equation (4.1) immediately implies (under periodic or no-flux boundary conditions) dissipation of the Fisher information (4.4). In this section we explore the corresponding dissipative structure on a discrete level. For ease of presentation and exposure of main ideas, we limit ourselves to the one dimensional case and periodic boundary conditions.

4.3.1 Discrete variational derivative method

In several papers [28, 49] before and later in the book [29], Furihata and Matsuo presented a structure preserving numerical scheme for large class of conservative and dissipative partial differential equations. Let us consider an evolution equation of the form

$$\partial_t n = -\frac{\delta \mathcal{E}[n]}{\delta n}\,, \quad x \in \mathbb{T}\,,\ t > 0\,, \tag{4.49}$$

where $\mathcal{E}$ is a given energy functional and $\delta\mathcal{E}[n]/\delta n$ denotes its variational derivative. Equation (4.49) is dissipative in the sense that

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}[n(t)] = \int_{\mathbb{T}} \frac{\delta \mathcal{E}[n]}{\delta n}\partial_t n \mathrm{d}x = -\int_{\mathbb{T}} \left(\frac{\delta \mathcal{E}[n]}{\delta n}\right)^2 \mathrm{d}x \le 0\,.$$

Observe that this dissipation property is again direct consequence of variational form (4.49) and the concrete form of the energy, and accordingly of the evolution equation, is irrelevant. Such dissipation properties usually have some physical meaning and physical solutions of equation (4.49) obey these laws. It is therefore desirable to construct numerical schemes which preserve the dissipative structure on a discrete level. Let $\mathbb{T}_N = \{x_i \ :\ i = 0, \ldots, N,\ x_0 \cong x_N\}$ denotes an equidistant discrete grid of mesh size h on the one dimensional torus $\mathbb{T} \cong [0, 1]$ and let $U^k \in \mathbb{R}^N$, such that U_i^k approximates $n(t_k, x_i)$ for $i = 0, \ldots, N-1$ and $k \ge 0$. First step is to define a discrete energy functional $\mathcal{E}_\mathrm{d} : \mathbb{R}^N \to \mathbb{R}$ as an approximation of the continuous energy functional $\mathcal{E}$. Applying a discrete variation procedure to $\mathcal{E}_\mathrm{d}$, one obtains discrete variational derivative, denoted by $\delta\mathcal{E}_\mathrm{d}/\delta(U^{k+1}, U^k)$. It is a vector of N components depending on values of U^{k+1} and U^k. For example, it can be defined[1] to satisfy the discrete chain rule

$$\mathcal{E}_\mathrm{d}[U^{k+1}] - \mathcal{E}_\mathrm{d}[U^k] = \sum_{i=0}^{N-1} \frac{\delta \mathcal{E}_\mathrm{d}}{\delta(U^{k+1}, U^k)}_i (U^{k+1} - U^k)_i h\,, \quad k \ge 0\,.$$

Finally, one defines a numerical scheme

$$\frac{1}{\tau}(U_i^{k+1} - U_i^k) = -\frac{\delta \mathcal{E}_\mathrm{d}}{\delta(U^{k+1}, U^k)}_i\,, \quad i = 0, \ldots, N-1\,,\ k \ge 0\,, \tag{4.50}$$

which by construction yields the discrete dissipation property, $\mathcal{E}_\mathrm{d}[U^{k+1}] \le \mathcal{E}_\mathrm{d}[U^k]$ for $k \ge 0$.

Let us now reconsider the above ideas for our DLSS equation

$$\partial_t n + \left(n \left(\frac{(\sqrt{n})_{xx}}{\sqrt{n}} \right)_x \right)_x = 0\,, \quad x \in \mathbb{T}\,,\ t > 0\,. \tag{4.51}$$

The variational derivative of the Fisher information $\mathcal{F}[n] = \int_{\mathbb{T}} (\sqrt{n})_x^2 \mathrm{d}x$ equals

$$\frac{\delta \mathcal{F}[n]}{\delta n} = -\frac{(\sqrt{n})_{xx}}{\sqrt{n}} \tag{4.52}$$

[1] The definition depends on quadrature rule used to define $\mathcal{E}_\mathrm{d}$. In the above example we took the simplest first-order quadrature rule.

and one immediately observes special variational form of equation (4.51),

$$\partial_t n + \left(n \left(\frac{\delta \mathcal{F}[n]}{\delta n} \right)_x \right)_x = 0 \,. \tag{4.53}$$

Integration by parts then automatically implies the dissipation of the Fisher information along solutions to (4.53),

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[n(t)] = \int_{\mathbb{T}} \frac{\delta \mathcal{F}[n]}{\delta n} \partial_t n \mathrm{d}x = - \int_{\mathbb{T}} n \left(\frac{\delta \mathcal{F}[n]}{\delta n} \right)_x^2 \mathrm{d}x \le 0 \,. \tag{4.54}$$

Introducing our standard change of variables $v = \sqrt{n}$, the Fisher information takes the form $\mathcal{F}[n] = \int_{\mathbb{T}} v_x^2 \mathrm{d}x$. In order to define discrete Fisher information, we first approximate the term

$$(v_x^2)|_{x=x_i} \approx \frac{1}{2}\left((\delta_i^+ V_i)^2 + (\delta_i^- V_i)^2 \right) \,, \quad i = 0, \dots N-1 \,,$$

where $v(x_i) \approx V_i$, and δ_i^+, δ_i^- denote the standard finite difference operators, difference forward and difference backward, respectively. Other choices of discretizations for v_x^2 are possible and allowable, but they eventually leed to another numerical scheme. We choose this approximation because of its symmetry. To approximate the integral of one-periodic functions w, we use the first-order quadrature rule $\sum_{i=0}^{N-1} w(x_i)h$. This rule is in fact of the second order, since due to periodic boundary conditions coincides the trapezoidal rule $(w(x_0) + w(x_N))h/2 + \sum_{i=1}^{N-1} w(x_i)h$. So we arrive to the definition of the discrete Fisher information functional, $\mathcal{F}_\mathrm{d} : \mathbb{R}^N \to \mathbb{R}$,

$$\mathcal{F}_\mathrm{d}[U] = \frac{1}{2} \sum_{i=0}^{N-1} \left((\delta_i^+ V_i)^2 + (\delta_i^- V_i)^2 \right) h \,, \tag{4.55}$$

where $U \in \mathbb{R}^N$ and $V_i = \sqrt{U_i}$ for $i = 0, \dots, N-1$.

Defining the discrete energy, next step is to obtain its discrete variational derivative. Applying the discrete variation procedure and using summation by parts formula (see [29, Proposition 3.2]) for periodic boundary conditions, we calculate:

$$\begin{aligned} \mathcal{F}_\mathrm{d}[U^{k+1}] - \mathcal{F}_\mathrm{d}[U^k] &= \frac{1}{2} \sum_{i=0}^{N-1} \left((\delta_i^+ V_i^{k+1})^2 - (\delta_i^+ V_i^k)^2 + (\delta_i^- V_i^{k+1})^2 - (\delta_i^- V_i^k)^2 \right) h \\ &= \frac{1}{2} \sum_{i=0}^{N-1} \big(\delta_i^+ (V_i^{k+1} + V_i^k) \delta_i^+ (V_i^{k+1} - V_i^k) \\ &\qquad + \delta_i^- (V_i^{k+1} + V_i^k) \delta_i^- (V_i^{k+1} - V_i^k) \big) h \\ &= - \sum_{i=0}^{N-1} \delta_i^{\langle 2 \rangle} (V_i^{k+1} + V_i^k)(V_i^{k+1} - V_i^k) h \\ &= - \sum_{i=0}^{N-1} \frac{\delta_i^{\langle 2 \rangle} (V_i^{k+1} + V_i^k)}{V_i^{k+1} + V_i^k} (U_i^{k+1} - U_i^k) h \,, \quad k \ge 0 \,, \end{aligned}$$

where $\delta_i^{\langle 2\rangle} w_i = \delta_i^+ \delta_i^- w_i = \delta_i^- \delta_i^+ w_i$ denotes the second-order central difference formula. The discrete variational derivative, denoted by $\delta\mathcal{F}_\mathrm{d}/\delta(U^{k+1}, U^k) \in \mathbb{R}^N$, is then defined componentwise by

$$\frac{\delta\mathcal{F}_\mathrm{d}}{\delta(U^{k+1}, U^k)_i} := -\frac{\delta_i^{\langle 2\rangle}(V_i^{k+1} + V_i^k)}{V_i^{k+1} + V_i^k}\,, \quad i = 0, \ldots, N-1\,. \tag{4.56}$$

Note that the discrete chain rule

$$\mathcal{F}_\mathrm{d}[U^{k+1}] - \mathcal{F}_\mathrm{d}[U^k] = \sum_{i=0}^{N-1} \frac{\delta\mathcal{F}_\mathrm{d}}{\delta(U^{k+1}, U^k)_i}(U_i^{k+1} - U_i^k)h\,,$$

holds and (4.56) is a Crank-Nicolson type approximation of the variational derivative (4.52).

Finally, the *discrete variational derivative method (DVDM for short)* for the DLSS equation is defined by the nonlinear system with unknowns $U_i^{k+1} = (V_i^{k+1})^2$,

$$\frac{1}{\tau}(U_i^{k+1} - U_i^k) = \delta_i^{\langle 1\rangle}\left(U_i^{k+1}\delta_i^{\langle 1\rangle}\left(\frac{\delta\mathcal{F}_\mathrm{d}}{\delta(U^{k+1}, U^k)_i}\right)\right)\,, \quad i = 0, \ldots, N-1\,,\ k \geq 0\,, \tag{4.57}$$

where $\delta_i^{\langle 1\rangle}$ denotes the central difference approximation of the first-order derivative at points x_i. We assume that an initial condition to equation (4.51) is given by a nonnegative function n_0, which is approximated by the projection on $\mathbb{T}_N$ and gives the starting values $U^0 \in \mathbb{R}^N$ for scheme (4.57).

Proof of Theorem 4.3. Let $n = v^2$ be a smooth positive solution to (4.51). By straightforward Taylor expansion calculations around (t_{k+1}, x_i) we obtain

$$\begin{aligned}
\left.\frac{\delta\mathcal{F}_\mathrm{d}}{\delta(n(t_{k+1}), n(t_k))}\right|_{x_i} &= -\frac{\delta_i^{\langle 2\rangle}(v(t_{k+1}, x_i) + v(t_k, x_i))}{v(t_{k+1}, x_i) + v(t_k, x_i)} \\
&= \left.\frac{v_{xx}}{v}\right|_{(t_{k+1}, x_i)} + O(\tau, h^2) \\
&= \left.\frac{\delta\mathcal{F}[n]}{\delta n}\right|_{(t_{k+1}, x_i)} + O(\tau, h^2)\,, \quad i = 0, \ldots, N-1\,,\ k \geq 0\,.
\end{aligned}$$

Similarly,

$$\left.\delta_i^{\langle 1\rangle}\left(n(t_{k+1})\delta_i^{\langle 1\rangle}\left(\frac{\delta\mathcal{F}_\mathrm{d}}{\delta(n(t_{k+1}), n(t_k))}\right)\right)\right|_{x_i} = \left.\left(n\left(\frac{\delta\mathcal{F}[n]}{\delta n}\right)_x\right)_x\right|_{(t_{k+1}, x_i)} + O(\tau, h^2)\,.$$

Thus, the local truncation error of the right hand side in (4.57) is of order $O(\tau, h^2)$. Since the left hand side is of order $O(\tau)$ in time and exact at spatial grid points x_i, the local truncation error of scheme (4.57) is of order $O(\tau, h^2)$.

In fact, we solve scheme (4.57) in terms of variables $V_i^k = \sqrt{U_i^k}$. Therefore, $U_i^k \geq 0$ for all $i = 0, \ldots, N-1$ and $k \geq 1$, and the discrete dissipation property follows immediately from the structure of the scheme and summation by parts formula,

$$\begin{aligned}\mathcal{F}_{\mathrm{d}}[U^{k+1}] - \mathcal{F}_{\mathrm{d}}[U^k] &= \sum_{i=0}^{N-1} \frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1}, U^k)_i}(U_i^{k+1} - U_i^k)h \\ &= -\tau \sum_{i=0}^{N-1} U_i^{k+1} \left(\delta_i^{\langle 1 \rangle} \left(\frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1}, U^k)_i} \right) \right)^2 h \leq 0 \,.\end{aligned}$$

The mass conservation is also an obvious direct consequence of the scheme. It remains to prove uniform boundedness of solutions. The energy decay implies a uniform bound on the discrete H^1-seminorm,

$$\sum_{i=0}^{N-1} (\delta_i^+ V_i^k)^2 h \leq \mathcal{F}_{\mathrm{d}}[U^0] < \infty \,.$$

According to the discrete Poincaré-Wirtinger inequality ([29, Lemma 3.3]), the latter implies

$$|V_i^k - 1|^2 \leq \sum_{i=0}^{N-1} (\delta_i^+ V_i^k)^2 h \leq C \quad \text{for all } i = 0, \ldots, N-1 \,, \ k \geq 1 \,,$$

where $C = \mathcal{F}_{\mathrm{d}}[U^0]$ is a positive constant independent of k. Finally, by the triangle inequality $|V_i^k| \leq \sqrt{C} + 1$ and thus $U_i^k \leq 2C + 2$ for all $i = 0, \ldots, N-1$ and $k \geq 1$. The last estimate prevents the blow-up of numerical solutions constructed by scheme (4.57). □

4.3.2 Temporally higher-order discrete variational derivative method

There are numerous ways of generalizing the above discrete variational derivative method. In order to stay in the spirit of Sections 4.2, we derive temporally higher-order discrete variational derivative methods, which are based on backward difference formulae and temporally higher-order approximations of the variational derivative. Let us introduce symmetric biquadratic form $f(\xi, \zeta) = (\xi^2 + \zeta^2)/2$, which represents both, the Fisher information $\mathcal{F}[n] = \int_{\mathbb{T}} f(v_x, v_x) \mathrm{d}x$ and the discrete Fisher information $\mathcal{F}_{\mathrm{d}}[U] = \sum_{i=0}^{N-1} f(\delta_i^+ V_i, \delta_i^- V_i)h$. The reason for introducing f lies in the following formal representation of the variational derivative,

$$\frac{\delta \mathcal{F}[n]}{\delta n} = -\frac{v_{xx}}{v} = \Big(-\partial_x \big(\partial_\xi f \big|_{\xi = v_x} \big) - \partial_x \big(\partial_\zeta f \big|_{\zeta = v_x} \big) \Big) \frac{1}{2v} \,. \tag{4.58}$$

This formula gives an idea how to approximate the variational derivative in general. First, let us denote with $\delta_k^{1,q}$ the q-th step backward difference operator at time point t_k (see Table 4.1). Discrete variational derivative of order q in time is defined componentwise by

$$\frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1}, \ldots, U^{k-q+1})_i} := \frac{1}{2V_i^{k+1}} \left(-\delta_i^- \left(\partial_\xi^{\mathrm{d}} f \right)_i - \delta_i^+ \left(\partial_\zeta^{\mathrm{d}} f \right)_i \right) \,, \quad k \geq q-1 \,, \tag{4.59}$$

where the discrete operators are in addition defined by

$$\begin{aligned}\left(\partial_\xi^{\mathrm{d}} f\right)_i &:= \partial_\xi f\big|_{\xi=\delta_i^+ V_i^{k+1}} + \mathbf{r}_{corr}\delta_{k+1}^{1,q}(\delta_i^+ U_i^{k+1}) \\ &= \delta_i^+ V_i^{k+1} + \mathbf{r}_{corr}\delta_{k+1}^{1,q}(\delta_i^+ U_i^{k+1})\,, \\ \left(\partial_\zeta^{\mathrm{d}} f\right)_i &:= \partial_\zeta f\big|_{\zeta=\delta_i^- V_i^{k+1}} + \mathbf{r}_{corr}\delta_{k+1}^{1,q}(\delta_i^- U_i^{k+1}) \\ &= \delta_i^- V_i^{k+1} + \mathbf{r}_{corr}\delta_{k+1}^{1,q}(\delta_i^- U_i^{k+1})\,,\end{aligned}$$

and $\mathbf{r}_{corr}$ is the so-called correction term, which is to be determined in order to satisfy the discrete chain rule

$$\delta_{k+1}^{1,q}\mathcal{F}_{\mathrm{d}}[U^{k+1}] = \sum_{i=0}^{N-1} \frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1},\ldots,U^{k-q+1})_i}\delta_{k+1}^{1,q}U_i^{k+1}h\,. \tag{4.60}$$

Observe that (4.59) is a discrete analog of (4.58) and the role of the correction term is not only to satisfy the discrete chain rule (4.60), but also to increase the temporal accuracy of the discrete variational derivative (see proof of Theorem 4.7 below). Straightforward computations with the above expressions using summation by parts formulae and assuming periodic boundary conditions yield

$$\frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1},\ldots,U^{k-q+1})_i} = -\frac{\delta_i^{\langle 2\rangle}V_i^{k+1}}{V_i^{k+1}} - \mathbf{r}_{corr}\frac{\delta_{k+1}^{1,q}\delta_i^{\langle 2\rangle}U_i^{k+1}}{V_i^{k+1}}\,,\quad k\ge q-1\,, \tag{4.61}$$

and

$$\mathbf{r}_{corr} = \frac{\delta_{k+1}^{1,q}\mathcal{F}_{\mathrm{d}}[U^{k+1}] - \sum_{i=0}^{N-1}\delta_i^+ V_i^{k+1}\delta_i^+\left(\frac{\delta_{k+1}^{1,q}U_i^{k+1}}{V_i^{k+1}}\right)h}{\sum_{i=0}^{N-1}(\delta_i^+\delta_{k+1}^{1,q}U_i^{k+1})\delta_i^+\left(\frac{\delta_{k+1}^{1,q}U_i^{k+1}}{V_i^{k+1}}\right)h}\,. \tag{4.62}$$

Temporally q-th order discrete variational derivative method (BDF-q DVDM for short) is then defined by the nonlinear system in unknowns $U_i^{k+1} = (V_i^{k+1})^2$,

$$\delta_{k+1}^{1,q}U_i^{k+1} = \delta_i^{\langle 1\rangle}\left(U_i^{k+1}\delta_i^{\langle 1\rangle}\left(\frac{\delta \mathcal{F}_{\mathrm{d}}}{\delta(U^{k+1},\ldots,U^{k-q+1})_i}\right)\right)\,,\quad i=0,\ldots,N-1\,,\ k\ge q-1\,. \tag{4.63}$$

The following theorem summarizes on assumptions and main properties of the scheme.

Theorem 4.7. *Let $N\in\mathbb{N}$, $U^0\in\mathbb{R}^N$ be nonnegative initial data and $U^l\in\mathbb{R}^N$ given starting values of the unit discrete mass, i.e. $\sum_{i=0}^{N-1}U_i^l h = 1$, and let $\mathcal{F}_{\mathrm{d}}[U^{q-1}]\le\ldots\le\mathcal{F}_{\mathrm{d}}[U^0]<\infty$. Numerical scheme (4.63) is consistent of order $(q,2)$ with respect to the time-space discretization. Let $(U^k)\subset(\mathbb{R}^N)^{\mathbb{N}}$, $(k\ge q)$ be sequence of solutions to scheme (4.63). Then $(U^k)\in l^\infty(\mathbb{R}^N)$, $\sum_{i=0}^{N-1}U_i^k h = 1$ for all $k\ge q$ and the discrete Fisher information is dissipated in the sense that it satisfies*

$$\delta_k^{1,q}\mathcal{F}_{\mathrm{d}}[U^k]\le 0\quad\text{for all } k\ge q\,. \tag{4.64}$$

Proof. Again let $n = v^2$ be a smooth positive solution to (4.51) and integer $q \geq 2$ (typically $q \leq 6$) the order of the backward difference formula. The left hand side of (4.63) is by assumption of order $O(\tau^q)$ in time and exact at spatial grid points x_i. Thus it remains to prove that the right hand side is of order $O(\tau^q, h^2)$. The following estimates are easily obtained by Taylor expansions around (t_{k+1}, x_i):

$$\delta_i^+ v(t_{k+1}, x_i) = v_x\big|_{(t_{k+1},x_i)} + \frac{h}{2} v_{xx}\big|_{(t_{k+1},x_i)} + O(h^2)\,, \tag{4.65}$$

$$\delta_i^- v(t_{k+1}, x_i) = v_x\big|_{(t_{k+1},x_i)} - \frac{h}{2} v_{xx}\big|_{(t_{k+1},x_i)} + O(h^2)\,, \tag{4.66}$$

$$-\frac{\delta_i^{\langle 2\rangle} v(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} = -\frac{v_{xx}}{v}\Big|_{(t_{k+1},x_i)} + O(h^2)\,, \tag{4.67}$$

$$\frac{\delta_{k+1}^{1,q}\delta_i^{\langle 2\rangle} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)} = \frac{n_{txx}}{v}\Big|_{(t_{k+1},x_i)} + O(\tau^q, h^2)\,, \tag{4.68}$$

$$\delta_i^+ \delta_{k+1}^{1,q} n(t_{k+1}, x_i) = n_{tx}\big|_{(t_{k+1},x_i)} + \frac{h}{2} n_{txx}\big|_{(t_{k+1},x_i)} + O(\tau^q, h^2)\,, \tag{4.69}$$

$$\delta_i^- \delta_{k+1}^{1,q} n(t_{k+1}, x_i) = n_{tx}\big|_{(t_{k+1},x_i)} - \frac{h}{2} n_{txx}\big|_{(t_{k+1},x_i)} + O(\tau^q, h^2)\,, \tag{4.70}$$

$$\delta_i^+ \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)}\right) = 2v_{tx}\big|_{(t_{k+1},x_i)} + h v_{txx}\big|_{(t_{k+1},x_i)} + O(\tau^q, h^2)\,, \tag{4.71}$$

$$\delta_i^- \left(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)}\right) = 2v_{tx}\big|_{(t_{k+1},x_i)} - h v_{txx}\big|_{(t_{k+1},x_i)} + O(\tau^q, h^2)\,. \tag{4.72}$$

Let us show that $\mathbf{r}_{corr} = \mathbf{r}_{\mathrm{n}}/\mathbf{r}_{\mathrm{d}}$ is of order $O(\tau^q, h^2)$. First we consider the denominator $\mathbf{r}_{\mathrm{d}}$. Note that due to periodic boundary conditions

$$\sum_{i=0}^{N-1} (\delta_i^+ \delta_{k+1}^{1,q} n(t_{k+1}, x_i))\delta_i^+ \Big(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)}\Big) h = \sum_{i=0}^{N-1} (\delta_i^- \delta_{k+1}^{1,q} n(t_{k+1}, x_i))\delta_i^- \Big(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)}\Big) h\,.$$

Hence,

$$\begin{aligned}\mathbf{r}_{\mathrm{d}} = \frac{1}{2}\sum_{i=0}^{N-1} \Bigg(&(\delta_i^+ \delta_{k+1}^{1,q} n(t_{k+1}, x_i))\delta_i^+ \Big(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)}\Big) \\ &+ (\delta_i^- \delta_{k+1}^{1,q} n(t_{k+1}, x_i))\delta_i^- \Big(\frac{\delta_{k+1}^{1,q} n(t_{k+1}, x_i)}{v(t_{k+1}, x_i)}\Big)\Bigg) h\,,\end{aligned}$$

and according to above estimates (4.69)–(4.72),

$$\mathbf{r}_{\mathrm{d}} = \sum_{i=0}^{N-1} n_{tx} v_{tx}\big|_{(t_{k+1},x_i)} h + O(\tau^q, h^2)\,. \tag{4.73}$$

Similarly we consider the nominator term $\mathbf{r}_{\mathrm{n}}$. Using (4.65)–(4.66), the first term can be estimated like

$$\begin{aligned}\delta^{1,q}_{k+1}\mathcal{F}_{\mathrm{d}}[n(t_{k+1})] &= \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\sum_{i=0}^{N-1}\big((\delta_i^+ v(t,x_i))^2 + (\delta_i^- v(t,x_i))^2\big)h\Big|_{t_{k+1}} + O(\tau^q)\\ &= 2\sum_{i=0}^{N-1} v_x v_{xt}\big|_{(t_{k+1},x_i)} h + O(\tau^q, h^2)\,. \end{aligned}\tag{4.74}$$

Again, due to periodic boundary conditions

$$\sum_{i=0}^{N-1}\delta_i^+ v(t_{k+1},x_i)\delta_i^+\Big(\frac{\delta^{1,q}_{k+1}n(t_{k+1},x_i)}{v(t_{k+1},x_i)}\Big)h = \sum_{i=0}^{N-1}\delta_i^- v(t_{k+1},x_i)\delta_i^-\Big(\frac{\delta^{1,q}_{k+1}n(t_{k+1},x_i)}{v(t_{k+1},x_i)}\Big)h\,,$$

and according to estimates (4.65)–(4.66) and (4.71)–(4.72),

$$\begin{aligned}&\frac{1}{2}\sum_{i=0}^{N-1}\Bigg(\delta_i^+ v(t_{k+1},x_i)\delta_i^+\Big(\frac{\delta^{1,q}_{k+1}n(t_{k+1},x_i)}{v(t_{k+1},x_i)}\Big) + \delta_i^- v(t_{k+1},x_i)\delta_i^-\Big(\frac{\delta^{1,q}_{k+1}n(t_{k+1},x_i)}{v(t_{k+1},x_i)}\Big)\Bigg)h\\ &\quad= 2\sum_{i=0}^{N-1} v_x v_{xt}\big|_{(t_{k+1},x_i)} h + O(\tau^q, h^2)\,. \end{aligned}\tag{4.75}$$

Thus, applying estimates (4.73)–(4.75) in (4.62) yields $\mathbf{r}_{corr} = O(\tau^q, h^2)$. Finally, estimates (4.67)–(4.68) imply

$$\begin{aligned}\frac{\delta\mathcal{F}_{\mathrm{d}}}{\delta(n(t_{k+1}),\ldots,n(t_{k+1-q}))}\Big|_{x_i} &= -\frac{\delta_i^{\langle 2\rangle}v(t_{k+1},x_i)}{v(t_{k+1},x_i)} - \mathbf{r}_{corr}\frac{\delta^{1,q}_{k+1}\delta_i^{\langle 2\rangle}n(t_{k+1},x_i)}{v(t_{k+1},x_i)}\\ &= \frac{\delta\mathcal{F}[n]}{\delta n}\Big|_{(t_{k+1},x_i)} + O(\tau^q,h^2)\,, \end{aligned}$$

which showes that the discrete variational derivative (4.61) is of order q in time. The rest of the proof follows the same steps as in the proof of Theorem 4.3, and the discrete dissipation property (4.64) is again direct consequence of the scheme. □

4.4 Numerical ilustrations

In this section we do numerical experiments with our aforementioned schemes. We consider equations (4.1) and (4.2) in space dimension $d = 1$ with periodic boundary conditions. Again, let $\mathbb{T}_N = \{x_i \,:\, i = 0,\ldots,N,\ x_0 \cong x_N\}$ denotes an equidistant spatial grid of mesh size $h = 1/N$ on the one dimensional torus $\mathbb{T} \cong [0,1]$. Let $\tau > 0$ be given time step and $U^k \in \mathbb{R}^N$ such that $U_i^k \approx n(t_k, x_i)$, where $t_k = k\tau$, $k \geq 0$ and $i = 0,\ldots,N-1$.

4.4.1 BDF-2 finite difference scheme

First we consider the onedimensional equation (4.2),

$$\partial_t n + \frac{1}{2}(n(\log n)_{xx})_{xx} = 0\,, \quad x \in \mathbb{T},\ t > 0\,, \quad n(0) = n_0\,,$$

which we solve with the scheme (4.7) — the BDF-2 method — using finite differences in space. The scheme is given by the nonlinear system of equations with unknowns $V_i^k = (U_i^k)^{\alpha/2}$ for $i = 0, \ldots, N-1$ and $k \geq 1$,

$$(V_i^1)^{2/\alpha-1}\big(V_i^1 - V_i^0\big) + \tau\delta_i^{\langle 2\rangle}\left((V_i^1)^{2/\alpha}\delta_i^{\langle 2\rangle}\log V_i^1\right) = 0\,, \quad i = 0, \ldots, N-1\,, \tag{4.76}$$

$$\begin{aligned}(V_i^{k+1})^{2/\alpha-1}\Big(\frac{3}{2}V_i^{k+1} - 2V_i^k + \frac{1}{2}V_i^{k-1}\Big)&\\ + \tau\delta_i^{\langle 2\rangle}\left((V_i^{k+1})^{2/\alpha}\delta_i^{\langle 2\rangle}\log V_i^{k+1}\right) &= 0\,, \quad i = 0, \ldots, N-1\,,\ k \geq 1.\end{aligned} \tag{4.77}$$

$$V_i^k = V_{i+lN}^k\,, \quad l \in \mathbb{Z}\,. \tag{4.78}$$

Above, a given value $\alpha \in [1, 3/2)$ belongs to the range of entropies for the onedimensional DLSS equation. We assume that initial data $(V_i^0)_{i=0}^{N-1}$, which approximates $n_0^{\alpha/2}$ is given by the projection on $\mathbb{T}_N$. The system (4.76) is the implicit Euler scheme, which is solved only once to initialize the BDF-2 scheme (4.77). Both systems of nonlinear equations, (4.76) and (4.77) with discrete periodic boundary conditions (4.78), can are solved by the Newton iterative method. In each time step $t_{k+1} = (k+1)\tau$, we take the solution from the previous time step t_k as an initial guess to compute the solution at the current time step t_{k+1}. In practice, only a few iterations (3 to 4) are enough to compute the solution of the system at each time step. The following example has been used to test the above BDF-2 scheme.

Example 4.8. Let the initial condition for equation (4.2) be $n_0(x) = 0.001 + \cos^{16}(\pi x)$. Other relevant parameters have the following values: the spatial mesh size $h = 0.005$ ($N = 200$), the time step $\tau = 10^{-6}$ and the terminal time $T = 5 \cdot 10^{-4}$.

Figure 4.1(a) showes the stability, in fact the decay, of the corresponding discrete α-functional for different values of α. Moreover, we observe even an exponential decay of the relative entropies, as shown in Figure 4.1(b). Although Theorem 4.1 doesn't provide even stability of the physical entropy E_1, numerical experiments however give expected decay of the discrete version $E_{1,\mathrm{d}}[U] = \sum_{i=0}^{N-1}(U_i(\log U_i - 1) + 1)h$. Interestingly, one also observes an exponential decay of the discrete Fisher information $\mathcal{F}_{\mathrm{d}}$ defined in Section 4.3.1.

Next, we want to consider temporal convergence of the BDF-2 finite difference scheme. We saw in Section 4.2.3 that for $\alpha = 1$, the time discrete BDF-2 scheme possesses the second-order convergence in time. In the fully discrete case (4.76)–(4.78) this may not be the case, since the monotonicity structure of the spatial operator has been destroyed by the discretization. However, Figure 4.2 showes that numerically estimated convergence rates for different parameters of α are close to 2. Numbers in the legend of Figure 4.2 are

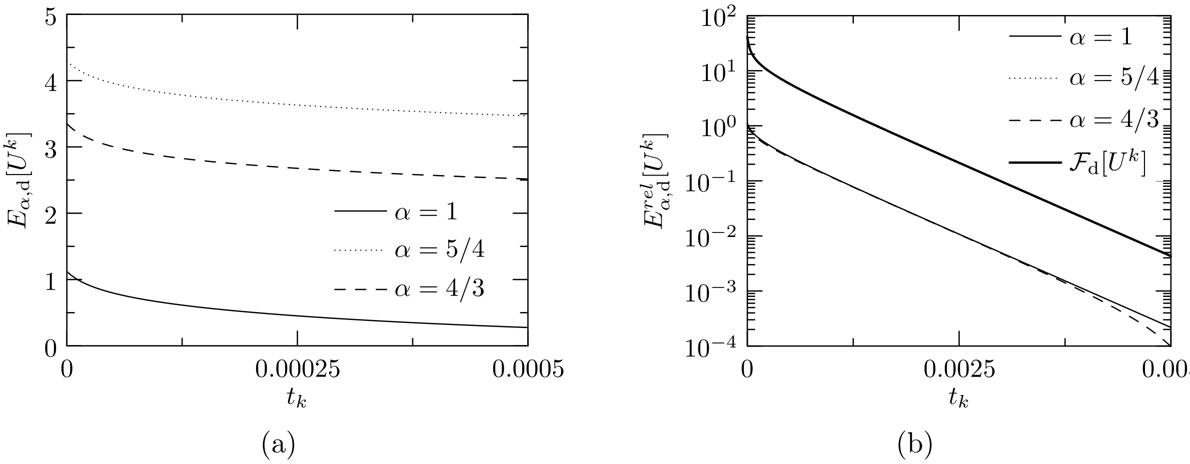


Figure 4.1: (a) Entropy stability (decay) for the BDF-2 finite difference scheme for different values of α. (b) Exponential decay of the relative entropy and the discrete Fisher information for the BDF-2 finite difference scheme.

averaged convergence rates obtaind by the linear regression method. Convergence of the method is meassured in the discrete l^2-norm

$$\|e_m\|_{l^2} := \left(h \sum_{i=0}^{N-1} (V_{e,i}^m - V_i^m)^2 \right)^{1/2}, \tag{4.79}$$

and numerical solutions are compared at the time instance $t_m = 5 \cdot 10^{-5}$. The exact solution V_e^m has been computed by method (4.76)–(4.78) using the very small time step $\tau = 10^{-10}$.

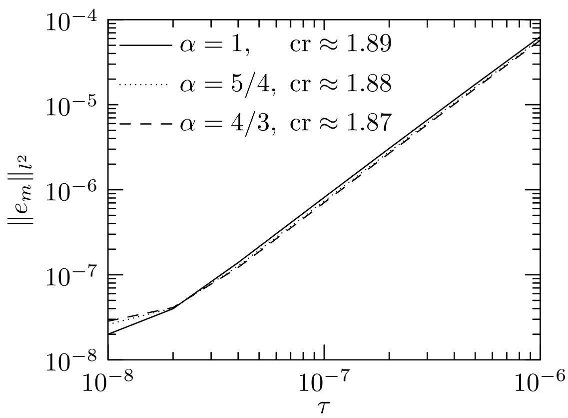


Figure 4.2: Temporal convergence rates of the BDF-2 finite difference scheme for different values of α.

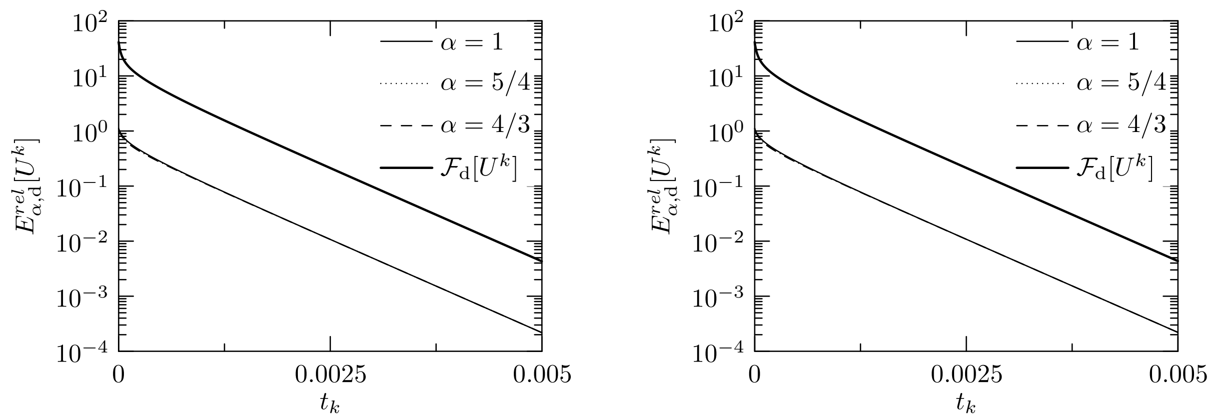
4.4.2 Discrete variational derivative methods

Here we present numerical results obtained for the discrete variational derivative methods introduced in the previous section. Recall equation (4.1) (in space dimension $d = 1$), which admits the particular variational form (4.53),

$$\partial_t n + \left(n \left(\frac{\delta \mathcal{F}[n]}{\delta n} \right)_x \right)_x = 0\,, \quad x \in \mathbb{T}\,,\ t > 0\,, \quad n(0) = n_0\,.$$

First, we consider the discrete variational derivative method (DVDM) given by scheme (4.57). The numerical test takes the same ingredients as in Example 4.8: the initial condition $n_0(x) = 0.001 + \cos^{16}(\pi x)$, grid size $h = 0.005$, time step $\tau = 10^{-6}$, but the bigger terminal time $T = 5 \cdot 10^{-3}$. We observe (Figure 4.3(a)) decay of the discrete Fisher information $\mathcal{F}_{\mathrm{d}}$, in fact an exponential decay, as well as an exponential decay of particular relative entripies $E^{rel}_{\alpha,\mathrm{d}}$.

Next, we employ the temporally higher-order variational derivative method (4.63) with discrete temporal operators $\delta_k^{1,2}$ (BDF-2) and $\delta_k^{1,3}$ (BDF-3). Initialization values for higher-order methods are computed by the DVDM and the BDF-2 method, respectively. Using the above inputs for the numerical simulation, the very same decay results for discrete functionals have been obtained (see Figure 4.3(b)).



(a) (b)

Figure 4.3: (a) Exponential decay of the discrete Fisher information and relative entropies for the DVDM. (b) Exponential decay of the discrete Fisher information and relative entropies for the BDF-2 DVDM.

Finally, we tested numerically the time convergence of discrete variational derivative methods. Figure 4.4 ilustrates the numerical error of the methods with respect to time step size τ. We took initial data n_0 as before, the mesh size $h = 0.01$ and we compared our numerical solutions in the l^2-norm (4.79) at the time instance $t_m = 5 \cdot 10^{-5}$. The exact solutions are computed by the respective methods taking the very small time step $\tau = 10^{-9}$. Table 4.2 gives estimated temporal convergence rates of the schemes, which are computed by the linear regression method for data from Figure 4.4. Note that the BDF-3 DVD method gives only slightly better results than the corresponding BDF-2 method. The reason is that the first step is initialized by only the first-order scheme (4.57) and this initialization error cannot be compensated due to higher-order accuracy of the local approximation. Obviously, one should use a higher-order one-step method for the initialization.

At this point, it should be mentiond that nonlinear systems in schemes (4.57) and (4.63), in all numerical experiments here, were solved by the NAG Toolbox routine `c05nb` [53], which proves to be at least three times faster than the standard MATLAB routine `fsolve`.

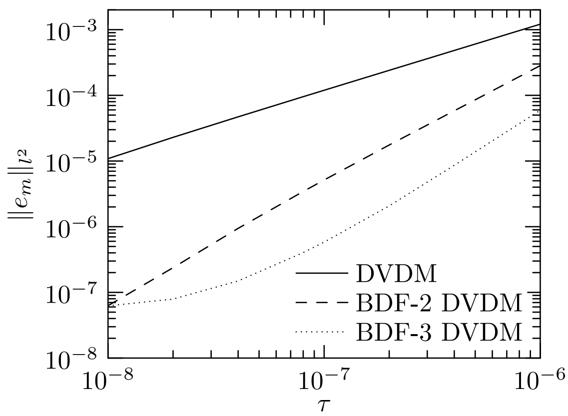


Figure 4.4: Numerical convergence rates of discrete variational derivative methods.

scheme	conv. rate
DVDM	1.020
BDF-2 DVDM	1.824
BDF-3 DVDM	1.977

Table 4.2: Estimated temporal convergence rates for discrete variational derivative methods.

Chapter 5

Conclusion and outlook

Conclusion

To conclude the thesis let us provide a brief overview of preceding chapters and main results therein.

In Chapter 2, a previously developed algebraic approach for proving entropy production inequalities is extended to deal with radially symmetric solutions for a class of higher-order evolution equations in multiple space dimensions. In application of the method, novel a priori estimates are derived for the thin-film equation, the fourth-order Derrida-Lebowitz-Speer-Spohn equation, and the sixth-order quantum diffusion equation.

Chapter 3 deals with the Cauchy problem for the sixth-order quantum diffusion equation, whose solutions describe the evolution of the charged particle density in a quantum fluid. The global-in-time existence of weak nonnegative solutions in two and three space dimensions under periodic boundary conditions has been proved. Moreover, these solutions are smooth and classical whenever the particle density is strictly positive, and the long-time convergence to the spatial homogeneous equilibrium at a universal exponential rate has been observed. The analysis strongly uses the Lyapunov property of the physical entropy.

Finally, Chapter 4 brings out novel approximations of the fourth-order Derrida-Lebowitz-Speer-Spohn equation. The semi-discrete two-step backward difference (BDF-2) method of the reformulated equation yields the discrete entropy stability property and second-order convergence of the method in a specific case. Particular variational structure of the equation has been used to introduce the discrete variational derivative method, which preserves dissipation of the Fisher information on a discrete level.

Outlook

The entropy construction method developed in Chapter 2 can be adapted for equations similar to (1.4), where the energy variable x — like the radial variable r in (2.12) — appears explicitly in the equation. For example, the dominating part on the right hand side of (1.4) at low energies and for large n is the cubic term in n. Hence, the nonlinear equation

$$\partial_t n = \frac{1}{\sqrt{x}}\Big[x^{13/2}n^4\Big(\frac{1}{n}\Big)_{xx}\Big]_{xx}\,, \quad x\in(0,L)\,,\ t>0\,, \tag{5.1}$$

describes the asymptotic dynamics of the condensate formation [33]. Corresponding physically motivated boundary conditions are

$$n^4\Big(\frac{1}{n}\Big)_{xx} = 0 \quad \text{and} \quad \Big[x^{13/2}n^4\Big(\frac{1}{n}\Big)_{xx}\Big]_x = 0 \quad \text{as} \quad x\to 0, L\,,$$

which directly imply the Lyapunov property of the functional $E_0[n] = \int_0^L \sqrt{x}\big(n - \log n\big)\mathrm{d}x$. In fact, this is the only entropy among α-functionals, naturally defined by

$$E_\alpha[n] = \frac{1}{\alpha(\alpha-1)}\int_0^L \sqrt{x}n^\alpha \mathrm{d}x\,, \quad \alpha\neq 0,1 \quad \text{and} \quad E_1[n] = \int_0^L \sqrt{x}\big(n\big(\log n - 1\big)+1\big)\mathrm{d}x\,.$$

Employing the homogeneous Neumann boundary condition $n_x = 0$ instead of the second-order condition, more can be done. However, since the Neumann boundary condition is from physical point of view completely irrelevant for the model at hand, the subsequent material is purely artistic work. First, let us write equation (5.1) in the form (cf. (2.12))

$$\partial_t n = \frac{1}{\sqrt{x}}\partial_x\big(x^\beta n^3 D_P[n,x]\big)\,,$$

where $\beta = 13/2$ and $P(\eta,\xi_1,\xi_2,\xi_3) = 2\beta\eta\xi_1^2 + 2\xi_1^3 - \beta\eta\xi_2 + 2\xi_1\xi_2 - \xi_3$ with η now representing $1/x$. Using the no-flux boundary condition, one easily calculates

$$\frac{\mathrm{d}}{\mathrm{d}t}E_\alpha[n(t)] = -\int_0^L x^\beta n^{\alpha+2} D_{S_0}[n]\mathrm{d}x \quad \text{with} \quad S_0(\eta,\xi) = \xi_1 P(\eta,\xi)\,.$$

Based on prescribed boundary conditions (cf. Section 2.2.2), we find a list of basic (linearly independent) shift polynomials

$$\begin{aligned}
T_1(\eta,\xi) &= \beta\eta\xi_1^3 + (\alpha-2)\xi_1^4 + 3\xi_1^2\xi_2\,,\\
T_2(\eta,\xi) &= \beta\eta\xi_1\xi_2 + (\alpha-1)\xi_1^2\xi_2 + \xi_2^2 + \xi_1\xi_3\,,\\
T_3(\eta,\xi) &= (\beta-1)\eta^2\xi_1^2 + (\alpha-1)\eta\xi_1^3 + 2\eta\xi_1\xi_2\,.
\end{aligned}$$

Eventually, we solve the decision problem of the type (2.19) and obtain the following result: *Let n be smooth positive solution to* (5.1) *satisfying homogeneous Neumann and no-flux boundary conditions at the boundary points $x = 0, L$. Then the functionals E_α defined above are entropies if $-(11+2\sqrt{33})/5 \le \alpha \le 1/3$. Moreover, if $-(11+2\sqrt{33})/5 < \alpha < 1/3$, then there exists $c > 0$, such that the estimate of the type (1.6) holds:*

$$\frac{\mathrm{d}}{\mathrm{d}t}E_\alpha[n(t)] + c\int_0^L x^{13/2}\Big[\big(n^{(\alpha+2)/2}\big)_{xx}^2 + \big(n^{(\alpha+2)/4}\big)_x^4\Big]\mathrm{d}x \le 0\,.$$

Concerning the sixth-order equation (3.1) studied in Chapter 3, we propose several questions that we find interesting to consider:

(i) With our entropy construction methods, we are able to prove the dissipation property (3.6) of the physical entropy $\mathcal{H}$ only in dimensions $d \leq 3$. Is $\mathcal{H}$ still a Lyapunov functional in higher dimensions $d \geq 4$?

(ii) Is the Fisher information $\mathcal{F}$ a Lyapunov functional for equation (3.1)? Our only result in this direction so far is a formal proof of dissipation of $\mathcal{F}$ in dimension $d = 1$, given in Appendix D.

(iii) Is the energy $\mathcal{E}$ (defined in (3.8)) monotonically decreasing along the weak solutions constructed in Section 3.4? If the answer is affirmative, then the additional hypotheses that the weak solution is energetic could be removed from Theorem 3.5.

(iv) Does (3.1) admit global weak solutions in dimensions $d \geq 4$? Even if we assume that an inequality of the form (3.6) continues to hold, it is far from clear how to rewrite the weak formulation (3.7) in a form that does not take advantage of Sobolev embeddings in low dimensions.

(v) If (3.1) is posed on $\mathbb{R}^d$ instead of $\mathbb{T}^d$, one readily verfies that there exists a family of self-similar solutions u_s, namely

$$u_s(t;x) = \lambda(t)^{-d} U\big(\lambda(t)^{-1}x\big) \quad \text{with} \quad \lambda(t) = (1+6t)^{1/6}$$

and the Gaussian profile

$$U(z) = \exp\Big(-\frac{|z|^2}{2\sqrt[3]{2}}\Big).$$

Do these "spreading Gaussians" play the same role for (3.1) as they do for the heat equation and for the DLSS equation? In other words, is U an attracting stationary solution of (3.1) after the self-similar rescaling with $x = \lambda(t)\xi$ and $t = (e^{6\tau}-1)/6$, and do arbitrary solutions converge to U at a universal exponential rate? In dimension $d = 1$, there is numerical evidence for an affirmative answer (see Appendix E).

Discrete variational derivative method, presented in Chapter 4 for the DLSS equation, has been employed to solve variety of conservative or dissipative nonlinear PDEs; for example, nonlinear Schrödinger equation, Klein-Gordon equation, Ginzburg-Landau equation, Cahn-Hilliard equation, etc [29]. However, it seems that the method has not been explored yet for dissipative equations of the type

$$\partial_t n = \operatorname{div}\left(\mathfrak{m}(u)\nabla\left(\frac{\delta\mathcal{E}[n]}{\delta n}\right)\right), \tag{5.2}$$

where $\mathfrak{m}$ is so-called mobility function (typically a power function) and $\mathcal{E}$ denotes corresponding energy functional. Equation (5.2), with appropriately defined $\mathfrak{m}$ and $\mathcal{E}$, includes porus-medium equation, thin-film equations and Wasserstein gradient flows in general. If appropriate boundary conditions are imposed, then $\mathcal{E}$ is dissipated along solutions to (5.2), and the key idea of the method is to preserve that property on a discrete level. It is straightforward to generalize the scheme (4.57) for equations of the type (5.2) on the onedimensional torus $\mathbb{T}$. Moreover, it might be fruitful to investigate on possible extensions of the discrete variational derivative method to the multidimensional case on more general domains. In principle, both basic concepts: finite volumes and finite elements could be considered.

Appendices

Appendix A

In this appendix we give a sketch of the derivation of the sixth-order equation (1.3). This equation is formally derived from an $O(\hbar^6)$ approximation of the generalized quantum drift-diffusion model of Degond et al. [21], where $\hbar$ is the scaled Planck constant. Without electric field, this model is given by

$$\partial_t n = \operatorname{div}(n\nabla A), \tag{A.1}$$

where the particle density $n(t;x)$ and the function $A(t;x)$ are related through the integral

$$n(t;x) = \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d} \operatorname{Exp}\left(A(t;x) - \frac{|p|^2}{2}\right) \mathrm{d}p, \quad x \in \mathbb{R}^d,\ t > 0.$$

Here, the so-called quantum exponential Exp is defined by $\operatorname{Exp}(a) = W(\exp(W^{-1}(a)))$, where $a(t;x,p)$ is a function in the phase-space, W is the Wigner transform, W^{-1} its inverse and exp is the operator exponential. For precise definitions and the derivation of the quantum drift-diffusion model we refer to [21].

The crucial step in the $O(\hbar^6)$ derivation of (A.1) is to determine an $O(\hbar^6)$ approximation of $\operatorname{Exp}(a)$ with $a(x,p) = A(t;x) - |p|^2/2$. To this end, we follow the strategy proposed in [21]. Define $F(z) = \operatorname{Exp}(za)$ and expand $F(z)$ formally as a series in $\hbar$, i.e. $F(z) = \sum_{k=0}^{\infty} \hbar^k F_k(z)$. The functions $F_k(z)$ can be computed by pseudo-differential calculus. For odd indices k, we have $F_k(z) = 0$, and for even indices we have to solve the following differential equation:

$$\frac{d}{dz}F_k(z) = a \circ_0 F_k(z) + a \circ_2 F_{k-2}(z) + \ldots + a \circ_k F_0(z), \quad z > 0,$$

with the initial condition $F_k(0) = \delta_{k0}$. The multiplication $\circ_n$ is defined for any two smooth functions ω_1 and ω_2 by (see also (5.19) in [21])

$$\omega_1 \circ_n \omega_2 = \sum_{|\alpha|+|\beta|=n} \left(\frac{i}{2}\right)^n \frac{(-1)^{|\beta|}}{\alpha!\beta!} \partial_x^\alpha \partial_p^\beta \omega_1 \partial_x^\beta \partial_p^\alpha \omega_2, \tag{A.2}$$

where $\alpha, \beta \in \mathbb{N}^d$ are multi-indices.

Let ∇^k denote the k-tensor of partial derivatives of order k, i.e.,

$$\left(\nabla_x^k \omega\right)_{i_1,i_2,\cdots,i_k} = \partial_x^{(i_1,i_2,\ldots,i_k)}\omega, \quad \left(\nabla_p^k \omega\right)_{j_1,j_2,\cdots,j_k} = \partial_p^{(j_1,j_2,\ldots,j_k)}\omega.$$

Lemma A.1. *It holds*

$$\omega_1 \circ_n \omega_2 = \frac{i^n}{2^n n!}\left(\sum_{k=0}^{n}(-1)^k \binom{n}{k}\left(\nabla_x^{n-k}\otimes\nabla_p^k\omega_1\right) : \left(\nabla_p^{n-k}\otimes\nabla_x^k\omega_2\right)\right), \tag{A.3}$$

where "$\otimes$" denotes the tensor product and ":" the component-wise inner product.

Proof. Let $k = |\beta| = \beta_1 + \cdots + \beta_d$ for $\beta \in \mathbb{N}^d$. According to the Schwartz rule, each partial derivative ∂_p^β appears in ∇_p^k on exactly $k!/\beta!$ positions, where $\beta! = \beta_1! \ldots \beta_d!$. Analogusly, for $|\alpha| = n-k$, each ∂_x^α appears at ∇_x^{n-k} on $(n-k)!/\alpha!$ positions. Thus, the expression $\partial_x^\alpha\partial_p^\beta$ appears in $\nabla_x^{n-k}\otimes\nabla_p^k$ on $(n-k)!k!/(\alpha!\beta!)$ positions, and the same number of appearance holds for the expression $\partial_x^\alpha\partial_p^\beta\partial_x^\beta\partial_p^\alpha$ in $(\nabla_x^{n-k}\otimes\nabla_p^k) : (\nabla_p^{n-k}\otimes\nabla_x^k)$. Using these combinatorial observations, formula (A.3) follows immediately. □

The functions $F_0(z)$ and $F_2(z)$ have already been calculated in [21]:

$$\begin{aligned}
F_0(z)(x,p) &= e^{za(x,p)}, \\
F_2(z)(x,p) &= \frac{1}{8}e^{za(x,p)}\Big(z^2\Delta_x A + \frac{z^3}{3}|\nabla_x A|^2 - \frac{z^3}{3}\nabla_x^2 A : p\otimes p\Big).
\end{aligned}$$

Thus, it remains to solve

$$\begin{aligned}
\frac{d}{dz}F_4(z) = a\circ_0 F_4(z) + a\circ_2 F_2(z) + a\circ_4 F_0(z) = a\cdot F_4(z) \\
&+ \frac{e^{za}}{192}\Big[z^5|\nabla A|^4 + 5z^4|\nabla A|^2\Delta A - 2z^5|\nabla A|^2(\nabla^2 A : p\otimes p) \\
&- 4z^4(\nabla^2 A : \nabla^2 A p\otimes p) + z^5(\nabla^2 A : p\otimes p)^2 + 2z^3\|\nabla^2 A\|^2 \\
&- 5z^4\Delta A(\nabla^2 A : p\otimes p) + 6z^3(\Delta A)^2 + 3z^2\Delta^2 A + z^3\Delta|\nabla A|^2 \\
&- z^3\Delta(\nabla^2 A : p\otimes p) + 6z^3\nabla A\cdot\nabla\Delta A + 2z^4\nabla A\cdot\nabla|\nabla A|^2 \\
&- 2z^4\nabla A\cdot\nabla(\nabla^2 A : p\otimes p)\Big] + \frac{\mathbf{e}^{za}}{384}\Big[z^4(\nabla^4 A : p\otimes p\otimes p\otimes p) \\
&- z^3(\nabla^4 A : (p\otimes p\otimes \mathbb{I})) - z^3(\nabla^4 A : p\otimes\nabla_p(p\otimes p)) \\
&- z^3(\nabla^4 A : \nabla_p(p\otimes p\otimes p)) + z^2(\nabla^4 A : \nabla_p(p\otimes\mathbb{I})) \\
&+ z^2(\nabla^4 A : \nabla_p^2(p\otimes p))\Big],
\end{aligned}$$

with $F_4(0) = 0$. In the above computations, we have exhaustively used Lemma A.1. By the variation-of-constants formula, we obtain

$$\begin{aligned}
F_4(1) = \frac{e^a}{384}\Big[&\frac{1}{3}|\nabla A|^4 + 2|\nabla A|^2\Delta A - \frac{2}{3}|\nabla A|^2(\nabla^2 A : p\otimes p)\\
&- \frac{8}{5}(\nabla^2 A : \nabla^2 A p\otimes p) + \frac{1}{3}(\nabla^2 A : p\otimes p)^2 + \|\nabla^2 A\|^2\\
&- 2\Delta A(\nabla^2 A : p\otimes p) + (\Delta A)^2 + 2\Delta^2 A + \frac{1}{2}\Delta|\nabla A|^2\\
&- \frac{1}{2}\Delta(\nabla^2 A : p\otimes p) + 3\nabla A\cdot\nabla\Delta A + \frac{4}{5}\nabla A\cdot\nabla|\nabla A|^2\\
&- \frac{4}{5}\nabla A\cdot\nabla(\nabla^2 A : p\otimes p) + \frac{1}{5}(\nabla^4 A : p\otimes p\otimes p\otimes p)\\
&- \frac{1}{4}\big((\nabla^4 A : (p\otimes p\otimes \mathbb{I})) + (\nabla^4 A : p\otimes \nabla_p(p\otimes p))\\
&+ (\nabla^4 A : \nabla_p(p\otimes p\otimes p))\big) + \frac{1}{3}\big((\nabla^4 A : \nabla_p(p\otimes \mathbb{I}))\\
&+ (\nabla^4 A : \nabla_p^2(p\otimes p))\big)\Big].
\end{aligned}$$

This gives us the $O(\hbar^6)$ expansion of the quantum exponential.

It remains to represent the density u as a function of A. We integrate F_0, F_2, and F_4 with respect to $p \in \mathbb{R}^d$ and employ the formulas

$$\begin{aligned}
\frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d} p_i p_j e^{A-|p|^2/2}\mathrm{d}p &= \frac{e^A}{(\sqrt{2\pi}\hbar)^d}\delta_{ij},\\
\frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d} p_r p_s p_i p_j e^{A-|p|^2/2}\mathrm{d}p &= \frac{e^A}{(\sqrt{2\pi}\hbar)^d}(\delta_{rs}\delta_{ij} + \delta_{ri}\delta_{sj} + \delta_{rj}\delta_{sj}),
\end{aligned}$$

where δ_{ij} denotes the Kronecker symbol. This gives

$$\begin{aligned}
n &= \frac{1}{(2\pi\hbar)^d}\int_{\mathbb{R}^d}(F_0(1) + \hbar^2 F_2(1) + \hbar^4 F_4(1))\mathrm{d}p + O(\hbar^6)\\
&= \frac{e^A}{(\sqrt{2\pi}\hbar)^d}\bigg(1 + \frac{\hbar^2}{24}\Big(2\Delta A + |\nabla A|^2\Big) + \frac{\hbar^4}{5760}\Big(5|\nabla A|^4 + 20|\nabla A|^2\Delta A\\
&\quad + \|\nabla^2 A\|^2 + 20(\Delta A)^2 + 24\Delta^2 A + \frac{15}{2}\Delta|\nabla A|^2 + 33\nabla A\cdot\nabla\Delta A\\
&\quad + 12\nabla A\cdot\nabla|\nabla A|^2\Big)\bigg) + O(\hbar^6).
\end{aligned}$$

To obtain an $\hbar$-expansion of A in terms of n, we insert the ansatz $A = A_0 + \hbar^2 A_2 + \hbar^4 A_4 +$

$O(\hbar^6)$ in the above expression for u. Equating equal powers of $\hbar$ yields the system

$$
\begin{aligned}
n &= \frac{e^{A_0}}{(\sqrt{2\pi})^d}, \quad 0 = A_2 + \frac{1}{24}\big(2\Delta A_0 + |\nabla A_0|^2\big), \\
0 &= A_4 + \frac{1}{2}A_2^2 + \frac{1}{24}A_2\big(2\Delta A_0 + |\nabla A_0|^2\big) + \frac{1}{12}\big(\Delta A_2 + \nabla A_0 \cdot \nabla A_2\big) \\
&\quad + \frac{1}{5760}\Big(5|\nabla A_0|^4 + 20|\nabla A_0|^2\Delta A_0 + \|\nabla^2 A_0\|^2 + 20(\Delta A_0)^2 \\
&\quad + 24\Delta^2 A_0 + \frac{15}{2}\Delta|\nabla A_0|^2 + 33\nabla A_0 \cdot \nabla\Delta A_0 + 12\nabla A_0 \cdot \nabla|\nabla A_0|^2\Big).
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
A_0 &= \log n + d\log(\sqrt{2\pi}), \quad A_2 = -\frac{1}{6}\frac{\Delta\sqrt{n}}{\sqrt{n}}, \\
A_4 &= \frac{1}{720}\Big(2\frac{\Delta^2 n}{n} - 3\frac{|\nabla n|^4}{u^4} + 4\nabla^2 n\nabla n \cdot \nabla n + 4\frac{\Delta n}{n}\frac{|\nabla n|^2}{n^2} - 4\frac{\nabla\Delta n}{n} \cdot \frac{\nabla n}{n} \\
&\quad - 2\Big(\frac{\Delta n}{n}\Big)^2 - \frac{\|\nabla^2 n\|^2}{n^2}\Big) = \frac{1}{360}\Big(\frac{1}{2}\|\nabla^2 \log n\|^2 + \frac{1}{n}\nabla^2 : (n\nabla^2 \log n)\Big).
\end{aligned}
$$

Finally, up to terms of order $O(\hbar^6)$, (A.1) becomes

$$
\partial_t n = \Delta n - \frac{\hbar^2}{6}\operatorname{div}\Big(n\nabla\Big(\frac{\Delta\sqrt{n}}{\sqrt{n}}\Big)\Big) + \frac{\hbar^4}{360}\operatorname{div}\Big(n\nabla\Big(\frac{1}{2}\|\nabla^2 \log n\|^2 + \frac{1}{n}\nabla^2 : (n\nabla^2 \log n)\Big)\Big).
$$

The second term on the right-hand side is the fourth-order operator of the DLSS equation. The sixth-order equation (1.3) is obtained by taking into account only the sixth-order expression and choosing $\hbar^4 = 360$.

Appendix B

The following `Mathematica` notebook has been used in the computer-aided proof of Theorem 2.3.

---

the sixth – order quantum diffusion equation

characteristic polynomial

```
In[1]:= S[{η_, ξ1_, ξ2_, ξ3_}] := ((α - 5) c1 + 6) ξ1^6 + (5 c1 + (α - 4) c2 - 18) ξ1^4 ξ2 + (3 c2 + 11) ξ1^2 ξ2^2 +
          (c2 + (α + 1) (α - 3) + 8) ξ1^3 ξ3 + (3 α - 5) ξ1 ξ2 ξ3 + ((α - 4) c6 + (d - 1) (c1 - 6)) η ξ1^5 +
          ((α - 3) c9 + (d - 2) c6 + (d - 1) (2 d - 7)) η^2 ξ1^4 + ((α - 3) c7 + 4 c6 + (d - 1) (c2 + 14)) η ξ1^3 ξ2 +
          ((d - 3) c9 - 2 (α - 2) (d - 1) + (d - 1) (3 d - 8)) η^3 ξ1^3 + (2 c7 + (α - 6) (d - 1)) η ξ1 ξ2^2 +
          ((α - 2) (d - 1) + 3 c9 + (d - 2) c7 - 3 (d - 1) (d - 4)) η^2 ξ1^2 ξ2 + (c7 - 3 (d - 1)) η ξ1^2 ξ3 +
          (d - 1)^2 η^4 ξ1^2 - 2 (d - 1)^2 η^3 ξ1 ξ2 - 2 (d - 1) η^2 ξ1 ξ3 + 2 (d - 1) η ξ2 ξ3 + (d - 1)^2 η^2 ξ2^2 + ξ3^2;
```

change of variables

```
In[2]:= ξ1 = η / ζ1;  ξ2 = ξ1^2 (ζ1 + ζ2);  ξ3 = ξ1^3 (ζ3 + 3 ζ1 ζ2);
```

choice of particular coefficients – integrations by parts

```
In[3]:= c7 = (d - 1) (α + 1/2);
        c9 = -c7;

In[5]:= Expand[S [{η, ξ1, ξ2, ξ3}] ζ1^6 / η^6 // FullSimplify]
```

characteristic polynomial in new variables

```
In[6]:= S1[{ζ1_, ζ2_, ζ3_}] :=
          6 - 5 c1 + c1 α - 12 ζ1 + 4 c1 ζ1 - 4 c2 ζ1 - 4 c6 ζ1 - 6 d ζ1 + c1 d ζ1 + c2 α ζ1 + c6 α ζ1 + 4 ζ1^2 + 2 c2 ζ1^2 +
          2 c6 ζ1^2 + 5 d ζ1^2 + c2 d ζ1^2 + c6 d ζ1^2 + 2 d^2 ζ1^2 - 18 ζ2 + 5 c1 ζ2 - 4 c2 ζ2 + c2 α ζ2 + 49 ζ1 ζ2/2 +
          8 c2 ζ1 ζ2 + 4 c6 ζ1 ζ2 + 25 d ζ1 ζ2/2 + c2 d ζ1 ζ2 - 7 α ζ1 ζ2/2 - 5/2 d α ζ1 ζ2 + 2 α^2 ζ1 ζ2 + d α^2 ζ1 ζ2 -
          5 ζ1^2 ζ2 - 15/2 d ζ1^2 ζ2 - 5/2 d^2 ζ1^2 ζ2 + 4 α ζ1^2 ζ2 + 4 d α ζ1^2 ζ2 + d^2 α ζ1^2 ζ2 + 11 ζ2^2 + 3 c2 ζ2^2 - 10 ζ1 ζ2^2 -
          5 d ζ1 ζ2^2 + 6 α ζ1 ζ2^2 + 3 d α ζ1 ζ2^2 + 4 ζ1^2 ζ2^2 + 4 d ζ1^2 ζ2^2 + d^2 ζ1^2 ζ2^2 + 5 ζ3 + c2 ζ3 - 2 α ζ3 + α^2 ζ3 -
          5 ζ1 ζ3/2 - 5 d ζ1 ζ3/2 + 2 α ζ1 ζ3 + d α ζ1 ζ3 - 5 ζ2 ζ3 + 3 α ζ2 ζ3 + 4 ζ1 ζ2 ζ3 + 2 d ζ1 ζ2 ζ3 + ζ3^2;
```

the discriminant with minus sign

```
In[7]:= Expand[- (D[S1[{ζ1, ζ2, ζ3}], ζ3] /. {ζ3 → 0})^2 + 4 S1[{ζ1, ζ2, 0}]]

Out[7]= - 1 - 20 c1 - 10 c2 - c2^2 + 20 α + 4 c1 α + 4 c2 α - 14 α^2 - 2 c2 α^2 + 4 α^3 - α^4 - 23 ζ1 + 16 c1 ζ1 - 11 c2 ζ1 -
         16 c6 ζ1 + d ζ1 + 4 c1 d ζ1 + 5 c2 d ζ1 - 30 α ζ1 + 4 c6 α ζ1 - 20 d α ζ1 - 2 c2 d α ζ1 + 13 α^2 ζ1 +
         9 d α^2 ζ1 - 4 α^3 ζ1 - 2 d α^3 ζ1 + 39 ζ1^2/4 + 8 c2 ζ1^2 + 8 c6 ζ1^2 + 15 d ζ1^2/2 + 4 c2 d ζ1^2 + 4 c6 d ζ1^2 +
         7 d^2 ζ1^2/4 + 10 α ζ1^2 + 15 d α ζ1^2 + 5 d^2 α ζ1^2 - 4 α^2 ζ1^2 - 4 d α^2 ζ1^2 - d^2 α^2 ζ1^2 - 22 ζ2 + 20 c1 ζ2 -
         6 c2 ζ2 - 50 α ζ2 - 2 c2 α ζ2 + 22 α^2 ζ2 - 6 α^3 ζ2 + 33 ζ1 ζ2 + 24 c2 ζ1 ζ2 + 16 c6 ζ1 ζ2 + 5 d ζ1 ζ2 +
         37 α ζ1 ζ2 + 23 d α ζ1 ζ2 - 12 α^2 ζ1 ζ2 - 6 d α^2 ζ1 ζ2 + 19 ζ2^2 + 12 c2 ζ2^2 + 30 α ζ2^2 - 9 α^2 ζ2^2
```

coefficients like in Lemma 3.1

```
d = 3; (*specify the dimension*)
a1 = -1 - 20 c1 - 10 c2 - c2^2 + 20 α + 4 c1 α + 4 c2 α - 14 α^2 - 2 c2 α^2 + 4 α^3 - α^4 // Simplify;
a2 = -23 ξ1 + 16 c1 ξ1 - 11 c2 ξ1 - 16 c6 ξ1 + d ξ1 + 4 c1 d ξ1 + 5 c2 d ξ1 - 30 α ξ1 + 4 c6 α ξ1 -
      20 d α ξ1 - 2 c2 d α ξ1 + 13 α^2 ξ1 + 9 d α^2 ξ1 - 4 α^3 ξ1 - 2 d α^3 ξ1 /. {ξ1 → 1} // Simplify;
a3 = 39 ξ1^2/4 + 8 c2 ξ1^2 + 8 c6 ξ1^2 + 15 d ξ1^2/2 + 4 c2 d ξ1^2 + 4 c6 d ξ1^2 + 7 d^2 ξ1^2/4 + 10 α ξ1^2 +
      15 d α ξ1^2 + 5 d^2 α ξ1^2 - 4 α^2 ξ1^2 - 4 d α^2 ξ1^2 - d^2 α^2 ξ1^2 /. {ξ1 → 1} // Simplify;
a4 = -22 ξ2 + 20 c1 ξ2 - 6 c2 ξ2 - 50 α ξ2 - 2 c2 α ξ2 + 22 α^2 ξ2 - 6 α^3 ξ2 /. {ξ2 → 1} // Simplify;
a5 = 19 ξ2^2 + 12 c2 ξ2^2 + 30 α ξ2^2 - 9 α^2 ξ2^2 /. {ξ2 → 1} // Simplify;
a6 = 33 ξ1 ξ2 + 24 c2 ξ1 ξ2 + 16 c6 ξ1 ξ2 + 5 d ξ1 ξ2 + 37 α ξ1 ξ2 +
      23 d α ξ1 ξ2 - 12 α^2 ξ1 ξ2 - 6 d α^2 ξ1 ξ2 /. {ξ1 → 1, ξ2 → 1} // Simplify;
```

eliminate existence quantifiers

```
Reduce[
  Exists[{c1, c2, c6}, a3 > 0 && (4 a3 a5 - a6^2 > 0 && 4 a1 a3 a5 - a3 a4^2 - a2^2 a5 - a1 a6^2 + a2 a4 a6 ≥ 0 ||
        4 a3 a5 - a6^2 == 0 && 2 a4 a3 - a2 a6 == 0 && 4 a3 a1 - a2^2 ≥ 0) || a3 == 0 && a2 == 0 &&
      a6 == 0 && (a5 > 0 && 4 a5 a1 - a4^2 ≥ 0 || a4 == 0 && a5 == 0 && a1 ≥ 0)]] // FullSimplify
```

```
Root[393 601 781 429 741 700 - 30 869 921 438 354 950 920 #1 + 909 136 653 589 444 589 613 #1^2 -
    13 067 554 891 693 074 455 322 #1^3 + 107 071 198 804 242 721 933 029 #1^4 -
    530 285 185 987 109 657 337 150 #1^5 + 1 485 065 531 007 236 342 067 360 #1^6 -
    903 670 068 054 124 067 973 182 #1^7 - 11 349 670 571 166 667 138 590 671 #1^8 +
    56 577 657 354 736 919 146 273 378 #1^9 - 147 230 360 918 572 718 046 770 295 #1^10 +
    231 738 416 778 937 419 353 125 992 #1^11 - 152 027 093 646 093 153 304 987 580 #1^12 -
    284 596 131 667 929 366 633 259 084 #1^13 + 1 101 664 331 459 877 604 997 419 944 #1^14 -
    2 005 868 470 113 009 076 388 148 352 #1^15 + 2 528 368 657 408 139 905 354 920 900 #1^16 -
    2 393 183 070 603 095 081 573 333 536 #1^17 + 1 741 484 151 169 186 832 842 089 152 #1^18 -
    974 340 654 437 711 767 044 765 696 #1^19 + 412 502 928 272 845 793 838 861 312 #1^20 -
    127 825 181 451 243 356 527 042 560 #1^21 + 27 303 715 635 205 678 822 932 480 #1^22 -
    3 581 686 556 834 839 599 513 600 #1^23 + 216 469 226 809 568 762 265 600 #1^24 &, 5] ≤ α ≤
 Root[393 601 781 429 741 700 - 30 869 921 438 354 950 920 #1 + 909 136 653 589 444 589 613 #1^2 -
    13 067 554 891 693 074 455 322 #1^3 + 107 071 198 804 242 721 933 029 #1^4 -
    530 285 185 987 109 657 337 150 #1^5 + 1 485 065 531 007 236 342 067 360 #1^6 -
    903 670 068 054 124 067 973 182 #1^7 - 11 349 670 571 166 667 138 590 671 #1^8 +
    56 577 657 354 736 919 146 273 378 #1^9 - 147 230 360 918 572 718 046 770 295 #1^10 +
    231 738 416 778 937 419 353 125 992 #1^11 - 152 027 093 646 093 153 304 987 580 #1^12 -
    284 596 131 667 929 366 633 259 084 #1^13 + 1 101 664 331 459 877 604 997 419 944 #1^14 -
    2 005 868 470 113 009 076 388 148 352 #1^15 + 2 528 368 657 408 139 905 354 920 900 #1^16 -
    2 393 183 070 603 095 081 573 333 536 #1^17 + 1 741 484 151 169 186 832 842 089 152 #1^18 -
    974 340 654 437 711 767 044 765 696 #1^19 + 412 502 928 272 845 793 838 861 312 #1^20 -
    127 825 181 451 243 356 527 042 560 #1^21 + 27 303 715 635 205 678 822 932 480 #1^22 -
    3 581 686 556 834 839 599 513 600 #1^23 + 216 469 226 809 568 762 265 600 #1^24 &, 6]
```

evaluate these roots numerically

```
% // N
```

```
0.347013 ≤ α ≤ 1.05174
```

Appendix C

Here we provide a collection of functional inequalities and other known results used throughout calculations in Chapters 3 and 4.

Lemma C.1. *Let $m \in \mathbb{N}$ be given. Then there exists a constant $C > 0$ such that for all $u \in H^m(\mathbb{T}^d)$,*

$$\|u\|_{H^m} \leq C\big(\|\nabla^m u\|_{L^2} + \|u\|_{L^2}\big).$$

Lemma C.2. *Let $m, n \in \mathbb{N}$ and $1 \leq p, r \leq \infty$ be given and assume that $n - d/r < m - d/p$. Then the Sobolev space $W^{m,p}(\mathbb{T}^d)$ embeds compactly into $W^{n,r}(\mathbb{T}^d)$. In the borderline case, if $n - d/r = m - d/p$ is not an integer, the embedding is still continuous.*

The following result is from [62, p.1034]).

Lemma C.3 (Gagliardo–Nirenberg inequality)**.** *Let $m,\ n \in \mathbb{N}_0$ with $m > n$ and let $1 \leq p, q, r \leq \infty$. Assume that there exists $\theta \in (0, 1)$ such that*

$$n - \frac{d}{r} = \theta\Big(m - \frac{d}{p}\Big) - (1-\theta)\frac{d}{q}.$$

There exists a constant $B > 0$ such that for all $u \in W^{m,p}(\mathbb{T}^d)$,

$$\|\nabla^n u\|_{L^r(\Omega)} \leq B\|u\|^{\theta}_{W^{m,p}}\|u\|^{1-\theta}_{L^q} \tag{C.1}$$

Estimates on square roots play a key role in the proofs of our results. The following result is a consequence of Théorème 1 (ii) in [47].

Lemma C.4. *Let $1 < p \leq \infty$. Then there exists a constant $C_{\mathrm{LV}} > 0$ such that for all nonnegative function $u \in W^{2,p}(\mathbb{T}^d)$,*

$$\|\sqrt{u}\|^2_{W^{1,2p}(\mathbb{T}^d)} \leq C_{\mathrm{LV}}\|u\|_{W^{2,p}(\mathbb{T}^d)}. \tag{C.2}$$

Proof. Let $\phi \in C^2(\mathbb{R})$ be a nonnegative cut-off function satisfying $\phi(x) = 1$ for $0 \leq x \leq 1$, and $\phi(x) = 0$ for $x \geq 2$ and for $x \leq -1$. Define accordingly $\phi_d \in C^2(\mathbb{R}^d)$ by

$$\phi_d(x_1, x_2, \ldots, x_d) = \phi(x_1)\phi(x_2)\cdots\phi(x_d). \tag{C.3}$$

Given $u \in W^{2,p}(\mathbb{T}^d)$, consider $w \in W^{2,p}(\mathbb{R}^d)$ with $w(x) = \phi_d(x)\,\mathrm{E}\,u(x)$; recall that $\mathrm{E}\,u$ is the periodic extension of u to $\mathbb{R}^d$. By definition of ϕ_d, we have $w(x) = \mathrm{E}\,u(x)$ for $x \in [0,1]^d$ and $\operatorname{supp} w \subset [-1,2]^d$. On one hand,

$$\begin{aligned}\|\,\mathrm{D}\sqrt{u}\|^{2p}_{L^{2p}(\mathbb{T}^d)} &= \sum_{j=1}^{d}\int_{[0,1]^d}|\partial_j\sqrt{\mathrm{E}\,u(x)}|^{2p}\,\mathrm{d}x \\ &\leq \sum_{j=1}^{d}\int_{\mathbb{R}^d}|\partial_j\sqrt{w(x)}|^{2p}\,\mathrm{d}x = \|\,\mathrm{D}\sqrt{w}\|^{2p}_{L^{2p}(\mathbb{R}^d)}.\end{aligned} \tag{C.4}$$

On the other hand, with constants A_p, $B_d > 0$,

$$
\begin{aligned}
\| \mathrm{D}^2 w\|_{L^p(\mathbb{R}^d)}^p &= \sum_{1\le j\le k\le d} \int_{\mathbb{R}^d} |\partial_{jk}^2 w(x)|^p \,\mathrm{d}x \\
&= \sum_{1\le j\le k\le d} \int_{\mathbb{R}^d} \left|\partial_{jk}^2\phi_d \,\mathrm{E}\, u + \partial_j\phi_d\partial_k \,\mathrm{E}\, u + \partial_k\phi_d\partial_j \,\mathrm{E}\, u + \phi_d\, \partial_{jk}^2 \,\mathrm{E}\, u\right|^p \mathrm{d}x \\
&\le A_p\|\phi_d\|_{C^2(\mathbb{R}^d)}^p \sum_{1\le j\le k\le d} \int_{[-1,2]^d} \big(|\,\mathrm{E}\, u|^p + |\partial_j \,\mathrm{E}\, u|^p + |\partial_j \,\mathrm{E}\, u|^p + |\partial_{jk}^2 \,\mathrm{E}\, u|^p\big) \,\mathrm{d}x \\
&\le A_pB_d\|\phi_d\|_{C^2(\mathbb{R}^d)}^p\|u\|_{W^{2,p}(\mathbb{T}^d)}^p. \qquad \text{(C.5)}
\end{aligned}
$$

By Théorème 1 (ii) in [47],

$$
\| \mathrm{D}\sqrt{w}\|_{L^{2p}(\mathbb{R}^d)}^{2p} \le K\| \mathrm{D}^2 w\|_{L^p(\mathbb{R}^d)}^p, \qquad \text{(C.6)}
$$

where $K > 0$ only depends on d and p. Then, combining (C.4) with (C.5) via (C.6), it follows that

$$
\| \mathrm{D}\sqrt{u}\|_{L^{2p}(\mathbb{T}^d)}^{2p} \le A_pB_dK\|\phi_d\|_{C^2(\mathbb{R}^d)}^d\|u\|_{W^{2,p}(\mathbb{T}^d)}^p.
$$

Finally, observe that, trivially,

$$
\|\sqrt{u}\|_{L^{2p}(\mathbb{T}^d)}^{2p} = \|u\|_{L^p(\mathbb{T}^d)}^p \le \|u\|_{W^{2,p}(\mathbb{T}^d)}^p.
$$

Hence, (C.2) holds with the constant

$$
C_{\mathrm{LV}} = \big(1 + A_pB_dK\|\phi_d\|_{C^2(\mathbb{R}^d)}^p\big)^{1/p},
$$

ending the proof. □

Next, we quote the key inequality in the existence proof of global weak solutions to the DLSS equation, proved in [36, Lemma 2.2]. It is in analogy to the inequality from Lemma 3.8 related to the sixth-order equation.

Lemma C.5. *Let $u \in H^2(\mathbb{T}^d)\cap W^{1,4}(\mathbb{T}^d)\cap L^\infty(\mathbb{T}^d)$ in dimension $d \ge 2$ be strictly positive. Then, for any $0 < \alpha < 2(d+1)/(d+2)$,*

$$
\frac{1}{2(\alpha-1)}\int_{\mathbb{T}^d} u^2\partial_{ij}^2(\log u)\partial_{ij}^2(u^{2(\alpha-1)})\mathrm{d}x \ge \kappa_\alpha \int_{\mathbb{T}^d} (\Delta u^\alpha)^2\mathrm{d}x\,, \qquad \text{(C.7)}
$$

if $\alpha \ne 1$, or

$$
\int_{\mathbb{T}^d} u^2\partial_{ij}^2(\log u)^2\mathrm{d}x \ge \kappa_1 \int_{\mathbb{T}^d} (\Delta u)^2\mathrm{d}x\,, \qquad \text{(C.8)}
$$

if $\alpha = 1$, respectively, where

$$
\kappa_\alpha = \frac{p(\alpha)}{\alpha^2(p(\alpha)-p(0))} \quad \text{and} \quad p(\alpha) = -\alpha^2 + \frac{2(d+1)}{d+2}\alpha - \Big(\frac{d-1}{d+2}\Big)^2. \qquad \text{(C.9)}
$$

Furthermore, if the stronger condition $(\sqrt{d}-1)^2/(d+2) < \alpha < (\sqrt{d}+1)^2/(d+2)$ holds, then $\kappa_\alpha > 0$.

The following result is proved in [37, Appendix]. It is needed to obtain strong convergence of the sequences $(\sqrt{u_n})$ or $(\sqrt[4]{u_n})$, given strong convergence of the sequence (u_n) and a uniform bound on $(\sqrt[4]{u_n})$ or $(\sqrt[6]{u_n})$, respectively.

Proposition C.6. *Let $0 < \beta < \gamma < \alpha < \infty$, $1 < p, q, r < \infty$ be given, where $\alpha p = \beta q = \gamma r$. Assume that (u_n) is a sequence of strictly positive functions on $\mathbb{T}^d$ with the following properties:*

1. *u_n^α converges strongly to u^α in $W^{1,p}(\mathbb{T}^d)$, and*
2. *u_n^β is bounded in $W^{1,q}(\mathbb{T}^d)$.*

Then u_n^γ converges strongly to u^γ in $W^{1,r}(\mathbb{T}^d)$.

The respective result holds for sequences of nonnegative functions $u_n : (0,T) \times \mathbb{T}^d \to \mathbb{R}$ upon replacing $W^{1,s}(\mathbb{T}^d)$ by $L^s(0,T;W^{1,s}(\mathbb{T}^d))$ for, respectively, $s = p, q, r$.

Finally, we recall a particular variant of the Leray–Schauder theorem that has been proven in [55].

Theorem C.7 (Leray–Schauder)**.** *Let X be a Banach space and let $B \subset X$ be a closed and convex set such that the zero element of X is contained in the interior of B. Furthermore, let $S : B \times [0,1] \to X$ be a continuous map such that its range $S(B \times [0,1])$ is relatively compact in X. Assume that $S(x,\sigma) \neq x$ for all $x \in \partial B$ and $\sigma \in [0,1]$ and that $S(\partial B \times \{0\}) \subset B$. Then there exists $x_0 \in B$ such that $S(x_0,1) = x_0$.*

Appendix D

In this appendix we provide a fromal proof of the Lyapunov property for the Fisher information along smooth positive solutions to the sixth-order quantum diffusion equation in space dimesion $d = 1$. The proof is based on the entropy construction method from [35].

Proposition D.1. *Let n be smooth and positive solution to equation* (3.1) *on the onedimesional torus $\mathbb{T}$. Then the Fisher information $\mathcal{F}[n] = \int_{\mathbb{T}} (\sqrt{n})_x^2 \mathrm{d}x$ is monotonically decreasing in time, i.e.*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[n(t)] \le 0 \quad \text{for all } t > 0\,.$$

Proof. According to Lemma 3.6, the sixth-order equation is for smooth positive solutions equivalent to

$$\partial_t n = (n(\log n)_{xxx})_{xxx} + 2(n(\log n)_{xx}^2)_{xx}\,,$$

and using the standard change of variables $\log n = y$, the latter becomes

$$\partial_t y = e^{-y}(e^y y_{xxx})_{xxx} + 2e^{-y}(e^y y_{xx}^2)_{xx}\,. \tag{D.1}$$

The Fisher information in new variable reads as

$$\mathcal{F}[n] = \int_{\mathbb{T}} (\sqrt{n})_x^2 \mathrm{d}x = \int_{\mathbb{T}} e^y y_x^2 \mathrm{d}x.$$

Integrating by parts, the time derivative of the Fisher information along solutions to (D.1) is calculated:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[n(t)] &= \frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathbb{T}} e^y y_x^2 \mathrm{d}x = \int_{\mathbb{T}} e^y (y_x^2 y_t + 2y_x y_{xt})\mathrm{d}x = -\int_{\mathbb{T}} e^y (y_x^2 + 2y_{xx}) y_t \mathrm{d}x \\ &= -\int_{\mathbb{T}} (y_x^2 + 2y_{xx})\big[(e^y y_{xxx})_{xxx} + 2(e^y y_{xx}^2)_{xx}\big]\mathrm{d}x \\ &= -\int_{\mathbb{T}} (y_x^2 + 2y_{xx})\big[e^y(y_x y_{xxx} + y_{xxxx} + 2y_{xx}^2)\big]_{xx}\mathrm{d}x \\ &= -\int_{\mathbb{T}} e^y (y_x^2 + 2y_{xx})_{xx}(y_x y_{xxx} + y_{xxxx} + 2y_{xx}^2)\mathrm{d}x \\ &= -2\int_{\mathbb{T}} e^y (y_{xx}^2 + y_x y_{xxx} + y_{xxxx})(y_x y_{xxx} + y_{xxxx} + 2y_{xx}^2)\mathrm{d}x \\ &= -2\int_{\mathbb{T}} e^y S_0(y_x, y_{xx}, \ldots)\mathrm{d}x\,,\end{aligned}$$

where the polynomial S_0 equals

$$S_0(\xi) = 2\xi_2^4 + 3\xi_1\xi_2^2\xi_3 + 3\xi_2^2\xi_4 + \xi_1^2\xi_3^2 + 2\xi_1\xi_3\xi_4 + \xi_4^2\,.$$

In order to prove the Lyapunov property for $\mathcal{F}$, we use integration by parts in a systematic way [35]. Symbol S_0 is of order 8, but only variables $\xi_1, \ldots, \xi_4$ appear in its definition. Thus, it is enough to consider only the following 8 integration by parts formulae and corresponding shift polynomials:

$$\begin{aligned}
I_1 &= \int_{\mathbb{T}} (e^y y_{xx}^2 y_{xxx})_x & &\rightsquigarrow & T_1(\xi) &= \xi_1\xi_2^2\xi_3 + 2\xi_2\xi_3^2 + \xi_2^2\xi_4,\\
I_2 &= \int_{\mathbb{T}} (e^y y_x y_{xxx}^2)_x & &\rightsquigarrow & T_2(\xi) &= \xi_1^2\xi_3^2 + \xi_2\xi_3^2 + 2\xi_1\xi_3\xi_4,\\
I_3 &= \int_{\mathbb{T}} (e^y y_x y_{xx}^3)_x & &\rightsquigarrow & T_3(\xi) &= \xi_1^2\xi_2^3 + \xi_2^4 + 3\xi_1\xi_2^2\xi_3,\\
I_4 &= \int_{\mathbb{T}} (e^y y_x^2 y_{xx} y_{xxx})_x & &\rightsquigarrow & T_4(\xi) &= \xi_1^3\xi_2\xi_3 + 2\xi_1\xi_2^2\xi_3 + \xi_1^2\xi_3^2 + \xi_1^2\xi_2\xi_4,\\
I_5 &= \int_{\mathbb{T}} (e^y y_x^3 y_{xx}^2)_x & &\rightsquigarrow & T_5(\xi) &= \xi_1^4\xi_2^2 + 3\xi_1^2\xi_2^3 + 2\xi_1^3\xi_2\xi_3,\\
I_6 &= \int_{\mathbb{T}} (e^y y_x^4 y_{xxx})_x & &\rightsquigarrow & T_6(\xi) &= \xi_1^5\xi_3 + 4\xi_1^3\xi_2\xi_3 + \xi_1^4\xi_4,\\
I_7 &= \int_{\mathbb{T}} (e^y y_x^5 y_{xx})_x & &\rightsquigarrow & T_7(\xi) &= \xi_1^6\xi_2 + 5\xi_1^4\xi_2^2 + \xi_1^5\xi_3,\\
I_8 &= \int_{\mathbb{T}} (e^y y_x^7)_x & &\rightsquigarrow & T_8(\xi) &= \xi_1^8 + 7\xi_1^6\xi_2.
\end{aligned}$$

These integration by parts formulae correspond to nonnegative integer solutions of the equation $p_1 + 2p_2 + 3p_3 + 4p_4 + 5p_5 + 6p_6 + 7p_7 = 7$ with $p_4 = \ldots = p_7 = 0$.

We are looking for a polynomial S of the form $S(\xi) = S_0(\xi) + \sum_{i=1}^{8} c_i T_i(\xi)$, which satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t} F[n(t)] = -\int_{\mathbb{T}} e^y S(y_x, y_{xx}, \ldots)\mathrm{d}x\,,$$

and there exist real coefficients c_i such that $S(\xi) \geq 0$ for all $\xi = (\xi_1, \xi_2, \xi_3, \xi_4) \in \mathbb{R}^4$. If such polynomial S, i.e. coefficients $c_i \in \mathbb{R}$ can be found, then this formally gives a proof of the Lyapunov property.

Firstly, the above decision problem can be optimized by using the sum of squares optimization tool available in MATLAB toolbox `yalmip` [48]. In particular, we obtain the following choice of coefficients to be useful:

$$c_2 = -2c_1, \quad c_3 = 0, \quad c_4 = \frac{1}{2}, \quad c_5 = \frac{1}{4}, \quad c_6 = -\frac{3}{50}, \quad c_7 = -\frac{1}{100}.$$

After changing polynomial variables to $x = \xi_2/\xi_1^2$, $y = \xi_3/\xi_1^3$ and $z = \xi_4/\xi_1^4$, we calculate $S(\xi) = \xi_1^8 S_{c_1,c_8}(x, y, z)$ with

$$\begin{aligned} S_{c_1,c_8}(x,y,z) = 2x^4 + \Big(\frac{3}{2} - 2c_1\Big)y^2 + z^2 + (c_1+4)x^2y + (c_1+3)x^2z + (2-4c_1)yz \\ + \frac{19}{25}xy + \frac{1}{2}xz + \frac{3}{4}x^3 + \frac{1}{5}x^2 + \Big(7c_8 - \frac{1}{100}\Big)x - \frac{7}{100}y - \frac{3}{50}z + c_8\,. \end{aligned}$$

Finally, it remains to solve the polynomial decision problem

$$\exists c_1, c_8 \in \mathbb{R} : \forall x, y, z \in \mathbb{R} : \; S_{c_1,c_8}(x,y,z) \geq 0\,.$$

This has been done by the computer algebra software `Mathematica` applying the command `Reduce`, which uses an implementation of CAD algoritham for quantifier eliminations. The result is affirmative and consequently, the Fisher information is a Lyapunov functional for equation (3.1). □

Appendix E

In the last appendix we provide a numerical evidence (in $d = 1$), which shows in favor of the question (v) (page 103) about the long-time asymptotics of the sixth-order equation (3.1) posed on $\mathbb{R}$. After the self-similar rescaling with $x = (1+6t)^{1/6}y$, $t = (e^{6s}-1)/6$ and equivalent reformulation according to Lemma 3.6, the function

$$v(s;y) := (1+6t)^{1/6}n(t;x)$$

solves the equation

$$\partial_s v = (v(\log v)_{yyy})_{yyy} + 2(v(\log v)_{yy}^2)_{yy} + (yv)_y\,, \quad y \in \mathbb{R}\,,\ s > 0\,. \tag{E.1}$$

One easily deduces the stationary solution of (E.1); $v_\infty(y) = \mathfrak{c}\exp(-y^2/2\sqrt[3]{2})$, where the positive parameter $\mathfrak{c}$ is chosen to adjust the mass according to given initial condition.

In order to perform numerical experiments we have to restrict our domain to a finite symmetric interval $(-L, L) \subset \mathbb{R}$, and for simplicity we impose periodic boundary conditions. Equation (E.1) is then discretized by the implicit Euler in time and standard finite differences in space:

$$\begin{aligned}\frac{V_i^{k+1}-V_i^k}{\tau} &= \delta_i^{\langle 3\rangle}(V_i^{k+1}\delta_i^{\langle 3\rangle}(\log V_i^{k+1})) + 2\delta_i^{\langle 2\rangle}\big(V_i^{k+1}(\delta_i^{\langle 2\rangle}(\log V_i^{k+1}))^2\big) \qquad \text{(E.2)}\\ &\quad + \frac{1}{4h^2}\big(V_{i+1}^{k+1}(y_{i+1}^2-y_i^2) + V_i^{k+1}(y_{i+1}^2-2y_i^2+y_{i-1}^2) - V_{i-1}^{k+1}(y_i^2-y_{i-1}^2)\big)\,,\\ V_i^{k+1} &= V_{i+lN}^{k+1}\,, \quad l \in \mathbb{Z}\,, \quad i = 0,\dots,N-1\,,\ k \geq 0\,, \qquad \text{(E.3)}\end{aligned}$$

where $V_i^k \approx v(s_k;y_i)$, $h = 2L/N$, $\tau > 0$ is a given time step and the finite difference operator $\delta_i^{\langle 3\rangle}$ is defined by

$$\delta_i^{\langle 3\rangle}V_i = \frac{1}{2h^3}(V_{i+2} - 2V_{i+1} + 2V_{i-1} - V_{i-2})\,.$$

Note that the convection term $(yv)_y$ is first substituted with $(\Theta_y v)_y$, where $\Theta = y^2/2$, and then discretized. For a given initial data $V^0 \approx v_0$, nonlinear system (E.2)–(E.3) is solved by the standard Newton iterative method, where we take the solution from the previous time step as an initial guess in the next step.

Example E.1. Numerical test presented here assumes the following: interval length $2L = 10$, mesh size $h = 0.05$, time step $\tau = 10^{-3}$ and initial condition $v_0(y) = \varepsilon(\sin(\pi y/L) + 3)$ with $\varepsilon = 0.0938$. Figures E.1(a)-(d) convincingly show convergence of numerical solutions $\{V^k\}_{k\geq 0}$ to certain stationary profile, which we denote by V^∞. Here we approximated V^∞ by V^{3000}.

Nevertheless, the observed convergence can be even further numerically explored. Let us introduce the perturbed entropy functional defined by

$$\widetilde{\mathcal{H}}[v] = \int_{\mathbb{R}} v\log v\,\mathrm{d}y + \frac{1}{2\sqrt[3]{2}}\int_{\mathbb{R}} y^2 v\,\mathrm{d}y\,.$$

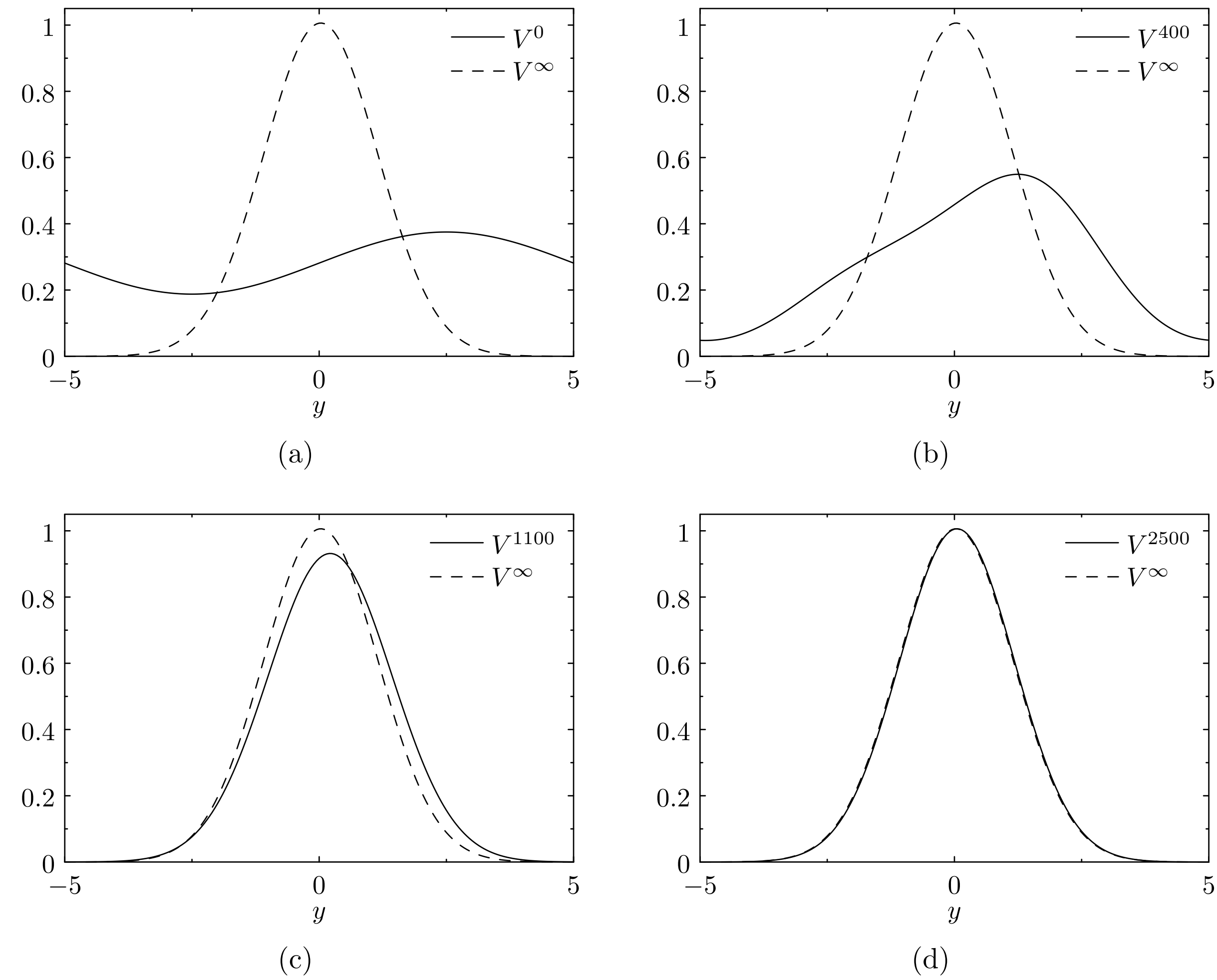


Figure E.1: Convergence of numerical solutions V^k of system (E.2)–(E.3) towards the stationary profile V^∞: (a) $s_0 = 0$, (b) $s_{400} = 0.4$, (c) $s_{1100} = 1.1$, (d) $s_{2500} = 2.5$.

Its definition is motivated in order to satisfy $\widetilde{\mathcal{H}}[v_\infty] = 0$ and we will use it to measure the convergence of numerical solutions $\{V^k\}_{k\geq 0}$ to the corresponding stationary profile V^∞. In fact, we have to reformulate $\widetilde{\mathcal{H}}$ slightly, since on finite intervals V^∞ is never the perfect Gaussian and thus $\widetilde{\mathcal{H}}[V^\infty] > 0$. Therefore, we adapt $\widetilde{\mathcal{H}}$ relatively to V^∞ by defining

$$\widetilde{\mathcal{H}}_{\mathrm{d}}[V] := \widetilde{\mathcal{H}}[V] - \widetilde{\mathcal{H}}[V^\infty]\,.$$

Above, $\widetilde{\mathcal{H}}[V]$ is to be understood in the sense of some quadrature rule, which approximates corresponding integrals. In our computations we use the composite Simpson's rule.

Figures E.2(a)-(b) below, show an exponential decay to zero of the perturbed entropy $\widetilde{\mathcal{H}}_{\mathrm{d}}$ along solutions $\{V^k\}_{k\geq 0}$ from Example E.1 and an exponential decay to zero of the L^1-norm of the sequence $\{V^k - V^\infty\}_{k\geq 0}$. The dashed lines indicate upper bounds for the convergence. These numerically established convergence results parallel to those obtained for the confined fast diffusion equation (second-order Fokker-Planck equation) [8] and for a family of confined nonlinear fourth-order equations [51]. Especially interesting result in [8] is the proof for sharp decay rate of the relative entropy along solutions to the fast diffusion equation, which has been performed via formal linearization of the equation aroud the stationary profile and applying a sharp Hardy-Poincaré inequality. The sharp decay rate equals -2Λ, where Λ denotes the optimal constant in the Hardy-Poincaré inequality and coincides with the spectral gap of the corresponding linear operator. Moreover, the optimal rates are saturated for translatations of the stationary profile [22].

Expanding a solution v of (E.1) in terms of an ε-perturbation w around v_∞,

$$v(s;y) = (1 + \varepsilon w(s;y))v_\infty(y)\,,$$

and keeping only first-order terms in ε, yields the linear equation for w,

$$\partial_s w + Lw = 0\,,$$

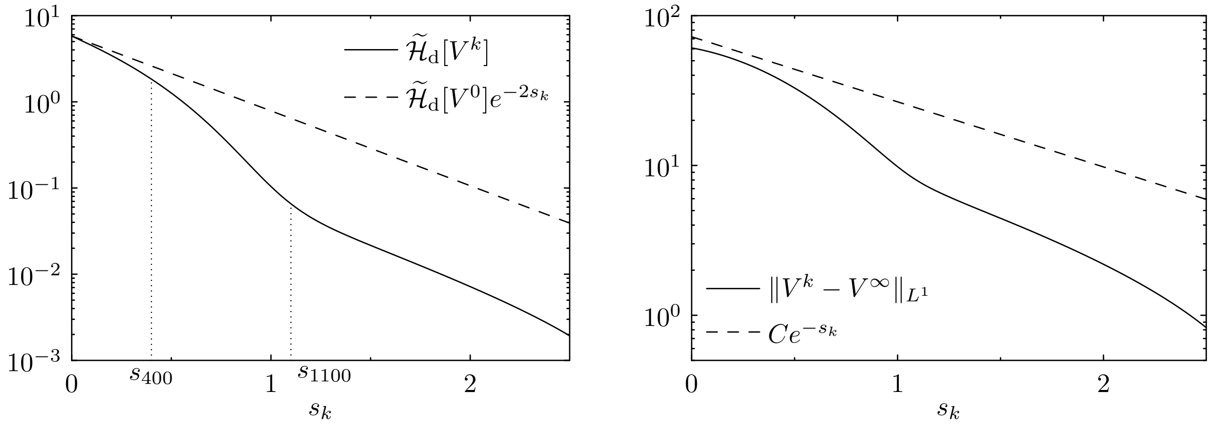
with $Lw = -\partial_y^6 w + \frac{3}{\sqrt[3]{2}} y\partial_y^5 w - (\frac{3}{\sqrt[3]{4}}y^2 + \frac{7}{\sqrt[3]{2}})\partial_y^4 w - (\frac{11}{\sqrt[3]{4}}y + \frac{1}{2}y^3)\partial_y^3 w - (3\sqrt[3]{2} - 2y^2)w_{yy} + yw_y$. Using additional change of variables $z = y/\sqrt[6]{2}$, operator L admits a Sturm-Liouville form [46],

$$Lw = -e^{z^2/2}\Big[2(e^{-z^2/2}w_{zzz})_{zzz} - 4\sqrt[3]{2}(e^{-z^2/2}w_{zz})_{zz} + \sqrt[3]{4}(e^{-z^2/2}w_z)_z\Big]\,.$$

Solutions of the eigenvalue problem $Lw = \lambda w$ are properly scaled Hermite polynomials

$$p_n(y) = 2^{n/6}H_n(y/\sqrt[6]{2})\,, \quad \text{where} \;\; H_n(z) = (-1)^n e^{z^2/2}\frac{\mathrm{d}^n}{\mathrm{d}z^n}e^{-z^2/2}\,,$$

with corresponding eigenvalues $\lambda_n = n^2(n+1)/2$. Obviously, the smallest nontrivial eigenvalue (spectral gap) is $\lambda_1 = 1$.



(a) (b)

Figure E.2: Exponential convergence of: (a) perturbed entropy functional $\widetilde{\mathcal{H}}_\mathrm{d}$, (b) L^1-norm with $C = 30(\widetilde{\mathcal{H}}_\mathrm{d}[V^0])^{1/2}$.

Next, observe the Figure E.2(a) and a kind of phase transition in decay of $\widetilde{\mathcal{H}}_{\mathrm{d}}$ around time points s_{400} and s_{1100}. Before the time s_{400} and after s_{1100}, $\widetilde{\mathcal{H}}_{\mathrm{d}}$ decays almost parallelly to the dashed line, which represents the exponential curve $\widetilde{\mathcal{H}}_{\mathrm{d}}[V_0]e^{-2s_k}$ in the semi-logarithmic plot. Figure E.1 and our simulations indicate that these temporal regions correspond to the translation dominated regime of the solution. Hence, in the spirit of results from [8, 22, 51], our numerical experiments suggest the optimal decay rates being $-2\lambda_1$ and $-\lambda_1$ for the perturbed entropy $\widetilde{\mathcal{H}}$ and L^1-norm, respectively.

Based on the above formal observations and obtained numerical results, we conclude the appendix with the following conjecture.

Conjecture. Let $v_0 \in L^1(\mathbb{R})$ be a nonnegative initial datum of finite entropy $\widetilde{\mathcal{H}}[v_0] < \infty$ and let v be solution to the rescaled quantum diffusion equation (E.1). Then v converges exponentially fast towards the respective Gaussian profile v_∞ in $L^1(\mathbb{R})$,

$$\|v(s) - v_\infty\|_{L^1} \leq C(\widetilde{\mathcal{H}}[v_0])^{1/2} e^{-s} \quad \text{for all} \quad s > 0\,,$$

where $C > 0$ depends only on v_0. Furthermore, the perturbed entropy functional $\widetilde{\mathcal{H}}$ decays along v at an exponential rate

$$\widetilde{\mathcal{H}}[v(s)] \leq \widetilde{\mathcal{H}}[v_0] e^{-2s} \quad \text{for all} \quad s > 0\,.$$

Bibliography

[1] M. G. Ancona. Diffusion-drift modelling of strong inversion layers. *COMPEL* 6 (1987), 11–18.

[2] S. Basu, R. Pollack, and M.-F. Roy. Algorithms in real algebraic geometry. Second edition. Algorithms and Computation in Mathematics, Vol. 10. Springer, Berlin, 2006.

[3] J. Becker and G. Grün. The thin-film equation: Recent advances and some new perspectives. *J. Phys.: Condens. Matter* 17 (2005), 291–307.

[4] F. Bernis and A. Friedman. Higher order nonlinear degenerate parabolic equations. *J. Diff. Eqs.* 83 (1990), 179–206.

[5] A. Bertozzi. The mathematics of moving contact lines in thin liquid films. *Notices Amer. Math. Soc.* 45 (1998), 689–697.

[6] M. Bertsch, R. Dal Passo, H. Garcke, and G. Grün. The thin viscous flow equation in higher space dimensions. *Adv. Diff. Eqs.* 3 (1998), 417–440.

[7] P. Bleher, J. Lebowitz, and E. Speer. Existence and positivity of solutions of a fourth-order nonlinear PDE describing interface fluctuations. *Comm. Pure Appl. Math.* 47 (1994), 923-942.

[8] M. Bonforte, J. Dolbeault, G. Grillo, and J. L. Vázquez. Sharp rates of decay of solutions to the nonlinear fast diffusion equation via functional inequalities. *Proc. Natl. Acad. Sci. USA* 107 (2010),16459–16464.

[9] M. Bukal, A. Jüngel and D. Matthes. A multidimensional sixth-order quantum diffusion equation. (*Submitted for publication.*)

[10] M. Bukal, A. Jüngel, and D. Matthes. Entropies for radially symmetric higher-order nonlinear diffusion equations. *Commun. Math. Sci.* 9 (2010), 353-382.

[11] M. Burger, H. Lin, and C. B. Schönlieb. Cahn–Hilliard Inpainting and a Generalization for Grayvalue Images. *SIAM J. Imaging Sci.* 2 (2009), 1129–1167.

[12] J. W. Cahn and J. E. Hilliard, Free energy of a nonuniform system. I. Interfacial free energy. *The Journal of Chemical Physics* 28 (1958), 258–267.

[13] J. A. Carrillo, A. Jüngel and S. Tang. Positive entropic schemes for a nonlinear fourth-order parabolic equation. *Discrete Contin. Dynam. Sys. B* 3 (2003), 1–20.

[14] J. A. Carrillo and G. Toscani. Long-time asymptotics for strong solutions of the thin-film equation. *Comm. Math. Phy.* 225 (2002), 551–571.

[15] L. Chen and M. Dreher. Quantum semiconductor models. In: M. Demuth, B.-W. Schulze, and I. Witt (eds.). *Partial Differential Equations and Spectral Theory*, Oper. Theory Adv. Appl. 211 (2011), 1-72.

[16] G. Collins. Quantifier elimination for real closed fields by cylindrical algebraic decomposition. Automata theory and formal languages (Second GI Conf., Kaiserslautern, 1975), pp. 134–183. Lecture Notes in Comput. Sci., Vol. 33, Springer, Berlin, 1975.

[17] P. Constantin, T. Dupont, R. E. Goldstein, L. P. Kadanoff, M. J. Shelley, and S. M. Zhou. Droplet breakup in a model of the Hele-Shaw cell. *Phys. Rev. E* 47 (1993), 4169–4181.

[18] R. Dal Passo, H. Garcke, and G. Grün. On a fourth order degenerate parabolic equation: global entropy estimates and qualitative behaviour of solutions. *SIAM J. Math. Anal.* 29 (1998), 321–342.

[19] G. Dahlquist. Error analysis for a class of methods for stiff non-linear initial value problems. *Numerical analysis (Proc. 6th Biennial Dundee Conf., Univ. Dundee, Dundee, 1975), Lecture Notes in Math., Vol. 506*, Springer, Berlin, 1976.

[20] G. Dahlquist. G-stability is equivalent to A-stability. *BIT Numerical Mathematics* 18 (1978), 384–401.

[21] P. Degond, F. Méhats, and C. Ringhofer. Quantum energy-transport and drift-diffusion models. *J. Stat. Phys.* 118 (2005), 625–665.

[22] J. Denzler and R. McCann. Fast diffusion to self-similarity: complete spectrum, long-time asymptotics and numerology. *Arch. Ration. Mech. Anal.* 175 (2005), 301–342.

[23] B. Derrida, J. Lebowitz, E. Speer, and H. Spohn. Fluctuations of a stationary nonequilibrium interface. *Phys. Rev. Lett.* 67 (1991), 165–168.

[24] B. Düring, D. Matthes, and P. Milisic. A gradient flow scheme for nonlinear fourth order equations. *Discrete Contin. Dyn. Syst. Ser. B*, 14 (2010), no. 3, 935–959.

[25] C. M. Elliott and Z. Songmu. On the Cahn-Hilliard equation. *Arch. Rational Mech. Anal.* 96 (1986), 339–357.

[26] J. Evans, V. Galaktionov, and J. R. King. Unstable sixth-order thin film equation: I. Blow-up similarity solutions. *Nonlinearity* 20 (2007), 1799–1841.

[27] J. C. Flitton and J. R. King. Moving-boundary and fixed-domain problems for a sixth-order thin-film equation. *Europ. J. Appl. Math.* 15 (2004), 713–754.

[28] D. Furihata. Finite difference schemes for $\frac{\partial u}{\partial t} = (\frac{\partial}{\partial x})^\alpha \frac{\delta G}{\delta u}$ that inherit energy conservation or dissipation property. *J. Comput. Phys* 156 (1999), 181–205.

[29] D. Furihata, T. Matsuo. Discrete Variational Derivative Method, *Chapman and Hall*, 2010.

[30] U. Gianazza, G. Savaré, and G. Toscani. The Wasserstein gradient flow of the Fisher information and the quantum drift-diffusion equation. *Arch. Ration. Mech. Anal.* 194 (2009), 133–220.

[31] D. Henry. *Geometric Theory of Semilinear Parabolic Equations.* Lect. Notes Math. 840. Springer, 1981.

[32] R. Jordan, D. Kinderlehrer, and F. Otto. The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Anal.* 29 (1998), 1–17.

[33] C. Josserand, Y.Pomeau, and S. Rica. Self-similar singularities in the kinetics of condensation. *J. of Low Temp. Physics* 145 (2006), 231–265.

[34] A. Jüngel. Quasi-hydrodynamic semiconductor equations. *Birkhäuser*, Basel, 2001.

[35] A. Jüngel and D. Matthes. An algorithmic construction of entropies in higher-order nonlinear PDEs. *Nonlinearity* 19 (2006), 633–659.

[36] A. Jüngel and D. Matthes. The Derrida-Lebowitz-Speer-Spohn equation: existence, non-uniqueness, and decay rates of the solutions. *SIAM J. Math. Anal.* 39 (2008), 1996–2015.

[37] A. Jüngel and J.-P. Milišić. A sixth-order nonlinear parabolic equation for quantum systems. *SIAM J. Math. Anal.* 41 (2009), 1472–1490.

[38] A. Jüngel and R. Pinnau. A positivity preserving numerical scheme for a nonlinear fourth-order parabolic equation. *SIAM J. Num. Anal.* 39 (2001), 385–406.

[39] A. Jüngel and R. Pinnau. Convergent semidiscretization of a nonlinear fourth order parabolic system. *Math. Model. Numer. Anal.* 37 (2003), 277–289.

[40] A. Jüngel and R. Pinnau. Global non-negative solutions of a nonlinear fourth-order parabolic equation for quantum systems. *SIAM J. Math. Anal.* 32 (2000), 760–777.

[41] A. Jüngel and I. Violet. First-order entropies for the Derrida-Lebowitz-Speer-Spohn equation. *Discrete Cont. Dyn. Sys. B* 8 (2007), 861–877.

[42] A. Jüngel and I. Violet. Mixed entropy estimates for the porous-medium equation with convection. *Discrete Contin. Dynam. Sys. B* 12 (2009), 783–796.

[43] J. King. The isolation oxidation of silicon: the reaction-controlled case. *SIAM J. Appl. Math.* 49 (1989), 10641080.

[44] M. D. Korzec, P. L. Evans, A. Münch, and B. Wagner. Stationary solutions of driven fourth- and sixth-order Cahn-Hilliard-type equations. *SIAM J. Appl. Math.* 69 (2008), 348–374.

[45] R. Laugesen. New dissipated energies for the thin film equation. *Comm. Pure Appl. Anal.* 4 (2005), 613–634.

[46] L. Littlejohn and A. Krall. Orthogonal Polynomials and Higher Order Singular Sturm-Liouville Systems. *Acta Applicande Mathematicae* 17 (1989), 99–170.

[47] P.-L. Lions and C. Villani. Régularité optimale de racines carrées. *C. R. Acad. Sci. Paris Sér. I Math.* 321 (1995), 1537–1541.

[48] J. Löfberg. YALMIP: A toolbox for modeling and optimization in MATLAB. In: *Proceedings of the CACSD Conference*, Taipei, Taiwan, IEEE (2004), 284-289.

[49] T. Matsuo and D. Furihata. Dissipative or conservative finite difference schemes for complex-valued nonlinear partial differential equations. *J. Comput. Phys* 171 (2001), 425–447.

[50] D. Matthes, A. Jüngel, and G. Toscani. Convex Sobolev inequalities derived from entropy dissipation. To appear in *Arch. Ration. Mech. Anal.*, 2010.

[51] D. Matthes, R. McCann, and G. Savaré. A family of nonlinear fourth order equations of gradient flow type. *Comm. Part. Diff. Eqs.* 34 (2009), no. 10-12, 1352–1397.

[52] T. Myers. Thin films with high surface tension. *SIAM Rev.* 40 (1998), 441-462.

[53] The Numerical Algorithms Group. NAG Toolbox for Matlab Function Document: c05nb. `http://www.nag.co.uk/numeric/MB/manual_22_1/pdf/C05/c05nb.pdf`.

[54] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations.* Springer, New York, 1983.

[55] A. Potter. An elementary version of the Leray-Schauder theorem. *J. London Math. Soc.* 5 (1972), 414–416.

[56] D. V. Semikoz and I. I. Tkachev. Condensation of bosons in the kinetic regime. *Phy. Rev. D* 55 (1997), 489–502.

[57] J. Simon. Compact sets in the space $L^p(0,T;B)$. *Ann. Mat. Pura Appl.* 146 (1987), 65–96.

[58] H. Spohn. Kinetics of the Bose-Einstein condensation. *Physica D* 239 (2010), 627–634.

[59] A. Tarski. *A Decision Method for Elementary Algebra and Geometry*. University of California Press, Berkeley, CA, 1951.

[60] C. Villani. Mass transportation, transportation inequalities and dissipative equations. In: M. C. Carvalho and J. Rodrigues (eds.). *Recent Advances in the Theory and Applications of Mass Transport*, pp. 95–109, Contemp. Math. 353. Amer. Math. Soc., Providence, 2004.

[61] D. Willett and J. Wong. On the discrete analogues of some generalizations of Gronwall's inequality. *Monatsh. Math.* 69 (1965), 362–367.

[62] E. Zeidler. *Nonlinear Functional Analysis and Its Applications*. Vol. IIB, Springer, New York, 1990.

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Curriculum vitae

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Occupation

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Winter term 2011/12	Teaching exercise course in *Partial Differential Equations*, TU Vienna.
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Skills

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Talks

Barcelona 06/2010	*On a nonlinear sixth-order quantum diffusion equation*, DSPDEs10, contributed talk.
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Other interests

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