Technische Universität München

Fakultät für Mathematik

Lehrstuhl für Dynamische Systeme

Fully variational Lagrangian discretizations for second and fourth order evolution equations

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Vollständiger Abdruck der von der Fakultät für Mathematik der Technischen Universität München zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften (Dr. rer. nat.)

genehmigten Dissertation.

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	3.	Univ.-Prof. Dr. Ansgar Jüngel Technische Universität Wien, Österreich (schriftliche Beurteilung)

Die Dissertation wurde am 17.06.2015 bei der Technischen Universität München eingereicht und durch die Fakultät für Mathematik am 07.09.2015 angenommen.

Dedicated to my late grandparents Herta, Hans and Helmut.

Abstract

The description of certain evolution equations as Wasserstein gradient flows attained great interest in the mathematical community in recent years, and opened new perspectives in analytical and numerical treatments of many problems with physical importance. In this thesis, a Lagrangian formulation is used to derive numerical schemes for a wide class of second and fourth order equations. The aim is to construct numerical solvers that inherit as many structure from the continuous flows as possible. This yields efficient, stable and easy-to-implement numerical schemes and further enables a successful study of the schemes' convergence, long-time asymptotics of discrete solutions and other qualitiative issues.

Zusammenfassung

Die Interpretation zahlreicher physikalisch interessanter Evolutionsgleichungen als Wasserstein-Gradientenflüsse wurde in den letzten Jahren mit großem Interesse in der mathematischen Fachwelt wahrgenommen, nicht zuletzt weil dies das Verständnis vieler physikalischer Prozesse verbesserte. In dieser Arbeit werden numerische Verfahren für eine weite Klasse von Gleichungen zweiter und vierter Ordnung beschrieben, welche auf eine Lagrange-Formulierung dieser Wasserstein Gradientenflüsse basieren. Bei der Diskretisierung wird insbesondere darauf geachtet die Struktur der Gradientenflüsse in den numerischen Verfahren beizubehalten, was zu effizienten und stabilen numerischen Schemata führt, die zusätzlich einfach zu implementieren sind. Der Erhalt von Struktureigenschaften der Gleichungen ermöglicht insbesondere die Konvergenz der Schemata, das Langzeitverhalten von diskreten Lösungen oder andere qualitative Eigenschaften zu untersuchen.

Contents

Acknowledgement

I would like to thank my PhD-supervisor Prof. Daniel Matthes for the great opportunity to work with him on this interesting project, for his support of my research, and for his valuable feedbacks. Without his progressive motivation and pushing, this thesis would not have been realized. I also want to thank him for allowing me the usage of many joint results for this thesis.

Thanks to Prof. Oliver Junge for many discussions about numerical optimization and other problems, and to give me the permission to use joint work in this thesis. I also want to thank the DFG Collaboration Research Center TRR 109, "Discretization in Geometry and Dynamics" for its support.

Thanks to my colleagues and friends at the faculty, especially to Florian Augustin, Sarah Rathbauer, Yuen au Yeung, David Sattlegger, Stephanie Troppmann and Katharina Schaar for helpful discussions on different topics to my work and for sweeten my stay at the university in Munich.

Many thanks to all my friends and colleagues who read through the first few versions of this thesis and gave me useful feedbacks and ideas to improve this work. With this in mind, if someone finds spelling errors or mistakes in mathematical contents, please contact Nicola Ondracek, Maximilian Streicher, Georg Wechslberger, Stephanie Troppmann, Katharina Schaar, Michael Möller, Michael Strobel, Anna Fiedler, Jonathan Zinsl, Stephanie Hertlein or my mother Grete.

I especially wish to thank my family — my mother Grete, my stepfather Franz, my siblings Sissi, Susi and Stix, my young nice Lenchen and my brother-in-law Thomas. Furthermore, i want to thank my close friends in Austria Johannes, Simon, Fabian, Gregor, Roman, Stefan, Robert S., Robert H., Peter, Philipp, Mathias, Roland, Erich, Rainer, and to those from Germany, Leo, Stephie, Werner and Dani.

Finally I want to thank my girlfriend Steffi for her love and her emotional support. Her support enabled me going through all ups and downs of this thesis.

CHAPTER 1

Introduction

The history of Wasserstein gradient flows began a long time ago when Monge formulated his optimal transportation problem in 1781. This problem quickly became popular and the Academy of Sciences in Paris ("l'Académie des Sciences") even offered a reward for its solution, which was then claimed by Appell [**App86**]. A relaxed formulation of Monge's problem was later introduced by Kantorovich in the forties of the 20th century [**Kan42, Kan04**]. In 1975, he received the Nobel Prize in Economic Science for his research on this topic. However, Kantorovich's representation of the optimal transportation problem initiated the definition of a metric on the set of (probability) measures — the Wasserstein distance.

It took another three decades until a link between certain evolution equations and the notion of optimal transportation was found. A first step in this direction was provided by the extensive work of De Giorgi, who studied time-discrete variational approaches for several evolution equations on general metric spaces, see for instance [**DG93**]. Then in [**JKO98**], Jordan, Kinderlehrer and Otto stated a semi-discrete (in time) variational scheme for the Fokker-Planck equation. The key observation was that the equation's evolution can be understood as a steepest descent for the free energy with respect to the Wasserstein distance. The geometric intuition has then been established and used for a rigorous analysis of the porous medium equation by Otto [**Ott01**] and was received with great interest in the mathematical community. The underlying idea for the temporal approximation in both works [**DG93**] and [**JKO98**] is the same, although they have been developed independently of each other. That is why the scheme was later known as the *JKO-scheme* (Jordan, Kinderlehrer and Otto) or the *minimizing movement scheme* (De Giorgi). In recent years, more and more evolution equations have been successfully reformulated as Wasserstein gradient flows, and the minimizing movement scheme became a popular tool for deriving fully discrete numerical schemes for a wide class of equations.

Optimal transportation and the Wasserstein distance

In what follows, we want to give a formal introduction into the topic of optimal transportation. For a more detailed explanation we refer to [**Vil03, Vil09**], which constitutes the main guide for this introductive section.

Let Ω_1, Ω_2 be two open domains in $\mathbb{R}^d$, $d \in \mathbb{N}$, and μ, ν two probability measures defined on Ω_1 and Ω_2, respectively. For the purposes of illustration, let us imagine that μ describes the allocation of some goods in Ω_1, whereas ν represents the needs of those goods in Ω_2. In order to satisfy the needs, we are interested in moving all goods from Ω_1 to Ω_2, but any transport is associated with some effort described by a convex cost function $c : \Omega_1 \times \Omega_2 \to \mathbb{R} \cup \{+\infty\}$. This means, heuristically spoken, that one has to "pay" $c(x, y)$ for the transport of a single good lying at $x \in \Omega_1$ to a point $y \in \Omega_2$. The optimal transportation problem is now formally stated as follows: *How can we transport all goods from Ω_1 to Ω_2 with minimal total cost?*

This problem can be written in a proper mathematical way that is known as the *Kantorovich optimal transportation problem*:

$$\text{Minimize} \quad I(\pi) := \int_{X\times Y} c(x,y)\,\mathrm{d}\pi(x,y) \quad \text{for} \quad \pi \in \Pi(\mu,\nu). \tag{1.1}$$

Here, $\Pi(\mu,\nu)$ is the set of all transport plans connecting μ and ν, which means that π is a measure on $X \times Y$ with marginals μ and ν,

$$\pi(A\times\Omega_2) = \mu(A) \quad \text{and} \quad \pi(\Omega_1 \times B) = \nu(B) \quad \text{for any measurable } A \subseteq \Omega_1, B \subseteq \Omega_2. \tag{1.2}$$

The restrictions in (1.2) assure that any good is transported from Ω_1 to Ω_2 by $\pi \in \Pi(\mu,\nu)$.

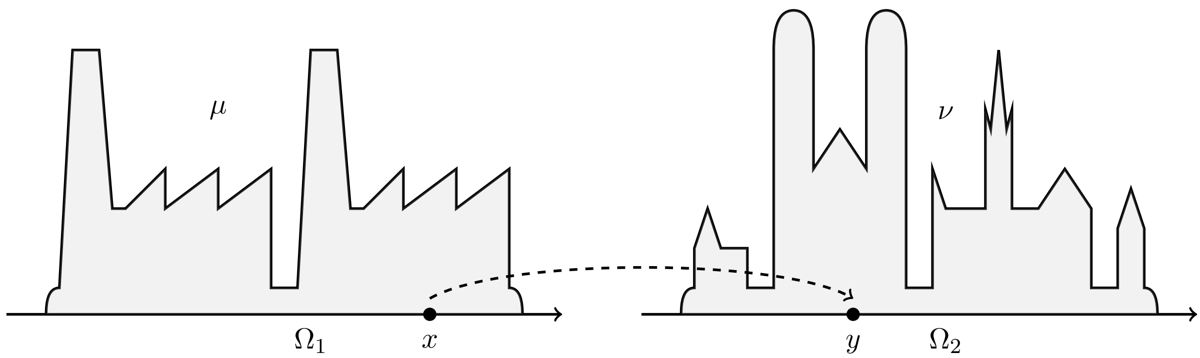


FIGURE 1.1. A schematic picture of the optimal transportation problem: How is it possible to transport all goods from Ω_1 to Ω_2 with minimal total cost?

In this thesis we are only considering the quadratic cost functional $c(x,y) := |x-y|^2$, which shall be fixed from now on. We further consider the case that both domains are equal, hence $\Omega = \Omega_1 = \Omega_2$. Let us assume in the following that the allocations of goods and of needs in Ω can vary. Then the above minimization problem can be formulated in terms of μ and ν, and the minimal cost transporting μ to ν can be interpreted as a value of the measures' distance:

Definition 1.1. *The L^2-Wasserstein distance between two probability measures μ,ν on Ω is defined by*

$$\mathcal{W}_2(\mu,\nu)^2 = \inf_{\pi\in\Pi(\mu,\nu)} I(\pi), \tag{1.3}$$

where $I(\pi)$ is given as in (1.1) *with $c(x,y) = |x-y|^2$.*

If μ and ν are absolutely continuous with respect to a fixed measure on Ω with densities u and v, then we henceforth write — by abuse of notation — $\mathcal{W}_2(u,v)$ instead of $\mathcal{W}_2(\mu,\nu)$.

As the definition suggests, one can analogously define L^p-Wasserstein distances for $p \geqslant 1$ and even for $p = +\infty$. However, we are always considering the case $p = 2$ and call the metric in (1.3) the *L^2-Wasserstein distance* or just *Wasserstein distance.*

L^2-Wasserstein gradient flows

In the forthcoming section, we want to give a brief and very formal introduction to L^2-Wasserstein gradient flows and motivate a link to solutions u to the *continuity equation*, i.e.

$$\partial_t u + \operatorname{div}\big(u\mathbf{v}\big) = 0 \quad \text{in } (0,+\infty)\times\Omega$$

with an arbitrary velocity field $\mathbf{v}$. The section's content is mostly inspired by the introductive Chapter 1.3 of [**AGS05**] that is essentially based on [**Amb95**] by Ambrosio. To motivate the connection between L^2-Wasserstein gradient flows and the continuity equation we mainly follow the ideas of [**Ott01**], which we recommend to the more interested reader.

Let us start with the Euclidean space $\mathbb{R}^d$ equipped with the scalar product $\langle\cdot,\cdot\rangle$ and the norm $\|\cdot\|_2$, which is the simplest setting for introducing the notion of gradient flows. We furthermore consider a smooth function $\mathcal{E}:\mathbb{R}^d\to\mathbb{R}$. Then the gradient $\nabla\mathcal{E}$ of $\mathcal{E}$ can be defined by validity of

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}\big(v(t)\big) = \left\langle \nabla\mathcal{E}\big(v(t)\big), \frac{\mathrm{d}}{\mathrm{d}t}v(t)\right\rangle \tag{1.4}$$

for any regular curve v with values in $\mathbb{R}^d$. We then say that a curve $u:(0,+\infty)\to\mathbb{R}^d$ is a *gradient flow along* $\mathcal{E}$, if it is a solution to

$$\frac{\mathrm{d}}{\mathrm{d}t}u(t) = -\nabla\mathcal{E}\big(u(t)\big). \tag{1.5}$$

From the geometrical point of view, a gradient flow always follows the direction in which $\mathcal{E}$ decreases at most, which is why $u(t)$ is also called a *curve of steepest descent* or *a curve of maximal slope.*

If one is interested in extending the notion of gradient flows to the more general setting of metric spaces, the characterization in (1.5) turns out to be disadvantageous, since a definition of a gradient as in (1.4) or of a time derivative is not available in general. Therefore we observe that a solution to (1.5) admits the equivalent representation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}\big(u(t)\big) \leqslant -\frac{1}{2}\left\|\frac{\mathrm{d}}{\mathrm{d}t}u(t)\right\|_2^2 - \frac{1}{2}\left\|\nabla\mathcal{E}\big(u(t)\big)\right\|_2^2. \tag{1.6}$$

This is more convenient for a generalization, since the first norm on the right-hand side of (1.6) can be replaced by the *metric derivative* $|u'|$ of u and the second one by a *strong upper gradient* g *for* $\mathcal{E}$, which are both purely metric objects. If V is a metric space and $\mathcal{E}$ is a functional defined on V, we then call an absolutely continuous curve $u:(0,+\infty)\to V$ a curve of maximal slope for $\mathcal{E}$ with respect to the strong upper gradient g, if

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}\big(u(t)\big) \leqslant -\frac{1}{2}\left|u'\right|^2(t) - \frac{1}{2}g(t)^2 \tag{1.7}$$

for almost every $t\in(0,+\infty)$. We are going to discuss the above objects and the resulting metric formulation of curves of maximal slopes more detailed in Section 3.5.

The link between L^2-Wasserstein gradient flows and the continuity equation. In this thesis we denote by $\mathcal{P}^r(\Omega)$ the set of all positive and integrable density functions on a certain domain $\Omega\subseteq\mathbb{R}^d$, $d\in\mathbb{N}$, with a fixed mass $M>0$. For the sake of simplicity, let us assume in this section that $M = 1$, hence densities in $\mathcal{P}^r(\Omega)$ are probability densities. The set $\mathcal{P}^r(\Omega)$ is known to be a differentiable manifold. Without going into any details, let us think of the tangent vector space on $\mathcal{P}^r(\Omega)$ at any point $u \in \mathcal{P}^r(\Omega)$ as follows

$$\operatorname{Tan}_u \mathcal{P}^r(\Omega) = \left\{ s : \Omega \to \mathbb{R}, \quad \text{such that} \quad \int_\Omega s \, \mathrm{d}x = 0 \right\}.$$

To define a L^2-Wasserstein gradient flow along a functional $\mathcal{E} : \mathcal{P}^r(\Omega) \to \mathbb{R} \cup \{+\infty\}$, one can exploit the metric structure of $(\mathcal{P}^r(\Omega), \mathcal{W}_2)$ and use (1.7). But in order to link L^2-Wasserstein gradient flows with the continuity equation, we want to motivate another approach. To this end, we are going to introduce a metric tensor g. There are infinitely many choices for g and any of them possibly induces another metric on $\mathcal{P}^r(\Omega)$, hence another gradient flow. An important obervation in [**Ott01**] was that one can choose a metric tensor g that induces the L^2-Wasserstein distance: Define the metric tensor $g_u : \operatorname{Tan}_u \mathcal{P}^r(\Omega) \times \operatorname{Tan}_u \mathcal{P}^r(\Omega)$ at the point $u \in \mathcal{P}^r(\Omega)$, such that

$$g_u(s_1, s_2) = \int_\Omega \langle \nabla p_1, \nabla p_2 \rangle \, u \, \mathrm{d}x,$$

where each tangent vector $s \in \operatorname{Tan}_u \mathcal{P}^r(\Omega)$ can be represented by a function $p : \Omega \to \mathbb{R}$ through the identity

$$s = -\operatorname{div}(u \nabla p).$$

The set of probability densities $\mathcal{P}^r(\Omega)$ equipped with the metric tensor g is known to form a Riemannian manifold, which is the required structure to define the notion of gradient flows. Consider for the moment an entropy/energy functional $\mathcal{E} : \mathcal{P}^r(\Omega) \to \mathbb{R} \cup \{+\infty\}$ that is assumed to be of the form

$$\mathcal{E}(u) = \int_\Omega \phi(u) \, \mathrm{d}x$$

with an integrand $\phi : [0, +\infty) \to \mathbb{R}$ that satisfies sufficient regularity assumptions, which we won't specify in this section. Following Otto's calculus in [**Ott01**], a gradient flow along $\mathcal{E}$ with respect to the L^2-Wasserstein distance is now formally written as

$$\partial_t u = -\operatorname{grad}_{\mathcal{W}_2} \mathcal{E}(u), \tag{1.8}$$

where the gradient is defined by the metric tensor and the (first) variational derivative of $\mathcal{E}$ through the identity

$$g_u \left(\operatorname{grad}_{\mathcal{W}_2} \mathcal{E}(u), s \right) = \frac{\delta \mathcal{E}(u)}{\delta u}[s] := \int_\Omega \phi'(u) s \, \mathrm{d}x$$

for any $s \in \operatorname{Tan}_u \mathcal{P}^r(\Omega)$. Note that this definition of the gradient is of the same kind as (1.4), since the variational derivative of $\mathcal{E}$ in direction s is attained by differentiating $\mathcal{E}(u(t))$ along curves of the form $u(t) = u + ts$. In terms of the metric tensor, the gradient flow equation in (1.8) has to be read as

$$g_u \left(\partial_t u, s \right) = -g_u \left(\operatorname{grad}_{\mathcal{W}_2} \mathcal{E}(u), s \right) \quad \text{for any } s \in \operatorname{Tan}_u \mathcal{P}^r(\Omega).$$

Explicitly, using the representation $s = -\operatorname{div}(u\nabla p)$, the gradient flow equation has the form

$$\int_\Omega \partial_t u\, p \,\mathrm{d}x - \int_\Omega \phi'(u) \operatorname{div}(u\nabla p) \,\mathrm{d}x = 0. \tag{1.9}$$

This representation of the L^2-Wasserstein gradient flow equation is the starting point of the investigations in this thesis. Indeed, (1.9) is nothing else than a weak formulation of the continuity equation with a special choice of the velocity field,

$$\partial_t u + \operatorname{div}\big(u\mathbf{v}(u)\big) = 0, \tag{1.10}$$

which is going to be the equation of our main interest in this thesis. The velocity field $\mathbf{v}(u)$ is a gradient field depending on the first variational derivative of $\mathcal{E}$ evaluated at u,

$$\mathbf{v}(u) = -\nabla\left(\frac{\delta\mathcal{E}(u)}{\delta u}\right). \tag{1.11}$$

Approximation of Wasserstein gradient flows by minimizing movement. We already mentioned [**JKO98**] by Jordan, Kinderlehrer and Otto, who derived a time-implicit semi-discrete scheme for a wide class of second order evolution equations by employing the equations' variational structure. Under certain assumptions on the functional $\mathcal{E}$, their scheme can be applied to equations that have the form of the continuity equation (1.10) with a velocity field as in (1.11).

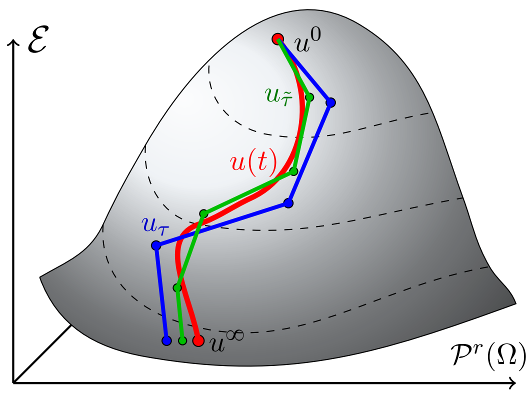


FIGURE 1.2. Schematic representation of a L^2-Wasserstein gradient flow and its approximations through the minimizing movement scheme

To this end, let $\tau > 0$ be a fixed time step size. Then the *minimizing movement scheme*, or *JKO-scheme*, for the continuity equation (1.10) can be formulated as follows: Starting with an initial datum $u^0 \in \mathcal{P}^r(\Omega)$, define recursively a sequence of density functions $(u_\tau^n)_{n=0}^\infty$ as the solutions of the following minimization problem

$$u_\tau^n := \operatorname*{arg\,min}_{u\in\mathcal{P}^r(\Omega)} \frac{1}{2\tau}\mathcal{W}_2(u, u_{\boldsymbol{\tau}}^{n-1})^2 + \mathcal{E}(u). \tag{1.12}$$

To guarantee the well-posedness of the minimizing movement scheme one has to guarantee the existence of a sequence that solves the minimization problem in (1.12). The solvability of the minimization problem is mostly attained by assuming a certain convexity property for the entropy/energy functional $\mathcal{E}$, but even this does not always have to be required, as one can see in some examples for fourth order equations.

Evolution equations with Wasserstein gradient flow structure

By now, many evolution equations with an important physical meaning have been shown to carry an underlying Wasserstein gradient flow structure. In this thesis, we are especially interested in second and fourth order equations as listed below. The gradient flow structure of the following equations is going to be discussed later in the corresponding chapters.

Drift-diffusion equation. In the case of second order evolution equations, we are considering a wide class of *drift-diffusion equations*, which are given by

$$\partial_t u = \Delta \mathrm{P}(u) + \mathrm{div}(u \nabla V).$$

The function P is in general assumed to be smooth with (super-) linear growth and V denotes a certain drift-potential. The most popular examples for equations of this form are the *heat equation* or *porous medium equations.* Nowadays, equations of this kind are well studied and results for existence or long-time behaviour can be found in almost every book about partial differential equations, we refer for instance to [**Eva10**].

The heat equation, which is the above equation with $\mathrm{P}(u) = u$ and mostly formulated without drift-potential V, describes the diffusion of heat in a homogeneous medium. If the observed domain Ω is bounded, solutions to the heat equation are known to attain a steady state that describes a total equilibration of the heat in the medium. Otherwise, if $\Omega = \mathbb{R}^d$, solutions of the heat equation propagate with infinite speed: For an initial distribution of heat u^0 at $t = 0$ that is possibly concentrated on a compact region, the solution $u(t)$ immediately becomes strictly positive on the whole domain as $t > 0$. Moreover, solutions asymptotically diverge like *Gaussians* as time goes to infinity.

For $\mathrm{P}(u) = u^m$ with $m > 1$, which turns the above equation into a porous medium equation with slow diffusion, the model describes the diffusion of gas in a porous medium, for instance. Similar to the heat equation before, solutions move towards an equilibrium in a bounded domain, but the asymptotic behaviour changes tremendously in case of an unbounded domain because of the solutions' finite speed of propagation. This can be exemplified in more detail studying a special class of self-similar solutions, the so-called *Barenblatt profiles*, which can be imagined as reversed paraboloids that are extended by zero in regions where the paraboloids are negative. For the reader more interested in this topic, we refer to [**Váz92**] which provides a mathematical overview about the theory of porous medium equations.

The asymptotic behaviour of the above equations is interesting insofar as certain fourth order equations share the same behaviour. This is going to be discussed in more detail in Chapter 4.

DLSS equation. The *DLSS equation* — also known as *quantum-drift-diffusion equation* — was first analyzed by Derrida, Lebowitz, Speer and Spohn in [**DLSS91a**, **DLSS91b**] and is given by

$$\partial_t u + \operatorname{div}\left(u\nabla\left(\frac{\Delta\sqrt{u}}{\sqrt{u}} + V\right)\right) = 0,$$

where V denotes a certain drift-potential. It rises from the Toom model [**DLSS91a**, **DLSS91b**] in one spatial dimension on the half-line $[0,+\infty)$ and was used to describe interface fluctuations therein. Moreover, the DLSS equation also finds application in semi-conductor physics, namely as a simplified model (low-temperature, field-free) for a quantum drift diffusion system for electron densities, see [**JP00**].

From the analytical point of view, a big variety of results in different settings has been developed over the last few decades. For results on existence and uniqueness, we refer for instance to [**BLS94**,**Fis13**,**GJT06**,**GST09**,**JM08**,**JP00**], and to [**CCT05**,**CT02a**,**CDGJ06**,**GST09**, **JM08**,**JT03**,**MMS09**] for qualitative and quantitative descriptions of the long-time behaviour. For the reader unfamiliar with the numerous analytical results on the DLSS equation, we refer to the review article [**JM10**] of Jüngel and Matthes, where the authors mentioned especially the existence of a nonnegative weak solution to the DLSS equation in higher dimension. The main reason that makes the research on this topic so nontrivial is the lack of comparison/maximum principles as available in the theory of second order equations. Unfortunately, the absence of these analytical tools should not be underestimated, as the work [**BLS94**] by Bleher et al. demonstrates. In [**BLS94**], the authors show that as long as a solution u to the DLSS equation is strictly positive, one can prove that it is even C^∞-smooth, but there are no results for regularity available from the moment when u touches zero. The question if strict positivity of the initial datum u^0 already implies strict positivity of solutions at any time is a difficult task and remains open until now, despite much effort and some recent progress in that direction, see [**Fis14**]. In order to deal with more general initial data, alternative theories for nonnegative weak solutions consistently gain in importance. Take for instance [**GST09**, **JM08**], where existence of weak solutions to the DLSS equation is shown on grounds of the a priori regularity estimate

$$\sqrt{u} \in L^2_{\mathrm{loc}}([0,+\infty); H^2(\mathbb{T}))$$

($\mathbb{T}$ stands for the torus in $\mathbb{R}^d$), by just considering nonnegative initial functions u^0 with finite Boltzmann entropy.

Thin film equation. The mathematical and physical literature devotes great attention to the family of *thin film equations* due to its physical importance. The general representation with a (potentially nonlinear) mobility function m is

$$\partial_t u + \operatorname{div}\big(m(u)\nabla\Delta u + u\nabla V\big) = 0.$$

Equations of this form give a dimension-reduced description of laminar flow with a free liquid-air-interface [**ODB97**]. In case of linear mobility $m(u) = u$ — which is the situation we are going to consider in this thesis — the thin film equation can also be used to describe the pinching of thin necks in a *Hele-Shaw* cell in one spatial dimension, hence it is sometimes referred to as the *Hele-Shaw flow*.

The analytical treatment of the fourth order degenerate thin film equations is far from trivial, but there exists a rich literature on this topic: One of the first results available in the mathematical literature was provided by Bernis and Friedman [**BF90**]. Later on a vast number of results to numerous mobility functions of physical meaning was treated in [**BDPGG98**]. A major problem in the equations' analysis is the lack of comparison/maximum principles, similar to the situation of the DLSS equation: In zones on which the solution u is strictly positive, the usage of classical parabolic theory yields C^∞-regularity. But there is no guarantee that solutions stay strictly positive, unfortunately. This is why one is typically interested in solutions that are *not* strictly positive but have a compact, time-dependent support. In the analysis of such nonnegative solutions the framework of energy and entropy methods play a key role, see for instance [**CU07, CT02b, GO01, LMS12**]. Using energy/entropy estimates, the gained regularity is usually something of the type $L^\infty_{\mathrm{loc}}([0,+\infty);H^1(\Omega)) \cap L^2_{\mathrm{loc}}([0,+\infty);H^2(\Omega))$, but no better. However, there are several other references to this topic, for instance Grün et al. [**BG15, DPGG98, Grü04**], concerning long-time behaviour of solutions and the nontrivial question of spreading behaviour of the support.

Aim of the thesis

In this thesis, the focus is on deriving structure-preserving and convergent numerical schemes for the second and fourth order evolution equations discussed above, which respect the equations' variational structure. For this purpose, I make use of the well-known fact that the equations' underlying L^2-Wasserstein gradient flows can be equivalently written as L^2-gradient flows using a Lagrangian formalism. The procedure in (1.12) then turns into a minimization problem on the set of transport maps. The main idea for deriving full discretizations for the evolution equations is to study the new "Lagrangian" minimization problem restricted to a finite-dimensional subspace of transport maps. The resulting Lagrangian numerical schemes provide an alternative perspective to "classical" Eulerian approaches: Instead of studying the differences in the altitude of discrete densities at fixed positions, the discrete evolution of fixed mass packages is considered, which is in accordance with the notion of optimal transport. Furthermore, discrete solutions to the presented particle schemes inherit various structural properties from the continuous flows by construction, like dissipation of the entropy/energy, mass and positivity preservation. The conservation of those properties and the preserved variational structure of the schemes (that basically results from the sophisticated adaptation of the minimizing procedure (1.12) in terms of transportation maps) are crucial for the analysis of convergence or long-time behaviour of discrete solutions. For instance, the dissipation of the respective entropy/energy easily yields at least a weak (with respect to the L^2-Wasserstein distance) compactness result following essentially the standard procedure developed in [**JKO98**].

In this thesis, I try to derive results for the convergence, the long-time behaviour or other qualitative properties of the schemes' solutions by exploiting the preserved variational structure. I am able to derive strong convergence of solutions to the schemes towards weak solutions of the respective equations at least in one spatial dimension, where I make use of one or more Lyapunov functionals to gain the essential a priori estimates. Also results on the long-time asymptotic of discrete solutions are going to be presented. In higher spatial dimensions, the variational formulation of the scheme and the preserved convexity of the considered entropies yield at least a stability result for the numerical approximation.

General notations and preliminary remarks

In this thesis, we always denote by Ω an open and especially connected subset of $\mathbb{R}^d$, $d \geqslant 1$, and call Ω a spatial domain. In addition we define for any given mass $M > 0$ the mass domain $\mathcal{M} := [0, M]$. Furthermore, $\mathbb{N}$ denotes the set of all positive natural numbers and we write $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.

Derivatives. Fix two integers $p, d \in \mathbb{N}$. In general, we denote by f' or $\frac{\mathrm{d}}{\mathrm{d}s} f$ the first and by $f^{(p)}$ or $\frac{\mathrm{d}^p}{\mathrm{d}s} f$ the pth derivative of a real-valued function $s \mapsto f(s)$ that is defined on a certain open subset of $\mathbb{R}$. If f is defined on a one-dimensional spatial domain Ω, then we sometimes use the notation f_x for the first derivative of f to specify that f only depends on the one-dimensional spatial domain Ω. Higher order derivations are then denoted by f_{xx}, f_{xxx} and so on.

Let us now consider a real-valued function $(x_1, \ldots, x_d) \mapsto f(x_1, \ldots, x_d)$ defined on an open subset of $\mathbb{R}^d$. Then we denote by $\partial_{x_1} f, \ldots, \partial_{x_d} f$ the partial derivatives of f with respect to the associated component. For notational simplicity, we will also write sometimes f_{x_k} or $\partial_k f$ for $\partial_{x_k} f$. For higher order partial derivatives, we use the notations

$$\partial_{x_k}^p f \quad \text{or} \quad \partial_{\underbrace{x_k \ldots x_k}_{p \text{ times}}} f$$

for $k \in \{1, \ldots, d\}$.

Let us now consider functions $f : \Omega \to \mathbb{R}$ and $\mathbf{v} = (\mathbf{v}_1, \ldots, \mathbf{v}_d)^T : \Omega \to \mathbb{R}^d$ on a spatial domain $\Omega \subseteq \mathbb{R}^d$ and write $x = (x_1, \ldots, x_d)^T$ for $x \in \Omega$. Then the spatial derivative of f is denoted by $\mathrm{D}\, f$ and we write $\mathrm{D}^p\, f$ for higher order derivatives. Of course, the gradient ∇f of f and the divergence of $\operatorname{div}(\mathbf{v})$ of $\mathbf{v}$ are given by

$$\nabla f = (\partial_{x_1} f, \ldots, \partial_{x_d} f)^T \quad \text{and} \quad \operatorname{div}(\mathbf{v}) = \sum_{k=1}^{d} \partial_{x_k} \mathbf{v}_k, \tag{1.13}$$

and we write $\Delta f = \operatorname{div}(\nabla f)$ for the Laplacian of f. We finally note that if f or $\mathbf{v}$ in addition depend on a time variable $t \in (0, +\infty)$, then the operators in (1.13) are understood to act only on the spatial variable $x \in \Omega$.

Spaces and norms. Let an arbitrary integer $d \in \mathbb{N}$ be given. Then we denote by $\langle \cdot, \cdot \rangle$ the standard inner product of two vectors, which induces the Euclidean norm $\|\vec{x}\|_2 = \sqrt{\langle \vec{x}, \vec{x} \rangle}$ on $\mathbb{R}^d$. We further write $\|\vec{x}\|_\infty = \max\{|x_k| : k = 1, \ldots, d\}$ for the maximum norm on $\mathbb{R}^d$.

For an arbitrary positive and integrable function $u : \Omega \to [0, +\infty)$ we introduce for any vector-valued function $f : \Omega \to \mathbb{R}^d$ the weighted L^p-norm

$$\|f\|_{L^p(\Omega; u)} := \left(\int_\Omega \|f(x)\|_2^p \, u(x) \, \mathrm{d}x \right)^{1/p} \quad \text{for any } p \in [1, +\infty).$$

All such functions with finite norm form the set $L^p(\Omega; u)$. For $p = +\infty$ we furthermore introduce analogously the set of essentially bounded functions $L^\infty(\Omega)$ with the norm

$$\|f\|_{L^\infty(\Omega)} := \operatorname*{ess\,sup}_{x\in\Omega} \|f(x)\|_\infty .$$

In the special case $p = 2$ the weighted L^2-norm is induced by the weighted scalar product

$$\langle f, g\rangle_u := \int_\Omega \langle f(x), g(x)\rangle\, u(x)\, \mathrm{d}x \quad \text{for all } f, g : \Omega \to \mathbb{R}^d.$$

To simplify the notation, we write $\langle\cdot,\cdot\rangle_1$, $\|\cdot\|_{L^p(\Omega)}$ and $L^p(\Omega)$, if the density u is equal to 1, hence if one integrates with respect to the Lebesgue measure. We further introduce the set $H^1(\Omega)$ of functions with finite H^1-norm that is defined for any function $f : \Omega \to \mathbb{R}$ by

$$\|f\|_{H^1(\Omega)} := \left(\|f\|^2_{L^2(\Omega)} + \|\partial_x f\|^2_{L^2(\Omega)}\right)^{1/2}.$$

Furthermore, we denote for any $p \in \mathbb{N}_0 \cup \{+\infty\}$ by $C^p(A; B)$ the set of all p-times continuously differentiable functions mapping $A \subseteq \mathbb{R}^d$ on $B \subseteq \mathbb{R}$. We also use $C(A; B)$ for $p = 0$. If $B = \mathbb{R}$, we just write $C^p(A)$. In addition we write $f \in C^p_c(A)$, if f is compactly supported in A and $f \in C^p(A)$.

Let us now consider continuous functions f that are defined on an interval $I \subseteq \mathbb{R}$ and have values in a metric space X equipped with a metric d. We introduce for $\alpha \in (0,1)$ the set $C^\alpha(I; X)$ of α-Hölder continuous (or just Hölder continuous) functions f that satisfy

$$\|f\|_{C^\alpha(I;X)} := \sup_{x\in I} \mathrm{d}(f(x), g) + \sup_{x,y\in I:\, x\neq y} \frac{\mathrm{d}(f(x), f(y))}{\|x-y\|_2^\alpha} < +\infty$$

for an arbitrary $g \in X$. Note that the boundedness of a function f with respect to $\|\cdot\|_{C^\alpha(I;X)}$ is independent of the choice of g. If the metric space X is equal to the Euclidean space $\mathbb{R}^d$ and $I = \Omega$ for a one-dimensional spatial domain Ω, we set $g = 0$ and simply write $\|\cdot\|_{C^\alpha(\Omega)}$ and $C^\alpha(\Omega)$.

Next, we assume any time interval $I \subseteq [0, +\infty)$, a certain vector space V with norm $\|\cdot\|_V$ and take a function f that depends on time and admits values in V. Then we write $f \in L^p(I; V)$, if

$$\|f\|_{L^p(I;V)} := \left(\int_I \|f(t)\|_V^p\, \mathrm{d}t\right)^{1/p} < \infty.$$

In addition to the above spaces, we write $f \in L^p_{\mathrm{loc}}(\Omega)$, $f \in H^1_{\mathrm{loc}}(\Omega)$ or $f \in C^\alpha_{\mathrm{loc}}(\Omega)$, if $f \in L^p(\mathcal{K})$, $f \in H^1(\mathcal{K})$ or $f \in C^\alpha(\mathcal{K})$ is satisfied for any compact subset $\mathcal{K} \subseteq \Omega$. Furthermore, if I is again a time interval and $f \in L^p(\mathcal{K}; V)$ is fulfilled for any compact subset $\mathcal{K} \subseteq I$, then we write $f \in L^p_{\mathrm{loc}}(I; V)$. Analogously we write $f \in C^\alpha_{\mathrm{loc}}(I; X)$ or $f \in L^p_{\mathrm{loc}}(I; V)$, if $f \in C^\alpha(\mathcal{K}; X)$ or $f \in L^p(\mathcal{K}; V)$, respectively, for any compact subset $\mathcal{K} \subseteq I$.

We recall that the *total variation* of a function $f \in L^1(a,b)$ defined on an interval (a,b) with $a, b \in \mathbb{R} \cup \{\pm\infty\}$, $a < b$, is given by

$$\mathrm{TV}\,[f] := \sup\left\{ \int_a^b f(x)\varphi'(x)\,\mathrm{d}x \,:\, \varphi \in \mathrm{Lip}(a,b),\ \text{compactly supported with } \sup_{x\in(a,b)} |\varphi(x)| \leqslant 1 \right\}, \tag{1.14}$$

where $\mathrm{Lip}(a,b)$ is the set of all Lipschitz-continuous functions. An analogue definition — most appropriate for functions $f : (a,b) \to \mathbb{R}$ that are piecewise smooth on intervals and only have jump discontinuities — is

$$\mathrm{TV}\,[f] = \sup\left\{ \sum_{j=1}^{J-1} |f(r_{j+1}) - f(r_j)| \,:\, J \in \mathbb{N},\ a < r_1 < r_2 < \cdots < r_J < b \right\}. \tag{1.15}$$

We further introduce the notation

$$[\![f]\!]_{\bar{x}} := \lim_{x\downarrow\bar{x}} f(x) - \lim_{x\uparrow\bar{x}} f(x)$$

for the height of the jump in the value of $f(x)$ at $x = \bar{x}$.

L^2-Wasserstein distance and the push-forward operator. Assume that a certain mass $M > 0$ is fixed. Then we introduce the set of regular densities with mass M,

$$\mathcal{P}^r(\Omega) := \left\{ u : \Omega \to [0, +\infty) : \int_\Omega u(x)\,\mathrm{d}x = M \right\}. \tag{1.16}$$

In addition, we define the set of regular densities with mass M and finite second moment as follows:

$$u \in \mathcal{P}_2^r(\Omega) \quad\iff\quad u \in \mathcal{P}^r(\Omega) \quad\text{and}\quad \int_\Omega |x|^2\, u(x)\,\mathrm{d}x < +\infty. \tag{1.17}$$

Note that in order to guarantee more flexibility in the numerical experiments we do *not* fix a certain mass M for the whole thesis. Nevertheless, we neglect M in the notation of $\mathcal{P}^r(\Omega)$ and $\mathcal{P}_2^r(\Omega)$ to simplify the heavy notation in the forthcoming chapters. Instead, we mention at the beginning of each chapter the considered mass to clarify which M is used in (1.16) and (1.17).

The Wasserstein distance on $\mathcal{P}^r(\Omega)$ is defined as in Definition 1.1 with the difference that we allow an arbitrary mass $M > 0$. Without going into any details about the topology on $\mathcal{P}^r(\Omega)$ that is induced by the Wasserstein distance $\mathcal{W}_2$, let us give a useful characterization of convergence in the metric space $(\mathcal{P}^r(\Omega), \mathcal{W}_2)$: A sequence of densities u_k converges towards u with respect to $\mathcal{W}_2$, if

$$\lim_{k\to\infty} \int_\Omega |x|^2 u_k(x)\,\mathrm{d}x = \int_\Omega |x|^2 u(x)\,\mathrm{d}x \qquad\text{and}\qquad \lim_{k\to\infty} \int_\Omega \varphi(x)u_k(x)\,\mathrm{d}x = \int_\Omega \varphi(x)u(x)\,\mathrm{d}x$$

for any continuous and bounded function $\varphi : \Omega \to \mathbb{R}$. We also say that u_k converges *weakly* towards u. We refer to [**AGS05**].

In this thesis a *transport map* or *transportation map* is always assumed to be a map from Ω to Ω that is at least measurable.

Next, let us introduce the *push-forward* operator: Let an arbitrary density $w \in \mathcal{P}^r(\Omega)$ and a transportation map $\mathbf{T} : \Omega \to \Omega$ be given. Then the *push-forward* $\mathbf{T}_\# w$ of $w \in \mathcal{P}^r(\Omega)$ through

$\mathbf{T}$ is defined by validity of

$$\int_{\mathbf{T}(\Omega)} \varphi(x)\mathbf{T}_{\#}w(x)\,\mathrm{d}x = \int_{\Omega} \varphi\big(\mathbf{T}(x)\big)w(x)\,\mathrm{d}x \tag{1.18}$$

for all continuous and bounded functions $\varphi : \Omega \to \mathbb{R}$. If the map $\mathbf{T} : \Omega \to \Omega$ is in addition injective and differentiable such that $\det \mathrm{D}\,\mathbf{T}(x) > 0$ for almost every $x \in \Omega$, then equation (1.18) allows an explicit representation for the push-forward,

$$\mathbf{T}_{\#}w = \frac{w}{\det \mathrm{D}\,\mathbf{T}} \circ \mathbf{T}^{-1} \tag{1.19}$$

for almost every $x \in \Omega$.

Reader's guide

The thesis is partitioned into two parts:

In Part 1, we assume the spatial domain Ω to be one-dimensional. In the introductive Chapter 2 we especially explain the Lagrangian formulation of Wasserstein gradient flows in one spatial dimension and introduce the general discrete setting that is required for our numerical schemes.

We start our numerical investigations by studying a class of second order evolution equations in Chapter 3 and provide three convergence results, each different in its nature: First, we gain a compactness result exploiting the dissipation of the entropy along discrete solutions, which suffices to pass to the limit in a discrete weak formulation. The main content of this proof is already published in a joint work with my PhD-supervisor Daniel Matthes [**MO14a**][1]. Second, a natural generalization of gradient flows in the setting of metric spaces — the notion of curves of maximal slopes — is translated and analyzed in the fully discrete case. We can show that solutions to our scheme for second order equations converge in this alternative formalism, using the framework of Γ-convergence. The third convergence result is based on a "consistency-stability"-argument.

Afterwards, we extend the numerical scheme to a family of fourth order equations in Chapter 4. The dissipation of entropy and energy functionals along discrete solutions and the long-time behaviour is analyzed, and the convergence of discrete stationary solutions to the respective continuous ones is proven. Chapter 4 is essentially based on a paper [**Osb14**] that I published online and have submitted. Furthermore, we show convergence of the scheme for the DLSS equation using both the entropy and energy dissipation under very weak assumptions on the initial density, see Chapter 5. The results of Chapter 5 are again joint work with my PhD-supervisor Daniel Matthes and can be found online [**MO14b**]. The paper [**MO14b**] is submitted and in revision.

Finally, an alternative numerical scheme for the thin film equation is presented in Chapter 6. Again by making use of two Lyapunov functionals, we obtain convergence of discrete solutions towards a weak formulation of the thin film equation. Chapter 6 is based on a submitted paper that is joint work with my PhD-supervisor Daniel Matthes.

[1] The journal can be found online at *http://journals.cambridge.org/action/displayJournal?jid=MZA* or *http://www.esaim-m2an.org/*

In the shorter Part 2, we are interested in the numerical treatment of evolution equations in two and higher dimensions. A scheme for a wide class of second order equations that is again based on a Lagrangian formulation of the minimizing movement scheme is derived, see Chapter 7. The presented approach is shown to preserve many structural properties from the continuous equations and a proof of the scheme's stability is provided. The presented content of Chapter 7 is part of recent research with Oliver Junge and my PhD-supervisor Daniel Matthes.

Among some concluding remarks in Chapter 8, a numerical scheme for fourth order equations on a two-dimensional domain is sketched. The basic idea is the same as in Chapter 4 for the one-dimensional case.

Part 1

One-dimensional case

CHAPTER 2

Preliminaries and Notation

In the first part of this thesis we are considering the case of a one-dimensional spatial domain $\Omega \subseteq \mathbb{R}$ that satisfies either $\Omega = (a, b)$ with $-\infty < a < b < +\infty$ or $\Omega = \mathbb{R}$. Hence we set $a = -\infty$ and $b = +\infty$ in the second case.

For the one-dimensional case, this preliminary chapter is intended to introduce some fundamental results about the L^2-Wasserstein distance and gradient flows in Lagrangian coordinates and provides the main idea for the ansatz of our discretization that is used in this thesis. An important observation that is one of our main motivations to introduce the Lagrangian point of view is, that the L^2-Wasserstein distance between two density functions possesses a convenient representation in terms of the densities' pseudo-inverse distribution functions, see Lemma 2.1 below. Therefore, we use Lagrangian coordinates to derive discrete submanifolds of $\mathcal{P}_2^r(\Omega)$, and the explicit representation of the L^2-Wasserstein distance then paves the way for various natural and easy-to-handle choices of discrete metrics on these submanifolds, see Section 2.2. Equipped with a suitable discretization of the space of density functions and the L^2-Wasserstein distance, continuous gradient flows can be translated into the discrete setting, which further leads to numerical schemes for the respective evolution equations, see Section 2.3.

2.1. Lagrangian coordinates

For each density u in the set of nonnegative density functions $\mathcal{P}_2^r(\Omega)$ with total mass M, one defines its *distribution function* $\mathrm{U} : \Omega \to [0, M]$ by

$$\mathrm{U}(x) = \int_a^x u(y)\,\mathrm{d}y. \tag{2.1}$$

For densities u that are not strictly positive, the distribution function U is not invertible. However, it makes sense to define the *pseudo-inverse distribution function* $\mathrm{X} : \mathcal{M} \to \overline{\Omega}$ on the mass-domain $\mathcal{M} = [0, M]$ for $u \in \mathcal{P}_2^r(\Omega)$ by

$$\mathrm{X}(\xi) = \inf\{x \in \Omega :\ \mathrm{U}(x) > \xi\} \quad \text{for all } \xi \in \mathcal{M}, \tag{2.2}$$

since it allows for a comfortable representation of the L^2-Wasserstein distance in one spatial dimension, see for instance [**Vil03**, Theorem 2.18]:

Lemma 2.1. *Let $u_0, u_1 \in \mathcal{P}_2^r(\Omega)$ have pseudo-inverse distribution functions $\mathrm{X}_0, \mathrm{X}_1 : \mathcal{M} \to \overline{\Omega}$. Then their Wasserstein distance amounts to*

$$\mathcal{W}_2(u_0, u_1) = \|\mathrm{X}_0 - \mathrm{X}_1\|_{L^2(\mathcal{M})}. \tag{2.3}$$

We also name X a *Lagrangian* or *Lagrangian map*. A characteristic property of a Lagrangian map is the validity of the following change of variables formula,

$$\int_\Omega \varphi(x)u(x)\,\mathrm{d}x = \int_{\mathcal{M}} \varphi\big(\mathrm{X}(\xi)\big)\,\mathrm{d}\xi, \tag{2.4}$$

that is fulfilled for every bounded and continuous test function φ.

Assume further $u \in \mathcal{P}_2^r(\Omega)$ to be a strictly positive density function. Then its corresponding pseudo-inverse distribution function is the well-defined inverse function of its distribution function. Thus $\mathrm{X} = \mathrm{U}^{-1}$, and X is an element of

$$\mathfrak{X} := \big\{\mathrm{X} \in \mathrm{Lip}(\mathcal{M};\overline{\Omega}) :\ a \leqslant \mathrm{X}(0) < \mathrm{X}(M) \leqslant b,\ \mathrm{X}\text{ strictly increasing}\big\},$$

where $\mathrm{Lip}(\mathcal{M};\overline{\Omega})$ is the set of locally Lipschitz-continuous functions on $\mathcal{M}$ with values in $\overline{\Omega}$. Owing to the Lipschitz-continuity of U and X, we can differentiate the identity $\mathrm{U} \circ \mathrm{X}(\xi) = \xi$ at almost every $\xi \in \mathcal{M}$ and obtain the relation

$$u(\mathrm{X}(\xi))\mathrm{X}_\xi(\xi) = 1 \qquad \text{for almost every } \xi \in \mathcal{M}. \tag{2.5}$$

2.1.1. The gradient flow in Lagrangian coordinates. As already mentioned in the introductive chapter before, we are interested in deriving fully discrete numerical schemes for evolution equations that carry a L^2-Wasserstein gradient flow structure.

In this part of the thesis we will consider integral functionals $\mathcal{E} : \mathcal{P}_2^r(\Omega) \to \mathbb{R} \cup \{+\infty\}$ of the form

$$\mathcal{E}(u) = \int_\Omega h(x, u, u_x)\,\mathrm{d}x \tag{2.6}$$

with an integrand $h : \Omega \times [0, +\infty) \times \mathbb{R} \to \mathbb{R}$ which is assumed to carry enough regularity to justify all the computations that follow. The variational derivative of the above functional $\mathcal{E}$ at $u \in \mathcal{P}_2^r(\Omega)$ is then given by (assuming u smooth enough)

$$\frac{\delta\mathcal{E}(u)}{\delta u} = h_r(x, u(x), u_x(x)) - \big(h_p(x, u(x), u_x(x))\big)_x,$$

where (x, r, p) denote the variables of h. For such a functional $\mathcal{E}$, we want to find a discretization for the continuity equation in (1.10) with the associated velocity field from (1.11). In one spatial dimension, (1.10) reads as follows: Find $u : (0, +\infty) \times \Omega \to [0, +\infty)$ such that

$$\partial_t u + \partial_x(u\mathbf{v}(u)) = 0 \quad \text{for } t > 0 \text{ and } x \in \Omega, \text{ where} \quad \mathbf{v}(u) = -\partial_x\left(\frac{\delta\mathcal{E}(u)}{\delta u}\right). \tag{2.7}$$

The starting point for our numerical approach of equation (2.7) is its *Lagrangian representation*. The reasons for using the Lagrangian point of view are essentially twofold: On the one hand, the Lagrangian representation of the L^2-Wasserstein distance from Lemma 2.1 allows an convenient calculation of the distance between arbitrary densities. On the other hand, the L^2-Wasserstein gradient flow for $\mathcal{E}$ turns into an L^2-gradient flow for $\mathfrak{E}(\mathrm{X}) := \mathcal{E}(u \circ \mathrm{X})$ that is

$$\partial_t \mathrm{X}(t, \xi) = \mathbf{v}(u) \circ \mathrm{X}(t, \xi) \quad \text{for } (t, \xi) \in (0, +\infty) \times \mathcal{M}, \tag{2.8}$$

which might be more convenient to handle as the original gradient flow, we refer for instance to [**CT04**] by Carrillo and Toscani. To make this nontrivial issue more comprehensible, let us link equation (2.7) and equation (2.8) by the following formal calculation:

Since each solution u of (2.7) is of mass M, its Lagrangian map $\mathrm{X} : (0, +\infty) \times \mathcal{M} \to \overline{\Omega}$ maps the mass domain $\mathcal{M}$ into $\overline{\Omega}$, so that

$$\xi = \int_a^{\mathrm{X}(t,\xi)} u(t,x)\,\mathrm{d}x, \tag{2.9}$$

for each $\xi \in \mathcal{M}$ and for any time t. Note especially that the left-hand side of (2.9) is independent of t. Applying a time derivative in equation (2.9) and using that u is a solution of the continuity equation in (2.7) hence yields

$$\begin{aligned} 0 &= \partial_t \mathrm{X}(t,\xi) u(t, \mathrm{X}(t,\xi)) + \int_a^{\mathrm{X}(t,\xi)} \partial_t u(t, \mathrm{X}(t,\xi))\,\mathrm{d}x \\ &= \partial_t \mathrm{X}(t,\xi) u(t, \mathrm{X}(t,\xi)) - \int_a^{\mathrm{X}(t,\xi)} \partial_x (u\mathbf{v}(u))(t,x)\,\mathrm{d}x \\ &= \big(\partial_t \mathrm{X}(t,\xi) - \mathbf{v}(u) \circ \mathrm{X}(t,\xi)\big) u(t, \mathrm{X}(t,\xi)), \end{aligned}$$

which induces (2.8).

2.1.2. Discretization in time. To study solutions to (2.8), one can for instance use a time discretization of (2.8) using Euler's implicit scheme, which turns out to be de facto equivalent to the minimizing movement scheme in (1.12).

To this end, it is necessary to introduce a decomposition of the real and nonnegative timeline $[0, +\infty)$, which shall be provided as follows: Fix a positive value $\tau > 0$ and introduce varying time step sizes $\boldsymbol{\tau} = (\tau_1, \tau_2, \ldots)$ with $\tau_n \in (0, \tau]$. Then a temporal decomposition of $[0, +\infty)$ with maximal step width τ is defined by

$$\{0 = t_0 < t_1 < \ldots < t_n < \ldots\}, \quad \text{where} \quad t_n := \sum_{j=1}^{n} \tau_j, \tag{2.10}$$

In addition we assume the time decomposition to be *quasi-uniform*, hence there exists a $\boldsymbol{\tau}$-independent constant $\overline{\alpha}_1 \in \mathbb{R}$, such that

$$\tau/\underline{\tau} < \overline{\alpha}_1, \quad \text{where } \underline{\tau} := \min_{n \in \mathbb{N}} \tau_n. \tag{2.11}$$

Henceforth, a temporal decomposition is always declared by the vector of time step sizes $\boldsymbol{\tau}$, which induces a partition of the time interval $[0, +\infty)$ by (2.10). For a fixed temporal decomposition with time step sizes $\boldsymbol{\tau} = (\tau_1, \tau_2, \ldots)$, a semi-discretization in time of (2.8) is attained by exploiting Euler's implicit scheme. This yields an approximative sequence of Lagrangian maps $(\mathrm{X}_{\boldsymbol{\tau}}^0, \mathrm{X}_{\boldsymbol{\tau}}^1, \ldots)$ recursively defined by

$$\mathrm{X}_{\boldsymbol{\tau}}^n := \operatorname*{arg\,min}_{\mathrm{X}} \mathfrak{E}_\tau(\tau_n, \mathrm{X}, \mathrm{X}_{\boldsymbol{\tau}}^{n-1}), \tag{2.12}$$

where the minimum is taken over all measurable transports mapping the mass domain $\mathcal{M}$ onto the spatial domain $\overline{\Omega}$, and

$$\mathfrak{E}_\tau(\sigma, \mathrm{X}, \mathrm{X}^*) := \frac{1}{2\sigma}\|\mathrm{X} - \mathrm{X}^*\|^2_{L^2(\mathcal{M})} + \mathfrak{E}(\mathrm{X}). \tag{2.13}$$

Especially in one spatial dimension, in which one has a close relation between the L^2-norm of Lagrangian maps and the L^2-Wasserstein distance of the associated density functions via (2.3), this minimization procedure turns out to yield a practical ansatz for deriving numerical schemes.

For later purposes, we introduce for a given temporal decomposition $\boldsymbol{\tau}$ a time interpolation as follows: If $(q_n)_{n=0}^{\infty}$ is a sequence with entries in an arbitrary metric space V, then its time interpolation $\{q\}_{\boldsymbol{\tau}} : [0, +\infty) \to V$ with respect to the decomposition $\boldsymbol{\tau}$ is defined by

$$\{q\}_{\boldsymbol{\tau}}(t) := \begin{cases} q_0 & \text{for t=0,} \\ q_n & \text{for } t \in (t_{n-1}, t_n]. \end{cases} \tag{2.14}$$

2.2. Spatial discretization – Ansatz space and discretized metric

Inside the space $\mathfrak{X}$ of inverse distribution functions, we define the finite-dimensional subspace $\mathfrak{X}_{\boldsymbol{\xi}}$ of those functions, which are piecewise affine with respect to a given partition $\boldsymbol{\xi}$ of $\mathcal{M}$ into sub-intervals that depend on a spatial decomposition parameter $K \in \mathbb{N}$. Correspondingly, there is a finite-dimensional submanifold $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ of $\mathcal{P}^r_2(\Omega)$ consisting of those densities, whose inverse distribution functions belong to $\mathfrak{X}_{\boldsymbol{\xi}}$. Densities in $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ are piecewise constant.

2.2.1. Ansatz space. Since we shall work simultaneously in the spaces $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ and $\mathfrak{X}_{\boldsymbol{\xi}}$, we need to introduce various notations. The notation in later sections becomes easier using the following sets of integers and half-integers between 0 and K that are

$$\mathbb{I}_K^+ = \{1, 2, \dots, K-1\}, \quad \mathbb{I}_K = \mathbb{I}_K^+ \cup \{0, K\} \quad \text{and} \quad \mathbb{I}_K^{1/2} = \left\{\frac{1}{2}, \frac{3}{2}, \dots, K - \frac{1}{2}\right\}.$$

We will now introduce the notations for our decomposition of the mass domain $\mathcal{M} = [0, M]$ and the spatial domain Ω. A vector $\boldsymbol{\xi} = (\xi_0, \dots, \xi_K)$ with entries ξ_j such that

$$0 = \xi_0 < \xi_1 < \dots < \xi_{K-1} < \xi_K = M$$

defines a partition of the mass domain $\mathcal{M}$ into K-many sub-intervals. We denote the lengths of the intervals by

$$\delta_{k-\frac{1}{2}} = \xi_k - \xi_{k-1} \quad \text{for all } k = 1, \dots, K.$$

We further set $\underline{\delta} = \min_{\kappa \in \mathbb{I}_K^{1/2}} \delta_\kappa$ and $\overline{\delta} = \max_{k \in \mathbb{I}_K^{1/2}} \delta_\kappa$. Let us further assume that $\underline{\delta}$ and $\overline{\delta}$ satisfy the following constraint on the mesh-ratio: There exists a K-independent constant $\overline{\alpha}_2 \in \mathbb{R}$, such that

$$\alpha_{\boldsymbol{\xi}} := \overline{\delta}/\underline{\delta} < \overline{\alpha}_2,$$

hence $\boldsymbol{\xi}$ is always chosen to be a *quasi-uniform* decompostion of the mass domain $\mathcal{M}$.

For a discretization of Ω, two situations arise depending on the boundedness of Ω:

(1) If Ω is a bounded domain, decompositions are given by the (non-equidistant) grids from

$$\mathfrak{x}_{\boldsymbol{\xi}} = \{\vec{\mathrm{x}} = (x_1, \ldots, x_{K-1}) : \ a < x_1 < \ldots < x_{K-1} < b\} \subseteq \Omega^{K-1}.$$

By definition, $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ is a vector with $K-1$ components, but we shall frequently use the convention that

$$x_0 = a \quad \text{and} \quad x_K = b. \tag{2.15}$$

(2) If $\Omega = \mathbb{R}$, we consider decompositions that are (non-equidistant) grids from

$$\mathfrak{x}_{\boldsymbol{\xi}} = \{\vec{\mathrm{x}} = (x_0, \ldots, x_K) : \ -\infty < x_0 < \ldots < x_K < +\infty\} \subseteq \Omega^{K+1}.$$

Compared to the previous situation, we just do not fix x_0 and x_K but let them move arbitrarily in $\mathbb{R}$. Consequently the number of degrees of freedom rises, hence $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ is a vector with $K+1$ components.

In any case, one obtains decompositions of Ω with $\mathfrak{x}_{\boldsymbol{\xi}} \subseteq \Omega^{\aleph}$, where the number of degrees of freedom $\aleph \in \mathbb{N}$ is given by

$$\aleph := \begin{cases} K-1 & \text{for bounded } \Omega, \\ K+1 & \text{for } \Omega = \mathbb{R}. \end{cases}$$

In the convex set $\mathfrak{X}$ of inverse distribution functions, we single out the $\aleph$-dimensional open and convex subset

$$\mathfrak{X}_{\boldsymbol{\xi}} := \{\mathrm{X} \in \mathfrak{X} : \ \mathrm{X} \text{ piecewise affine on each } [\xi_{k-1}, \xi_k], \text{ for } k = 1, \ldots, K\}.$$

There is a one-to-one correspondence between grid vectors $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ and inverse distribution function $\mathrm{X} \in \mathfrak{X}_{\boldsymbol{\xi}}$, explicitly given by

$$\mathrm{X} = \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] = \sum_{k \in \mathbb{I}_K} x_k \theta_k, \tag{2.16}$$

where the $\theta_k : \mathcal{M} \to \mathbb{R}$ are the usual affine hat functions with $\theta_k(\xi_\ell) = \delta_{k,\ell}$, i.e.

$$\theta_k(\xi) = \begin{cases} (\xi - \xi_{k-1})/\delta_{k-\frac{1}{2}}, & \text{if } 1 \leqslant k \leqslant K \text{ and } \xi \in [\xi_{k-1}, \xi_k], \\ (\xi_{k+1} - \xi)/\delta_{k+\frac{1}{2}}, & \text{if } 0 \leqslant k \leqslant K-1 \text{ and } \xi \in (\xi_k, \xi_{k+1}], \\ 0, & \text{otherwise.} \end{cases}$$

Due to this particular relation between the set $\mathfrak{x}_{\boldsymbol{\xi}}$ and the Lagrangian maps in $\mathfrak{X}_{\boldsymbol{\xi}}$, we are going to call vectors in $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ *Lagrangian vectors*. Furthermore, the locally constant density function $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] \in \mathcal{P}_2^r(\Omega)$ associated to $\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ is

$$\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](x) = \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa \mathbf{1}_{(x_{\kappa-\frac{1}{2}}, x_{\kappa+\frac{1}{2}}]}(x), \tag{2.17}$$

where we define

$$\vec{\mathrm{z}} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] = (z_{1/2}, \ldots, z_{K-1/2}) \quad \text{with weights} \quad z_\kappa = \frac{\delta_\kappa}{x_{\kappa+\frac{1}{2}} - x_{\kappa-\frac{1}{2}}}. \tag{2.18}$$

The choice of $\vec{\mathrm{z}}$ is such that each interval $(x_{\kappa-\frac{1}{2}}, x_{\kappa+\frac{1}{2}}]$ contains a total mass of δ_κ. The function $\mathbf{1}$ in (2.17) denotes the indicator function given by

$$\mathbf{1}_A(x) = \begin{cases} 1 & \text{for } x \in A \cap \Omega, \\ 0 & \text{for } x \notin A \cap \Omega, \end{cases}$$

for any subset A of $\mathbb{R}$. Depending on the domain Ω, we introduce the following convention:

$$z_{-\frac{1}{2}} = \begin{cases} z_{\frac{1}{2}} & \text{for bounded } \Omega, \\ 0 & \text{for } \Omega = \mathbb{R} \end{cases} \quad \text{and} \quad z_{K+\frac{1}{2}} = \begin{cases} z_{K-\frac{1}{2}} & \text{for bounded } \Omega, \\ 0 & \text{for } \Omega = \mathbb{R} \end{cases}. \tag{2.19}$$

This convention reflects the no-flux boundary conditions in case of a bounded domain Ω, whereas it mimics the compact support of the locally constant density $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ if $\Omega = \mathbb{R}$.

We finally introduce the associated $\aleph$-dimensional submanifold

$$\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega) := \mathbf{u}_{\boldsymbol{\xi}}[\mathfrak{x}_{\boldsymbol{\xi}}] = \{u \in \mathcal{P}^r_2(\Omega) \ : \ u = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] \text{ for some } \vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}\} \subseteq \mathcal{P}^r_2(\Omega)$$

as the image of the injective map $\mathbf{u}_{\boldsymbol{\xi}} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$.

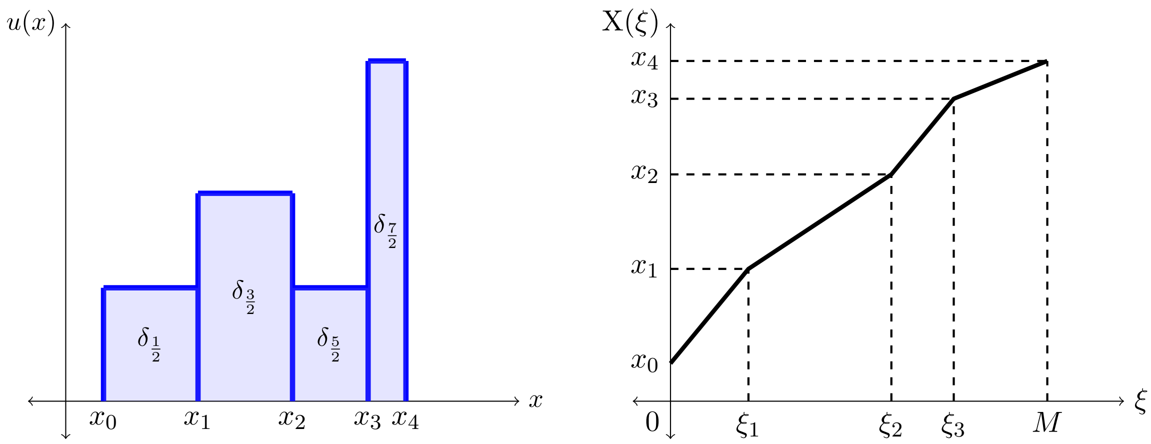


FIGURE 2.1. A typical density function $u \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ (left) with inverse distribution function $\mathrm{X} \in \mathfrak{X}_{\boldsymbol{\xi}}$ (right).

2.2.2. A metric on the ansatz space. Below, we illustrate the idea for definitions of "Wasserstein-like" metrics $\mathrm{d}_{\boldsymbol{\xi}}$ on the ansatz space $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$. The restriction of the genuine L^2-Wasserstein distance $\mathcal{W}_2$ to $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ appears as a natural candidate for $\mathrm{d}_{\boldsymbol{\xi}}$. Due to the convenient representation of $\mathcal{W}_2$ in one spatial dimension, see Lemma 2.1, the reduction of $\mathcal{W}_2$ on the discrete submanifold $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ induces a homogeneous quadratic form in terms of $\mathfrak{x}_{\boldsymbol{\xi}}$. More precisely, one attains the following result:

Lemma 2.2. *Fix a discretization* $\boldsymbol{\xi}$*, and let* $u^0, u^1 \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ *have representations* $u^0 = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^0]$ *and* $u^1 = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^1]$ *with* $\vec{\mathrm{x}}^0, \vec{\mathrm{x}}^1 \in \mathfrak{x}_{\boldsymbol{\xi}}$*, respectively. Then*

$$\mathcal{W}_2(u^0, u^1)^2 = (\vec{\mathrm{x}}^0 - \vec{\mathrm{x}}^1)^T \mathrm{W}_2 (\vec{\mathrm{x}}^0 - \vec{\mathrm{x}}^1) \tag{2.20}$$

with a symmetric tridiagonal matrix $\mathrm{W}_2 \in \mathbb{R}^{\aleph\times\aleph}$*. The coefficients* $[\mathrm{W}_2]_{kl}$ *of* W_2 *are given by*

$$[\mathrm{W}_2]_{kl} = \int_\Omega \theta_k(\xi)\theta_l(\xi)\,\mathrm{d}\xi = \frac{1}{6}\begin{cases} 2(\delta_{k+\frac12} + \delta_{k-\frac12}), & l = k \\ \delta_{k+\frac12}, & l = k+1 \\ 0, & else \end{cases}, \tag{2.21}$$

for any $l \geqslant k$ *with*

$$k, l \in \mathbb{I}_K^\aleph = \begin{cases} \mathbb{I}_K^+ & \text{for bounded } \Omega, \\ \mathbb{I}_K & \text{for } \Omega = \mathbb{R}. \end{cases}$$

We further use the convention that $\delta_{-\frac12} = \delta_{K+\frac12} = 0$ *in* (2.21)*. Moreover,* W_2 *satisfies*

$$\frac{1}{6}\sum_{k\in\mathbb{I}_K^\aleph}(\delta_{k-\frac12} + \delta_{k+\frac12})v_k^2 \leqslant v^T \mathrm{W}_2 v \leqslant \frac12 \sum_{k\in\mathbb{I}_K^\aleph}(\delta_{k-\frac12} + \delta_{k+\frac12})v_k^2. \tag{2.22}$$

for every $v \in \mathbb{R}^\aleph$

Proof. The first statement of this lemma follows by straight-forward calculations. To prove (2.22), we consider that $\aleph = K+1$, since the other case then easily follows by restriction. So let $v \in \mathbb{R}^{K+1}$ be given and observe that

$$3v^T \mathrm{W}_2 v = \sum_{k=0}^K (\delta_{k-\frac12} + \delta_{k+\frac12})v_m^2 + \sum_{k=1}^K \delta_{k-\frac12} v_k v_{k-1}.$$

Applying Young's inequality to the second sum yields together with a rearrangement of the sums

$$-\frac12 \sum_{k=0}^K (\delta_{k-\frac12} + \delta_{k+\frac12})v_k^2 \leqslant \sum_{k=1}^K \delta_{k-\frac12} v_k v_{k-1} \leqslant \frac12 \sum_{k=0}^K (\delta_{k-\frac12} + \delta_{k+\frac12})v_k^2.$$

□

The above result points out that

$$\mathrm{d}_{\boldsymbol{\xi}}(u^0, u^1) = (\vec{\mathrm{x}}^0 - \vec{\mathrm{x}}^1)^T \mathrm{W} (\vec{\mathrm{x}}^0 - \vec{\mathrm{x}}^1) \quad \text{for any } u^0 = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^0] \text{ and } u^1 = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^1] \tag{2.23}$$

with $\mathrm{W} = \mathrm{W}_2$ is obviously the most natural choice for $\mathrm{d}_{\boldsymbol{\xi}}$, since it gives the right value for the L^2-Wasserstein distance between two locally constant density functions. Nevertheless, we are going to see in later chapters that another choice for W in (2.23) can also lead to a satisfying metric on $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$, as long as W satisfies

$$c_1 \vec{\mathrm{v}}^T \mathrm{W} \vec{\mathrm{v}} \leqslant \vec{\mathrm{v}}^T \mathrm{W}_2 \vec{\mathrm{v}} \leqslant c_2 \vec{\mathrm{v}}^T \mathrm{W} \vec{\mathrm{v}} \tag{2.24}$$

for any $\vec{\mathrm{v}} \in \mathbb{R}^\aleph$ and $\boldsymbol{\xi}$-independent constants $c_1, c_1 > 0$. Such a condition for W is crucial for the study of weak compactness (with respect to the L^2-Wasserstein distance) of $\mathrm{d}_{\boldsymbol{\xi}}$-bounded subsets of $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$.

In particular, we are going to study two different options for $\mathrm{d}_{\boldsymbol{\xi}}$ in this thesis:

(1) In case of *second order* evolution equations (Chapter 3), we consider a non-equidistant mass decomposition $\boldsymbol{\xi}$, and choose the metric $\mathrm{d}_{\boldsymbol{\xi}}$ induced by the tridiagonal matrix defined in (2.21).

(2) In case of *fourth order* evolution equations (Chapter 4-6), we are always going to consider an equidistant mass decomposition of the form

$$\boldsymbol{\xi} = (0, \delta, \ldots, (K-1)\delta, M) \tag{2.25}$$

with $\delta = MK^{-1}$ for a certain integer $K \in \mathbb{N}$, and choose $\mathrm{d}_{\boldsymbol{\xi}}$ induced by $\mathrm{W} = \delta\mathbb{I}$. Here, $\mathbb{I} \in \mathbb{R}^{\aleph\times\aleph}$ denotes the identity matrix.

Considering an equidistant mass decomposition as in (2.25), it is easy to check by a slight change of the proof of (2.22) in Lemma 2.2 that $\mathrm{W} = \delta\mathbb{I}$ satisfies (2.24) with the constants $c_1 = \frac{1}{6}$ and $c_2 = 1$.

Once one has fixed a matrix $\mathrm{W} \in \mathbb{R}^{\aleph\times\aleph}$ as mentioned above, one can define a metric $\mathrm{d}_{\boldsymbol{\xi}}$ on $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ through (2.23). With the rescaled scalar product $\langle\cdot,\cdot\rangle_{\boldsymbol{\xi}}$ and norm $\|\cdot\|_{\boldsymbol{\xi}}$ defined for $\vec{\mathrm{v}}, \vec{\mathrm{w}} \in \mathbb{R}^{\aleph}$ by

$$\langle\vec{\mathrm{v}}, \vec{\mathrm{w}}\rangle_{\boldsymbol{\xi}} = \vec{\mathrm{v}}^T\mathrm{W}\vec{\mathrm{w}} \quad \text{and} \quad \|\vec{\mathrm{v}}\|_{\boldsymbol{\xi}} = \langle\vec{\mathrm{v}}, \vec{\mathrm{v}}\rangle_{\boldsymbol{\xi}}^{1/2}, \tag{2.26}$$

the distance $\mathrm{d}_{\boldsymbol{\xi}}$ is conveniently written as

$$\mathrm{d}_{\boldsymbol{\xi}}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^0], \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^1]) = \|\vec{\mathrm{x}}^1 - \vec{\mathrm{x}}^0\|_{\boldsymbol{\xi}}.$$

Note that

$$\frac{1}{6}\|\vec{\mathrm{x}}^0 - \vec{\mathrm{x}}^1\|_{\boldsymbol{\xi}} \leqslant \|\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^1] - \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^0]\|_{L^2(\mathcal{M})} \leqslant \|\vec{\mathrm{x}}^0 - \vec{\mathrm{x}}^1\|_{\boldsymbol{\xi}},$$

is then trivially satisfied for both choices $\mathrm{W} = \mathrm{W}_2$ and $\mathrm{W} = \delta\mathbb{I}$. Therefore, the metrics $\mathcal{W}_2$ and $\mathrm{d}_{\boldsymbol{\xi}}$ are equivalent in $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$, i.e.

$$\frac{1}{6}\mathrm{d}_{\boldsymbol{\xi}}(u^0, u^1) \leqslant \mathcal{W}_2(u^0, u^1) \leqslant \mathrm{d}_{\boldsymbol{\xi}}(u^0, u^1) \tag{2.27}$$

for any $u^0, u^1 \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$.

We shall not elaborate further on the point in which sense the thereby defined metric $\mathrm{d}_{\boldsymbol{\xi}}$ depending on W is a good approximation of the L^2-Wasserstein distance on $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$. However, the respective results in the following chapters validate our choices a posteriori. For results concerning the Γ-convergence of discretized transport metrics to the Wasserstein distance see [**GM13**].

2.2.3. Functions on the metric space $(\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega), \mathrm{d}_{\boldsymbol{\xi}})$. When discussing functions on the submanifold $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ in the following, we always assume that these are given in the form $f : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$. We denote the first derivative of f by $\partial_{\vec{\mathrm{x}}} f : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}^{\aleph}$ and the second one by $\partial^2_{\vec{\mathrm{x}}} f : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}^{\aleph\times\aleph}$, where the components are given through

$$[\partial_{\vec{\mathrm{x}}} f(\vec{\mathrm{x}})]_k = \partial_{x_k} f(\vec{\mathrm{x}}) \quad \text{and} \quad [\partial^2_{\vec{\mathrm{x}}} f(\vec{\mathrm{x}})]_{k,l} = \partial_{x_k}\partial_{x_l} f(\vec{\mathrm{x}}). \tag{2.28}$$

Example 2.3. *Each component* z_κ *of* $\vec{z} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{x}]$ *is a function on* $\mathfrak{x}_{\boldsymbol{\xi}}$*, and*

$$\partial_{\vec{x}} z_\kappa = -z_\kappa^2 \frac{\mathbf{e}_{\kappa+\frac{1}{2}} - \mathbf{e}_{\kappa-\frac{1}{2}}}{\delta_\kappa}. \tag{2.29}$$

Here, $\mathbf{e}_k \in \mathbb{R}^{\aleph}$ *denotes the* k*th canonical unit vector, hence*

$$\langle \mathbf{e}_k, \vec{y} \rangle = y_k \quad \text{for any vector } \vec{y} \in \mathbb{R}^{\aleph} \text{ with entries } y_k \text{ and } k \in \mathbb{I}_K^{\aleph}. \tag{2.30}$$

If Ω *is bounded, hence* $\aleph = K - 1$*, we use the convention* $\mathbf{e}_0 = \mathbf{e}_K = 0$*.*

Assume for the moment that a matrix $\mathrm{W} \in \mathbb{R}^{\aleph \times \aleph}$ is fixed and take the associated rescaled scalar product $\langle \cdot, \cdot \rangle_{\boldsymbol{\xi}}$ as defined in (2.26). Then we introduce the gradient

$$\nabla_{\boldsymbol{\xi}} f(\vec{x}) = \mathrm{W}^{-1} \partial_{\vec{x}} f(\vec{x}),$$

where the scaling by W^{-1} is chosen such that

$$\langle \vec{v}, \nabla_{\boldsymbol{\xi}} f(\vec{x}) \rangle_{\boldsymbol{\xi}} = \sum_{k \in \mathbb{I}_K^{\aleph}} v_k \partial_{x_k} f(\vec{x})$$

for arbitrary vectors $\vec{v} \in \mathbb{R}^{\aleph}$.

2.3. The basic idea for a numerical scheme

In the following section, we first want to discuss the general strategy of deriving numerical schemes to (2.7) in this Part 1, see Subsection 2.3.1 below. We then present in Subsection 2.3.2 some preliminary results for solutions to the schemes that inherit the special structure of the chosen approach.

2.3.1. Fully discretization. The general idea for deriving numerical schemes — independently of the equation's order — is a discretization of the minimizing movement scheme in Lagrangian coordinates.

So fix a pair $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$, consisting of a temporal decomposition $\boldsymbol{\tau}$ described as in (2.10), and a spatial decomposition $\boldsymbol{\xi}$ of the mass domain $\mathcal{M}$ as before in Section 2.2. We further fix a discrete metric $\mathrm{d}_{\boldsymbol{\xi}}$ on $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ as mentioned above in the Subsection 2.2.2, which is induced by a matrix W satisfying (2.24).

In view of (2.13), it is hence necessary to find a discretization $\mathbf{E}$ of the entropy $\mathfrak{E}$ in terms of Lagrangian vectors $\mathfrak{x}_{\boldsymbol{\xi}}$. The choice of such a functional strongly depends on the specific character of $\mathfrak{E}$. Take for instance an entropy of the form $\mathfrak{E}(\mathrm{X}) = \int_{\mathcal{M}} \psi(\partial_\xi \mathrm{X})\,\mathrm{d}\xi$ for any function $\psi : (0, +\infty) \to \mathbb{R}$, then a natural candidate for $\mathbf{E}$ is the restriction $\mathbf{E}(\vec{x}) = \mathfrak{E}(\partial_\xi \mathbf{X}_{\boldsymbol{\xi}}[\vec{x}])$ for any $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$. But we will also consider entropies with integrands depending on higher derivatives of X that call for a more sophisticated choice of $\mathbf{E}$.

However, let us assume for the moment that an adequate discretization of $\mathfrak{E} : \mathfrak{X} \to \mathbb{R}$ is given by the functional $\mathbf{E} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$. Furthermore, fix a discrete metric $\mathrm{d}_{\boldsymbol{\xi}}$ accordingly to the previous Section 2.2. Then a natural discretization of the minimizing movement scheme in terms of Lagrangian maps is gained by the following iterative procedure: Starting from a given $\vec{x}_\Delta^0 \in \mathfrak{x}_{\boldsymbol{\xi}}$, we define recursively a sequence $\vec{x}_\Delta = (\vec{x}_\Delta^0, \vec{x}_\Delta^1, \ldots)$ by choosing each vector $\vec{x}_\Delta^n$ as a global minimizer of $\vec{x} \mapsto \mathbf{E}_\Delta(\tau_n, \vec{x}, \vec{x}_\Delta^{n-1})$ with $\mathbf{E}_\Delta : (0,\tau] \times \mathfrak{x}_{\boldsymbol{\xi}} \times \mathfrak{x}_{\boldsymbol{\xi}}$ defined by

$$\mathbf{E}_\Delta(\sigma, \vec{x}, \vec{x}^*) = \frac{1}{2\sigma} \|\vec{x} - \vec{x}^*\|_{\boldsymbol{\xi}}^2 + \mathbf{E}(\vec{x}). \tag{2.31}$$

It is ad hoc not clear, if the functional $\vec{x} \mapsto \mathbf{E}_\Delta(\tau_n, \vec{x}, \vec{x}_\Delta^n)$ even possesses a global minimizer, but this can mostly be guaranteed by choosing $\tau > 0$ sufficiently small. However, for the sake of simplicity, let us assume for the rest of this section the existence of $\tau > 0$, such that $\vec{x} \mapsto \mathbf{E}_\Delta(\sigma, \vec{x}, \vec{x}^*)$ attains at least one global minimizer for any $\vec{x}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$ and $\sigma \in (0,\tau]$.

In practice, one wishes to define $\vec{x}_\Delta$ as — preferably unique — solution of the system of Euler-Lagrange equations associated to $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{x}_\Delta^{n-1})$, which leads to the implicit Euler time stepping:

$$\frac{\vec{x} - \vec{x}_\Delta^{n-1}}{\tau_n} = -\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}). \tag{2.32}$$

If a solution $\vec{x}_\Delta$ of iteratively defined minimizers of (2.31) indeed solves the system of Euler-Lagrange equations (2.32) is strongly dependent on the choice of $\mathbf{E}$ and on the maximal time step size τ, and is a highly nontrivial claim.

2.3.2. Entropy dissipation and weak compactness. Let us assume in this subsection that $\vec{x}_\Delta = (\vec{x}_\Delta^0, \vec{x}_\Delta^1, \ldots)$ is a sequence of Lagrangian vectors that successively solve the minimization problem (2.31). Furthermore, denote by $u_\Delta = (\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}_\Delta^0], \mathbf{u}_{\boldsymbol{\xi}}[\vec{x}_\Delta^1], \ldots)$ its corresponding sequence of density functions.

The above minimization procedure turns out to carry many powerful properties which positively effect the analysis of iteratively defined sequences of minimizers $\vec{x}_\Delta$. As a direct consequence one can even prove compactness of the corresponding sequence of density functions u_Δ, at least in a weak sense.

But before we come to this, let us show the following.

Lemma 2.4. *The sequence $\vec{x}_\Delta = (\vec{x}_\Delta^0, \vec{x}_\Delta^1, \ldots)$ of iteratively defined minimizers of the functional $\vec{x} \mapsto \mathbf{E}_\Delta(\tau_n, \vec{x}, \vec{x}_\Delta^{n-1})$ satisfies*

$$\mathbf{E}(\vec{x}_\Delta^n) \leqslant \mathbf{E}(\vec{x}_\Delta^0) \quad \textit{for all } n \geqslant 0, \tag{2.33}$$

$$\left\|\vec{x}_\Delta^{\overline{n}} - \vec{x}_\Delta^{\underline{n}}\right\|_{\boldsymbol{\xi}}^2 \leqslant 2\mathbf{E}(\vec{x}_\Delta^0)\,(t_{\overline{n}} - t_{\underline{n}}) \quad \textit{for all } \overline{n} \geqslant \underline{n} \geqslant 0. \tag{2.34}$$

If in addition $\vec{x}_\Delta$ solves the system of Euler-Lagrange equations (2.32), then for any $N \in \mathbb{N}$

$$\sum_{n=1}^{N} \tau_n \left\| \frac{\vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}}{\tau_n} \right\|_{\boldsymbol{\xi}}^2 = \sum_{n=1}^{N} \tau_n \left\|\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}_\Delta^n)\right\|_{\boldsymbol{\xi}}^2 \leqslant 2\mathbf{E}(\vec{x}_\Delta^0). \tag{2.35}$$

Proof. The monotonicity (2.33) follows (by induction on n) from the definition of $\vec{x}_\Delta^n$ as minimizer of $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{x}_\Delta^{n-1})$:

$$\mathbf{E}(\vec{x}_\Delta^n) \leqslant \frac{1}{2\tau_n} \left\|\vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2 + \mathbf{E}(\vec{x}_\Delta^n) = \mathbf{E}_\Delta(\tau_n, \vec{x}_\Delta^n, \vec{x}_\Delta^{n-1}) \leqslant \mathbf{E}_\Delta(\tau_n, \vec{x}_\Delta^{n-1}, \vec{x}_\Delta^{n-1}) = \mathbf{E}(\vec{x}_\Delta^{n-1}).$$

Moreover, summation of these inequalities from $n = \underline{n} + 1$ to $n = \overline{n}$ yields

$$\sum_{n=\underline{n}+1}^{\overline{n}} \frac{\tau_n}{2} \left[\frac{\left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}}{\tau_n} \right]^2 \leqslant \mathbf{E}(\vec{x}_\Delta^{\underline{n}}) - \mathbf{E}(\vec{x}_\Delta^{\overline{n}}) \leqslant \mathbf{E}(\vec{x}_\Delta^0).$$

For $\underline{n} = 0$ and $\overline{n} \to \infty$, we immediately get (2.35) using (2.32). If instead we combine the estimate with Jensen's inequality, we obtain

$$\left\| \vec{x}_\Delta^{\overline{n}} - \vec{x}_\Delta^{\underline{n}} \right\|_{\boldsymbol{\xi}} \leqslant \sum_{n=\underline{n}+1}^{\overline{n}} \tau_n \frac{\left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}}{\tau_n} \leqslant \left(\sum_{n=\underline{n}+1}^{\overline{n}} \tau_n \left[\frac{\left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}}{\tau_n} \right]^2 \right)^{1/2} \left(t_{\overline{n}} - t_{\underline{n}} \right)^{1/2},$$

which leads to (2.34). □

Throughout Part I of this thesis, we are going to use for a sequence $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ consisting of a temporal decomposition $\boldsymbol{\tau}$ and a spatial decomposition $\boldsymbol{\xi}$ the short-hand notation

$$\Delta \to 0,$$

meaning that $\tau \to 0$ and $\overline{\delta} \to 0$ in the limit. For the sake of notational simplicity, denote henceforth by $\vec{x}_\Delta$ and u_Δ not only the sequences of vectors $\vec{x}_\Delta^n$ and densities u_Δ^n, respectively, but also the sequences defined by the assignements $\Delta \to \vec{x}_\Delta$ and $\Delta \to u_\Delta$.

Proposition 2.5. *Assume that $\mathbf{E}(\vec{x}_\Delta^0) \leqslant \overline{\mathcal{E}}$ uniformly in Δ for a fixed constant $\overline{\mathcal{E}} > 0$. Then for any $T > 0$, there exists a function $u_* \in C^{1/2}([0,T]; \mathcal{P}_2^r(\Omega))$ and a subsequence of Δ (still denoted by Δ), such that $\{u_\Delta\}_{\boldsymbol{\tau}}(t) \to u_*(t)$ in $\mathcal{P}_2^r(\Omega)$ uniformly with respect to time $t \in [0,T]$ as $\Delta \to 0$.*

Proof. Fix any $T > 0$. We can use the same techniques as in [**AGS05**, Theorem 11.1.6] thanks to the result in (2.27): By connecting every pair of sequenced discrete values $u_\Delta^{n-1}, u_\Delta^n$ with a constant speed geodesic, i.e.

$$\langle u_\Delta \rangle_{\boldsymbol{\tau}}(t) := \mathbf{u}_{\boldsymbol{\xi}} \left[\frac{t - t_{n-1}}{\tau_n} \vec{x}_\Delta^n + \frac{t_n - t}{\tau_n} \vec{x}_\Delta^{n-1} \right] \qquad \text{for } t \in (t_{n-1}, t_n],$$

we obtain a family of Lipschitz-continuous curves satisfying for any $s, t \in (t_{n-1}, t_n]$

$$\begin{aligned} &\mathcal{W}_2(\langle u_\Delta \rangle_{\boldsymbol{\tau}}(s), \langle u_\Delta \rangle_{\boldsymbol{\tau}}(t))^2 \\ &= \int_{\mathcal{M}} \left| \left(\frac{s - t_{n-1}}{\tau_n} \mathbf{X}_\Delta^n + \frac{t_n - s}{\tau_n} \mathbf{X}_\Delta^{n-1} \right) - \left(\frac{t - t_{n-1}}{\tau_n} \mathbf{X}_\Delta^n + \frac{t_n - t}{\tau_n} \mathbf{X}_\Delta^{n-1} \right) \right|^2 \mathrm{d}\xi \\ &= \left(\frac{s-t}{\tau_n} \right)^2 \int_{\mathcal{M}} \left| \mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1} \right|^2 \mathrm{d}\xi = \left(\frac{s-t}{\tau_n} \right)^2 \mathcal{W}_2(u_\Delta^n, u_\Delta^{n-1})^2. \end{aligned}$$

Then for arbitrary $s, t \in [0,T]$, $s < t$ and $n, m \in \mathbb{N}$ such that $s \in (t_{n-1}, t_n]$ and $t \in (t_m, t_{m+1}]$, we get together with (2.34) and the metric equivalence (2.27)

$$\begin{aligned} \mathcal{W}_2(\langle u_\Delta \rangle_{\boldsymbol{\tau}}(s), \langle u_\Delta \rangle_{\boldsymbol{\tau}}(t)) &\leqslant \mathcal{W}_2(\langle u_\Delta \rangle_{\boldsymbol{\tau}}(s), u_\Delta^n) + \mathcal{W}_2(u_\Delta^n, u_\Delta^m) + \mathcal{W}_2(u_\Delta^m, \langle u_\Delta \rangle_{\boldsymbol{\tau}}(t)) \\ &\leqslant \frac{t_n - s}{\tau_n} \mathcal{W}_2(u_\Delta^{n-1}, u_\Delta^n) + \mathcal{W}_2(u_\Delta^n, u_\Delta^m) + \frac{t - t_m}{\tau_{m+1}} \mathcal{W}_2(u_\Delta^m, u_\Delta^{m+1}) \quad (2.36) \\ &\leqslant \sqrt{s - t}\, C, \end{aligned}$$

where $C > 0$ just depends on $\overline{\mathcal{E}}$. Analogously one proves

$$\mathcal{W}_2(\{u_\Delta\}_{\boldsymbol{\tau}}(t), \langle u_\Delta\rangle_{\boldsymbol{\tau}}(t)) \leqslant \sqrt{\tau} C \quad \text{for any } t \in [0,T]$$

with another Δ-independent constant $C > 0$. We can therefore invoke the Arzelà-Ascoli Theorem A.1, which yields the relative compactness of the family $\langle u_\Delta\rangle_{\boldsymbol{\tau}}$ in $C^0([0,T]; \mathcal{P}_2^r(\Omega))$. Hence there exists $u_* \in C^{1/2}([0,T]; \mathcal{P}_2^r(\Omega))$, such that

$$\sup_{t\in[0,T]} \mathcal{W}_2(\langle u_\Delta\rangle_{\boldsymbol{\tau}}(t), u_*(t)) \longrightarrow 0$$

and

$$\sup_{t\in[0,T]} \mathcal{W}_2(\{u_\Delta\}_{\boldsymbol{\tau}}(t), u_*(t)) \leqslant \sqrt{\tau} C + \sup_{t\in[0,T]} \mathcal{W}_2(\langle u_\Delta\rangle_{\boldsymbol{\tau}}(t), u_*(t)) \longrightarrow 0$$

as $\Delta \to 0$. This proves the claim. $\square$

CHAPTER 3

Second order drift-diffusion equation

The contents of Sections 3.1–3.4 of this chapter and especially the main results in Theorem 3.3 and Theorem 3.4 are already published in a joint work with my PhD-supervisor Daniel Matthes [**MO14a**][1]

3.1. Introduction

In the following chapter, we propose and study a fully discrete Lagrangian scheme for the following nonlinear drift-diffusion equation with no-flux boundary conditions on the bounded interval $\Omega = (a, b)$,

$$\partial_t u = \partial_{xx}\mathrm{P}(u) + \partial_x(uV_x) \quad \text{for } t > 0 \text{ and } x \in \Omega, \tag{3.1}$$

$$\partial_x\mathrm{P}(u) + uV_x = 0 \quad \text{for } t > 0 \text{ and } x \in \partial\Omega, \tag{3.2}$$

$$u = u^0 \geqslant 0 \quad \text{at } t = 0, \tag{3.3}$$

where $V : \overline{\Omega} \to \mathbb{R}$ is assumed to be in $C^2(\Omega)$ and $\mathrm{P} : [0, +\infty) \to [0, +\infty)$ is a nonnegative and monotonically increasing function that satisfies the following assumptions:

- One can find a strictly convex function $\phi : [0, +\infty) \to \mathbb{R}$ with $\phi(0) = 0$, such that
$$\mathrm{P}(r) = r\phi'(r) - \phi(r). \tag{3.4}$$
- $r \mapsto \mathrm{P}(r)$ is linear or has superlinear growth. In addition, we assume the existence of an integer $p \geqslant 1$ and of constants $\underline{c}, \overline{c}, \underline{d}, \overline{d} \in (0, +\infty)$, such that
$$\mathrm{P}(r)^2 \geqslant \underline{c}r^p - \underline{d} \quad \text{and} \quad \mathrm{P}(r)/r \leqslant \overline{c}r^p + \overline{d}. \tag{3.5}$$
for any $r \in (0, +\infty)$.

Typical examples for P satisfying the above conditions are $\mathrm{P}(r) = r$ (*heat equation*) or $\mathrm{P}(r) = r^m$ for $m > 1$ (*porous medium equation* with slow diffusion).

Furthermore, the initial datum u^0 is assumed to be integrable with total mass $M > 0$, i.e.

$$\int_\Omega u^0(x)\,\mathrm{d}x = M,$$

which shall be fixed for the rest of this chapter. This means especially that $u^0 \in \mathcal{P}_2^r(\Omega)$ with $\mathcal{P}_2^r(\Omega)$ as defined in (1.17).

Remark 3.1. *The technical assumptions in* (3.5) *are only minor restrictions for the choice of* P*. In fact, these assumptions mainly assure that* $\mathrm{P}(r)$ *does not behave "too badly" close to* $r = 0$*,*

[1] The journal can be found online at *http://journals.cambridge.org/action/displayJournal?jid=MZA* or *http://www.esaim-m2an.org/*

and that P *does not increase exponentially fast as* $r \to +\infty$*. However, one can get rid of* (3.5) *by considering a CFL-condition for the temporal and spatial decompositions, which fixes a relation between* τ *and* $\overline{\delta}$*. A proof including such a CFL-condition was done in [**MO14a**]. This is why we are going to present an alternative approach that involves the assumptions* (3.5)*, which are less restrictive than a CFL-condition.*

Studies on Lagrangian schemes for (3.1) are widespread in the literature. MacCamy and Sokolovsky [**MS85**] presented already a discretization that is almost identical to ours, for (3.1) with $\mathrm{P}(u) = u^2$ and $V \equiv 0$. Another pioneering work in this direction is the paper by Russo [**Rus90**], who compares several (semi-)Lagrangian discretizations in the linear case $\mathrm{P}(u) = u$; extensions to two spatial dimensions are also discussed. Later, Budd et al. [**BCHR99**] used a moving mesh to capture self-similar solutions of the porous medium equation on the whole line. We further refer to [**BCW10**] by Burger et al., describing a numerical scheme for nonlinear diffusion equations using a mixed finite element method.

The connection between Lagrangian schemes and the gradient flow structure of equation (3.1) was investigated by Kinderlehrer and Walkington [**KW99**] and in a series of unpublished theses [**Roe04**,**Lev02**]. In a recent paper by Westdickenberg and Wilkening [**WW10**], a similar scheme for (3.1) is obtained as a by-product in the process of designing a structure preserving discretization for the Euler equations.

In the aforementioned works, numerical schemes are defined and used in experiments; qualitative properties and convergence are not studied analytically. Some analytical investigations have been carried out by Gosse and Toscani [**GT06a**]: For a Lagrangian scheme with explicit time discretization, they prove comparison principles and rigorously discuss stability and consistency.

Similar approaches are also available for chemotaxis systems [**BCC08**], for non-local aggregation equations [**CM10**, **CW**], and for convolution-diffusion equations [**GT06b**].

3.1.1. Gradient flow structure. The link between equation (3.1) and the continuity equation in (2.7) (or (1.10), respectively) is given by the entropy

$$\mathcal{E}(u) = \int_\Omega \phi(u(x))\,\mathrm{d}x + \int_\Omega u(x)V(x)\,\mathrm{d}x, \tag{3.6}$$

which corresponds to (2.6) using the integrand $h(x,r,p) = \phi(r) + rV(x)$. The induces velocity field is then given in terms of the first variational derivative of $\mathcal{E}$ by

$$\mathbf{v}(u) = -\partial_x\big(\phi'(u) + V\big) = -\left(\frac{\partial_x \mathrm{P}(u)}{u} + V_x\right). \tag{3.7}$$

As we have mentioned in the introduction, this means that a solution to (3.1) satisfying the no-flux boundary condition (3.2) can be interpreted as a L^2-Wasserstein gradient flow in the potential landscape of the entropy $\mathcal{E}$, see [**Ott01**]. Written in terms of Lagrangian coordinates

X, the L^2-Wasserstein gradient flow for $\mathcal{E}$ turns into an L^2-gradient flow for

$$\begin{aligned}\mathcal{E}(u\circ \mathrm{X}) &= \int_{\mathcal{M}} \phi\left(\frac{1}{\partial_\xi \mathrm{X}(\xi)}\right) \partial_\xi \mathrm{X}(\xi)\,\mathrm{d}\xi + \int_{\mathcal{M}} V\big(\mathrm{X}(\xi)\big)\,\mathrm{d}\xi \\ &= \int_{\mathcal{M}} \psi\big(\partial_\xi \mathrm{X}(\xi)\big)\,\mathrm{d}\xi + \int_{\mathcal{M}} V\big(\mathrm{X}(\xi)\big)\,\mathrm{d}\xi,\end{aligned}$$

with the integrand $\psi : (0,+\infty) \to \mathbb{R}$ defined by $\psi(s) = s\phi(1/s)$. Here we used the change of variables $x = \mathrm{X}(\xi)$ and relation (2.5) under the integral in (3.6). Using that $\partial_t \mathrm{X} = \mathbf{v}(u)\circ \mathrm{X}$, see (2.8) from Section 2.1.1, it is easily verified that this L^2-gradient flow has the form

$$\partial_t \mathrm{X} = \partial_\xi \psi'(\partial_\xi \mathrm{X}) - V_x(\mathrm{X}). \tag{3.8}$$

Indeed, using that $\psi'(s^{-1}) = -\mathrm{P}(s)$, which follows from (3.4), one achieves

$$\partial_t \mathrm{X} = \mathbf{v}(u)\circ \mathrm{X} = -\left(\frac{\partial_x \mathrm{P}(u)}{u} + V_x\right)\circ \mathrm{X} = -\partial_\xi \mathrm{P}(u\circ \mathrm{X}) - V_x(\mathrm{X}) = \partial_\xi \psi'(\partial_\xi \mathrm{X}) - V_x(\mathrm{X}).$$

Let us finally remark that the functional $\mathcal{E}$ is λ-convex along geodesics in $\mathcal{W}_2$ with

$$\lambda = \min_{x\in\overline{\Omega}} V_{xx}(x), \tag{3.9}$$

which has been first observed by McCann [**McC97**]. Consequently, the L^2-Wasserstein gradient flow is λ-contractive.[2] Hence, two solutions u, v converge ($\lambda > 0$) or diverge ($\lambda < 0$) at most at an exponential rate of λ with respect to $\mathcal{W}_2$, i.e.,

$$\mathcal{W}_2(u(t), v(t)) \leqslant \mathcal{W}_2(u^0, v^0)e^{-\lambda t} \quad \text{for all } t > 0. \tag{3.10}$$

3.1.2. Description of the numerical scheme. We are now going to present a numerical scheme for (3.1) using the gradient flow representation in (3.8), which is practical, stable and easy to implement.

Before we come to the proper definition of the numerical scheme, we fix a spatio-temporal discretization parameter $\Delta = (\boldsymbol{\tau};\boldsymbol{\xi})$ as follows: For a given $\tau > 0$, introduce varying time step sizes $\boldsymbol{\tau} = (\tau_1, \tau_2, \ldots)$ with $\tau_n \in (0,\tau]$, then a time decomposition of $[0,+\infty)$ is defined by $(t_n)_{n=0}^\infty$ with $t_n := \sum_{j=1}^n \tau_j$ as in (2.10). As spatial discretization, fix $K \in \mathbb{N}$ and introduce an arbitrary but quasi-uniform spatial decomposition $\boldsymbol{\xi} = (\xi_0, \ldots, \xi_K)$ of the mass domain $\mathcal{M}$ as in Subsection 2.2.1. Furthermore, fix the discrete metric $\mathrm{d}_{\boldsymbol{\xi}}$ on $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ that is induced by the matrix W_2 from (2.21), hence $\mathrm{d}_{\boldsymbol{\xi}}(u,v) = \mathcal{W}_2(u,v)$ for any locally constant density functions $u, v \in \mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$.

Our numerical scheme is now defined as a discretization of equation (3.8):

Numerical scheme. *Fix a discretization parameter $\Delta = (\boldsymbol{\tau};\boldsymbol{\xi})$. Then a numerical scheme for (3.1) is defined as follows:*

(1) *For $n = 0$, fix an initial sequence of monotone values $\vec{\mathrm{x}}_\Delta^0 := (x_1^0, \ldots, x_{K-1}^0) \in \mathfrak{x}_{\boldsymbol{\xi}}$ and set $x_0^0 = a$ and $x_K^0 = b$ by convention. The vector $\vec{\mathrm{x}}_\Delta^0$ describes a non-equidistant decomposition of $\overline{\Omega} = [a,b]$.*

[2] Note that λ-contractivity with $\lambda < 0$ is a weaker property than contractivity of the flow. Indeed, trajectories may diverge, but not faster than in (3.10).

(2) *For $n \geqslant 1$, recursively define Lagrangian vectors $\vec{x}_\Delta^n = (x_1^n, \dots, x_{K-1}^n) \in \mathfrak{x}_{\boldsymbol{\xi}}$ as solutions to the $K-1$ equations*

$$\begin{aligned} \frac{1}{\tau_n}\big[\mathrm{W}_2(\vec{x} - \vec{x}_\Delta^{n-1})\big]_k =& \psi'\Big(\frac{x_{k+1}-x_k}{\delta_{k+\frac{1}{2}}}\Big) - \psi'\Big(\frac{x_k - x_{k-1}}{\delta_{k-\frac{1}{2}}}\Big) \\ & - \int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{x}](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi, \end{aligned} \tag{3.11}$$

with $k = 1, \dots, K-1$. We later show in Proposition 3.9 that the solvability of the system (3.11) *is guaranteed.*

The above procedure (1) − (2) *yields a sequence of monotone vectors $\vec{x}_\Delta := (\vec{x}_\Delta^0, \vec{x}_\Delta^1, \dots, \vec{x}_\Delta^n, \dots)$, and each entry $\vec{x}_\Delta^n$ defines a spatial decomposition of the compact interval $[x_0^n, x_K^n] \subseteq \overline{\Omega}$, $n \in \mathbb{N}$. Fixing an index $k \in \{1, \dots, K\}$, the sequence $n \mapsto x_k^n$ defines a discrete temporal evolution of spatial grid points in Ω, and if one assigns each interval $[x_{k-1}^n, x_k^n]$ a constant mass package $\delta_{k-\frac{1}{2}}$, the map $n \mapsto [x_{k-1}^n, x_k^n]$ characterizes the temporal movement of mass. Hence $\vec{x}_\Delta$ is uniquely related to a sequence of locally constant density functions $u_\Delta := (u_\Delta^0, u_\Delta^1, \dots, u_\Delta^n, \dots)$, where each function $u_\Delta^n : \Omega \to \mathbb{R}_+$ fulfills*

$$u_\Delta^n(x) = \mathbf{u}_{\boldsymbol{\xi}}[\vec{x}_\Delta^n] = \sum_{\kappa \in \mathbb{I}_K^{1/2}} \frac{\delta}{x_{\kappa+\frac{1}{2}}^n - x_{\kappa-\frac{1}{2}}^n} \mathbf{1}_{(x_{\kappa-\frac{1}{2}}, x_{\kappa+\frac{1}{2}}]}(x),$$

according to the definition of $\mathbf{u}_{\boldsymbol{\xi}}$ in (2.17).

Remark 3.2. *In order to satsify the initial condition that $u(0, \cdot) = u^0$ in* (3.3)*, a suitable choice of the initial grid $\vec{x}_\Delta^0$ is required. One can for instance define $\vec{x}_\Delta^0$ such that each grid point satisfies*

$$\xi_k = \int_{x_{k-1}^0}^{x_k^0} u^0(x)\,\mathrm{d}x$$

for $k = 1, \dots, K-1$. It is easy to verify that the corresponding local density converges towards u^0 with respect to the L^2-Wasserstein distance, see for instance Lemma 3.24.

At the first glance, it seems unclear in which sense (3.11) is a discretization of the L^2-gradient flow from (3.8). To motivate the above approach, multiply (3.8) by a locally affine hat function θ_k and integrate with respect to ξ, then integration by parts yields

$$\begin{aligned} \int_{\mathcal{M}} \partial_t \mathrm{X}\theta_k\,\mathrm{d}\xi &= -\int_{\mathcal{M}} \psi'(\partial_\xi \mathrm{X})\partial_\xi\theta_k\,\mathrm{d}\xi - \int_{\mathcal{M}} V_x(\mathrm{X})\theta_k\,\mathrm{d}\xi \\ &= \frac{1}{\delta_{k+\frac{1}{2}}}\int_{\xi_k}^{\xi_{k+1}} \psi'(\partial_\xi\mathrm{X})\,\mathrm{d}\xi - \frac{1}{\delta_{k-\frac{1}{2}}}\int_{\xi_{k-1}}^{\xi_k} \psi'(\partial_\xi\mathrm{X})\,\mathrm{d}\xi - \int_{\mathcal{M}} V_x(\mathrm{X})\theta_k\,\mathrm{d}\xi. \end{aligned}$$

For this equation, we apply a finite element discretization by replacing X with a discrete Lagrangian map $\mathbf{X}_{\boldsymbol{\xi}}[\vec{x}]$. Then a discretization of the time derivative using the respective difference quotient, and the identity $[\mathrm{W}_2]_{kl} = \int_{\mathcal{M}} \theta_k\theta_l\,\mathrm{d}\xi$ immediately yields (3.11).

Note that there are infinitely many (and maybe more "obvious") ways to discretize the right-hand side in (3.8). However, the one in (3.11) can be derived as a natural restriction of the L^2-Wasserstein gradient flow in the potential landscape of the original entropy $\mathcal{E}$, and hence provides the crucial a priori estimate for the discrete-to-continuous limit using the dissipation of the entropy along discrete solutions. This circumstance is going to be discussed later in Section 3.2.1.c in more detail.

From now on we denote a solution to the above scheme by $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}_\Delta^0, \vec{\mathrm{x}}_\Delta^1, \ldots)$ and its corresponding sequence of densities by $u_\Delta = (u_\Delta^0, u_\Delta^1, \ldots)$, where the components $\vec{\mathrm{x}}_\Delta^n$ and u_Δ^n correlate through the map $\mathbf{u}_\Delta : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$.

3.1.3. Main results. For the moment, fix a discretization parameter $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$.

Let us further introduce a "discretized" version of the entropy $\mathcal{E}$ on the set of Lagrangian vectors $\mathfrak{x}_{\boldsymbol{\xi}}$ by

$$\mathbf{E}(\vec{\mathrm{x}}) := \mathcal{E}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]) = \sum_{\kappa \in \mathbb{I}_K^{1/2}} \delta_\kappa \psi\left(\frac{x_{\kappa+\frac{1}{2}} - x_{\kappa-\frac{1}{2}}}{\delta_\kappa}\right) + \int_{\mathcal{M}} V\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big)\,\mathrm{d}\xi, \tag{3.12}$$

which is nothing else than the restriction of $\mathcal{E}$ to the set of piecewise constant density functions in the language of Lagrangian vectors.

Our first result pictures the qualitative properties of discrete solutions to (3.11).

Theorem 3.3. *Assume that $\tau^{-1} + \lambda > 0$. From any initial density $u_\Delta^0 = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^0]$ with Lagrangian vector $\vec{\mathrm{x}}_\Delta^0$, a sequence $\vec{\mathrm{x}}_\Delta^n$ satisfying* (3.11) *can be constructed by inductively defining $\vec{\mathrm{x}}_\Delta^n$ as the* unique *global minimizer of*

$$\vec{\mathrm{x}} \mapsto \frac{1}{2\tau_n} \left\| \vec{\mathrm{x}} - \vec{\mathrm{x}}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 + \mathbf{E}(\vec{\mathrm{x}}). \tag{3.13}$$

The sequence of associated densities $u_\Delta = (u_\Delta^0, u_\Delta^1, \ldots)$ with entries $u_\Delta^n = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^n]$ then has the following properties:

- Positivity and conservation of mass: *For each $n \in \mathbb{N}$, u_Δ^n is a strictly positive function and has mass equal to M.*
- Dissipation: *The entropy $\mathcal{E}$ is dissipated, i.e. $\mathcal{E}(u_\Delta^n) \leqslant \mathcal{E}(u_\Delta^{n-1})$.*
- Contraction: *If v_Δ is another sequence solving recursively* (3.13)*, then*

$$\mathcal{W}_2(u_\Delta^n, v_\Delta^n) \leqslant e^{-\frac{\lambda}{1+\lambda\tau} t_n} \mathcal{W}_2(u_\Delta^0, v_\Delta^0). \tag{3.14}$$

Positivity, conservation of mass, and dissipation of the entropy follow immediately from the scheme's construction, while the contraction property and even well-posedness are nontrivial claims.

The main theorem of this chapter is the proof of convergence, which can be formulated as follows.

Theorem 3.4. *Let a strictly positive initial density u^0 be given. Furthermore, choose Lagrangian vectors $\vec{\mathrm{x}}_\Delta^0$ such that $u_\Delta^0 = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^0]$ converges to u^0 weakly in $L^1(\Omega)$ as $\Delta \to 0$ and*

$$\overline{\mathcal{E}} := \sup_\Delta \mathcal{E}(u_\Delta^0) < +\infty. \tag{3.15}$$

For each Δ, construct a discrete approximation $\vec{\mathrm{x}}_\Delta$ according to the procedure described in (3.11)*. Then there exist a subsequence of u_Δ (still denoted by Δ) and a limit function u_* in $C^{1/2}_{\mathrm{loc}}([0,+\infty);\mathcal{P}^r_2(\Omega))$ such that:*

- *$\{u_\Delta\}_\tau$ converges to u_* strongly in $L^1_{\mathrm{loc}}([0,+\infty)\times\Omega)$.*
- *u_* satisfies the following weak formulation of* (3.1)*:*

$$\int_0^\infty \int_\Omega u_* \partial_t \varphi \,\mathrm{d}x\,\mathrm{d}t + \int_0^\infty \int_\Omega \mathrm{P}(u_*)\partial_{xx}\varphi - u_* V_x \partial_x \varphi \,\mathrm{d}x\,\mathrm{d}t = 0, \tag{3.16}$$

for any test function $\varphi \in C^\infty((0,+\infty)\times\Omega)$ with compact support in $(0,+\infty)\times\overline{\Omega}$ and $\partial_x\varphi(t,a) = \partial_x\varphi(t,b) = 0$.

Remark 3.5. *The consistency and stability calculations in Section 3.6, see especially Proposition 3.32, provide a rate of convergence of order $\tau + \overline{\delta}^2$, if solutions to* (3.1) *are assumed to be sufficiently smooth, see Remark 3.30. Numerical experiments confirm the analytically observed rate, see Section 3.7.*

At this point we want to remark that the above convergence result even holds true if one neglects the strict positivity of the initial density u^0. For this, one has to choose strictly positive density functions u^0_Δ that converge weakly towards u^0 and satisfy an upper bound as in (3.15). The resulting sequence of strictly positive densities u_Δ that is gained by the numerical scheme then still converges strongly towards a density u_* solving the weak formulation of (3.1). As the proof of Theorem 3.4 will show, one of the main ingredients of the compactness results is the uniform boundedness of the initial approximation u^0_Δ. A more detailed argumentation can be found in [**MO14a**].

Furthermore, using the abstract notion of Γ-convergence we show in in Section 3.5 that the limit curve u_* is a *curve of maximal slope*, which constitutes the natural generalization of a gradient flow in the setting of metric spaces [**AGS05**, **ALS06**, **Ort05**, **Ser11**].

Theorem 3.6. *In addition to the assumptions in Theorem 3.4, assume that λ as defined in* (3.9) *satisfies $\lambda \geqslant 0$. Then the limit curve $u_* \in C^{1/2}_{\mathrm{loc}}([0,+\infty);\mathcal{P}^r_2(\Omega))$ of Theorem 3.4 is a curve of maximal slope for $\mathcal{E}$, hence u_* especially satisfies*

$$\frac{1}{2}\int_0^t |u_*'|^2(r)\,\mathrm{d}r + \frac{1}{2}\int_0^t |\partial\mathcal{E}|^2(u_*(r))\,\mathrm{d}r = \mathcal{E}(u_*(0)) - \mathcal{E}(u_*(t))$$

for any $t \in [0,+\infty)$. The proper definitions of $|u_*'|$, $|\partial\mathcal{E}|(u_*(r))$ and of the notion of curves of maximal slope are listed in Definition 3.20, see Section 3.5.

3.1.4. Key estimates. In what follows, we give a formal outline for the derivation of the main a priori estimate for the fully discrete solutions.

The first main estimate is related to the gradient flow structure of (3.1): It is the potential flow of the entropy $\mathcal{E}$ with respect to the L^2-Wasserstein distance $\mathcal{W}_2$. The consequences, which are immediate from the abstract theory of gradient flows [**AGS05**], are that $t \mapsto \mathcal{E}(u(t))$ is monotone, and that each solution "curve" $t \mapsto u(t)$ is globally Hölder-$\frac{1}{2}$-continuous with respect to $\mathcal{W}_2$. In order to carry over these properties to our discretization, the latter is constructed as a gradient flow of a flow potential $\mathbf{E}$ with respect to a particular metric $\mathrm{d}_{\boldsymbol{\xi}}$ on the space of locally constant density functions, see Section 3.2.1.c below for more details.

The second main estimate is a discrete interpretation of the following a priori estimate, which is essential in the continuous theory of well-posedness of (6.1): Solutions to (3.1) dissipate the entropy $\mathcal{E}$ and the respective estimate is formally derived by an integration by parts (assuming $V = 0$),

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(u) = -\int_\Omega \phi'(u)\partial_{xx}\mathrm{P}(u)\,\mathrm{d}x = \int_\Omega u\big(\partial_x\phi'(u)\big)^2\,\mathrm{d}x,$$

where we again use the identity (3.4). Adapting this estimate in terms of locally constant density functions, the best one can hope for is a control on the total variation instead of the derivative, see Proposition 3.13. Nevertheless, this is the perfect regularity estimate to obtain our main compactness result stated in Proposition 3.16.

3.2. Discretization in space and time

3.2.1. Properties of the entropy — continuous and discrete case.

3.2.1.a. The entropy in Lagrangian coordinates. To study the scheme's properties, it is essential to get an idea of the continuous entropy $\mathcal{E}$ rewritten in terms of Lagrangian coordinates. As already mentioned in Section 3.1.1 before, a change of variables $x = \mathrm{X}(\xi)$ under the integral of $\mathcal{E}$ yields $\mathcal{E}(u) = \mathfrak{E}(\mathrm{X})$ for any density $u \in \mathcal{P}_2^r(\Omega)$ with pseudo-inverse distribution function X, where

$$\mathfrak{E}(\mathrm{X}) := \int_{\mathcal{M}} \psi\big(\partial_\xi \mathrm{X}(\xi)\big)\,\mathrm{d}\xi + \int_{\mathcal{M}} V\big(\mathrm{X}(\xi)\big)\,\mathrm{d}\xi, \tag{3.17}$$

and $\psi(s) = s\phi(1/s)$. Due to the requirements on P and ϕ, it turns out that ψ satisfies

$$\psi'(s) = \phi(s^{-1}) - s^{-1}\phi'(s^{-1}) = -\mathrm{P}(s^{-1}), \quad \text{and} \quad \psi''(s) = s^{-2}\mathrm{P}'(s^{-1}) > 0. \tag{3.18}$$

Thus ψ is a strictly convex function. Furthermore, ψ gets arbitraryly large close to zero, i.e.

$$\lim_{s\downarrow 0}\psi(s) = \psi(1) + \lim_{s\downarrow 0}\int_s^1 \mathrm{P}(\sigma^{-1})\,\mathrm{d}\sigma = \psi(1) + \lim_{r\to\infty}\int_1^r \frac{\mathrm{P}(\rho)}{\rho^2}\,\mathrm{d}\rho = +\infty, \tag{3.19}$$

where the last equality is a result of the linearity of P, respectively of P's superlinear growth. This behaviour of ψ is crucial to prove the well-posedness of (3.11), but before we come to this, we are going to show the following lemma.

Lemma 3.7. *The functional $\mathfrak{E}$ is bounded from below,*

$$\mathfrak{E}(\mathrm{X}) \geqslant \underline{\mathcal{E}} := M\left(\psi\Big(\frac{b-a}{M}\Big) + \lambda\right), \tag{3.20}$$

and it is λ-convex on $\mathfrak{X}$ with the λ given in (3.9)*, i.e.*

$$\mathfrak{E}\big((1-s)\mathrm{X}^0 + s\mathrm{X}^1\big) \leqslant (1-s)\mathfrak{E}(\mathrm{X}^0) + s\mathfrak{E}(\mathrm{X}^1) - \frac{\lambda s(1-s)}{2}\|\mathrm{X}^0 - \mathrm{X}^1\|^2_{L^2(\mathcal{M})} \tag{3.21}$$

for all $\mathrm{X}^0, \mathrm{X}^1 \in \mathfrak{X}$ *and every* $s \in [0,1]$.

Proof. Since ψ is convex, the lower bound follows by Jensen's inequality:

$$\mathfrak{E}(\mathrm{X}) \geqslant M\psi\bigg(\int_{\mathcal{M}} \partial_\xi \mathrm{X}(\xi)\frac{\mathrm{d}\xi}{M}\bigg) + \int_{\mathcal{M}} \min_{x\in\Omega} V(x)\,\mathrm{d}\xi.$$

By definition of λ, this yields (3.20). Next, let $\mathrm{X}^0, \mathrm{X}^1 \in \mathfrak{X}$ and $s \in [0,1]$ be given. Again by the convexity of $\psi : (0,+\infty) \to \mathbb{R}$, it follows in particular that

$$\int_{\mathcal{M}} \psi\big((1-s)\partial_\xi \mathrm{X}^0(\xi) + s\partial_\xi \mathrm{X}^1(\xi)\big)\,\mathrm{d}\xi \leqslant (1-s)\int_{\mathcal{M}} \psi\big(\partial_\xi \mathrm{X}^0(\xi)\big)\,\mathrm{d}\xi + s\int_{\mathcal{M}} \psi\big(\partial_\xi \mathrm{X}^1(\xi)\big)\,\mathrm{d}\xi.$$

By using Taylor expansions, one gets for arbitrary $y, z \in \Omega$ and $s \in [0,1]$

$$\begin{aligned} V(y) \geqslant& V\big((1-s)y+sz\big) + sV_x\big((1-s)y+sz\big)(y-z) + \frac{\lambda}{2}s^2(y-z)^2 \quad \text{and} \\ V(z) \geqslant& V\big((1-s)y+sz\big) + (1-s)V_x\big((1-s)y+sz\big)(z-y) + \frac{\lambda}{2}(1-s)^2(y-z)^2. \end{aligned}$$

Adding the first inequality multiplied by $(1-s)$ to the second multiplied by s yields

$$V\big((1-s)y+sz\big) \leqslant (1-s)V(y) + sV(z) - \frac{\lambda}{2}s(1-s)(y-z)^2.$$

In combination, this implies inequality (3.21). □

3.2.1.b. The discretized entropy. The restriction of the energy $\mathfrak{E}$ from (3.17) to the subspace $\mathfrak{X}_{\boldsymbol{\xi}}$ is naturally associated to the functional $\mathbf{E} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ with

$$\mathbf{E}(\vec{\mathrm{x}}) = \mathbf{E}(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]) = \mathcal{E}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]),$$

which was already defined in (3.12). Rememeber the explicit representation of $\mathbf{E}$,

$$\mathbf{E}(\vec{\mathrm{x}}) = \sum_{k=1}^{K} \delta_{k-\frac{1}{2}}\psi\bigg(\frac{x_k - x_{k-1}}{\delta_{k-\frac{1}{2}}}\bigg) + \int_{\mathcal{M}} V\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big)\,\mathrm{d}\xi,$$

for every $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. Note especially that by the linearity of the map $\vec{\mathrm{x}} \mapsto \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, the functional $\mathbf{E}$ inherits the boundedness and convexity from $\mathfrak{E}$. It is further easy to verify that the gradient vector $\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}}) = \big[\partial_{x_k}\mathbf{E}(\vec{\mathrm{x}})\big]_{k=1}^{K-1} \in \mathbb{R}^{K-1}$ is given by

$$\big[\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}})\big]_k = -\psi'\bigg(\frac{x_{k+1}-x_k}{\delta_{k+\frac{1}{2}}}\bigg) + \psi'\bigg(\frac{x_k - x_{k-1}}{\delta_{k-\frac{1}{2}}}\bigg) + \int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi. \tag{3.22}$$

Using once again that $\psi'(s^{-1}) = -\mathrm{P}(s)$ and $\vec{\mathrm{z}} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, a more compact representation of the gradient is provided by

$$\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}}) = \sum_{\kappa\in\mathbb{I}_K^{1/2}} \delta_\kappa \mathrm{P}(z_\kappa)\frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta_\kappa} + \sum_{k\in\mathbb{I}_K^+}\bigg(\int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi\bigg)\mathbf{e}_k, \tag{3.23}$$

where $\mathbf{e}_k \in \mathbb{R}^{K-1}$ denotes the kth canonical unit vector with the convention $\mathbf{e}_0 = \mathbf{e}_K = 0$, as in Example 2.3. The Hessian matrix $\partial_{\vec{\mathrm{x}}}^2\mathbf{E}(\vec{\mathrm{x}}) = \big[\partial_{x_m x_k}\mathbf{E}(\vec{\mathrm{x}})\big]_{m,k=1}^{K-1} \in \mathbb{R}^{(K-1)\times(K-1)}$ is symmetric with

$$\partial_{\vec{x}}^2 \mathbf{E}(\vec{x}) = \sum_{\kappa \in \mathbb{I}_K^{1/2}} \delta_\kappa \mathrm{P}'(z_\kappa) z_\kappa^2 \left(\frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta_\kappa} \right) \left(\frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta_\kappa} \right)^T + \sum_{k,l \in \mathbb{I}_K^+} \left(\int_{\mathcal{M}} V_{xx}\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{x}](\xi)\big) \theta_k(\xi) \theta_l(\xi) \, \mathrm{d}\xi \right) \mathbf{e}_k \mathbf{e}_l^T \tag{3.24}$$

Lemma 3.8. $\mathbf{E}$ *is bounded from below by* $\underline{\mathcal{E}}$ *defined in* (3.20). *Further, it is* λ*-convex with respect to the quadratic structure induced by* W_2*, i.e.,* $\partial_{\vec{x}}^2 \mathbf{E}(\vec{x}) - \lambda \mathrm{W}_2$ *is positive semi-definite for arbitrary* $\vec{x}^0 \in \mathfrak{x}_{\boldsymbol{\xi}}$*. Consequently,*

$$\left\langle \vec{x}^1 - \vec{x}^0, \nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}^1) - \partial_{\vec{x}} \mathbf{E}(\vec{x}^0) \right\rangle_{\boldsymbol{\xi}} \geqslant \lambda \left\| \vec{x}^1 - \vec{x}^0 \right\|_{\boldsymbol{\xi}}^2 \tag{3.25}$$

is satisfied for every $\vec{x}^0, \vec{x}^1 \in \mathfrak{x}_{\boldsymbol{\xi}}$*.*

Proof. Boundedness from below is a consequence of (3.20) and the definition of $\mathbf{E}$ by restriction of $\mathfrak{E}$. Convexity is a direct consequence of the convexity (3.21) of $\mathfrak{E}$, taking into account (2.20) and (2.21), and that $\vec{x} \mapsto \mathbf{X}_{\boldsymbol{\xi}}[\vec{x}]$ is a linear map. The estimate (3.25) is obtained by Taylor expansion. ☐

3.2.1.c. Interpretation of the scheme as a discrete Wasserstein gradient flow. Throughout this section, we fix a pair $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ consisting of a spatial decomposition $\boldsymbol{\xi}$ of the mass domain $\mathcal{M}$ and varying time step sizes $\boldsymbol{\tau} = (\tau_1, \tau_2, \ldots)$ that induces a temporal decomposition of $[0, +\infty)$ by

$$\{0 = t_0 < t_1 < \ldots < t_n < \ldots\}, \quad \text{where} \quad t_n := \sum_{j=1}^n \tau_j,$$

with $\tau_n \in (0, \tau]$ and $\tau > 0$.

Starting from the discretized entropy $\mathbf{E}$ we approximate the spatially discrete gradient flow equation

$$\partial_t \vec{x} = -\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}) \tag{3.26}$$

also in time, using minimizing movements. For each $\vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$, introduce the *Yosida-regularized entropy* $\mathbf{E}_\Delta(\cdot, \cdot, \vec{y}) : [0, \tau] \times \mathfrak{x}_{\boldsymbol{\xi}}$ by

$$\mathbf{E}_\Delta(\sigma, \vec{x}, \vec{y}) = \frac{1}{2\sigma} \left\| \vec{x} - \vec{y} \right\|_{\boldsymbol{\xi}}^2 + \mathbf{E}(\vec{x}). \tag{3.27}$$

A fully discrete approximation $\vec{x}_\Delta = (\vec{x}_\Delta^0, \vec{x}_\Delta^1, \ldots)$ of (3.26) is now defined inductively from a given initial datum $\vec{x}_\Delta^0$ by choosing each $\vec{x}_\Delta^n$ as a global minimizer of $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{x}_\Delta^{n-1})$. Below, we prove that such a minimizer always exists (see Proposition 3.9).

For practical applications, one would like the sequence $\vec{x}_\Delta$ to be the unique solution of the Euler-Lagrange equations associated to $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{x}_\Delta^{n-1})$, which leads to the implicit Euler time stepping

$$\frac{\vec{x} - \vec{x}_\Delta^{n-1}}{\tau_n} = -\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}), \tag{3.28}$$

which is exactly the same as (3.11) from the defintion of our scheme in Section 3.1.2. Equivalence of (3.28) and the minimization problem is guaranteed at least for sufficiently small $\tau > 0$, as the following Proposition shows.

Proposition 3.9. *Assume that $\tau^{-1} + \lambda > 0$ with $\lambda \in \mathbb{R}$ defined in (3.9), and let $u^0_\Delta = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^0_\Delta]$ in $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ be given. Then there are sequences $u_\Delta = (u^0_\Delta, u^1_\Delta, \ldots)$ and $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}^0_\Delta, \vec{\mathrm{x}}^1_\Delta, \ldots)$, uniquely related by the map $\mathbf{u}_{\boldsymbol{\xi}} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ from (2.17), such that $u^n_\Delta \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ is the unique minimizer of $\mathcal{E}_\tau(\tau_n, \cdot, u^{n-1}_\Delta)$ on $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$, and $\vec{\mathrm{x}}^n_\Delta$ is the unique minimizer of $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$, for every $n \in \mathbb{N}$. Moreover, $\vec{\mathrm{x}}^n_\Delta$ is the unique solution in $\mathfrak{x}_{\boldsymbol{\xi}}$ to the system of Euler-Lagrange equations*

$$\frac{1}{\tau_n}(\vec{\mathrm{x}} - \vec{\mathrm{x}}^{n-1}_\Delta) = -\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{\mathrm{x}}), \tag{3.29}$$

with $\partial_{\vec{\mathrm{x}}} \mathbf{E}(\vec{\mathrm{x}})$ explicitly given in (3.22).

Proof. Fix $n \in \mathbb{N}$. It suffices to prove that $\vec{\mathrm{x}} \mapsto \mathbf{E}_\Delta(\tau_n, \vec{\mathrm{x}}, \vec{\mathrm{x}}^{n-1}_\Delta)$ has a unique minimizer in the open set $\mathfrak{x}_{\boldsymbol{\xi}}$. To this end, observe that

$$\mathbf{E}_\Delta(\tau_n, \vec{\mathrm{x}}, \vec{\mathrm{x}}^{n-1}_\Delta) = \mathbf{E}(\vec{\mathrm{x}}) - \frac{\lambda}{2} \left\| \vec{\mathrm{x}} - \vec{\mathrm{x}}^{n-1}_\Delta \right\|^2_{\boldsymbol{\xi}} + \frac{1}{2}(\tau_n^{-1} + \lambda) \left\| \vec{\mathrm{x}} - \vec{\mathrm{x}}^{n-1}_\Delta \right\|^2_{\boldsymbol{\xi}}$$

for every $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. From Lemma 3.7, we know that the sum of the first two terms on the right-hand side constitutes a convex function in $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. Since $\tau_n^{-1} + \lambda > 0$ for any $n \in \mathbb{N}$, and since W_2 is positive definite by Lemma 2.2, the last term is strictly convex. Thus, $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$ possesses at most one critical point in $\mathfrak{x}_{\boldsymbol{\xi}}$.

Let further $(\vec{\mathrm{x}}^j)_{j=0}^\infty$ be a minimizing sequence for $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$ in $\mathfrak{x}_{\boldsymbol{\xi}}$. Since each of the $K-1$ components x^j_k belongs to the compact interval $\overline{\Omega}$, we may assume without loss of generality that $\vec{\mathrm{x}}^j$ converges to some $\vec{\mathrm{x}}^* \in \overline{\Omega}^{K-1}$. It remains to prove that $\vec{\mathrm{x}}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$. Since $(\vec{\mathrm{x}}^j)_{j=0}^\infty$ is a minimizing sequence, $\mathbf{E}_\Delta(\tau_n, \vec{\mathrm{x}}^j, \vec{\mathrm{x}}^{n-1}_\Delta)$ is bounded. Hence one obtains for arbitrary $\iota \in \mathbb{I}_K^{1/2}$ by Jensen's inequality that

$$\begin{aligned} C &\geqslant \frac{1}{2\tau_n} \left\| \vec{\mathrm{x}}^j - \vec{\mathrm{x}}^{n-1}_\Delta \right\|^2_{\boldsymbol{\xi}} + \sum_{\kappa \in \mathbb{I}_K^{1/2}} \delta_\kappa \psi\left(\frac{x^j_{\kappa+\frac{1}{2}} - x^j_{\kappa-\frac{1}{2}}}{\delta_\kappa} \right) + \int_{\mathcal{M}} V\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^j](\xi)\big)\,\mathrm{d}\xi \\ &\geqslant \delta_\iota \psi\left(\frac{x^j_{\iota+\frac{1}{2}} - x^j_{\iota-\frac{1}{2}}}{\delta_\iota} \right) + (M - \delta_\iota)\psi\left(\frac{b - a - (x^j_{\iota+\frac{1}{2}} - x^j_{\iota-\frac{1}{2}})}{M - \delta_\iota} \right) + M\lambda. \end{aligned}$$

Since $\psi(s) \to \infty$ for $s \downarrow 0$, this implies that $x^j_{\iota+\frac{1}{2}} - x^j_{\iota-\frac{1}{2}} \geqslant \epsilon\delta_\iota > 0$ with some $\epsilon > 0$ for all j, and thus also $x^*_{\iota+\frac{1}{2}} - x^*_{\iota-\frac{1}{2}} \geqslant \epsilon\delta_\iota > 0$, implying $\vec{\mathrm{x}}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$. By continuity of $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$ on $\mathfrak{x}_{\boldsymbol{\xi}}$, it follows that $\vec{\mathrm{x}}^*$ is a minimizer. Consequently, $\mathbf{E}_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$ possesses a unique critical point in $\mathfrak{x}_{\boldsymbol{\xi}}$, thus the corresponding Euler-Lagrange equations (3.29) are uniquely solvable. ☐

Remark 3.10. *The above proof especially shows that $\vec{\mathrm{x}} \mapsto \mathbf{E}_\Delta(\sigma, \vec{\mathrm{x}}, \vec{\mathrm{y}})$ is $(\sigma^{-1} + \lambda)$-convex for any $\sigma \in (0, \tau]$ and any $\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}}$.*

3.2.1.d. Metric contraction. The above results show impressively the importance of the scheme's structural preservation, and as we are going to prove in this section, the inherited convexity of $\mathbf{E}$ from $\mathfrak{E}$ is the key-ingredient for the discrete analogue (3.14) of the metric contraction in (3.10). The following proposition is a first step towards (3.14) of Theorem 3.3,

Proposition 3.11. *If $v_\Delta = (v_\Delta^0, v_\Delta^1, \dots)$ is any other discrete solution of the numerical scheme, then*

$$(1 + 2\lambda\tau_n)\mathcal{W}_2(u_\Delta^n, v_\Delta^n)^2 \leqslant \mathcal{W}_2\big(u_\Delta^{n-1}, v_\Delta^{n-1}\big)^2 \tag{3.30}$$

for all $n \in \mathbb{N}$.

Proof. For $\vec{\mathrm{x}}_\Delta$, $\vec{\mathrm{y}}_\Delta$ such that $u_\Delta^n = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^n]$, and $v_\Delta^n = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_\Delta^n]$ for any $n \in \mathbb{N}$, we know by Proposition 3.9 that

$$\mathrm{W}_2(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1}) = -\tau_n \partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}}_\Delta^n), \quad \text{and} \quad \mathrm{W}_2(\vec{\mathrm{y}}_\Delta^n - \vec{\mathrm{y}}_\Delta^{n-1}) = -\tau_n \partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}_\Delta^n).$$

Substracting these equations, we obtain

$$\mathrm{W}_2(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{y}}_\Delta^n) + \tau_n\big(\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}}_\Delta^n) - \partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}_\Delta^n)\big) = \mathrm{W}_2(\vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{y}}_\Delta^{n-1}). \tag{3.31}$$

Since W_2 is a positive-definite and symmetric matrix, one can find a symmetric and again positive-definite matrix denoted by $\mathrm{W}_2^{1/2}$ — its square root — such that $\mathrm{W}_2^{1/2}\mathrm{W}_2^{1/2} = \mathrm{W}_2$. As a next step, we multiply (3.31) with $\mathrm{W}_2^{-1/2}$ and take the norm on both sites in (3.31), then we obtain

$$\begin{aligned}(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{y}}_\Delta^n)^T\mathrm{W}_2(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{y}}_\Delta^n) + 2\tau_n(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{y}}_\Delta^n)^T\big(\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}}_\Delta^n) - \partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}_\Delta^n)\big)&\\ \leqslant (\vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{y}}_\Delta^{n-1})^T\mathrm{W}_2(\vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{y}}_\Delta^{n-1}).&\end{aligned}$$

Combining this with the convexity property (3.25), we arrive at the recursive relation

$$(1 + 2\lambda\tau_n)(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{y}}_\Delta^n)^T\mathrm{W}_2(\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{y}}_\Delta^n) \leqslant (\vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{y}}_\Delta^{n-1})^T\mathrm{W}_2(\vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{y}}_\Delta^{n-1}).$$

Iteration of this estimate and application of (2.21) yields (3.30). ☐

This result establishes the basis for the proof of the exponential decay rate given in Theorem 3.3. Effectively, (3.14) is just an application of the following version of the dicrete Gronwall lemma: Assume $(c_n)_{n=0}^\infty$ and $(y_n)_{n=0}^\infty$ to be sequences with values in $(0, +\infty)$, which satisfy $(1 + c_n)y_n \leqslant y_{n-1}$ for any $n \in \mathbb{N}$. Then

$$y_n \leqslant y_0 e^{-\sum_{k=0}^{n-1} \frac{c_k}{1+c_k}} \quad \text{for any } n \in \mathbb{N}.$$

This statement can be easily proven by induction. Therefore, one attains (3.14) and together with Proposition 3.9 all claims of Theorem 3.3 are proven.

3.3. A priori estimates and compactness

Throughout this section, we consider a sequence $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ of discretization parameters such that $\overline{\delta} \to 0$ and $\tau \to 0$ in the limit, formally denoted by $\Delta \to 0$. Furthermore, we assume that a fully discrete solution $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}_\Delta^0, \vec{\mathrm{x}}_\Delta^1, \dots)$ is given for each Δ-mesh, defined by (3.11).

3.3.1. Entropy inequalities. The following estimates for the entropy $\mathbf{E}$ are immediate conclusions from Lemma 2.4.

Lemma 3.12. *Let $\vec{\mathrm{x}}_\Delta$ be a solution of the numerical scheme. Then for every $N \in \mathbb{N}$,*

$$\sum_{n=1}^{N} \frac{1}{2\tau_n} \left\| \vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 \leqslant \mathbf{E}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{E}(\vec{\mathrm{x}}_\Delta^N), \tag{3.32}$$

$$\sum_{n=1}^{N} \frac{\tau_n}{2} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{\mathrm{x}}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 \leqslant \mathbf{E}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{E}(\vec{\mathrm{x}}_\Delta^N). \tag{3.33}$$

3.3.2. Bound on the total variation. Below, we derive a bound on the time-integrated *total variation* of the considered discrete solution u_Δ which is independent of the discretization Δ. This bound provides the key a priori estimate for the convergence proof in the next section. The use of total variation (instead of Sobolev norms) is natural in our context, since it can be directly evaluated on the piecewise constant profiles u_Δ^n.

Recall the definition (1.14) of the total variation of a function $f \in L^1(\Omega)$. If f is a piecewise constant function, taking values f_k on intervals $(x_{k-1}, x_k]$, with our usual convention $a = x_0 < x_1 < \cdots < x_K = b$, then the integral in (1.14) amounts to

$$\int_\Omega f(x)\varphi'(x)\,\mathrm{d}x = \sum_{k=1}^{K} \big[f(x)\varphi(x)\big]_{x=x_{k-1}+0}^{x_k-0} = \sum_{k=1}^{K-1} (f_k - f_{k+1})\varphi(x_k),$$

where we have used that $\varphi(a) = \varphi(b) = 0$. Consequently, for such f the supremum in (1.14) equals

$$\mathrm{TV}\,[f] = \sum_{k=1}^{K-1} |f_{k+1} - f_k| \tag{3.34}$$

and is attained for every $\varphi \in \mathrm{Lip}(\Omega)$ with $\varphi(x_k) = \mathrm{sgn}(f_k - f_{k+1})$ at $k = 1, \ldots, K-1$.

Proposition 3.13. *Assume u_Δ to be a solution of the numerical scheme. Then*

$$\int_0^T \mathrm{TV}\,[\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})]^2 \leqslant \mathcal{C}(T), \tag{3.35}$$

for every time horizon $T > 0$, where

$$\mathcal{C}(T) = 2M^2\big[2(\overline{\mathcal{E}} - \underline{\mathcal{E}}) + T \sup_{x\in\Omega} |V_x(x)|^2\big]. \tag{3.36}$$

Proof. Fix a time index n. Furthermore, let $\vec{\mathrm{y}} \in \mathbb{R}^{K-1}$ with components $y_k \in [-1, 1]$ be given, where we use the convention that $y_0 = y_K = 0$. Then, in view of (3.23), we have for $\vec{\mathrm{z}}_\Delta^n = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^n]$ that

$$\begin{aligned} \langle \nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{\mathrm{x}}_\Delta^n), \vec{\mathrm{y}} \rangle_{\boldsymbol{\xi}} &= \sum_{\kappa \in \mathbb{I}_K^{1/2}} \delta_\kappa \mathrm{P}(z_\kappa^n) \frac{y_{\kappa-\frac12} - y_{\kappa+\frac12}}{\delta_\kappa} + \sum_{k\in\mathbb{I}_K^+} \Big(\int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi \Big) y_k \\ &= \sum_{k\in\mathbb{I}_K^+} \big(\mathrm{P}(z_{k+\frac12}^n) - \mathrm{P}(z_{k-\frac12}^n)\big) y_k + \sum_{k\in\mathbb{I}_K^+} \Big(\int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi \Big) y_k, \end{aligned} \tag{3.37}$$

remember $y_0 = y_K = 0$. Respecting that $\|\vec{y}\|_{\boldsymbol{\xi}} \leqslant M\|\vec{y}\|_\infty$ we can take the supremum over all $\vec{y}$ with $\|\vec{y}\|_\infty \leqslant 1$ in (3.37). Then the Cauchy-Schwarz inequality yields

$$\sup_{\|\vec{y}\|_\infty \leqslant 1} \sum_{k \in \mathbb{I}_K^+} \big(\mathrm{P}(z^n_{k+\frac{1}{2}}) - \mathrm{P}(z^n_{k-\frac{1}{2}})\big) y_k \leqslant M \,\|\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}^n_\Delta)\|_{\boldsymbol{\xi}} + M \sup_{x\in\Omega} |V_x(x)|,$$

where the supremum on the left-hand side is attained for the vector $\vec{y} \in \mathbb{R}^{K-1}$ with components $y_k = \mathrm{sgn}(\mathrm{P}(z^n_{k+\frac{1}{2}}) - \mathrm{P}(z^n_{k-\frac{1}{2}}))$ at $k = 1, \ldots, K-1$. Due to (3.34) and

$$u^n_\Delta = \sum_{\kappa \in \mathbb{I}_K^{1/2}} z^n_\kappa \mathbf{1}_{(x^n_{\kappa-\frac{1}{2}}, x^n_{\kappa+\frac{1}{2}}]}(x),$$

we conclude that

$$\mathrm{TV}\left[\mathrm{P}(u^n_\Delta)\right] \leqslant M \,\|\nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{x}^n_\Delta)\|_{\boldsymbol{\xi}} + M \sup_{x\in\Omega} |V_x(x)|.$$

To obtain (3.35), take the square on both sides, sum the resulting inequalities from $n = 1$ to $n = N$ with a sufficiently large integer $N \in \mathbb{N}$ with $T > \sum_{n=1}^N \tau_n$, and apply the energy estimate (3.33). □

The above result yields in combination with (3.5) the following corollary for the time interpolation $\{u_\Delta\}_{\boldsymbol{\tau}}$ of u_Δ, remember definition (2.14).

Corollary 3.14. *Assume u_Δ to be a solution of the numerical scheme. Then for any $T > 0$ one can find a constant $C > 0$ independent of Δ, such that $\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})/\{u_\Delta\}_{\boldsymbol{\tau}}$ is uniformly bounded in $L^1([0,T] \times \Omega)$.*

Proof. Fix any time horizon $T > 0$. First note that the above bound on the total variation of $\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})$ in (3.35) yields the uniform boundedness of $\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})$ in $L^2([0,T]; L^\infty(\Omega))$, hence there exists a constant $C > 0$ such that

$$\int_0^T \|\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})\|^2_{L^\infty(\Omega)} \,\mathrm{d}t \leqslant C.$$

Due to the first assumption on P in (3.5), we immediately get that

$$\underline{c} \int_0^T \|\, \{u_\Delta\}_{\boldsymbol{\tau}} \,\|^p_{L^\infty(\Omega)} \,\mathrm{d}t \leqslant \int_0^T \|\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})\|^2_{L^\infty(\Omega)} \,\mathrm{d}t + T(b-a)\underline{d} \leqslant C + T(b-a)\underline{d}, \tag{3.38}$$

hence $\{u_\Delta\}_{\boldsymbol{\tau}}$ is uniformly bounded in $L^p([0,T]; L^\infty(\Omega))$. Finally apply the second inequality in (3.5), then

$$\int_0^T \left\| \frac{\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})}{\{u_\Delta\}_{\boldsymbol{\tau}}} \right\|_{L^\infty(\Omega)} \mathrm{d}t \leqslant \overline{c} \int_0^T \|\, \{u_\Delta\}_{\boldsymbol{\tau}} \,\|^p_{L^\infty(\Omega)} \,\mathrm{d}t + T(b-a)\overline{d}.$$

This shows the assumption due to the (3.38). □

3.3.3. Convergence of time interpolant. In this section, we prove Theorem 3.4. Let an arbitrary time horizon $T > 0$ and an initial condition $u^0 \in \mathcal{P}_2^r(\Omega)$ with $\mathcal{E}(u^0) < \infty$ be given. Accordingly, we denote by $N_{\boldsymbol{\tau}}$ is the smallest integer with $\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n > T$. Throughout this section, we assume all the hypotheses of Theorem 3.4:

- The initial conditions $u_\Delta^0 \in \mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ converge to u^0 weakly in $L^1(\Omega)$.
- Uniform boundedness with respect to the discretization Δ,

$$\alpha_{\boldsymbol{\xi}} \leqslant \overline{\alpha}_2 < \infty, \quad \mathcal{E}(u_\Delta^0) \leqslant \overline{\mathcal{E}} < \infty.$$

Denote by u_Δ the corresponding discrete solutions obtained as in Proposition 3.9, then the following weak convergence result is a well-known consequence of the energy estimate (3.32).

Proposition 3.15. *Every subsequence of $\{u_\Delta\}_{\boldsymbol{\tau}}$ contains a sub-subsequence that converges locally uniformly with respect to time in $\mathcal{W}_2$ to a limit curve $u_* \in C^{1/2}_{\mathrm{loc}}([0,+\infty);\mathcal{P}_2^r(\Omega))$.*

Proof. Fix $T > 0$, then we can apply Proposition 2.5 due to the entropy estimates in (3.32) and (3.33), which yields the locally uniform convergence of $\{u_\Delta\}_{\boldsymbol{\tau}}$ with respect to time $t \in [0,T]$ in $\mathcal{W}_2$ to a limit curve $u_T \in C^{1/2}([0,T];\mathcal{P}_2^r(\Omega))$. Clearly, the argument applies to every choice of $T > 0$. Using a diagonal argument, one constructs a limit curve $u_* \in C^{1/2}_{\mathrm{loc}}([0,+\infty);\mathcal{P}_2^r(\Omega))$ such that u_T is the restriction of u_* to $[0,T]$.

□

A stronger compactness result is needed for the convergence proof.

Proposition 3.16. *Every subsequence of $\{u_\Delta\}_{\boldsymbol{\tau}}$ contains a sub-subsequence (still denoted by $\{u_\Delta\}_{\boldsymbol{\tau}}$), such that for any $T > 0$*

$$\{u_\Delta\}_{\boldsymbol{\tau}} \longrightarrow u_* \quad \textit{strongly in } L^1([0,T]\times\Omega),$$
$$\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}}) \longrightarrow \mathrm{P}(u_*) \quad \textit{strongly in } L^1([0,T]\times\Omega),$$

where u_* is the limit curve from Proposition 3.15.

The proof of this proposition is an application of the Aubin-Lions compactness principle. Specifically, we use:

Theorem 3.17. *[Adapted from Theorem 2 in [**RS03**]] Assume for any time horizon $T > 0$ that:*

(1) *There is a* normal coercive integrand $\mathfrak{F} : L^1(\Omega) \to [0,\infty]$, *i.e., $\mathfrak{F}$ is measurable, lower semi-continuous and has compact sublevels in $L^1(\Omega)$, for which the following is true:*

$$\sup_\Delta \int_0^T \mathfrak{F}\big(\{u_\Delta\}_{\boldsymbol{\tau}}(t)\big)\,\mathrm{d}t < \infty. \tag{3.39}$$

(2) *The $\{u_\Delta\}_{\boldsymbol{\tau}}$ are integral equicontinuous with respect to $\mathcal{W}_2$,*

$$\lim_{h\downarrow 0}\sup_\Delta \int_0^{T-h} \mathcal{W}_2\big(\{u_\Delta\}_{\boldsymbol{\tau}}(t+h),\{u_\Delta\}_{\boldsymbol{\tau}}(t)\big)\,\mathrm{d}t = 0. \tag{3.40}$$

Then the sequence $(\{u_\Delta\}_{\boldsymbol{\tau}})_\Delta$ is relatively compact in $L^1_{\mathrm{loc}}([0,+\infty)\times\Omega)$.

Let $\mathfrak{F} : L^1(\Omega) \to \mathbb{R} \cup \{+\infty\}$ be given by $\mathfrak{F}(u) = \mathrm{TV}\,[\mathrm{P}(u)]^2$ — possibly $+\infty$ — if u is nonnegative with $\int_\Omega u(x)\,\mathrm{d}x = M$, and by $+\infty$ otherwise.

Lemma 3.18. *$\mathfrak{F}$ is lower semi-continuous and has relatively compact sublevels.*

Proof. Let $A_C := \mathfrak{F}^{-1}((-\infty; c]) \subseteq L^1(\Omega)$ be a sublevel of $\mathfrak{F}$. By [**Giu84**, Theorem 1.19], the set $B_C := \{\mathrm{P}(u) \,|\, u \in A_C\}$ is relatively compact in $L^1(\Omega)$; here we use the fact that our domain Ω is an interval, so that $\mathrm{TV}\,[\mathrm{P}(u)]^2 \leqslant C$ and $\int_\Omega u(x)\,\mathrm{d}x = M$ induce a uniform bound on the BV-norm of $\mathrm{P}(u)$. Thus, if $(u_\ell)_{\ell=0}^\infty$ is a sequence in A_C, converging to u_0 in $L^1(\Omega)$, then also $(\mathrm{P}(u_\ell))_{\ell=0}^\infty$ converges to $\mathrm{P}(u_0)$ in $L^1(\Omega)$. By lower semi-continuity of the total variation $\mathrm{TV}\,[\cdot]$ [**Giu84**, Theorem 1.9], the lower semi-continuity of $\mathfrak{F}$ follows.

To conclude compactness of A_C, it suffices to prove that the mapping $u \mapsto \mathrm{P}(u)$ is $L^1(\Omega)$-continuously invertible. For that, let a sequence $(f_\ell)_{\ell=0}^\infty$ in B_C be given, which converges to some f_0 in $L^1(\Omega)$. Since the map $r \mapsto \mathrm{P}(r)$ is strictly increasing, positive, and continuous with superlinear growth it possesses a strictly increasing, positive and continuous inverse with sublinear growth. Hence, there is a uniquely determined sequence of functions $u_\ell \in A_C$ such that $\mathrm{P}(u_\ell) = f_\ell$ for all $\ell \in \mathbb{N}$, and a unique $u_0 \in A_C$ with $\mathrm{P}(u_0) = f_0$. We wish to show that u_ℓ converges to u_0 in $L^1(\Omega)$. By standard arguments, we can assume without loss of generality that the f_ℓ converge to f_0 pointwise a.e. By continuous invertibility of $r \mapsto \mathrm{P}(r)$, the u_l converge to u_0 pointwise a.e. Moreover, by construction,

$$\sup_{\ell \in \mathbb{N}} \int_\Omega \mathrm{P}(u_\ell(x))\,\mathrm{d}x = \sup_{\ell \in \mathbb{N}} \int_\Omega f_\ell(x)\,\mathrm{d}x < \infty,$$

so we can invoke Vitali's Theorem — recall the superlinear growth of P — to conclude strong convergence of u_ℓ to u_0. □

Proof of Proposition 3.16. Fix any arbitrary time horizon $T > 0$. It suffices to show that every subsequence of $\{u_\Delta\}_{\boldsymbol{\tau}}$ contains a sub-subsequence which is relatively compact. In view of Proposition 3.15, we may thus assume — without loss of generality — that $\{u_\Delta\}_{\boldsymbol{\tau}}$ converges uniformly with respect to $t \in [0,T]$ in $\mathcal{P}_2^r(\Omega)$ to a curve $u_* \in C^{1/2}([0,T]; \mathcal{P}_2^r(\Omega))$. The verification of (3.40) is easily gained by following the analogue proof of [**DFM14**, Proposition 4.8] step-by-step. Furthermore, the estimate in (3.39) is a direct consequence of the regularity estimate (3.35). Thus Theorem 3.17 provides relative compactness of $\{u_\Delta\}_{\boldsymbol{\tau}}$ in $L^1([0,T] \times \Omega)$. Since L^1-convergence implies weak convergence, it actually follows that $\{u_\Delta\}_{\boldsymbol{\tau}}$ converges to u_* in $L^1([0,T] \times \Omega)$. Without loss of generality, we may even assume that $\{u_\Delta\}_{\boldsymbol{\tau}}$ converges to u_* a.e. on $[0,T] \times \Omega$. By continuity of P, also $\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})$ converges to $\mathrm{P}(u_*)$ a.e. on $[0,T] \times \Omega$. Furthermore, (3.34) implies

$$\int_0^T \int_\Omega \mathrm{P}\big(\{u_\Delta\}_{\boldsymbol{\tau}}(t,x)\big)^2\,\mathrm{d}x\,\mathrm{d}t \leqslant 2(b-a) \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \Big[\mathrm{P}\Big(\frac{M}{b-a}\Big)^2 + \mathrm{TV}\,[\mathrm{P}(u_\Delta^n)]^2 \Big],$$

which is Δ-uniformly bounded because of the regularity estimate (3.35). We can finally invoke Vitali's Theorem to conclude that $\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})$ tends to $\mathrm{P}(u_*)$ in $L^1([0,T] \times \Omega)$, due to the growth property of P. □

3.4. Weak formulation and the limit equation

It is easily verified by applying integration by parts that a weak formulation of (3.1) with the no-flux boundary conditions can be stated as follows: Find $u : [0, +\infty) \times \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$, such that

$$\int_0^\infty \int_\Omega u\rho\eta' \,\mathrm{d}x\,\mathrm{d}t + \int_0^\infty \int_\Omega \mathrm{P}(u)\rho''\eta - uV_x\rho'\eta \,\mathrm{d}x\,\mathrm{d}t = 0, \tag{3.41}$$

for any test function $\rho \in C^\infty(\Omega)$ with $\rho'(a) = \rho'(b) = 0$ and any $\eta \in C_c^\infty((0, +\infty))$. Note especially that the weak formulation (3.16) is equivalent to (3.41). Simply observe that any $\varphi \in C^\infty((0, +\infty) \times \Omega)$ can be approximated by linear combinations of products $\eta(t)\rho(x)$ with functions $\eta \in C^\infty((0, +\infty))$ and $\rho \in C^\infty(\Omega)$.

An alternative way to derive this weak formulation is obtained by studying the variation of the entropy $\mathcal{E}$ along a Wasserstein gradient flow generated by an arbitrary test function ρ, which describes a transport along the velocity field ρ'. The corresponding entropy functional is $\Phi(u) = \int_\Omega \rho(x)u(x)\,\mathrm{d}x$.

The aim of this section is to show that the limit curve u_* from Proposition 3.16 satisfies this weak formulation and attains the initial datum u^0 weakly as $t \downarrow 0$. To this end, the idea from the continuous case can be adapted to derive a discrete analogue of the weak formulation for our variational numerical scheme. Henceforth, fix an arbitrary spatial test function $\rho \in C^\infty(\Omega)$ with $\rho'(a) = \rho'(b) = 0$ and choose $\varpi > 0$, such that

$$\|\rho\|_{C^4(\Omega)} = \sum_{k=0}^{4} \|\rho^{(k)}\|_{C^0(\Omega)} \leqslant \varpi. \tag{3.42}$$

As already mentioned, we can use the same variational methods as in [**MO14a**] to show that $\{u_\Delta\}_{\boldsymbol{\tau}}$ inherits a discrete analogue to the weak formulation (3.41). Hence, we study the variations of the entropy $\mathbf{E}$ along the vector field $\vec{\mathrm{v}}(\vec{\mathrm{x}})$ generated by the potential

$$\boldsymbol{\Phi}(\vec{\mathrm{x}}) = \int_{\mathcal{M}} \rho(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}])\,\mathrm{d}\xi$$

for any arbitrary smooth function $\rho \in C^\infty(\Omega)$ with $\rho'(a) = \rho'(b) = 0$. That is why we define

$$\vec{\mathrm{v}}(\vec{\mathrm{x}}) = \nabla_{\boldsymbol{\xi}}\boldsymbol{\Phi}(\vec{\mathrm{x}}), \quad \text{where} \quad \left[\partial_{\vec{\mathrm{x}}}\boldsymbol{\Phi}(\vec{\mathrm{x}})\right]_k = \int_{\mathcal{M}} \rho'(\mathbf{X}(\xi))\theta_k(\xi)\,\mathrm{d}\xi, \quad k = 1, \ldots, K-1. \tag{3.43}$$

Later on, we will use the compactness results from Proposition 3.16 to pass to the limit, which yields our main result in Theorem 3.4.

The proof of this theorem will be treated in two essential steps

(1) We show the validity of a discrete weak formulation for $\{u_\Delta\}_{\boldsymbol{\tau}}$, using a discrete flow interchange estimate.
(2) Then we pass to the limit using Proposition 3.16.

Lemma 3.19 (discrete weak formulation). *For any $\rho \in C^\infty(\Omega)$ with $\rho'(a) = \rho'(b) = 0$ and $\eta \in C_c^\infty((0, +\infty))$, the solution $\vec{\mathrm{x}}_\Delta^n$ with $u_\Delta^n = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^n]$ of the minimization problem* (3.13) *fulfills*

$$\sum_{n=0}^{\infty} \tau_n\eta(t_n)\frac{\boldsymbol{\Phi}(\vec{\mathrm{x}}_\Delta^n) - \boldsymbol{\Phi}(\vec{\mathrm{x}}_\Delta^{n-1})}{\tau_n} - \eta(t_n)\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} = \mathcal{O}(\tau) + \mathcal{O}(\bar{\delta}^{\frac{1}{2}}), \tag{3.44}$$

where we use the short-hand notation

$$\rho'(\vec{\mathrm{x}}) := \big(\rho'(x_1), \dots, \rho'(x_{K-1})\big)\,.$$

Proof. As a first step, we prove that both vectors $\rho'(\vec{\mathrm{x}})$ and $\vec{\mathrm{v}}(\vec{\mathrm{x}})$ almost coincide for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$, i.e.

$$\big\|\vec{\mathrm{v}}(\vec{\mathrm{x}}) - \rho'(\vec{\mathrm{x}})\big\|_{\boldsymbol{\xi}}^2 \leqslant \overline{\delta}\varpi^2\overline{\alpha}_2(b-a)^2. \tag{3.45}$$

Hence, denote by $\mathbf{X} = \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ the corresponding Lagrangian map of $\vec{\mathrm{x}}$ and choose any $k = 1, \dots, K-1$, then a Taylor expansion shows that

$$\rho'\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big) = \rho'(x_k) + \rho''(\hat{x})(x_k - x_{k-1})\theta_{k-1}(\xi) \tag{3.46}$$

$$= \rho'(x_{k-1}) + \rho''(\check{x})(x_k - x_{k-1})\theta_k(\xi) \tag{3.47}$$

for all $\xi \in [\xi_{k-1}, \xi_k]$, where $\hat{x}, \check{x} \in \Omega$ denote suitable intermediate values depending on ξ. Multiply (3.46) by θ_k, multiply (3.47) by θ_{k-1}, and sum these up to obtain that

$$\rho'\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\big) = \rho'(x_k)\theta_k(\xi) + \rho'(x_{k-1})\theta_{k-1}(\xi) + R_k(\xi) \tag{3.48}$$

where the error term R_k fulfills, recalling (3.42),

$$\begin{aligned}\int_{\mathcal{M}} |R_k(\xi)|\,\mathrm{d}\xi &\leqslant \varpi(x_k - x_{k-1})\int_{\xi_{k-1}}^{\xi_k} \theta_k(\xi)\theta_{k-1}(\xi)\,\mathrm{d}\xi + \varpi(x_{k+1} - x_k)\int_{\xi_k}^{\xi_{k+1}} \theta_k(\xi)\theta_{k+1}(\xi)\,\mathrm{d}\xi \\ &\leqslant \frac{\varpi\overline{\delta}}{6}\big((x_k - x_{k-1}) + (x_{k+1} - x_k)\big).\end{aligned} \tag{3.49}$$

Furthermore, define the vector $\vec{\mu} = \mathrm{W}_2(\vec{\mathrm{v}}(\vec{\mathrm{x}}) - \rho'(\vec{\mathrm{x}}))$, then each component of $\vec{\mu}$ is given by

$$\mu_k = \int_{\xi_{k-1}}^{\xi_{k+1}} \left(\rho'\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\big) - \sum_{j=k-1}^{k+1} \rho'(x_j)\theta_j\right)\theta_k\,\mathrm{d}\xi,$$

due to $[\mathrm{W}_2]_{k,j} = \int_{\mathcal{M}} \theta_k\theta_j\,\mathrm{d}\xi$. Substitute (3.48) and (3.49) into the integral, then Young's inequality yields the bound

$$|\mu_k|^2 \leqslant \frac{\varpi^2\overline{\delta}^2}{18}\big((x_k - x_{k-1})^2 + (x_{k+1} - x_k)^2\big)$$

for every $k = 1, \dots, K-1$. Recalling the lower estimate on W_2 in (2.22), it follows for $\nu = \mathrm{W}_2^{-1}\mu$ that

$$\begin{aligned}\big\|\vec{\mathrm{v}}(\vec{\mathrm{x}}) - \rho'(\vec{\mathrm{x}})\big\|_{\boldsymbol{\xi}}^2 &= \mu^T\mathrm{W}_2^{-1}\mu \leqslant \frac{6}{\underline{\delta}}\sum_{k=1}^{K-1}\mu_k^2 \leqslant \overline{\delta}\frac{\varpi^2\overline{\alpha}_2}{3}\sum_{k=1}^{K-1}\big((x_k - x_{k-1})^2 + (x_{k+1} - x_k)^2\big) \\ &\leqslant \overline{\delta}\varpi^2\overline{\alpha}_2(b-a)^2,\end{aligned}$$

proving our claim (3.45).

Let us now invoke the proof of (3.44). A Taylor expansion of ρ for $\mathrm{X}, \mathrm{X}' \in \mathfrak{X}$ yields

$$\rho(\mathrm{X}) - \rho(\mathrm{X}') - \frac{\varpi}{2}(\mathrm{X} - \mathrm{X}')^2 \leqslant \rho'(\mathrm{X})(\mathrm{X} - \mathrm{X}'),$$

which implies for $X' = \mathbf{X}_{\boldsymbol{\xi}}[\vec{x}_\Delta^{n-1}]$ and $X = \mathbf{X}_{\boldsymbol{\xi}}[\vec{x}_\Delta^{n}]$ by integration

$$\begin{aligned}\mathbf{\Phi}(\vec{x}_\Delta^n) - \mathbf{\Phi}(\vec{x}_\Delta^{n-1}) - \frac{\varpi}{2}\left\|\vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2 &\leqslant \sum_{k=1}^{K-1}[\vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}]_k \int_{\mathcal{M}} \rho'(\mathbf{X}_{\boldsymbol{\xi}}[\vec{x}_\Delta^n])\theta_k(\xi)\,\mathrm{d}\xi \\ &= \left\langle \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}, \nabla_{\boldsymbol{\xi}}\mathbf{\Phi}(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} \\ &= \tau_n \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \nabla_{\boldsymbol{\xi}}\mathbf{\Phi}(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}}.\end{aligned} \tag{3.50}$$

Owing to (3.45), the last term can be estimated as follows,

$$\begin{aligned}\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \nabla_{\boldsymbol{\xi}}\mathbf{\Phi}(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} &= \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} + \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \vec{v}(\vec{x}_\Delta^n) - \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} \\ &\leqslant \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} + \left\|\nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n)\right\|_{\boldsymbol{\xi}} \left\|\vec{v}(\vec{x}_\Delta^n) - \rho'(\vec{x}_\Delta^n)\right\|_{\boldsymbol{\xi}} \\ &\leqslant \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} + \sqrt{\delta}\varpi(b-a)\left\|\nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n)\right\|_{\boldsymbol{\xi}}.\end{aligned} \tag{3.51}$$

Inequality (3.50) in combination with (3.51) then yields after multiplication with $\eta(t_n)$ and summation over $n \in \mathbb{N}$,

$$\begin{aligned}&\left|\sum_{n=1}^{\infty} \tau_n \eta(t_n)\left(\frac{\mathbf{\Phi}(\vec{x}_\Delta^n) - \mathbf{\Phi}(\vec{x}_\Delta^{n-1})}{\tau_n} - \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n\right\rangle_{\boldsymbol{\xi}}\right)\right| \\ \leqslant &\|\eta\|_{C^0([0,+\infty)}\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\frac{\varpi}{2}\left\|\vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2 + \|\eta\|_{C^0([0,T])}\sqrt{\delta}\varpi(b-a)\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\left\|\nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n)\right\|_{\boldsymbol{\xi}}.\end{aligned}$$

The right-hand side is of order $\mathcal{O}(\tau) + \mathcal{O}(\overline{\delta}^{\frac{1}{2}})$, due to (3.32) and (3.33). An analogue calculation replacing ρ with $-\rho$ leads finally to (3.44). ☐

Proof of Theorem 3.4. It still remains to prove that the limit curve from Proposition 3.16 complies with the weak formulation in (3.16)

To this end, we want to pass to the limit in the discrete weak formulation in (3.44). As an immediate observation, we note that

$$\begin{aligned}\sum_{n=1}^{\infty}\tau_n\eta(t_n)\frac{\mathbf{\Phi}(\vec{x}_\Delta^n) - \mathbf{\Phi}(\vec{x}_\Delta^n)}{\tau_n} &= \sum_{n=1}^{\infty}\tau_n\eta(t_n)\int_{\mathcal{M}}\frac{\rho(\mathbf{X}_\Delta^n) - \rho(\mathbf{X}_\Delta^{n-1})}{\tau_n}\,\mathrm{d}\xi \\ &= -\sum_{n=1}^{\infty}\tau_n\frac{\eta(t^{n+1}) - \eta(t_n)}{\tau_n}\int_\Omega \rho(x)\left\{u_\Delta\right\}_{\boldsymbol{\tau}}(t_n,x)\,\mathrm{d}x \\ &\longrightarrow -\int_0^\infty\int_\Omega \eta'(t)\rho(x)u_*(t,x)\,\mathrm{d}x\,\mathrm{d}t,\end{aligned}$$

as $\Delta \to 0$. So the proof of Theorem 3.4 is done, as soon as we know that

$$\sum_{n=1}^{\infty}\tau_n\eta(t_n)\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} \longrightarrow -\int_0^\infty\int_\Omega \mathrm{P}(u_*)\rho''\eta - u_*V_x\rho'\eta\,\mathrm{d}x\,\mathrm{d}t, \tag{3.52}$$

as $\Delta \to 0$. So assume $\operatorname{supp}\eta \subseteq [0,T]$ for any $T > 0$, and fix $N_{\boldsymbol{\tau}} \in \mathbb{N}$ such that $\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n > T$. First observe that (3.22) implies for any integer $n = 1, \dots, N_{\boldsymbol{\tau}}$

$$\big\langle \nabla_{\boldsymbol{\xi}} \mathbf{E}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}} = -\sum_{k=1}^{K-1} \left[\psi'\Big(\frac{x_{k+1}^n - x_k^n}{\delta_{k+\frac12}}\Big) - \psi'\Big(\frac{x_k^n - x_{k-1}^n}{\delta_{k-\frac12}}\Big) \right] \rho'(x_k^n)$$
$$+ \int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^n]\big) \sum_{k=1}^{K-1} \rho'(x_k^n)\theta_k \,\mathrm{d}\xi = A_1^n + A_2^n.$$

We consider both terms on the right-hand side separately. Using that $\psi'(1/r) = -\mathrm{P}(r)$ and that $\rho'(a) = \rho'(b) = 0$, we see that the first term equals

$$A_1^n = \sum_{k=1}^{K} \psi'\Big(\frac{x_k^n - x_{k-1}^n}{\delta_{k-\frac12}}\Big)\big(\rho'(x_k^n) - \rho'(x_{k-1}^n)\big) = -\sum_{k=1}^{K} \int_{x_{k-1}^n}^{x_k^n} \mathrm{P}\Big(\frac{\delta_{k-\frac12}}{x_k^n - x_{k-1}^n}\Big)\rho''(\hat{x}_k)\,\mathrm{d}x,$$

with a suitable $\hat{x}_k \in (x_{k-1}^n, x_k^n)$ by the intermediate value theorem. Multiplying A_1^n with $\tau_n\eta(t_n)$ and summing over $n = 1, \dots, N$ yields

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \eta(t_n) A_1^n = \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \eta(t_n) \int_\Omega \mathrm{P}\big(u_\Delta^n\big)\rho''(x)\,\mathrm{d}x\,\mathrm{d}t + R_1, \tag{3.53}$$

where the residuum fulfills due to $|\rho''(\hat{x}_k) - \rho''(x)| \leqslant \varpi(x_k^n - x_{k-1}^n)$ for any $x \in (x_{k-1}^n, x_k^n)$

$$|R_1| \leqslant \varpi \|\eta\|_{C^0([0,T])} \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \sum_{k=1}^{K} \mathrm{P}(u_\Delta^n)(x_k^n - x_{k-1}^n)^2$$
$$\leqslant \overline{\delta}\varpi \|\eta\|_{C^0([0,T])} \int_0^T \int_\Omega \frac{\mathrm{P}(\{u_\Delta\}_{\boldsymbol{\tau}})}{\{u_\Delta\}_{\boldsymbol{\tau}}}\,\mathrm{d}x\,\mathrm{d}t.$$

Here we used that

$$u_\Delta^n(x) = z_{k-\frac12}^n = \frac{\delta_{k-\frac12}}{x_k^n - x_{k-1}^n}$$

for any $x \in (x_{k-1}^n, x_k^n]$ and $k = 1, \dots, K$. Hence the residuum vanishes as $\Delta \to 0$, due to Corollary 3.14. For the second term A_2^n, we perform a change of variables:

$$\int_{\xi_{k-1}^n}^{\xi_k^n} V_x\big(x_k^n\theta_k + x_{k-1}^n\theta_{k-1}\big)\big(\rho'(x_k^n)\theta_k + \rho'(x_{k-1}^n)\theta_{k-1}\big)\,\mathrm{d}\xi = \int_{x_{k-1}^n}^{x_k^n} V_x(x)\rho'(\check{x})\frac{\delta_{k-\frac12}}{x_k^n - x_{k-1}^n}\,\mathrm{d}x,$$

with some intermediate value $\check{x} \in (x_{k-1}^n, x_k^n)$. Summation over $k = 1, \dots, K$ again provides due to a Taylor expansion ρ' in $\check{x}$

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \eta(t_n) A_2^n = \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \eta(t_n) \int_\Omega V_x(x)\rho'(x)u_\Delta^n(x)\,\mathrm{d}x + R_2, \tag{3.54}$$

with a residuum that is bounded by

$$|R_2| \leqslant \varpi T(b-a)\|\eta\|_{C^0([0,T])} \max_{x\in\overline{\Omega}} |V_x|.$$

Combining (3.53), (3.54), and the compactness result in Proposition 3.16 finally gives (3.52). □

3.5. An alternative proof using Γ-convergence

In this section, we are going to discuss an alternative proof of convergence for the special case $\lambda \geqslant 0$ that can be obtained by exploiting the equation's variational structure more deeply. In particular, the theory on perturbed λ-contractive gradient flows developed by Serfaty [**Ser11**] and Ortner [**Ort05**] indicates an alternative route towards the same goal, making use of the machinery of Γ-convergence.

Before we can claim the main result of this section, we have to define an equivalent notion of solutions to the L^2-Wasserstein gradient flow equation, see [**AGS05**, Theorem 11.1.3].

Definition 3.20. *We call a function $u : [0, +\infty) \to \mathcal{P}_2^r(\Omega)$ a* curve of maximal slope for $\mathcal{E}$ *if it satisfies the following two conditions:*

(1) *u is* (locally) absolutely continuous*: There exists a function $A \in L^2_{\mathrm{loc}}([0, +\infty))$, such that*

$$\mathcal{W}_2(u(s), u(t)) \leqslant \int_s^t A(r)\,\mathrm{d}r,$$

for all $s, t \in [0, +\infty)$

(2) *u fulfills*

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E}(u(t)) \leqslant -\frac{1}{2}\left|u'\right|^2(t) - \frac{1}{2}\left|\partial\mathcal{E}\right|^2(u(t)), \tag{3.55}$$

where $|u'|$ is the metric derivative *of u and $|\partial\mathcal{E}|(u)$ is the* local slope *of $\mathcal{E}$ at u,*

$$\left|u'\right|(t) := \lim_{h\to 0}\frac{\mathcal{W}_2(u(t+h), u(t))}{h} \quad \textit{and} \quad \left|\partial\mathcal{E}\right|(u) := \limsup_{v\to u}\frac{\left(\mathcal{E}(u) - \mathcal{E}(v)\right)^+}{\mathcal{W}_2(u, v)}.$$

The formalism of curves of maximal slope constitutes the natural generalization of a gradient flow in the setting of metric spaces [**AGS05**, Theorem 11.1.3], and is well studied for the non-discretized set $\mathcal{P}_2^r(\Omega)$, see for instance [**AGS05**, **ALS06**, **Ort05**, **Ser11**] and others.

Our definition of a curve of maximal slope slightly differs from the typical one from the literature, see for instance [**AGS05**, Definition 1.3.2], where a *strong upper gradient for $\mathcal{E}$* is used in (3.55) instead of the local slope. However, one can show that the local slope $|\partial\mathcal{E}|$ is a strong upper gradient for $\mathcal{E}$ due to the λ-convexity of $\mathcal{E}$ and the additional assumption that $\lambda \geqslant 0$. More precisely, the local slope $|\partial\mathcal{E}|$ satisfies

$$\left|\mathcal{E}(u(s)) - \mathcal{E}(u(t))\right| \leqslant \int_s^t \left|\partial\mathcal{E}\right|(u(r))\left|u'\right|(r)\,\mathrm{d}r \tag{3.56}$$

for any locally absolutely continuous curve $u : [0, +\infty) \to \mathcal{P}_2^r(\Omega)$ and for any $s, t \in [0, +\infty)$ with $s < t$, which essentially is the definition of a strong upper gradient according to [**AGS05**, Defintion 1.2.1]. This inequality is a nontrivial result that is a consequence of [**AGS05**, Theorem 2.4.9] and [**AGS05**, Theorem 1.2.5]: The first theorem guarantees that the local slope and the *global slope* coincide if $\mathcal{E}$ is λ-convex with some $\lambda \geqslant 0$. Since the global slope is not needed in this thesis, we refer to [**AGS05**, Definition 1.2.4] for a proper definition. The second theorem shows that the global slope of $\mathcal{E}$ is a strong upper gradient for $\mathcal{E}$ in terms of (3.56), if $\mathcal{E}$ is lower semi-continuous. Note that the lower semi-continuity of $\mathcal{E}$ results from the continuity of its integrand ϕ, see [**AGS05**, Remark 9.3.8].

As a consequence of (3.56) one obtains in particular that

$$\mathcal{E}(u(s)) - \mathcal{E}(u(t)) \leqslant \frac{1}{2}\int_s^t |u'|^2(r)\,\mathrm{d}r + \frac{1}{2}\int_s^t |\partial\mathcal{E}|^2(u(r))\,\mathrm{d}r \tag{3.57}$$

for any locally absolutely continuous curve $u : [0,+\infty) \to \mathcal{P}_2^r(\Omega)$ and for $s,t \in [0,+\infty)$ with $s < t$.

Remark 3.21. *If u is a curve of maximal slope for $\mathcal{E}$, then one has equality in* (3.55) *owing to* (3.57)*.*

The aim of this section is to proof Theorem 3.6, which was essentially formulated as follows.

Theorem 3.22. *In addition to the assumptions in Theorem 3.4, assume that $\mathcal{E}$ is λ-convex according to the definition in* (3.21) *with $\lambda \geqslant 0$. Then the limit curve $u_* \in C^{1/2}_{\mathrm{loc}}([0,+\infty);\mathcal{P}_2^r(\Omega))$ of Theorem 3.4 is a curve of maximal slope for $\mathcal{E}$, hence u_* especially satisfies for any $t \in [0,+\infty)$ the equality*

$$\frac{1}{2}\int_0^t |u_*'|^2(r)\,\mathrm{d}r + \frac{1}{2}\int_0^t |\partial\mathcal{E}|^2(u_*(r))\,\mathrm{d}r = \mathcal{E}(u_*(0)) - \mathcal{E}(u_*(t)). \tag{3.58}$$

Remark 3.23. *Note that Theorem 3.22 is essentially a conclusion of the strong convergence result in Theorem 3.4 and [**AGS05**, Theorem 11.1.3]. Nevertheless, it is interesting from the analytical point of view to apply the notion of* Γ*-convergence* directly *to solutions of our scheme, which demonstrates once more the particular structural preservation of our approximation.*

The proof of Theorem 3.22 is discussed in the following two subsections. Before we can treat the content of the above theorem, we introduce a discrete local slope for the entropy $\mathcal{E}$ in terms of Lagrangian vectors in Subsection 3.5.1 and prove its lower semi-continuity. Making use of this new object, we can show that a solution to our numerical scheme indeed converges towards a curve of maximal slope. For this purpose, a similar strategy as developed in [**Ser11**] and [**Ort05**] is applied, see Subsection 3.5.2.

3.5.1. Lower semi-continuity of the entropy and discrete local slope. Lower semi-continuity is one of the main ingredients for any kind of Γ-convergence proof. It turns out that under the assumptions on the entropy, $\mathcal{E}$ and $\partial\mathcal{E}$ accomplish this essential property, i.e. for any $u \in \mathcal{P}_2^r(\Omega)$ and arbitrary sequence $(u_k)_{k=0}^\infty$ of density functions converging towards u in $\mathcal{W}_2$, one obtains

$$\liminf_{k\to\infty} \mathcal{E}(u_k) \geqslant \mathcal{E}(u) \quad \text{and} \quad \liminf_{k\to\infty} |\partial\mathcal{E}|(u_k) \geqslant |\partial\mathcal{E}|(u). \tag{3.59}$$

The lower semi-continuity of $\mathcal{E}$ results from the continuity of its integrand ϕ, see [**AGS05**, Remark 9.3.8]. We further refer to Section 4.1 of [**ALS06**] and especially to Example 4.4 within. However, for our purpose we just need the lower semi-continuity of $\mathcal{E}$.

All attempts to translate a Γ-convergence proof into the discrete case stand or fall by transferring those powerful properties to the discrete case. One of the main questions in this context is the following: Is it even possible to approximate each density function $u \in \mathcal{P}_2^r(\Omega)$ by functions of the discrete submanifolds $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$? The following lemma gives a positive answer.

Lemma 3.24. *Let us denote by $\bigcup_{\boldsymbol{\xi}} \mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ the union of all finite-dimensional submanifolds $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega) \subseteq \mathcal{P}_2^r(\Omega)$ with spatial decompositions $\boldsymbol{\xi}$ as described in Section 2.2. Then $\bigcup_{\boldsymbol{\xi}} \mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ is dense in $\mathcal{P}_2^r(\Omega)$ with respect to the L^2-Wasserstein distance. In particular, for any density $u \in \mathcal{P}_2^r(\Omega)$ an approximating sequence $\vec{\mathrm{x}}_{\boldsymbol{\xi}}$ of Lagrangian vectors in $\mathfrak{x}_{\boldsymbol{\xi}}$ can be explicitly given by*

$$\vec{\mathrm{x}}_{\boldsymbol{\xi}} \in \mathfrak{x}_{\boldsymbol{\xi}} \text{ with components that satisfy } \int_{x_{k-1}}^{x_k} u(s)\,\mathrm{d}s = \delta_{k-\frac{1}{2}}, \tag{3.60}$$

so that $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_{\boldsymbol{\xi}}] \to u$ with respect to the L^2-Wasserstein distance as $\overline{\delta} \to 0$.

Proof. To prove the above assertion, we will reformulate it in terms of Lagrangian coordinates. For any decomposition $\boldsymbol{\xi}$ introduce a projection map $\pi_{\boldsymbol{\xi}} : \mathfrak{X} \to \mathfrak{X}_{\boldsymbol{\xi}}$ on the space of Lagrangian maps, such that for all $\mathrm{X} \in \mathfrak{X}$.

$$\pi_{\boldsymbol{\xi}}[\mathrm{X}] = \sum_{k \in \mathbb{I}_K} x_k \theta_k(\xi), \quad \text{with } x_k = \mathrm{X}(\xi_k),\ k = 1, \ldots, K-1, \text{ and } x_0 = a,\, x_K = b.$$

Note that $\pi_{\boldsymbol{\xi}} : \mathfrak{X} \to \mathfrak{X}_{\boldsymbol{\xi}}$ is well-defined, although $\mathrm{X} \in \mathfrak{X}$ does not have to be continuous. The reason for this is the possibility to evaluate any function $\mathrm{X} \in \mathfrak{X}$ at least at any point $\xi \in [0, M)$, thanks to definition (2.2). If we can show

$$\|(\mathrm{id} - \pi_{\boldsymbol{\xi}})\mathrm{X}\|_{L^2(\mathcal{M})} \leqslant \sqrt{\overline{\delta}}(b-a) \tag{3.61}$$

for any $\mathrm{X} \in \mathfrak{X}$, then the lemma is proven, since the associated sequence $u_{\boldsymbol{\xi}}$ of density functions with Lagrangian maps $\pi_{\boldsymbol{\xi}}[\mathrm{X}]$ fulfills

$$\mathcal{W}_2(u, u_{\boldsymbol{\xi}}) = \|\pi_{\boldsymbol{\xi}}[\mathrm{X}] - \mathrm{X}\|_{L^2(\mathcal{M})} \longrightarrow 0$$

as $\overline{\delta} \to 0$, due to (2.3). For the proof of (3.61), note first that X and $\pi_{\boldsymbol{\xi}}[\mathrm{X}]$ are monotonically increasing. Thus, for any $\xi \in (\xi_{k-1}, \xi_k]$

$$|\mathrm{X}(\xi) - \pi_{\boldsymbol{\xi}}[\mathrm{X}](\xi)| \leqslant \begin{cases} \big(\mathrm{X}(\xi_k) - \mathrm{X}(\xi_{k-1})\big), & k = 2, \ldots, K-1, \\ \big(\mathrm{X}(\xi_1) - a\big), & k = 1, \\ \big(b - \mathrm{X}(\xi_{K-1})\big), & k = K. \end{cases} .$$

Therefore one obtains $|\mathrm{X}(\xi) - \pi_{\boldsymbol{\xi}}[\mathrm{X}](\xi)| \leqslant (b-a)$ for any $\xi \in \mathcal{M}$, which further yields

$$\begin{aligned} \|(\mathrm{id} - \pi_{\boldsymbol{\xi}})\mathrm{X}\|_{L^2(\mathcal{M})}^2 &= \sum_{k=1}^{K} \int_{\xi_{k-1}}^{\xi_k} |\mathrm{X}(\xi) - \pi_{\boldsymbol{\xi}}[\mathrm{X}](\xi)|^2 \,\mathrm{d}\xi \\ &\leqslant \overline{\delta}(b-a) \left[\sum_{k=2}^{K-1} \big(\mathrm{X}(\xi_k) - \mathrm{X}(\xi_{k-1})\big) + \big(\mathrm{X}(\xi_1) - a\big) + \big(b - \mathrm{X}(\xi_{K-1})\big) \right] \\ &= \overline{\delta}(b-a)^2. \end{aligned}$$

This proves (3.61) and closes the proof. □

For the forthcoming calculations we want to introduce a discrete counterpart to the local slope of $|\partial\mathcal{E}|$: For any $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$, define the *discrete local slope* $|\partial_{\boldsymbol{\xi}}\mathbf{E}|$ of $\mathbf{E}$ at $\vec{x}$ by

$$|\partial_{\boldsymbol{\xi}}\mathbf{E}|\,(\vec{x}) = \limsup_{\vec{y}\in\mathfrak{x}_{\boldsymbol{\xi}}:\vec{y}\to\vec{x}} \frac{\big(\mathbf{E}(\vec{x}) - \mathbf{E}(\vec{y})\big)^+}{\|\vec{x}-\vec{y}\|_{\boldsymbol{\xi}}}, \tag{3.62}$$

The main challenge in this section is now to prove that the discrete local slope $|\partial_{\boldsymbol{\xi}}\mathbf{E}|$ of $\mathbf{E}$ satisfies a discrete formulation of the lower semi-continuity similar to the one in (3.59). Therefor, we are going to derive an alternative representation to (3.62) for the discrete local slope, which is more convenient for analytical treatments as (3.62).

For this purpose we first analyze $|\partial\mathcal{E}|$: Note that the functional $u \mapsto \mathcal{E}_\tau(\sigma, u, v)$ given by

$$\mathcal{E}_\tau(\tau, u, v) = \frac{1}{2\sigma}\mathcal{W}_2(u,v)^2 + \mathcal{E}(u)$$

is $(\sigma^{-1} + \lambda)$-convex for any $v \in \mathcal{P}_2^r(\Omega)$ and any $\sigma \in (0,\tau)$, which is a consequence of the λ-convexity of $\mathcal{E}$ and the representation

$$\mathcal{E}_\tau(\sigma, u, v) = \mathcal{E}(u) - \frac{\lambda}{2}\mathcal{W}_2(u,v)^2 + \frac{1}{2}(\sigma^{-1}+\lambda)\mathcal{W}_2(u,v)^2.$$

This property allows the alternative representation of the local slope $|\partial\mathcal{E}|\,(u)$ through

$$|\partial\mathcal{E}|\,(u) = \sup_{v\in\mathcal{P}_2^r(\Omega):v\neq u}\left(\frac{\mathcal{E}(u)-\mathcal{E}(v)}{\mathcal{W}_2(u,v)} + \frac{\lambda}{2}\mathcal{W}_2(u,v)\right)^+. \tag{3.63}$$

A proof of this claim can be found in [**AGS05**, Theorem 2.4.9] and can be easily adapted to the discrete setting. Indeed, the $(\sigma^{-1}+\lambda)$-convexity of the functional $\vec{x} \mapsto \mathbf{E}_\Delta(\sigma, \vec{x}, \vec{y})$ for any $\vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$ and $\sigma \in (0,\tau)$ (see Remark 3.10) and the metric equality $\|\vec{x}-\vec{y}\|_{\boldsymbol{\xi}} = \mathcal{W}_2(\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}], \mathbf{u}_{\boldsymbol{\xi}}[\vec{y}])$ from (2.20) yield that one can repeat the proof [**AGS05**, Theorem 2.4.9] step-by-step to show that

$$|\partial_{\boldsymbol{\xi}}\mathbf{E}|\,(\vec{x}) = \sup_{\vec{y}\in\mathfrak{x}_{\boldsymbol{\xi}}:\vec{y}\neq\vec{x}}\left(\frac{\mathbf{E}(\vec{x})-\mathbf{E}(\vec{y})}{\|\vec{x}-\vec{y}\|_{\boldsymbol{\xi}}} + \frac{\lambda}{2}\|\vec{x}-\vec{y}\|_{\boldsymbol{\xi}}\right)^+. \tag{3.64}$$

To verify (3.64), one can also argue as follows: Since Theorem 2.4.9 in [**AGS05**] is stated for arbitrary metric spaces, it is in particular applicable to the space $(\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega), \mathrm{d}_{\boldsymbol{\xi}})$.

The proof of the following lemma relies on the method used in [**Ort05**, Proposition 13].

Lemma 3.25. *For any $u \in \mathcal{P}_2^r(\Omega)$, there exists a sequence of Lagrangian vectors $\vec{x}_{\boldsymbol{\xi}}$, such that $\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}_{\boldsymbol{\xi}}] = u_{\boldsymbol{\xi}} \to u$ with respect to the L^2-Wasserstein distance and*

$$\mathcal{E}(u_{\boldsymbol{\xi}}) \longrightarrow \mathcal{E}(u) \tag{3.65}$$

as $\overline{\delta} \to 0$. Moreover, the discrete local slope is lower semi-continuous with respect to the L^2-Wasserstein distance in the following sence: If $\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}_{\boldsymbol{\xi}}] \to u$ with respect to the L^2-Wasserstein distance for any sequence $\vec{x}_{\boldsymbol{\xi}}$, then

$$\liminf_{\overline{\delta}\to 0} |\partial_{\boldsymbol{\xi}}\mathbf{E}|\,(\vec{x}_{\boldsymbol{\xi}}) \geqslant |\partial\mathcal{E}|\,(u). \tag{3.66}$$

Proof. To prove (3.65) we take any $u \in \mathcal{P}_2^r(\Omega)$ with $\mathcal{E}(u) < +\infty$ — otherwise the proof is trivial. So for any arbitrary decomposition $\boldsymbol{\xi}$, define a sequence $\vec{\mathrm{x}}_{\boldsymbol{\xi}}$ with components as in (3.60), then the corresponding sequence of densities $u_{\boldsymbol{\xi}} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_{\boldsymbol{\xi}}]$ converges towards u w.r.t $\mathcal{W}_2$, see Lemma 3.24. Therefore we get

$$\begin{aligned}\mathcal{E}(u_{\boldsymbol{\xi}}) &= \sum_{k=1}^{K} \int_{x_{k-1}}^{x_k} \phi\left(\frac{\delta_k}{x_k - x_{k-1}}\right) \mathrm{d}x = \sum_{k=1}^{K} (x_k - x_{k-1}) \phi\left(\frac{1}{x_k - x_{k-1}} \int_{x_{k-1}}^{x_k} u(s)\,\mathrm{d}s\right) \\ &\leqslant \sum_{k=1}^{K} \int_{x_{k-1}}^{x_k} \phi\big(u(s)\big)\,\mathrm{d}s = \mathcal{E}(u),\end{aligned}$$

using Jensen's inequality. Taking the lim sup of both sides yields $\limsup_{\overline{\delta}\to 0} \mathcal{E}(u_{\boldsymbol{\xi}}) \leqslant \mathcal{E}(u)$ and since $\mathcal{E}$ is lower semi-continous, we especially obtain $\lim_{\overline{\delta}\to 0} \mathcal{E}(u_\Delta) = \mathcal{E}(u)$.

To prove (3.66) it is essential to use the representation of the local slope as in (3.63), which guarantees the existence of a sequence $(v_j)_{j=0}^{\infty}$ that satisfies

$$|\partial \mathcal{E}|(u) = \lim_{j\to\infty} \left(\frac{\mathcal{E}(u) - \mathcal{E}(v_j)}{\mathcal{W}_2(u, v_j)} + \frac{\lambda}{2} \mathcal{W}_2(u, v_j)\right)^+ .$$

Furthermore, define sequences $\vec{\mathrm{x}}_{\boldsymbol{\xi}}$ and $\vec{\mathrm{y}}_{j,\boldsymbol{\xi}}$ according to Lemma 3.24, such that $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_{\boldsymbol{\xi}}]$ converges to u and $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_{j,\boldsymbol{\xi}}]$ to v_j for any $j \in \mathbb{N}$, both with respect to the L^2-Wasserstein distance. By means of (3.65) and the equality $\mathcal{W}_2(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_{\boldsymbol{\xi}}], \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_{j,\boldsymbol{\xi}}]) = \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}$ we get

$$\begin{aligned}|\partial \mathcal{E}|(u) &= \lim_{j\to\infty} \left(\frac{\liminf_{\overline{\delta}\to 0} \mathbf{E}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}) - \lim_{\overline{\delta}\to 0} \mathbf{E}(\vec{\mathrm{y}}_{j,\boldsymbol{\xi}})}{\lim_{\overline{\delta}\to 0} \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}} + \lim_{\overline{\delta}\to 0} \frac{\lambda}{2} \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}\right)^+ \\ &\leqslant \lim_{j\to\infty} \liminf_{\overline{\delta}\to 0} \left(\frac{\mathbf{E}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}) - \mathbf{E}(\vec{\mathrm{y}}_{j,\boldsymbol{\xi}})}{\|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}} + \frac{\lambda}{2} \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}\right)^+ .\end{aligned}$$

For further estimation, note that

$$\begin{aligned}&\liminf_{\overline{\delta}\to 0} \left(\frac{\mathbf{E}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}) - \mathbf{E}(\vec{\mathrm{y}}_{j,\boldsymbol{\xi}})}{\|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}} + \frac{\lambda}{2} \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}\right)^+ \\ &\leqslant \liminf_{\overline{\delta}\to 0} \sup_{j\in\mathbb{N}} \left(\frac{\mathbf{E}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}) - \mathbf{E}(\vec{\mathrm{y}}_{j,\boldsymbol{\xi}})}{\|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}} + \frac{\lambda}{2} \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}\right)^+ \qquad \text{for any } j \in \mathbb{N},\end{aligned}$$

so taking the limit with respect to j in the last inequality we get due to (3.64)

$$|\partial \mathcal{E}|(u) \leqslant \liminf_{\overline{\delta}\to 0} \sup_{j\in\mathbb{N}} \left(\frac{\mathbf{E}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}) - \mathbf{E}(\vec{\mathrm{y}}_{j,\boldsymbol{\xi}})}{\|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}} + \frac{\lambda}{2} \|\vec{\mathrm{x}}_{\boldsymbol{\xi}} - \vec{\mathrm{y}}_{j,\boldsymbol{\xi}}\|_{\boldsymbol{\xi}}\right)^+ \leqslant \liminf_{\overline{\delta}\to 0} |\partial_{\boldsymbol{\xi}} \mathbf{E}|(\vec{\mathrm{x}}_{\boldsymbol{\xi}}).$$

□

3.5.2. The convergence result. A reader familiar with the theory in [**AGS05**, Part 1] or [**Ser11**, **Ort05**] will observe that the strategy used below is closely related to the one in [**Ser11**] and [**Ort05**].

From now on, we will always make the following assumptions, which are essentially the same as in Theorem 3.3 and 3.4:

- We assume $\boldsymbol{\tau}$ fine enough, i.e.
$$\tau^{-1} + \lambda > 0. \tag{3.67}$$
- We suppose that the initial discretization u_Δ^0 of u^0 is chosen such that
$$\mathcal{W}_2(u_\Delta^0, u^0) \longrightarrow 0, \quad \mathcal{E}(u_\Delta^0) \longrightarrow \mathcal{E}(u^0), \tag{3.68}$$
as $\Delta \to 0$ and $\mathcal{E}(u_\Delta^0) \leqslant \overline{\mathcal{E}}$ for fixed $\overline{\mathcal{E}} > 0$.

Note that the first point (3.67) guarantees the existence of minimizers. The second one is an essential tool for the proof of the subsection's main theorem.

In this subsection, let $\vec{\mathrm{x}}_\Delta$ be a solution of the numerical scheme in (3.11), which especially satisfies (3.13) from Theorem 3.3. Furthermore, denote by u_Δ the respective sequence of locally constant density functions, which converges towards a limit curve $u_* \in C^{1/2}_{\mathrm{loc}}([0,+\infty); \mathcal{P}_2^r(\Omega))$ as $\Delta \to 0$, see Theorem 3.4.

Before we can formulate the next lemma, we have to introduce some additional notation for the solution $\vec{\mathrm{x}}_\Delta$:

Definition 3.26 (discrete metric derivative and discrete De Giorgi's variational interpolation). *Suggest $\vec{\mathrm{x}}_\Delta$ to be a solution of our scheme in* (3.11)*. Then for any $n \in \mathbb{N}$ and $t \in (t_{n-1}, t_n]$, the* discrete metric derivative *of $\vec{\mathrm{x}}_\Delta$ is given by*
$$\left\lfloor \vec{\mathrm{x}}'_\Delta \right\rfloor(t) := \frac{\left\| \vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}}{\tau_n}. \tag{3.69}$$
Moreover, define the De Giorgi's variational interpolation *by*
$$\vec{\mathrm{x}}_\Delta^t := \operatorname*{arg\,min}_{\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}} \mathbf{E}_\Delta(t - t_{n-1}, \vec{\mathrm{x}}, \vec{\mathrm{x}}_\Delta^{n-1}) \quad \text{for } t \in (t_{n-1}, t_n],\ n \in \mathbb{N}, \tag{3.70}$$
and introduce similarly to the discrete metric derivative the map $G_\Delta : (0,+\infty) \to \mathbb{R}_+$,
$$G_\Delta(t) = \frac{\left\| \vec{\mathrm{x}}_\Delta^t - \vec{\mathrm{x}}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}}{t - t_{n-1}} \quad \text{for any } t \in (t_{n-1}, t_n]. \tag{3.71}$$

Lemma 3.27. *Suppose that $\vec{\mathrm{x}}_\Delta$ is a solution to our scheme in* (3.11)*, thus especially solves successively the discrete minimizing movement scheme in* (3.11)*. Then*
$$\frac{1}{2}\int_{t_{n-1}}^{t_n} \left\lfloor \vec{\mathrm{x}}'_\Delta \right\rfloor^2(t)\,\mathrm{d}t + \frac{1}{2}\int_{t_{n-1}}^{t_n} |G_\Delta(t)|^2\,\mathrm{d}t \leqslant \mathbf{E}(\vec{\mathrm{x}}_\Delta^{n-1}) - \mathbf{E}(\vec{\mathrm{x}}_\Delta^n) \tag{3.72}$$
for any $t \in \big((n-1)\tau, n\tau\big]$, $n \in \mathbb{N}$. Furthermore, there exists a subsequence of $\vec{\mathrm{x}}_\Delta$, not relabeled, a non-increasing function $\varphi : [0,+\infty) \to [-\infty, \infty]$ and functions $A, G \in L^2_{\mathrm{loc}}([0,+\infty))$, such that for any $T > 0$
$$\left\lfloor \vec{\mathrm{x}}'_\Delta \right\rfloor \longrightarrow A \text{ weakly in } L^2([0,T]) \text{ and } A \geqslant \left|u'_*\right| \text{ almost everywhere,} \tag{3.73}$$
$$\mathbf{E}(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(t)) \longrightarrow \varphi(t) \geqslant \mathcal{E}(u(t)) \text{ for any } t \in [0,T], \tag{3.74}$$
$$|\partial_{\boldsymbol{\xi}}\mathbf{E}|(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(t)) \longrightarrow G \text{ weakly in } L^2([0,T]) \tag{3.75}$$

as $\Delta \to 0$*. Here,* u_* *denotes the limit curve from Proposition 3.16 that is in addition locally absolutely continuous, i.e.* $\mathcal{W}_2(u_*(s), u_*(t)) \leqslant \int_s^t A(r)\,\mathrm{d}r$ *for any* $s < t$*.*

Proof. Equation (3.72) immediately follows from (A.3), see Lemma A.5, and the previous definitions of the discrete metric derivative (3.69) and of G_Δ in (3.71).

Summing over $n \in \mathbb{N}$ in (3.72) yields

$$\frac{1}{2}\int_0^\infty \lfloor \vec{\mathrm{x}}'_\Delta \rfloor^2 (t)\,\mathrm{d}t + \frac{1}{2}\int_0^\infty |G_\Delta(t)|^2\,\mathrm{d}t \leqslant \overline{\mathcal{E}} - \underline{\mathcal{E}},$$

where $\underline{\mathcal{E}}$ is the lower bound of $\mathfrak{E}$ (and therefore of $\mathcal{E}$ and $\mathbf{E}$ as well), see (3.20). Hence $\lfloor \vec{\mathrm{x}}'_\Delta \rfloor$ is uniformly bounded in $L^2([0, +\infty))$. Therefore a weakly convergent subsequence and a limit function $A \in L^2_{\mathrm{loc}}([0, +\infty))$ exist, such that the first statement in (3.73) is satisfied. Furthermore, the above estimate can be combined with the definition of G_Δ in (3.71) and the slope estimate (A.2) from Lemma A.5. This yields

$$\frac{1}{2}\int_0^\infty |\partial_{\boldsymbol{\xi}} \mathbf{E}| \left(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(t)\right)\mathrm{d}t \leqslant \overline{\mathcal{E}} - \underline{\mathcal{E}},$$

and proves the existence of $G \in L^2_{\mathrm{loc}}([0, +\infty))$, such that (3.75) holds true. On top of that, one can apply Helly's Theorem A.2 on the sequence of non-increasing functions $t \mapsto \mathbf{E}(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(t))$, which guarantees the existence of a non-increasing function $\varphi(t)$ with the limit property in (3.74). That especially proves (3.74) due to the lower semi-continuity of $\mathcal{E}$.

It still remains to prove the estimate $A \geqslant |u'_*|$. For this, introduce for any time $t \in [0, +\infty)$

$$n^-_\Delta(t) = \max\{j : t \geqslant \sum_{n=1}^{j} \tau_n\} \quad \text{and} \quad n^+_\Delta(t) = \min\{j : t \leqslant \sum_{n=1}^{j} \tau_n\}.$$

Then (2.20) and the definition of $\lfloor \vec{\mathrm{x}}'_\Delta \rfloor$ yield for any $s < t$

$$\begin{aligned}\mathcal{W}_2(\{u_\Delta\}_{\boldsymbol{\tau}}(s), \{u_\Delta\}_{\boldsymbol{\tau}}(t)) \leqslant \sum_{j=n^-_\Delta(s)+1}^{n^+_\Delta(t)} \mathcal{W}_2(u^j_\Delta, u^{j-1}_\Delta) &= \sum_{j=n^-_\Delta(s)+1}^{n^+_\Delta(t)} \tau_j \frac{\left\| \vec{\mathrm{x}}^j_\Delta - \vec{\mathrm{x}}^{j-1}_\Delta \right\|_{\boldsymbol{\xi}}}{\tau_j} \\ &= \int_{t_{n^-_\Delta(s)}}^{t_{n^+_\Delta(t)}} \lfloor u'_\Delta \rfloor (r)\,\mathrm{d}r.\end{aligned}$$

Passing to the limit on both sides as $\Delta \to 0$ yields $\mathcal{W}_2(u_*(s), u_*(t)) \leqslant \int_s^t A(r)\,\mathrm{d}(r)$. □

Owing to the above convergence results and the lim/lim inf-properties in (3.65) and (3.66), we can now give a proof of the main convergence result of this section, Theorem 3.22.

Proof of Theorem 3.22. Making use of the above results in Lemma 3.27 and the lower semi-continuity of the discrete slope in (3.66) yield for any $t \in [0, +\infty)$

$$\begin{aligned}
&\frac{1}{2}\int_0^t \left|u_*'\right|^2(r)\,\mathrm{d}r + \frac{1}{2}\int_0^t |\partial\mathcal{E}|^2(u_*(r))\,\mathrm{d}r + \mathcal{E}(u_*(t)) \\
\leqslant &\frac{1}{2}\int_0^t A^2(r)\,\mathrm{d}r + \liminf_{\Delta\to 0}\frac{1}{2}\int_0^t |\partial_{\boldsymbol{\xi}}\mathbf{E}|^2\left(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(r)\right)\mathrm{d}r + \varphi(t) \\
\leqslant &\liminf_{\Delta\to 0}\left(\frac{1}{2}\int_0^t \left\lfloor\vec{\mathrm{x}}_\Delta'\right\rfloor^2(r)\,\mathrm{d}r + \frac{1}{2}\int_0^t |G_\Delta(r)|^2\,\mathrm{d}r + \mathbf{E}(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(t))\right) \\
\leqslant &\limsup_{\Delta\to 0}\left(\frac{1}{2}\int_0^t \left\lfloor\vec{\mathrm{x}}_\Delta'\right\rfloor^2(r)\,\mathrm{d}r + \frac{1}{2}\int_0^t |G_\Delta(r)|^2\,\mathrm{d}r + \mathbf{E}(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(t))\right) \\
= &\limsup_{\Delta\to 0}\mathbf{E}(\{\vec{\mathrm{x}}_\Delta\}_{\boldsymbol{\tau}}(0)) = \limsup_{\Delta\to 0}\mathcal{E}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_\Delta^0]) = \mathcal{E}(u^0).
\end{aligned} \tag{3.76}$$

Furthermore, one has that

$$\mathcal{E}(u^0) - \mathcal{E}(u_*(t)) \leqslant \int_0^t |\partial\mathcal{E}|^2(u_*(r))\,\mathrm{d}r + \int_0^t \left|u_*'\right|^2(r)\,\mathrm{d}r,$$

due to (3.57). This yields equality in (3.76) and consequently (3.58). □

3.6. Consistency and stability

In the following, we are going to show that our numerical scheme is consistent and stable. This can further be used to prove an alternative convergence result to the one we already stated in Theorem 3.4.

For the rest of this section we fix an arbitrary time horizon $T > 0$ and define for any temporal decomposition $\boldsymbol{\tau}$ an integer $N_{\boldsymbol{\tau}} \in \mathbb{N}$ such that $T \leqslant \sum_{n=0}^{N_{\boldsymbol{\tau}}} \tau_n \leqslant (T+1)$ is fulfilled.

As a first step, we prove the scheme's consistency which means in particular the following:

Proposition 3.28. *Assume* $\mathrm{X} \in C^p([0,T] \times \mathcal{M})$ *with* $p \geqslant 4$ *to be a smooth solution of the Lagrangian formulation of* (3.1)*, i.e.*

$$\partial_t \mathrm{X} = \partial_\xi \psi'(\partial_\xi \mathrm{X}) - V_x(\mathrm{X}). \tag{3.77}$$

Let $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ *be a family of discretization parameters, such that any spatial decomposition* $\boldsymbol{\xi}$ *satisfies*

$$\delta_{k+\frac{1}{2}} - \delta_{k-\frac{1}{2}} = \mathcal{O}(\overline{\delta}^2) \quad \textit{for any } k = 1, \ldots, K-1. \tag{3.78}$$

Furthermore, denote by $\vec{\mathrm{y}}_\Delta$ *the restriction of* X *to the respective meshes, given by* $\mathrm{y}_k^n = \mathrm{X}(t_n, x_k)$ *for any* $n \in \mathbb{N}_0$ *and* $k = 1, \ldots, K-1$.

Then $\vec{\mathrm{y}}_\Delta$ *satisfies the system of Euler-Lagrange equations* (3.29) *with an error of order* $\mathcal{O}(\tau) + \mathcal{O}(\overline{\delta}^2) + \mathcal{O}(\overline{\delta}^p/\underline{\tau})$. *More precisely, the sequence of vectors* $\vec{\gamma}_\Delta = (\vec{\gamma}_\Delta^1, \ldots, \vec{\gamma}_\Delta^{N_{\boldsymbol{\tau}}})$ *with* $\vec{\gamma}_\Delta^n \in \mathbb{R}^{K-1}$ *and components*

$$\gamma_k^n := \frac{\mathrm{y}_k^n - \mathrm{y}_k^{n-1}}{\tau_n} + \left[\nabla_{\boldsymbol{\xi}}\mathbf{E}_{\boldsymbol{\xi}}(\vec{\mathrm{y}}_\Delta^n)\right]_k,$$

satisfies

$$\mathsf{err} := \max_{n=1}^{N_{\boldsymbol{\tau}}} \|\vec{\gamma}^n_\Delta\|_{\boldsymbol{\xi}} \leqslant C(\tau + \overline{\delta}^2 + \overline{\delta}^p/\underline{\tau}), \tag{3.79}$$

with $\overline{\delta} = \max_{k\in\mathbb{I}_K^{1/2}} \delta_\kappa$ *and* $\underline{\tau} = \min_{n\in\mathbb{N}} \tau_n$ *as defined in* (2.11)

Remark 3.29. *Note that the requirement* (3.78) *is naturally induced by the smoothness of solution* X*, if one chooses* $\boldsymbol{\xi}$ *such that the initial grid* $\vec{\mathrm{y}}^0_\Delta$ *on* Ω *is uniform, i.e.* $\delta_x := (\mathrm{y}^0_k - \mathrm{y}^0_{k-1})$ *is independent of* k*. Then a Taylor expansion on the associated distribution function* U *of* X *around the point* x^0_k *yields due to* (2.1) *and* (2.9)

$$\delta_{k+\frac{1}{2}} - \delta_{k-\frac{1}{2}} = \mathrm{U}(\mathrm{y}^0_{k+1}) - 2\mathrm{U}(\mathrm{y}^0_k) + \mathrm{U}(\mathrm{y}^0_{k-1}) = \delta_x^2 \mathrm{U}''(\mathrm{y}^0_k) + \mathcal{O}(\delta_x^3) = \mathcal{O}(\overline{\delta}^2),$$

since the smoothness of $\partial_\xi \mathrm{X}(0,\xi_k)$ *yields* $\delta_x = \mathcal{O}(\overline{\delta})$

Remark 3.30. *The term* $\mathcal{O}(\overline{\delta}^p/\underline{\tau})$ *in* err *indicates a certain CFL-condition for the temporal and spatial decompositions, but this can be neglected for sufficiently smooth solutions* X *of* (3.77)*.*

To make the proof of the above claim more readable, we introduce the following — more technical — lemma.

Lemma 3.31. *Consider the same assumption as before in Proposition 3.28. Then for any* $k = 1,\dots,K-1$ *and* $n = 1,\dots,N_{\boldsymbol{\tau}}$ *the residuum*

$$R^n := \frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2}\partial_t \mathrm{X}(t_n,\xi_k) + \big[\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}^n_\Delta)\big]_k \tag{3.80}$$

fulfills $|R^n| \leqslant C\overline{\delta}^3$*.*

Proof. In view of equation (3.77), the claim that $|R^n| \leqslant C\overline{\delta}^3$ is equivalent to

$$\big[\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}^n_\Delta)\big]_k = -\frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2}\big(\partial_\xi \psi'(\partial_\xi \mathrm{X})(t_n,\xi_k) - V_x(\mathrm{X}(t_n,\xi_k))\big) + \mathcal{O}(\overline{\delta}^3) \tag{3.81}$$

With this in mind, remember the explicit representation of $\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}^n_\Delta)$ in (3.22), that is

$$\big[\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}_\Delta)\big]_k = -\psi'\bigg(\frac{\mathrm{y}^n_{k+1} - \mathrm{y}^n_k}{\delta_{k+\frac{1}{2}}}\bigg) + \psi'\bigg(\frac{\mathrm{y}^n_k - \mathrm{y}^n_{k-1}}{\delta_{k-\frac{1}{2}}}\bigg) + \int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi$$

for each $k = 1,\dots,K-1$ and $n = 1,\dots,N_{\boldsymbol{\tau}}$. Let us treat both terms separately. First note that the definition of $\vec{\mathrm{x}}_\Delta$ and a Taylor expansion yield

$$\frac{\vec{\mathrm{y}}^n_{k\pm1} - \vec{\mathrm{y}}^n_k}{\delta_{k\pm\frac{1}{2}}} = \partial_\xi \mathrm{X}(t_n,\xi_k) \pm \frac{\delta_{k\pm\frac{1}{2}}}{2}\partial_\xi^2 \mathrm{X}(t_n,\xi_k) + \frac{\delta^2_{k\pm\frac{1}{2}}}{6}\partial_\xi^3 \mathrm{X}(t_n,\xi_k) + \mathcal{O}(\overline{\delta}^3),$$

hence

$$
\begin{aligned}
&-\psi'\bigg(\frac{\mathrm{y}_{k+1}^n-\mathrm{y}_k^n}{\delta_{k+\frac12}}\bigg)+\psi'\bigg(\frac{\mathrm{y}_k^n-\mathrm{y}_{k-1}^n}{\delta_{k-\frac12}}\bigg)\\
=&-\psi'\left(\partial_\xi \mathrm{X}(t_n,\xi_k)+\frac{\delta_{k+\frac12}}{2}\partial_\xi^2\mathrm{X}(t_n,\xi_k)+\frac{\delta_{k+\frac12}^2}{6}\partial_\xi^3\mathrm{X}(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3)\right)\\
&+\psi'\left(\partial_\xi \mathrm{X}(t_n,\xi_k)-\frac{\delta_{k-\frac12}}{2}\partial_\xi^2\mathrm{X}(t_n,\xi_k)+\frac{\delta_{k-\frac12}^2}{6}\partial_\xi^3\mathrm{X}(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3)\right).
\end{aligned}
\tag{3.82}
$$

A further Taylor expansion for the function ψ' then shows that

$$
\begin{aligned}
&\psi'\left(\partial_\xi \mathrm{X}(t_n,\xi_k)\pm\frac{\delta_{k\pm\frac12}}{2}\partial_\xi^2\mathrm{X}(t_n,\xi_k)+\frac{\delta_{k\pm\frac12}^2}{6}\partial_\xi^3\mathrm{X}(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3)\right)\\
=&\psi'(\partial_\xi\mathrm{X}(t_n,\xi_k))\pm\psi''(\partial_\xi\mathrm{X}(t_n,\xi_k))\left(\frac{\delta_{k\pm\frac12}}{2}\partial_\xi^2\mathrm{X}(t_n,\xi_k)+\frac{\delta_{k\pm\frac12}^2}{6}\partial_\xi^3\mathrm{X}(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3)\right)\\
&+\frac12\psi'''(\partial_\xi\mathrm{X}(t_n,\xi_k))\left(\frac{\delta_{k\pm\frac12}}{2}\partial_\xi^2\mathrm{X}(t_n,\xi_k)+\frac{\delta_{k\pm\frac12}^2}{6}\partial_\xi^3\mathrm{X}(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3)\right)^2+\mathcal{O}(\overline{\delta}^3)\\
=&\psi'(\partial_\xi\mathrm{X}(t_n,\xi_k))\pm\frac{\delta_{k\pm\frac12}}{2}\psi''\left(\partial_\xi\mathrm{X}(t_n,\xi_k)\right)\partial_\xi^2\mathrm{X}(t_n,\xi_k)+\frac{\delta_{k\pm\frac12}^2}{6}\psi''\left(\partial_\xi\mathrm{X}(t_n,\xi_k)\right)\partial_\xi^3\mathrm{X}(t_n,\xi_k)\\
&+\frac{\delta_{k\pm\frac12}^2}{8}\psi'''\left(\partial_\xi\mathrm{X}(t_n,\xi_k)\right)(\partial_\xi^2\mathrm{X})^2(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3),
\end{aligned}
\tag{3.83}
$$

Combining (3.82) with (3.83), we obtain due to the assumption on the decomposition $\boldsymbol{\xi}$ in (3.78) that

$$
\begin{aligned}
&-\psi'\bigg(\frac{\mathrm{y}_{k+1}^n-\mathrm{y}_k^n}{\delta_{k+\frac12}}\bigg)+\psi'\bigg(\frac{\mathrm{y}_k^n-\mathrm{y}_{k-1}^n}{\delta_{k-\frac12}}\bigg)\\
=&-\frac{\delta_{k+\frac12}+\delta_{k-\frac12}}{2}\psi''\left(\partial_\xi\mathrm{X}(t_n,\xi_k)\right)\partial_\xi^2\mathrm{X}(t_n,\xi_k)-\frac{\delta_{k+\frac12}^2-\delta_{k-\frac12}^2}{6}\psi''\left(\partial_\xi\mathrm{X}(t_n,\xi_k)\right)\partial_\xi^3\mathrm{X}(t_n,\xi_k)\\
&-\frac{\delta_{k+\frac12}^2-\delta_{k-\frac12}^2}{8}\psi'''\left(\partial_\xi\mathrm{X}(t_n,\xi_k)\right)(\partial_\xi^2\mathrm{X})^2(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3)\\
=&-\frac{\delta_{k+\frac12}+\delta_{k-\frac12}}{2}\partial_\xi\psi'(\partial_\xi\mathrm{X})(t_n,\xi_k)+\mathcal{O}(\overline{\delta}^3),
\end{aligned}
\tag{3.84}
$$

where the last term corresponds to the first term in (3.81).

For the second term of $\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}_\Delta^n)$ we once again use the smoothness of X and a Taylor expansion,

$$
\begin{aligned}
\int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_\Delta^n](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi=\int_{\mathcal{M}}\Big(&V_x(\mathrm{X}(t_n,\xi_k))+V_{xx}(\mathrm{X}(t_n,\xi_k))\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_\Delta^n](\xi)-\mathrm{X}(t_n,\xi_k)\big)\\
&+\frac12 V_{xxx}(\check{x})\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_\Delta^n](\xi)-\mathrm{X}(t_n,\xi_k)\big)^2\Big)\theta_k(\xi)\,\mathrm{d}\xi
\end{aligned}
$$

where $\check{x}$ lies between $\mathrm{X}(t_n, \xi_{k-1})$ and $\mathrm{X}(t_n, \xi_{k+1})$. Due to

$$\int_{\mathcal{M}} \theta_k(\xi)\,\mathrm{d}\xi = \frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2}$$

we further obtain the representation

$$\int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi = \frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2} V_x(\mathrm{X}(t_n, \xi_k)) \tag{3.85}$$

$$+ V_{xx}(\mathrm{X}(t_n, \xi_k)) \int_{\mathcal{M}} \big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi) - \mathrm{X}(t_n, \xi_k)\big)\theta_k(\xi)\,\mathrm{d}\xi \tag{3.86}$$

$$+ \int_{\mathcal{M}} \frac{1}{2} V_{xxx}(\check{x})\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi) - \mathrm{X}(t_n, \xi_k)\big)^2\theta_k(\xi)\,\mathrm{d}\xi. \tag{3.87}$$

The first term in (3.85) is the second term in (3.81) and it is easly seen by a Taylor expansion that the third term in (3.87) has to be of order $\mathcal{O}(\overline{\delta}^3)$. Therefore we have to study the second term (3.86). To this aim, note that the locally affine function $\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta]$ satisfies

$$\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi) = \begin{cases} \mathrm{X}(t_n, \xi_k) + \big(\mathrm{X}(t_n, \xi_{k-1}) - \mathrm{X}(t_n, \xi_k)\big)\theta_{k-1}(\xi) & \text{for } \xi \in [\xi_{k-1}, \xi_k], \\ \mathrm{X}(t_n, \xi_k) + \big(\mathrm{X}(t_n, \xi_{k+1}) - \mathrm{X}(t_n, \xi_k)\big)\theta_{k+1}(\xi) & \text{for } \xi \in (\xi_{k-1}, \xi_k], \end{cases}$$

and therefore

$$\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi) - \mathrm{X}(t_n, \xi_k) = \begin{cases} \big(\mathrm{X}(t_n, \xi_{k-1}) - \mathrm{X}(t_n, \xi_k)\big)\theta_{k-1}(\xi) & \text{for } \xi \in [\xi_{k-1}, \xi_k], \\ \big(\mathrm{X}(t_n, \xi_{k+1}) - \mathrm{X}(t_n, \xi_k)\big)\theta_{k+1}(\xi) & \text{for } \xi \in (\xi_{k-1}, \xi_k]. \end{cases} \tag{3.88}$$

Furthermore, another Taylor expansion shows that

$$\mathrm{X}(t_n, \xi_k) - \mathrm{X}(t_n, \xi_{k\pm 1}) = \mp \delta_{k\pm\frac{1}{2}} \partial_\xi \mathrm{X}(t_n, \xi_k) + \mathcal{O}(\overline{\delta}^2). \tag{3.89}$$

Hence inserting (3.88) and (3.89) into the second term (3.86), one attains

$$\begin{aligned} &V_{xx}(\mathrm{X}(t_n, \xi_k)) \int_{\mathcal{M}} \big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^n_\Delta](\xi) - \mathrm{X}(t_n, \xi_k)\big)\theta_k(\xi)\,\mathrm{d}\xi \\ =& V_{xx}(\mathrm{X}(t_n, \xi_k)) \int_{\xi_{k-1}}^{\xi_k} \big(\mathrm{X}(t_n, \xi_{k-1}) - \mathrm{X}(t_n, \xi_k)\big)\theta_{k-1}(\xi)\theta_k(\xi)\,\mathrm{d}\xi \\ &+ V_{xx}(\mathrm{X}(t_n, \xi_k)) \int_{\xi_k}^{\xi_{k+1}} \big(\mathrm{X}(t_n, \xi_{k+1}) - \mathrm{X}(t_n, \xi_k)\big)\theta_{k+1}(\xi)\theta_k(\xi)\,\mathrm{d}\xi \\ =& V_{xx}(\mathrm{X}(t_n, \xi_k)) \left(\frac{\delta^2_{k+\frac{1}{2}} - \delta^2_{k-\frac{1}{2}}}{6} \partial_\xi \mathrm{X}(t_n, \xi_k) \right) + \mathcal{O}(\overline{\delta}^3), \end{aligned} \tag{3.90}$$

where we used in the last equation that

$$\int_{\mathcal{M}} \theta_k(\xi)\theta_{k\pm 1}(\xi)\,\mathrm{d}\xi = \frac{\delta_{k\pm\frac{1}{2}}}{6}$$

for any $k \in \{1, \dots, K-1\}$. Putting all results for the terms (3.85) - (3.87) together, we finally conclude that

$$\int_{\mathcal{M}} V_x\big(\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}_\Delta^n](\xi)\big)\theta_k(\xi)\,\mathrm{d}\xi = \frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2} V_x(\mathrm{X}(t_n, \xi_k)) + \mathcal{O}(\overline{\delta}^3),$$

which in particular shows in combination with (3.84) the claim in (3.81). ☐

Proof of Proposition 3.28. To get the required rate on the error, one has to investigate

$$\big[\mathrm{W}_2\vec{\gamma}_\Delta^n\big]_k = \frac{1}{\tau_n}\big[\mathrm{W}_2(\vec{\mathrm{y}}_\Delta^n - \vec{\mathrm{y}}_\Delta^{n-1})\big]_k + \big[\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}_\Delta^n)\big]_k.$$

The main challenge is to simplify the term $\big[\mathrm{W}_2(\vec{\mathrm{y}}_\Delta^n - \vec{\mathrm{y}}_\Delta^{n-1})\big]_k$. For this purpose, remember the definition of the matrix W_2 in (2.21) which satisfies for arbitrary $\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}}$

$$6[\mathrm{W}_2\vec{\mathrm{y}}]_k = \begin{cases} \delta_{k-\frac{1}{2}} y_{k-1} + 2(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}) y_k + \delta_{k+\frac{1}{2}} y_{k+1} & \text{for } k = 2, \dots, K-2, \\ 2(\delta_{\frac{3}{2}} + \delta_{\frac{1}{2}}) y_1 + \delta_{\frac{3}{2}} y_2 & \text{for } k = 1, \\ \delta_{K-\frac{1}{2}} y_{K-2} + 2(\delta_{K-\frac{1}{2}} + \delta_{K-\frac{3}{2}}) y_{K-1} & \text{for } k = K-1. \end{cases} \tag{3.91}$$

Let us first fix an index $k \in \{2, \dots, K-2\}$. Furthermore, define the intermediate point

$$\bar{\xi}_k := \xi_k + \frac{\delta_{k+\frac{1}{2}} - \delta_{k-\frac{1}{2}}}{3} \in [\xi_{k-1}, \xi_{k+1}],$$

which is chosen such that

$$\delta_{k-\frac{1}{2}}(\xi_{k-1} - \bar{\xi}_k) + 2(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}})(\xi_k - \bar{\xi}_k) + \delta_{k+\frac{1}{2}}(\xi_{k+1} - \bar{\xi}_k) = 0. \tag{3.92}$$

Then a Taylor expansion yields for any $n = 1, \dots, N_{\boldsymbol{\tau}}$

$$\mathrm{X}(t_n, \xi) = \mathrm{X}(t_n, \bar{\xi}_k) + \partial_\xi \mathrm{X}(t_n, \bar{\xi}_k)(\xi - \bar{\xi}_k) + \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!}(\xi - \bar{\xi}_k)^l + \mathcal{O}(\overline{\delta}^p) \tag{3.93}$$

remember $\mathrm{X} \in C^p([0,T] \times \mathcal{M})$. Let us now consider $\mathrm{W}_2\vec{\mathrm{y}}_\Delta^n$ for any $n = 1, \dots, N_{\boldsymbol{\tau}}$, then one attains due to (3.91)

$$6[\mathrm{W}_2\vec{\mathrm{y}}_\Delta^n]_k = \delta_{k-\frac{1}{2}}\mathrm{X}(t_n, \xi_{k-1}) + 2(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}})\mathrm{X}(t_n, \xi_k) + \delta_{k+\frac{1}{2}}\mathrm{X}(t_n, \xi_{k+1}).$$

Applying (3.92) and (3.93) further yields

$$\begin{aligned} 6\big[\mathrm{W}_2\vec{\mathrm{y}}_\Delta^n\big]_k = {} & \delta_{k-\frac{1}{2}} \left(\mathrm{X}(t_n, \bar{\xi}_k) + \partial_\xi \mathrm{X}(t_n, \bar{\xi})(\xi_{k-1} - \bar{\xi}_k) + \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!}(\xi_{k-1} - \bar{\xi}_k)^l \right) \\ & + 2(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}) \left(\mathrm{X}(t_n, \bar{\xi}_k) + \partial_\xi \mathrm{X}(t_n, \bar{\xi})(\xi_k - \bar{\xi}_k) + \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!}(\xi_k - \bar{\xi}_k)^l \right) \\ & + \delta_{k+\frac{1}{2}} \left(\mathrm{X}(t_n, \bar{\xi}_k) + \partial_\xi \mathrm{X}(t_n, \bar{\xi})(\xi_{k+1} - \bar{\xi}_k) + \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!}(\xi_{k+1} - \bar{\xi}_k)^l \right) \\ & + \mathcal{O}(\overline{\delta}^{p+1}) \\ = {} & 3(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}})\mathrm{X}(t_n, \bar{\xi}_k) + A_k^n + \mathcal{O}(\overline{\delta}^{p+1}) \end{aligned}$$

with

$$A_k^n = 2(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}) \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!} (\xi_k - \bar{\xi}_k)^l$$
$$+ \delta_{k-\frac{1}{2}} \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!} (\xi_{k-1} - \bar{\xi}_k)^l + \delta_{k+\frac{1}{2}} \sum_{l=2}^{p-1} \frac{\partial_\xi^l \mathrm{X}(t_n, \bar{\xi}_k)}{l!} (\xi_{k+1} - \bar{\xi}_k)^l.$$

The same calculation can be done for $n-1$ instead of n, thus one obtains

$$\frac{1}{\tau_n} \big[\mathrm{W}_2(\vec{\mathrm{y}}_\Delta^n - \vec{\mathrm{y}}_\Delta^{n-1})\big]_k = \frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2\tau_n} \big(\mathrm{X}(t_n, \bar{\xi}_k) - \mathrm{X}(t_{n-1}, \bar{\xi}_k)\big) + \frac{A_k^n - A_k^{n-1}}{6\tau_n} + \mathcal{O}(\overline{\delta}^{p+1}/\underline{\tau}). \tag{3.94}$$

First note, that one can apply Taylor expansions with respect to time in each summand of A_k^n, which yields

$$\frac{A_k^n - A_k^{n-1}}{6\tau_n} = \mathcal{O}(\overline{\delta}^3). \tag{3.95}$$

Next, another two Taylor expansions lead to

$$\frac{\mathrm{X}(t_n, \bar{\xi}_k) - \mathrm{X}(t_{n-1}, \bar{\xi}_k)}{\tau_n} = \partial_t \mathrm{X}(t_n, \xi_k) + (\bar{\xi}_k - \xi_k)\partial_t\partial_\xi \mathrm{X}(t_n, \xi_k) + \mathcal{O}(\tau) + \mathcal{O}(\overline{\delta}^2). \tag{3.96}$$

Combining (3.94), (3.95) and (3.96) with the identity $\bar{\xi}_k - \xi_k = \frac{\delta_{k+\frac{1}{2}} - \delta_{k-\frac{1}{2}}}{3}$ in (3.92) yields

$$\begin{aligned}\big[\mathrm{W}_2\vec{\gamma}_\Delta^n\big]_k &= \frac{1}{\tau_n}\big[\mathrm{W}_2(\vec{\mathrm{y}}_\Delta^n - \vec{\mathrm{y}}_\Delta^{n-1})\big]_k + \big[\partial_{\vec{\mathrm{x}}} \mathbf{E}(\vec{\mathrm{y}}_\Delta^{n+1})\big]_k \\ &= \frac{\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}}{2} \partial_t \mathrm{X}(t_n, \xi_k) + \frac{\delta_{k+\frac{1}{2}}^2 - \delta_{k-\frac{1}{2}}^2}{2} \partial_t\partial_\xi \mathrm{X}(t_n, \xi_k) + \big[\partial_{\vec{\mathrm{x}}} \mathbf{E}(\vec{\mathrm{y}}_\Delta^{n+1})\big]_k \\ &\quad + \mathcal{O}(\overline{\delta}\tau) + \mathcal{O}(\overline{\delta}^3) + \mathcal{O}(\overline{\delta}^{p+1}/\underline{\tau}).\end{aligned}$$

An analogue calculation shows the same result for the indices $k = 1$ and $k = K-1$. Therefore, as a result of Lemma 3.31 and the assumption on the spatial decomposition $\boldsymbol{\xi}$ in (3.78), we conclude that

$$\|\mathrm{W}_2\vec{\gamma}_\Delta^n\|_\infty \leqslant C(\overline{\delta}\tau + \overline{\delta}^3 + \overline{\delta}^{p+1}/\underline{\tau})$$

independently of n. Gerschgorin's Theorem yields $\frac{2\underline{\delta}}{3} \leqslant \mu \leqslant \overline{\delta}$ for any eigenvalue μ of W_2 and therefore $\|\mathrm{W}_2^{-\frac{1}{2}}\|_2 \leqslant \sqrt{\frac{3}{2\underline{\delta}}}$. As an immediate consequence, one obtains

$$\|\mathrm{W}_2^{\frac{1}{2}}\vec{\gamma}_\Delta^n\|_2 = \|\mathrm{W}_2^{-\frac{1}{2}}\mathrm{W}_2\vec{\gamma}_\Delta^n\|_2 \leqslant \sqrt{\frac{3}{2\underline{\delta}}}\sqrt{K-1}\|\mathrm{W}_2\vec{\gamma}_\Delta^n\|_\infty \leqslant \sqrt{\frac{3}{2}}\overline{\alpha}_2(\tau + \overline{\delta}^2 + \overline{\delta}^p/\underline{\tau})$$

for any $n \in \mathbb{N}$ and furthermore by Cauchy-Schwarz inequality

$$\mathsf{err} = \max_{n=1}^{N_\tau} \|\vec{\gamma}_\Delta^n\|_{\boldsymbol{\xi}} \leqslant \max_{n=1}^{N_\tau} \sqrt{\big\langle\vec{\gamma}_\Delta^n, \mathrm{W}_2\vec{\gamma}_\Delta^n\big\rangle} \leqslant \max_{n=1}^{N_\tau} \|\mathrm{W}_2^{\frac{1}{2}}\vec{\gamma}_\Delta^n\|_2 \leqslant \sqrt{\frac{3}{2}}\overline{\alpha}_2(\tau + \overline{\delta}^2 + \overline{\delta}^p/\underline{\tau}).$$

□

Proposition 3.32 (Stability). *Let $\Delta = (\boldsymbol{\tau};\boldsymbol{\xi})$ be a family of discretization parameters, such that any spatial decomposition $\boldsymbol{\xi}$ satisfies* (3.78) *and any temporal decomposition $\boldsymbol{\tau}$ is chosen fine enough, i.e. $1+\lambda\tau_n \neq 0$ for any $n = 1,\dots,N_{\boldsymbol{\tau}}$. For each Δ, assume u_Δ to be a solution of the numerical scheme as described in Section 3.1.2. Furthermore, let $u : [0,T]\times\Omega \to [0,+\infty)$ be a smooth solution of* (3.1) *such that $\mathrm{X} \in C^p([0,T]\times\mathcal{M})$ with $p \geqslant 4$ solves* (3.77)*. Moreover, define the sequence $\mathrm{u}_\Delta = (\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^0_\Delta], \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{y}}^1_\Delta], \dots)$ with $\vec{\mathrm{y}}_\Delta$ defined as in Proposition 3.28. Then*

$$\mathcal{W}_2(\mathrm{u}_\Delta, u^n_\Delta)^2 \leqslant \left(\mathcal{W}_2(\mathrm{u}^0_\Delta, u^0_\Delta)^2 + t_n \frac{1+\tau}{1+2\tau_\lambda}\mathsf{err}^2\right) e^{t_n \frac{1-2\lambda}{1+2\tau_\lambda}}, \tag{3.97}$$

where err *is the error of consistency defined in* (3.79) *and $\tau_\lambda := \inf_{n\in\mathbb{N}}(\lambda\tau_n)$. Moreover,*

$$\sup_{t\in[0,T]} \mathcal{W}_2(\{\mathrm{u}_\Delta\}_{\boldsymbol{\tau}}, \{u^n_\Delta\}_{\boldsymbol{\tau}}) \leqslant C(\tau + \overline{\delta}^2 + \overline{\delta}^p/\underline{\tau}) \tag{3.98}$$

is satisfied as long as $\mathcal{W}_2(\mathrm{u}^0_\Delta, u^0_\Delta) \leqslant C\overline{\delta}^2$.

Proof. The proof follows the same idea as the one of (3.30). From Proposition 3.9 and Proposition 3.28, we know that

$$\vec{\mathrm{y}}^n_\Delta - \vec{\mathrm{y}}^{n-1}_\Delta + \tau_n \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{\mathrm{y}}^n_\Delta) = \tau_n\vec{\gamma}^n_\Delta \quad \text{and} \quad \vec{\mathrm{x}}^n_\Delta - \vec{\mathrm{x}}^{n-1}_\Delta + \tau_n \nabla_{\boldsymbol{\xi}}\mathbf{E}(\vec{\mathrm{x}}^n_\Delta) = 0.$$

Multiply both equations with $\mathrm{W}_2^{1/2}$ and substract them, then

$$\mathrm{W}_2^{1/2}(\vec{\mathrm{y}}^n_\Delta - \vec{\mathrm{x}}^n_\Delta) + \tau_n \mathrm{W}_2^{-1/2}\big(\partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{y}}^n_\Delta) - \partial_{\vec{\mathrm{x}}}\mathbf{E}(\vec{\mathrm{x}}^n_\Delta)\big) = \mathrm{W}_2^{1/2}(\vec{\mathrm{y}}^{n-1}_\Delta - \vec{\mathrm{x}}^{n-1}_\Delta) + \tau_n \mathrm{W}_2^{1/2}\vec{\gamma}^n_\Delta.$$

As a next step, take the norm on both sides, then the convexity property (3.25) and Young's inequality yield

$$\begin{aligned}(1+2\lambda\tau_n)\left\|\vec{\mathrm{y}}^n_\Delta - \vec{\mathrm{x}}^n_\Delta\right\|^2_{\boldsymbol{\xi}} &\leqslant \left\|\vec{\mathrm{y}}^{n-1}_\Delta - \vec{\mathrm{x}}^{n-1}_\Delta\right\|^2_{\boldsymbol{\xi}} + \tau_n^2\left\|\vec{\gamma}^n_\Delta\right\|^2_{\boldsymbol{\xi}} + 2\tau_n\left\langle \vec{\mathrm{y}}^{n-1}_\Delta - \vec{\mathrm{x}}^{n-1}_\Delta, \vec{\gamma}^n_\Delta\right\rangle_{\boldsymbol{\xi}} \\ &\leqslant (1+\tau_n)\left\|\vec{\mathrm{y}}^{n-1}_\Delta - \vec{\mathrm{x}}^{n-1}_\Delta\right\|^2_{\boldsymbol{\xi}} + \tau_n(1+\tau_n)\left\|\vec{\gamma}^n_\Delta\right\|^2_{\boldsymbol{\xi}}.\end{aligned}$$

Due to the elemental equality $\frac{1+\tau_n}{1+2\lambda\tau_n} = 1 + \frac{\tau_n(1-2\lambda)}{1+2\lambda\tau_n}$, we finally conclude that

$$\begin{aligned}\left\|\vec{\mathrm{x}}^n_\Delta - \vec{\mathrm{y}}^n_\Delta\right\|^2_{\boldsymbol{\xi}} &\leqslant \left(1 + \frac{\tau_n(1-2\lambda)}{1+2\tau_n\lambda}\right)\left\|\vec{\mathrm{x}}^{n-1}_\Delta - \vec{\mathrm{y}}^{n-1}_\Delta\right\|^2_{\boldsymbol{\xi}} + \frac{\tau_n(1+\tau_n)}{1+2\tau_n\lambda}\left\|\vec{\gamma}^n_\Delta\right\|^2_{\boldsymbol{\xi}} \\ &\leqslant \left\|\vec{\mathrm{x}}^0_\Delta - \vec{\mathrm{y}}^0_\Delta\right\|^2_{\boldsymbol{\xi}} + \sum_{k=0}^{n-1}\tau_{k+1}\frac{(1-2\lambda)}{1+2\tau_k\lambda}\left\|\vec{\mathrm{x}}^k_\Delta - \vec{\mathrm{y}}^k_\Delta\right\|^2_{\boldsymbol{\xi}} + \sum_{k=0}^{n-1}\tau_{k+1}\frac{(1+\tau_k)}{1+2\tau_k\lambda}\left\|\vec{\gamma}^{k+1}_\Delta\right\|^2_{\boldsymbol{\xi}},\end{aligned}$$

which proves (3.97) due to the discrete Gronwall Lemma A.3. The statement in (3.98) is a consequence of (3.97) and the order of consistency (3.79). □

This result provides an alternative proof of convergence, since we have already seen in Lemma 3.24 that $\{\mathrm{u}_\Delta\}_{\boldsymbol{\tau}}$ converges towards the smooth solution u of (3.1) with respect to the L^2-Wasserstein distance, at least pointwise in time.

3.7. Numerical results

In all numerical experiments below, we used an equidistant time decomposition $\boldsymbol{\tau}$, i.e. $\tau_n = \tau$ for all $n \in \mathbb{N}$.

3.7.1. Implementation.

3.7.1.a. Choice of the initial condition. The numerical scheme is phrased in Lagrangian coordinates: The discretization $\boldsymbol{\xi} = (\xi_0, \xi_1, \ldots, \xi_K)$ of the reference domain $\mathcal{M}$ is fixed, whereas the corresponding grid points $\vec{\mathrm{x}}^n = (x_1^n, \ldots, x_{K-1}^n) \in \mathfrak{x}_{\boldsymbol{\xi}}$ on the interval Ω evolve in (discrete) time. In the numerical experiments that follow, our choice for the discretization of the initial condition is to use an equidistant grid $\vec{\mathrm{x}}^0$ with K vertices on Ω,

$$x_k^0 = a + k(b-a)/K,$$

and an accordingly adapted mesh $\boldsymbol{\xi}$ on $\mathcal{M}$, with

$$\xi_k = \mathrm{U}^0(x_k^0), \quad \text{where} \quad \mathrm{U}^0(x) = \int_a^x u^0(y)\,\mathrm{d}y \quad \text{for all } x \in \Omega$$

is the initial datum's distribution function. This discretization has the property that

$$\int_{x_{k-1}^0}^{x_k^0} u^0(x)\,\mathrm{d}x = \int_{x_{k-1}^0}^{x_k^0} u_\Delta^0(x)\,\mathrm{d}x \quad \text{for all } k = 1, \ldots, K.$$

3.7.1.b. Time stepping. Each time step in the numerical scheme consists of solving the system of Euler-Lagrange equations (3.11). In practice, this is done with a damped Newton method, which guarantees that the constraint $\vec{\mathrm{x}}_\Delta^n \in \mathfrak{x}_{\boldsymbol{\xi}}$ — i.e. that $a < x_1^n < \cdots < x_{K-1}^n < b$ — is propagated from the $n-1$st to the nth iterate. Remember that we are looking for the unique root in $\mathfrak{x}_{\boldsymbol{\xi}}$ of the functional

$$\partial_{\vec{\mathrm{x}}} \mathbf{E}_\Delta(\tau, \vec{\mathrm{x}}, \vec{\mathrm{x}}_\Delta^{n-1}) = \frac{1}{\tau} \mathrm{W}_2(\vec{\mathrm{x}} - \vec{\mathrm{x}}_\Delta^{n-1}) + \partial_{\vec{\mathrm{x}}} \mathbf{E}(\vec{\mathrm{x}}),$$

which defines the nth time iterate $\vec{\mathrm{x}}_\Delta^n$. For the evaluation of $\partial_{\vec{\mathrm{x}}} \mathbf{E}_\Delta(\tau, \vec{\mathrm{x}}, \vec{\mathrm{x}}_\Delta^{n-1})$ and its Jacobian

$$\partial_{\vec{\mathrm{x}}}^2 \mathbf{E}_\Delta(\tau, \vec{\mathrm{x}}, \vec{\mathrm{x}}_\Delta^{n-1}) = \frac{1}{\tau} \mathrm{W}_2 + \partial_{\vec{\mathrm{x}}}^2 \mathbf{E}(\vec{\mathrm{x}}),$$

an explicit expression for the integrals

$$\partial_{x_k} \left(\int_{\mathcal{M}} V \circ \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\,\mathrm{d}\xi \right) = \int_{\mathcal{M}} V_x \circ \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] \theta_k(\xi)\,\mathrm{d}\xi$$

is needed. Denoting by $\mathfrak{V}$ an anti-derivative of V, one finds after integration by parts that

$$\begin{aligned} \int_{\xi_{k-1}}^{\xi_k} V_x \circ \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] \theta_k(\xi)\,\mathrm{d}\xi &= \frac{\delta_{k-\frac{1}{2}}}{x_k - x_{k-1}} \int_{x_{k-1}}^{x_k} V_x(x) \frac{x - x_{k-1}}{x_k - x_{k-1}}\,\mathrm{d}x \\ &= \frac{\delta_{k-\frac{1}{2}}}{x_k - x_{k-1}} \left(V(x_k) - \frac{\mathfrak{V}(x_k) - \mathfrak{V}(x_{k-1})}{x_k - x_{k-1}} \right), \end{aligned}$$

and an analogue expression for the integral from ξ_k to ξ_{k+1}. In combination, we obtain

$$\partial_{x_k}\int_{\mathcal{M}} V\circ\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)\,\mathrm{d}\xi = \frac{-\delta_{k-\frac12}}{(x_k-x_{k-1})^2}\big(\mathfrak{V}(x_k)-\mathfrak{V}(x_{k-1})\big)+\frac{\delta_{k+\frac12}}{(x_{k+1}-x_k)^2}\big(\mathfrak{V}(x_{k+1})-\mathfrak{V}(x_k)\big) + V(x_k)\left(\frac{\delta_{k-\frac12}}{x_k-x_{k-1}}-\frac{\delta_{k+\frac12}}{x_{k+1}-x_k}\right),$$

and furthermore for any $k,m\in\{1,\dots,K-1\}$,

$$\partial_{x_m}\partial_{x_k}\left(\int_{\mathcal{M}} V\circ\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\,\mathrm{d}\xi\right) = \begin{cases} \frac{2\delta_{k-\frac12}}{(x_k-x_{k-1})^3}\big(\mathfrak{V}(x_k)-\mathfrak{V}(x_{k-1})\big)+\frac{2\delta_{k+\frac12}}{(x_{k+1}-x_k)^3}\big(\mathfrak{V}(x_{k+1})-\mathfrak{V}(x_k)\big) \\ -2V(x_k)\left(\frac{\delta_{k-\frac12}}{(x_k-x_{k-1})^2}+\frac{\delta_{k+\frac12}}{(x_{k+1}-x_k)^2}\right)-V_x\left(\frac{\delta_{k-\frac12}}{(x_k-x_{k-1})^2}-\frac{\delta_{k+\frac12}}{(x_{k+1}-x_k)^2}\right), & m=k \\ -\frac{2\delta_{k-\frac12}}{(x_k-x_{k-1})^3}\big(\mathfrak{V}(x_k)-\mathfrak{V}(x_{k-1})\big)+\frac{\delta_{k-\frac12}}{(x_k-x_{k-1})^2}\left(V(x_k)+V(x_{k-1})\right), & m=k-1 \\ 0, & \text{otherwise.}\end{cases}$$

This enables an explicit representation for the Hessian $\partial^2_{\vec{\mathrm{x}}}\mathbf{E}_\Delta(\tau,\vec{\mathrm{x}},\vec{\mathrm{x}}^{n-1}_\Delta)$, using (3.24).

3.7.2. Numerical experiments. The following numerical experiments are performed for the porous medium equation with quadratic nonlinearity,

$$\partial_t u = \partial_{xx}u^2+\partial_x(V_x u),$$

on the interval $\Omega=(a,b)=(-1,1)$. For the potential V, we choose $V(x)=-\frac{1}{\pi}\cos(\pi x)$, and as initial datum, we take the following function of unit mass $M=1$:

$$u^0(x)=C\big(-\cos(2\pi x)+1.5\big)\big((x+0.5)^4+1\big)\quad\text{with}\quad C=\frac{240-280\pi^2+423\pi^4}{80\pi^4}. \tag{3.99}$$

3.7.2.a. Reference Solution. Our numerical reference resolution is calculated with $K=5000$ spatial grid points and a time step size $\tau=10^{-2}$. Figure 3.1/left shows snapshots of the reference solution's spatial density after the first couple of time steps. One observes the typical behaviour for nonlinear drift diffusion equations: On a very short time scale, diffusion reduces the extrema of the initial mass distribution; subsequently, the drift dominates and transports the mass towards the equilibrium (dotted line) on a longer time scale. Figure 3.1/right displays the corresponding particle trajectories in the Lagrangian picture, i.e. how the points x_k^n move with (discrete) time n for fixed k.

3.7.2.b. Fixed τ. In a first series of experiments, we fix the time step $\tau=10^{-2}$ and vary the number of spatial grid points K. In Figure 3.2/left, the corresponding L^1-distances to the reference solution u_{ref} obtained in 3.7.2.a above are shown as a function of time. Figure 3.2/right shows the L^1-errors at $T=0.2$. The observed convergence rate is of order K^{-2}, which corresponds to the analytically observed rate from Section 3.6.

3.7.2.c. Fixed K. Next, we study the decay of the L^1-error under refinement of the temporal discretization for fixed $K=400$. In Figure 3.3/left, the error is plotted at the fixed terminal

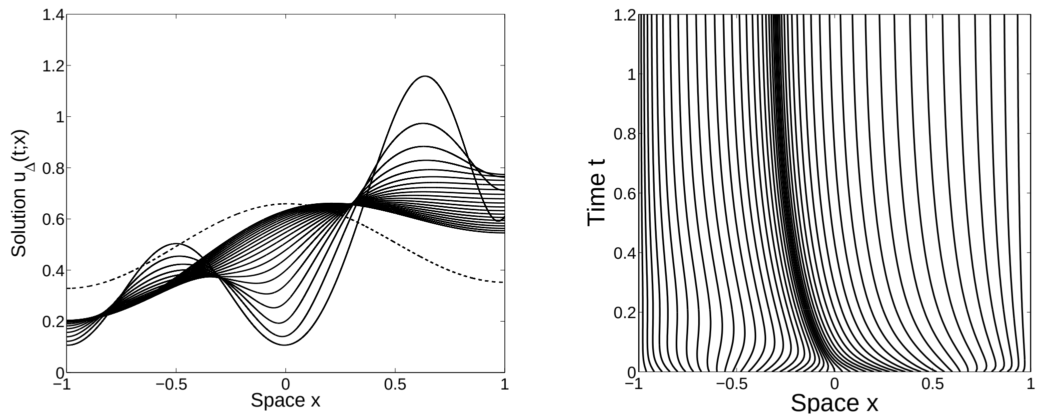


FIGURE 3.1. Left: evolution of the (reference) solution u_Δ with initial condition (3.99) at times $t = 0, \tau, \dots, 20\tau = 0.2$, with time step size $\tau = 10^{-2}$ and $K = 5000$ grid points. The dotted line shows the stationary solution. Right: associated particle trajectories.

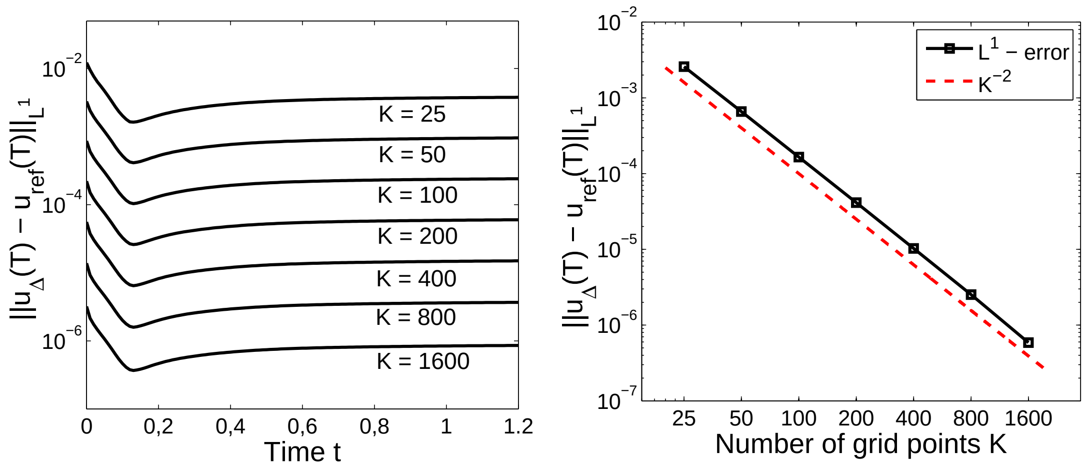
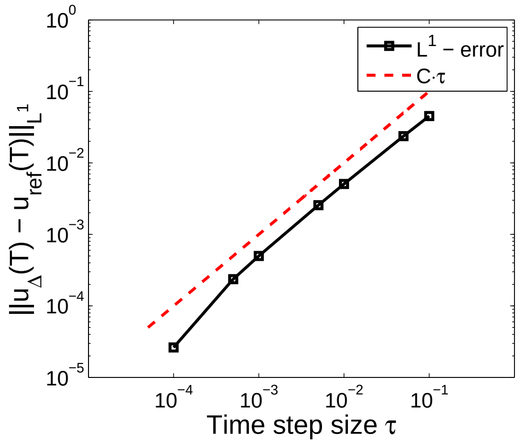


FIGURE 3.2. Numerical error analysis with fixed time step $\tau = 10^{-2}$, using $K = 25, 50, 100, 200, 400, 800, 1600$ grid points. Left: evolution of the L^1-error $\| \{u_\Delta\}_{\boldsymbol{\tau}} (t) - u_{\text{ref}}(t)\|_{L^1(\Omega)}$. Right: order of convergence at terminal time $T = 0.2$.

time $T = 0.2$ for various choices of τ. The observed order of convergence is τ, which is again in agreement with the consistency result in Section 3.6.

3.7.2.d. Weakly convergent initial datum. In order to illustrate that it sufficies to approximate the original initial condition u^0 by its discretizations u^0_Δ just *weakly* in $L^1(\Omega)$, we use perturbed discrete initial data $u^0_{\Delta,\varepsilon}$ that are biased by high-frequency oscillations of fixed amplitude 0.1, as indicated in Figure 3.3/right. As expected, the perturbation already becomes almost invisible after the first time step, and the discrete solution $u_{\Delta,\varepsilon}$ is indistinguishable from the one computed with unperturbed initial conditions u^0_Δ.



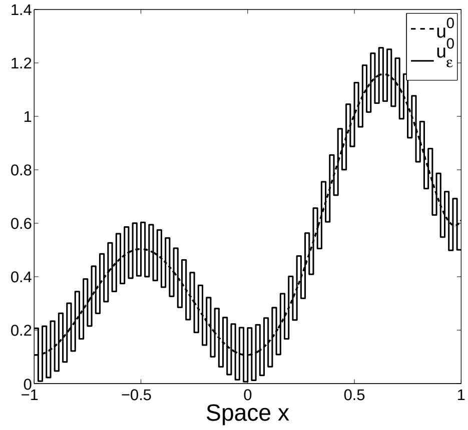


FIGURE 3.3. Left: numerical error analysis with fixed $K = 400$. We analyze the L^1-error $\| \{u_\Delta\}_{\boldsymbol{\tau}} (T) - u_{\text{ref}}(T)\|_{L^1(\Omega)}$ at terminal time $T = 0.2$ using $\tau = 10^{-4}, 5\cdot 10^{-4}, 10^{-3}, 5\cdot 10^{-3}, 10^{-2}, 5\cdot 10^{-2}, 10^{-1}$. Right: initial condition $u^0_{\Delta,\varepsilon}$ with high frequency perturbation.

3.7.2.e. A discontinuous initial datum. For the last two series of experiments, we change the initial condition u^0. This first series is carried out with the discontinuous inital datum

$$u^0(x) = \begin{cases} 0.1, & \text{if } |x| > 0.75 \text{ or } |x| < 0.25, \\ 0.9, & \text{otherwise.} \end{cases} \tag{3.100}$$

As in experiment 3.7.2.b we fix a time step size that is $\tau = 5 \cdot 10^{-3}$ and vary the number of grid points K. Figure 3.4/right displays the observed L^1-error at final time $T = 0.2$. In contrast to experiment 3.7.2.b, the approximation error is zero initially, since the step function u^0 can be discretized exactly. However, the error jumps to a positive value in the first time step and shows a very similar qualitative behaviour to that in experiment 3.7.2.b. Although the observed error at final time $T = 0.2$ is slightly larger than the one of experiment 3.7.2.b, the order of convergence is again K^{-2}.

3.7.2.f. A merely nonnegative initial datum. For this last series of experiment, we consider the initial condition

$$u^0(x) = \big(-\cos(2\pi x) + 1.5\big)\big((x+0.5)^4 + 1\big) \times \begin{cases} -(x-0.5)(x+0.5) & \text{for } |x| \leqslant 0.5 \\ 0 & \text{for } |x| > 0.5, \end{cases} \tag{3.101}$$

which vanishes outside of the subinterval $[-0.5, 0.5] \subseteq \Omega$. The numerical scheme is not directly applicable to u^0, but to any of its strictly positive approximations $u^0 + \varepsilon$, see Figure 3.5/left. As already mentioned in Section 3.1.3 one can expect the sequence of solutions with initial densities $u^0 + \varepsilon$ to converge towards the solution of (3.1) with the nonpositive density u^0 as $\varepsilon \to 0$ and $\Delta \to 0$. The qualitative numerical results at $T = 0.6$ for various choices of $\varepsilon > 0$ are given in Figure 3.5/right.

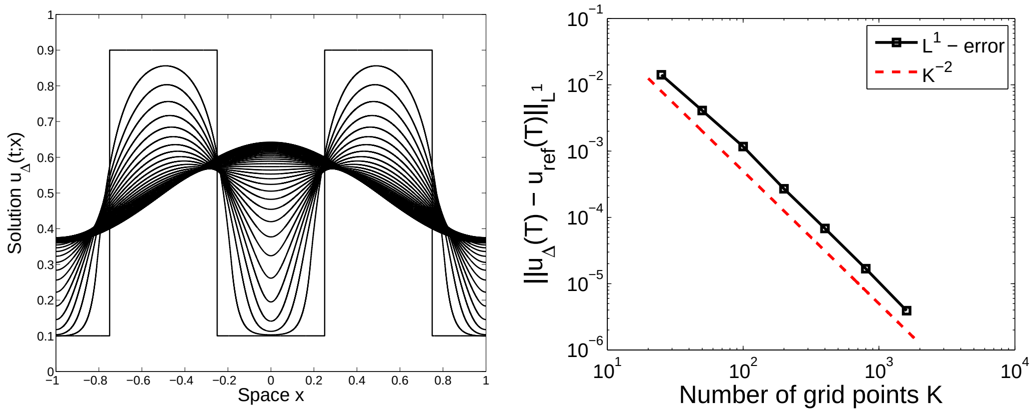


FIGURE 3.4. Left: evolution of the solution u_Δ with initial condition (3.100) at times $t = 0, \tau, \ldots, 40\tau = 0.2$, with time step $\tau = 5 \cdot 10^{-3}$ and $K = 5000$ grid points. Right: numerical error analysis for discrete solutions with the discontinuous initial datum from (3.100), using a fixed time step $5 \cdot \tau = 10^{-3}$ and varying $K = 25, 50, 100, 200, 400, 800, 1600$.

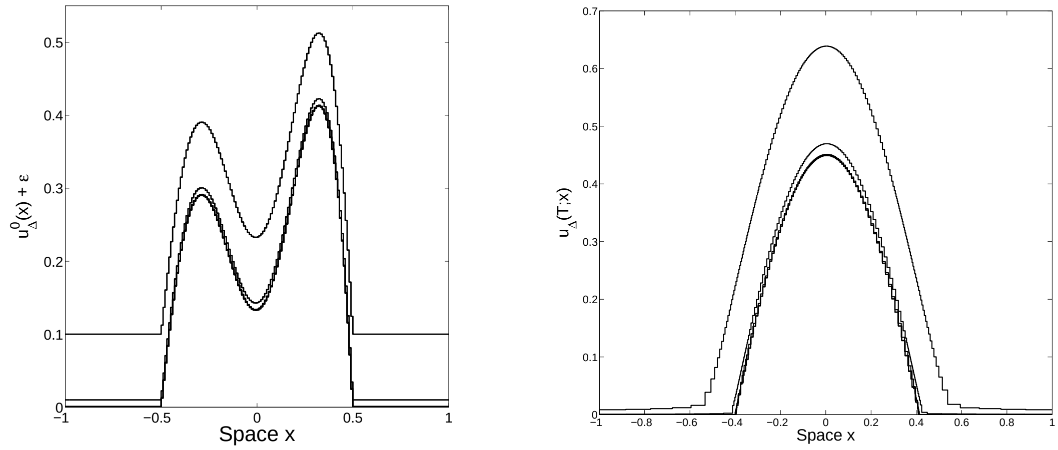


FIGURE 3.5. The merely nonnegative initial condition u^0 from (3.101) is approximated by strictly positive data $u^0 + \varepsilon$. Left: discrete initial profiles for $\varepsilon = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}, 10^{-5}$. Right: qualitative behaviour of corresponding discrete solutions at $T = 0.6$, using $\tau = 10^{-3}$, $K = 200$.

CHAPTER 4

A family of fourth order equations

The content of this chapter is based on a submitted paper, see [**Osb14**] for a preprint. The proof of Theorem 4.4 is based on a submitted paper that is joint work with my PhD-supervisor Daniel Matthes [**MO14b**]. This paper is currently in revision.

4.1. Introduction

In this chapter, we are going to study a fully discrete Lagrangian scheme for a family of nonlinear fourth order equations of the type

$$\partial_t u + \partial_x\big(u\partial_x(u^{\alpha-1}\partial_{xx}u^\alpha)\big) + \lambda\partial_x(xu) = 0 \quad \text{for } t > 0 \text{ and } x \in \Omega, \tag{4.1}$$

$$u = u^0 \geqslant 0 \quad \text{at } t = 0. \tag{4.2}$$

We are going to study both cases for the spatial domain Ω as discussed in Chapter 2, hence $\Omega = (a, b)$ is bounded or $\Omega = \mathbb{R}$. In case of a bounded domain $\Omega = (a, b)$ we consider in addition no-flux boundary conditions which are

$$\partial_x u = 0, \quad u\, u\partial_x(u^{\alpha-1}\partial_{xx}u^\alpha) + \lambda xu = 0 \quad \text{for } t > 0 \text{ and } x \in \partial\Omega. \tag{4.3}$$

The initial density $u^0 \geqslant 0$ is assumed to be integrable with total mass $M > 0$, and we assume that $M = 1$ for reasons of simplification. Depending on the spatial domain, we consider the following additional requirements for the initial density:

(1) If Ω is bounded, then we assume u^0 to be strictly positive.
(2) If $\Omega = \mathbb{R}$, then we suppose that u^0 is compactly supported and strictly positive on its support $\operatorname{supp}(u^0)$, which is assumed to be an interval.

In any case, we have that $u^0 \in \mathcal{P}_2^r(\Omega)$ by means of (1.17).

We are especially interested in the long-time behaviour of discrete solutions and their rate of decay towards equilibrium. For the exponent in (4.1), we consider values $\alpha \in [\frac{1}{2}, 1]$, and assume $\lambda \geqslant 0$. The most famous examples for parabolic equations described by (4.1) are the so-called *DLSS equation* for $\alpha = \frac{1}{2}$, (first analyzed by Derrida, Lebowitz, Speer and Spohn in [**DLSS91a**,**DLSS91b**] with application in semiconductor physics) and the *thin film equation* for $\alpha = 1$ — indeed, for other values of α, references are very rare in the literature, except the paper [**MMS09**] by Matthes, McCann and Savaré.

Due to the physically motivated origin of equation (4.1) (especially for $\alpha = \frac{1}{2}$ and $\alpha = 1$), it is not surprising that solutions to (4.1) carry many structural properties as for instance nonnegativity, the conservation of mass and the dissipation of (several) entropy functionals. In Section 4.2.1, we are going to list more properties of solutions to (4.1). For the numerical approximation of solutions to (4.1), it is hence natural to ask for structure-preserving discretizations that inherit at least some of those properties. A minimum criteria for such a scheme should be the preservation of nonnegativity, which can already be a difficult task, if standard discretizations are used. So far, many (semi-)discretizations for certain equations described by (4.1) have been proposed in the literature, and most of them keep some basic structural properties of the equation's underlying nature. Take for example [**BEJ14, CJT03, JP01, JV07**], where positivity appears as a conclusion of Lyaponov functionals — a logarithmic/power entropy [**BEJ14, CJT03, JP01**] or some variant of a (perturbed) information functional. But there is only a little number of examples, where structural properties of equation (4.1) are adopted from the discretization by construction. A very first try in this direction was a fully Lagrangian approach for the DLSS equation by Düring, Matthes and Pina [**DMM10**], which is based on its L^2-Wasserstein gradient flow representation and thus preserves nonnegativity and dissipation of the Fisher information.

4.1.1. Gradient flow structure. As in the case of second order equations described in Chapter 3, there is a natural connection between the continuity equation (2.7) and the equations in (4.1) that is given by the α-dependent family of *perturbed information functionals*

$$\mathcal{F}_{\alpha,\lambda}(u) = \frac{1}{2\alpha}\int_\Omega \big(\partial_x u^\alpha\big)^2\,\mathrm{d}x + \frac{\lambda}{2}\int_\Omega |x|^2 u(x)\,\mathrm{d}x. \tag{4.4}$$

So if we consider the functional $\mathcal{E} = \mathcal{F}_{\alpha,\lambda}$ in (2.6), hence $h(x,r,p) = \frac{\alpha}{2}r^{2(\alpha-1)}|p|^2 + \frac{\lambda}{2}|x|^2 r$, then the induced velocity field for the continuity equation in (2.7) is given by

$$\mathbf{v}(u) = \partial_x(u^{\alpha-1}\partial_{xx}u^\alpha) + \lambda x \tag{4.5}$$

and the continuity equation equals (4.1). Therefore, solutions to (4.1) can be interpreted as L^2-Wasserstein gradient flows in the potential landscape of the entropies $\mathcal{F}_{\alpha,\lambda}$, see [**DM08**] by Denzler and McCann. This issue was further considered by Gianazza, Savaré and Toscani [**GST09**] in the case $\alpha = \frac{1}{2}$, and by Giacomelli and Otto [**GO01, Ott98**] for $\alpha = 1$.

Similar to the second order equations in Chapter 3, the L^2-Wasserstein gradient flows along $\mathcal{F}_{\alpha,\lambda}$ further allow an interpretation as L^2-gradient flows along the functionals

$$\mathcal{F}_{\alpha,\lambda}(u\circ \mathrm{X}) = \frac{1}{2\alpha}\int_{\mathcal{M}} \left[\partial_\xi\left(\frac{1}{\partial_\xi \mathrm{X}}\right)^\alpha\right]^2 \frac{1}{\partial_\xi \mathrm{X}}\,\mathrm{d}\xi + \frac{\lambda}{2}\int_{\mathcal{M}} \mathrm{X}^2\,\mathrm{d}\xi,$$

where X is the pseudo-inverse distribution function of u. Those L^2-gradient flows have the form

$$\partial_t \mathrm{X} = \frac{2\alpha}{2\alpha+1}\partial_\xi\big(\mathrm{Z}^{\alpha+\frac{3}{2}}\partial_{\xi\xi}\mathrm{Z}^{\alpha+\frac{1}{2}}\big) + \lambda \mathrm{X}, \quad \text{where} \quad \mathrm{Z}(t,\xi) := \frac{1}{\partial_\xi \mathrm{X}(t,\xi)} = u\big(t,\mathrm{X}(t,\xi)\big). \tag{4.6}$$

This identity is formally verified using that $\partial_t \mathrm{X} = \mathbf{v}(u)\circ \mathrm{X}$, see (2.8) from Section 2.1.1: The explicit representation of $\mathbf{v}(u)$ from (4.5) yields

$$\begin{aligned}\partial_t \mathrm{X} = \mathbf{v}(u)\circ \mathrm{X} &= \partial_x(u^{\alpha-1}\partial_{xx}u^\alpha)\circ \mathrm{X} + \lambda \mathrm{X} = \partial_\xi\big((u\circ \mathrm{X})^{\alpha-1}(\partial_{xx}u^\alpha)\circ \mathrm{X}\big)\mathrm{Z} + \lambda \mathrm{X}\\ &= \partial_\xi\left(\mathrm{Z}^\alpha\partial_\xi\big(\partial_\xi(\mathrm{Z}^\alpha)\mathrm{Z}\big)\right)\mathrm{Z} + \lambda \mathrm{X}.\end{aligned}$$

From this point on, elementary calculations show that this equation is equivalent to (4.6).

4.1.2. Description of the numerical scheme. The following family of numerical schemes for the highly nonlinear equations (4.1) is based on a finite element discretization of (4.6) with local linear spline interpolants, so it is kind of the simplest discretization procedure possible. Note in addition that the schemes' formulations are almost the same for both situations, bounded domain or $\Omega = \mathbb{R}$, and just differ by means of (2.19). However, we are going to show later in Section 4.2.2.b that our numerical approximation is equivalent to a natural restriction of a L^2-Wasserstein gradient flow in the potential landscape of the discretized version of the perturbed information functional $\mathcal{F}_{\alpha,\lambda}$.

Let us fix a spatio-temporal discretization parameter $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ in the following way: Given $\tau > 0$, introduce varying time step sizes $\boldsymbol{\tau} = (\tau_1, \tau_2, \ldots)$ with $\tau_n \in (0, \tau]$, and define a time decomposition $(t_n)_{n=0}^{\infty}$ of $[0, +\infty)$ as in (2.10). As spatial discretization we fix $K \in \mathbb{N}$ and introduce an equidistant spatial decomposition of the mass domain $\mathcal{M}$, so one gets $\boldsymbol{\xi} = (\xi_0, \ldots, \xi_K)$ with $\xi_k = k\delta$ for any $k = 0, \ldots, K$ and the k-independent mesh size $\delta = MK^{-1}$. We further fix the discrete metric $\mathrm{d}_{\boldsymbol{\xi}}$ on $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ that is induced by the matrix $\mathrm{W} = \delta\mathbb{I} \in \mathbb{R}^{\aleph\times\aleph}$, hence we especially have

$$\langle \vec{\mathrm{v}}, \vec{\mathrm{w}} \rangle_{\boldsymbol{\xi}} = \delta \langle \vec{\mathrm{v}}, \vec{\mathrm{w}} \rangle \quad \text{and} \quad \|\vec{\mathrm{v}}\|_{\boldsymbol{\xi}} = \sqrt{\delta \langle \vec{\mathrm{v}}, \vec{\mathrm{v}} \rangle},$$

for any $\vec{\mathrm{v}}, \vec{\mathrm{w}} \in \mathbb{R}^{\aleph}$. Further introduce the central first and second order finite difference operators $\mathrm{D}^1_{\boldsymbol{\xi}}$ and $\mathrm{D}^2_{\boldsymbol{\xi}}$ that associate difference quotients depending on an extended "doubled-grid" in the following way: For each vector of the form $\vec{\mathrm{y}} = (y_{-\frac{1}{2}}, y_0, y_{\frac{1}{2}}, y_1, \ldots, y_{K-1}, y_{K-\frac{1}{2}}, y_K, y_{K+\frac{1}{2}})$ we have

$$\begin{aligned} [\mathrm{D}^1_{\boldsymbol{\xi}}\, \vec{\mathrm{y}}]_k &= (y_{k+\frac{1}{2}} - y_{k-\frac{1}{2}})/\delta \quad \text{for} \quad k = 0, \ldots, K \quad \text{and} \\ [\mathrm{D}^2_{\boldsymbol{\xi}}\, \vec{\mathrm{y}}]_\kappa &= (y_{\kappa+1} - 2y_\kappa + y_{\kappa-1})/\delta^2 \quad \text{for} \quad \kappa = \frac{1}{2}, \ldots, K - \frac{1}{2}. \end{aligned} \tag{4.7}$$

Our numerical scheme is now defined as a standard discretization of equation (4.6):

Numerical scheme. *Fix a discretization parameter* $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$. *Then for any* $(\alpha, \lambda) \in [\frac{1}{2}, 1] \times [0, +\infty)$ *a numerical scheme for* (4.1) *is recursively given as follows:*

(1) *For* $n = 0$, *fix an initial Lagrangian vector* $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}} \subseteq \Omega^{\aleph}$. *If* Ω *is bounded, then we fix* $x_0 = a$ *and* $x_K = b$ *in accordance with* (2.15).

(2) *For* $n \geqslant 1$, *recursively define Lagrangian vectors* $\vec{\mathrm{x}}^n_\Delta \in \mathfrak{x}_{\boldsymbol{\xi}}$ *as solutions to the system with a number of* $\aleph$ *equations given by*

$$\frac{x_k^n - x_k^{n-1}}{\tau_n} = \frac{2\alpha}{(2\alpha+1)}\, \mathrm{D}^1_{\boldsymbol{\xi}} \Big[(z^n)^{\alpha+\frac{3}{2}} [\mathrm{D}^2_{\boldsymbol{\xi}} (\vec{\mathrm{z}}^n)^{\alpha+\frac{1}{2}}] \Big]_k + \lambda x_k, \tag{4.8}$$

where $k \in \mathbb{I}^{\aleph}_K$. *The values* $z^n_{\ell-\frac{1}{2}} \geqslant 0$ *are defined as in* (2.18) *with convention* (2.19). *We later show in Proposition 4.6 that the solvability of the system* (4.8) *is guaranteed.*

From now on we denote a solution to the above scheme by $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}^0_\Delta, \vec{\mathrm{x}}^1_\Delta, \ldots)$ and its corresponding sequence of densities by $u_\Delta = (u^0_\Delta, u^1_\Delta, \ldots)$, where the components $\vec{\mathrm{x}}^n_\Delta$ and u^n_Δ correlate through the map $\mathbf{u}_{\boldsymbol{\xi}} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$.

We will see later in Section 4.2.1, that the information functional $\mathcal{F}_{\alpha,\lambda}$ can be derived using the dissipation of the entropy

$$\mathcal{H}_{\alpha,\lambda}(u) = \int_\Omega \varphi_\alpha(u)\,\mathrm{d}x + \frac{\Lambda_{\alpha,\lambda}}{2}\int_\Omega |x|^2 u(x)\,\mathrm{d}x, \quad \text{where} \quad \varphi_\alpha(s) := \begin{cases} \Theta_\alpha \frac{s^{\alpha+1/2}}{\alpha-1/2}, & \alpha\in(\frac12,1] \\ \Theta_{1/2} s\ln(s), & \alpha=\frac12 \end{cases},$$

with constants $\Theta_\alpha := \sqrt{2\alpha}/(2\alpha+1)$ and $\Lambda_{\alpha,\lambda} := \sqrt{\lambda/(2\alpha+1)}$. As replacements for the entropy $\mathcal{H}_{\alpha,\lambda}$ and the perturbed information functional $\mathcal{F}_{\alpha,\lambda}$, we introduce

$$\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}) := \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} f_\alpha(z_\kappa) + \frac{\Lambda_{\alpha,\lambda}}{2}\delta\sum_{k\in\mathbb{I}_K}|x_k|^2, \quad \text{with} \quad f_\alpha(s) := \begin{cases} \Theta_\alpha \frac{s^{\alpha-1/2}}{\alpha-1/2}, & \alpha\in(\frac12,1] \\ \Theta_{1/2}\ln(s), & \alpha=\frac12 \end{cases} \tag{4.9}$$

and

$$\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}) := \Theta_\alpha^2\delta\sum_{k\in\mathbb{I}_K}\left(\frac{z_{k+\frac12}^{\alpha+\frac12} - z_{k-\frac12}^{\alpha+\frac12}}{\delta}\right)^2 + \frac{\lambda}{2}\delta\sum_{k\in\mathbb{I}_K}|x_k|^2. \tag{4.10}$$

Remember that $x_0 = a$ and $x_K = b$ are fixed if Ω is bounded.

4.1.3. Familiar schemes. As already mentioned before in Chapter 3, the idea to derive numerical schemes respecting the Wasserstein gradient flow structure of second order equations is not new in the literature.

This circumstance changes dramatically if one is interested in the numerical treatment of fourth order equations as in (4.1). In fact, we are just aware of a little number of schemes concerning the limiting cases $\alpha = \frac12$ and $\alpha = 1$. Especially, Lagrangian schemes for fourth order equations are relatively rare.

For the quantum drift diffusion equation, $\alpha = \frac12$, we mention the paper [**DMM10**] by Düring, Matthes and Pina. The fully discrete scheme described therein is — as far as we know — the only one available in the literature that inherits the equations gradient flow structure. The authors translate (4.1) for $\alpha = \frac12$ into its Lagrangian formulation and generate a proper solution of the minimizing movement scheme on a submanifold of the set of density functions. Hence the scheme produces a discrete mass-preserving solution at any time iteration, which dissipates the Fisher information and adapts the naturally given L^2-Wasserstein gradient flow structure from the continuous into the discrete setting. Another work that contains at least some parallels to the above approach is [**PU99**], where a scheme for the bipolar (stationary) quantum drift-diffusion model is presented, which is based on a quasi-gradient method.

In case of $\alpha = 1$, alternative Lagrangian discretizations for (6.1) or related thin film type equations have been proposed in [**CN10**, **GT06b**], but only dissipation of the energy has been studied there, and no rigorous convergence analysis has been carried out. As far as we know, there is only a little number of publications that make use of the dissipation of more than one entropy/energy functional to gain compactness results. Take for instance [**Grü03**,**GR00**,**ZB00**], where the authors even prove convergence in higher dimensions, but only on regions where the obtained limit curve is strictly positive.

4.1.4. Main results. In this section, fix a discretization $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ with $\tau, \delta > 0$.

All analytical results that will follow, arise from the very fundamental observation that solutions to the scheme defined in Section 4.1.2 can be successively derived as minimizers of the *discrete minimizing movement scheme*

$$\vec{\mathrm{x}} \mapsto \frac{1}{2\tau_n} \left\| \vec{\mathrm{x}} - \vec{\mathrm{x}}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}), \tag{4.11}$$

see Proposition 4.6. An immediate consequence of the minimization procedure is that solutions $\vec{\mathrm{x}}_\Delta^n$ dissipate the functional $\mathbf{F}_{\alpha,\lambda}$.

4.1.4.a. Results for $\Omega = \mathbb{R}$. Concerning the long-time behaviour of solutions $\vec{\mathrm{x}}_\Delta$, remarkable similarities to the continuous case appear, if $\Omega = \mathbb{R}$. Assuming first the case $\lambda > 0$, it turns out that the unique minimizer $\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min}$ of $\mathbf{H}_{\alpha,\lambda}$ is even a minimizer of the discrete information functional $\mathbf{F}_{\alpha,\lambda}$, and the corresponding set of density functions $u_{\boldsymbol{\xi}}^{\min} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min}]$ converges for $\delta \to 0$ towards a Barenblatt-profile $\mathrm{b}_{\alpha,\lambda}$ or Gaussian $\mathrm{b}_{1/2,\lambda}$, respectively, that is defined by

$$\mathrm{b}_{\alpha,\lambda} = \left(\mathsf{a} - \mathsf{b}|x|^2\right)_+^{1/(\alpha-1/2)}, \quad \mathsf{b} = \frac{\alpha - 1/2}{\sqrt{2\alpha}} \Lambda_{\alpha,\lambda} \quad \text{for } \alpha > 1/2 \text{ and} \tag{4.12}$$

$$\mathrm{b}_{1/2,\lambda} = \mathsf{a} e^{-\Lambda_{1/2,\lambda}|x|^2} \quad \text{for } \alpha = 1/2, \tag{4.13}$$

where $\mathsf{a} \in \mathbb{R}$ is chosen to conserve unit mass. Beyond this, solutions $\vec{\mathrm{x}}_\Delta^n$ satisfying (4.8) converge as $n \to \infty$ towards a minimizer $\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min}$ of $\mathbf{F}_{\alpha,\lambda}$ with an exponential decay rate which is "asymptotically equal" to the one obtained in the continuous case. The above results are merged in the following theorems:

Theorem 4.1. *For $\lambda > 0$, any sequence of vectors $\vec{\mathrm{x}}_\Delta$ satisfying* (4.11) *dissipates the entropies $\mathbf{H}_{\alpha,\lambda}$ and $\mathbf{F}_{\alpha,\lambda}$ at least exponentially, i.e.*

$$\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n) - \mathbf{H}_{\alpha,\lambda}^{\min} \leqslant \left(\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{H}_{\alpha,\lambda}^{\min}\right) e^{-\frac{2\lambda}{1+\lambda\tau} t_n}, \quad \textit{and} \tag{4.14}$$

$$\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n) - \mathbf{F}_{\alpha,\lambda}^{\min} \leqslant \left(\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{F}_{\alpha,\lambda}^{\min}\right) e^{-\frac{2\lambda}{1+\lambda\tau} t_n}, \tag{4.15}$$

with $\mathbf{H}_{\alpha,\lambda}^{\min} = \mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})$ and $\mathbf{F}_{\alpha,\lambda}^{\min} = \mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})$. The associated sequence of densities u_Δ furthermore satisfies

$$\|u_\Delta^n - u_{\boldsymbol{\xi}}^{\min}\|_{L^1(\Omega)}^2 \leqslant c_{\alpha,\lambda} \left(\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{H}_{\alpha,\lambda}^{\min}\right) e^{-\frac{2\lambda}{1+\lambda\tau} t_n} \tag{4.16}$$

for any time step $n \in \mathbb{N}$, where $c_{\alpha,\lambda} > 0$ depends only on α, λ.

Theorem 4.2. *Assume $\lambda > 0$. Then the sequence of minimizers $u_{\boldsymbol{\xi}}^{\min}$ satisfies*

$$u_{\boldsymbol{\xi}}^{\min} \longrightarrow \mathrm{b}_{\alpha,\lambda}, \ \textit{strongly in } L^p(\Omega) \textit{ for any } p \geqslant 1 \tag{4.17}$$

as $\delta \to 0$.

Let us now consider the zero-confinement case $\lambda = 0$. In the continuous setting, the long-time behaviour of solutions to (4.1) with $\lambda = 0$ can be studied by a rescaling of solutions to (4.1) with $\lambda > 0$. We are able to translate this method into the discrete case and derive a discrete counterpart of [**MMS09**, Corollary 5.5], which describes the intermediate asymptotics of solutions that approach self-similar Barenblatt profiles as $t \to \infty$.

Theorem 4.3. *Assume $\lambda = 0$ and take a sequence of vectors $\vec{\mathrm{x}}_\Delta^n$ satisfying* (4.11)*. Then there exists a constant $c_\alpha > 0$ depending only on α, such that*

$$\|u_\Delta^n - \mathrm{b}_{\Delta,\alpha,0}^n\|_{L^1(\Omega)} \leqslant c_\alpha \sqrt{\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{H}_{\alpha,1}^{\min}}(R_\Delta^n)^{-1}, \quad \textit{with} \quad R_\Delta^n := \big(1 + a_\tau(2\alpha+3)t_n\big)^{\frac{1}{b_\tau(2\alpha+3)}},$$

where $\mathrm{b}_{\Delta,\alpha,0}^n$ is a rescaled discrete Barenblatt profile and $a_\tau, b_\tau > 0$, such that $a_\tau, b_\tau \to 1$ for $\tau \to 0$, see Section 4.3.3 for more details.

In view of the results about the long-time behaviour of discrete solutions, we want to point out that the ideas for the proofs of Theorem 4.1 and 4.3 are mainly guided by the techniques developed in [**MMS09**]. The remarkable observation in this chapter is the fascinating structure preservation of our discretization, which allows us to adapt nearly any calculation from the continuous theory for the discrete setting.

4.1.4.b. Results for bounded $\Omega = (a,b)$. In the special case that $\alpha = \frac{1}{2}$ and Ω is bounded, we can even prove convergence of the discrete solution towards a weak solution of (4.1) under very weak requirements on the initial datum.

Theorem 4.4. *Fix $\alpha = \frac{1}{2}$ and let a nonnegative initial condition u^0 with $\mathcal{H}_{1/2,\lambda}(u^0) < \infty$ be given. Choose initial conditions $\vec{\mathrm{x}}_\Delta^0$ such that u_Δ^0 converges to u^0 weakly as $\Delta \to 0$, and*

$$\overline{\mathcal{H}}_{\alpha,\lambda} := \sup_\Delta \mathbf{H}_{1/2,\lambda}(\vec{\mathrm{x}}_\Delta^0) < \infty \quad \textit{and} \quad \lim_{\Delta\to 0}(\tau+\delta)\mathbf{F}_{1/2,\lambda}(\vec{\mathrm{x}}_\Delta^0) = 0.$$

For each Δ, construct a discrete approximation $\vec{\mathrm{x}}_\Delta$ according to the procedure described in (4.8) *above. Then, there are a subsequence with $\Delta \to 0$ and a limit function $u_* \in C((0,+\infty)\times\Omega)$ such that:*

- *$\{u_\Delta\}_\tau$ converges to u_* locally uniformly on $(0,+\infty)\times\Omega$,*
- *$\sqrt{u_*} \in L^2_{\mathrm{loc}}((0,+\infty); H^1(\Omega))$,*
- *u_* satisfies the following weak formulation of* (4.1) *with $\alpha = \frac{1}{2}$:*

$$\int_0^\infty \int_\Omega \partial_t\varphi\, u_* \,\mathrm{d}x\,\mathrm{d}t + \int_\Omega \varphi(0,x)u^0(x)\,\mathrm{d}x + \int_0^\infty N(u_*,\varphi)\,\mathrm{d}t = 0,$$

  with

$$N(u,\varphi) := \frac{1}{2}\int_\Omega \partial_{xxx}\varphi\,\partial_x u + 4\partial_{xx}\varphi\,\big(\partial_x\sqrt{u}\big)^2\,\mathrm{d}x,$$

  for every test function $\varphi \in C^\infty([0,+\infty)\times\Omega)$ that is compactly supported in $[0,+\infty)\times\overline{\Omega}$ and satisfies $\partial_x\varphi(t,a) = \partial_x\varphi(t,b) = 0$ for any $t \in [0,+\infty)$.

The proof of this theorem is long and contains many technical difficulties, this is why we are going to treat it in the subsequent Chapter 5.

4.2. Discretization in space and time

In this section, we try to get a better intuition of the scheme in Section 4.1.2. Foremost, we will derive (4.8) as a discrete system of Euler-Lagrange equations of a variational problem that rises from a L^2-Wasserstein gradient flow restricted to a discrete submanifold $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ of the space of probability measures $\mathcal{P}_2^r(\Omega)$ on Ω. This is why the numerical scheme in Section 4.1.2 satisfies several discrete analogues of the structural properties of equation (4.1), which are going to be discussed in the subsequent section. We will point out that some of the inherited properties are obtained by construction (for instance preservation of mass and dissipation of the entropy), where others are caused by the underlying dicsrete gradient flow structure and the smart choice of the discrete L^2-Wasserstein distance.

If $\Omega = \mathbb{R}$, it is possible to prove that the entropy and the information functional share the same minimizer even in the discrete case, and solutions to the discrete gradient flow converge with an exponential rate to this stationary state. The proof of this observation is more sophisticated, that is why we dedicate an own section (Section 4.3) to the treatment of this special property.

4.2.1. The information functionals as the auto-dissipation of the entropies. The family of fourth order equations (4.1) carries a bunch of remarkable structural properties. The most fundamental one is the conservation of mass, i.e. $t \mapsto \|u(t,\cdot)\|_{L^1(\Omega)}$ is a constant function for $t \in [0,+\infty)$ and attains the value $M = \|u^0\|_{L^1(\Omega)}$. This is a naturally given property, if one interprets solutions to (4.1) as gradient flows in the potential landscape of the perturbed information functional

$$\mathcal{F}_{\alpha,\lambda}(u) = \frac{1}{2\alpha}\int_\Omega \left(\partial_x u^\alpha\right)^2 \mathrm{d}x + \frac{\lambda}{2}\int_\Omega |x|^2 u(x)\,\mathrm{d}x, \tag{4.18}$$

equipped with the L^2-Wasserstein distance $\mathcal{W}_2$. As an immediate consequence, $\mathcal{F}_{\alpha,\lambda}$ is a Lyapunov functional, and one can find infinitely many other (formal) Lyapunov functionals at least for special choices of α — see [**BLS94**, **CCT05**, **JM06**] for $\alpha = \frac{1}{2}$ or [**BG15**, **CT02b**, **GO01**] for $\alpha = 1$. Apart from $\mathcal{F}_{\alpha,\lambda}$, one of the most important of such Lyapunov functionals is given by the $\Lambda_{\alpha,\lambda}$-convex entropy

$$\mathcal{H}_{\alpha,\lambda}(u) = \int_\Omega \varphi_\alpha(u)\,\mathrm{d}x + \frac{\Lambda_{\alpha,\lambda}}{2}\int_\Omega |x|^2 u(x)\,\mathrm{d}x, \quad \varphi_\alpha(s) = \begin{cases} \Theta_\alpha \frac{s^{\alpha+1/2}}{\alpha-1/2}, & \alpha \in (\frac{1}{2},1] \\ \Theta_{1/2} s\ln(s), & \alpha = \frac{1}{2} \end{cases}. \tag{4.19}$$

It turns out that the functionals $\mathcal{F}_{\alpha,\lambda}$ and $\mathcal{H}_{\alpha,\lambda}$ are not just Lyapunov functionals, but share numerous remarkable similiarities. One can indeed see (4.1) as a higher order extension of the second order *porous media/heat equation* [**JKO98**]

$$\partial_s v = \Theta_\alpha \partial_{xx}(v^{\alpha+1/2}) + \Lambda_{\alpha,\lambda}\partial_x(xu), \tag{4.20}$$

which corresponds to the L^2-Wasserstein gradient flow of $\mathcal{H}_{\alpha,\lambda}$. But in view of our numerical approximation, the most interesting connection between the functionals $\mathcal{F}_{\alpha,\lambda}$ and $\mathcal{H}_{\alpha,\lambda}$ is the following: The unperturbed functional $\mathcal{F}_{\alpha,0}$, i.e. $\lambda = \Lambda_{\alpha,\lambda} = 0$, equals the dissipation of $\mathcal{H}_{\alpha,0}$ along its own gradient flow,

$$\mathcal{F}_{\alpha,0}(v(s)) = -\frac{\mathrm{d}}{\mathrm{d}s}\mathcal{H}_{\alpha,0}(v(s)), \tag{4.21}$$

where $\partial_s v = \Theta_\alpha \partial_{xx}(v^{\alpha+1/2})$. In view of the gradient flow structure, this relation makes equation (4.1) the “big brother” of the porous media/heat equation (4.20), and implies many structural consequences, see for instance [**DM08**, **MMS09**]. For instance, the λ-convexity of $\mathbf{H}_{\alpha,\lambda}$ in combination with (4.21) paves the way for useful a priori estimates that lead to compactness results as in [**MMS09**]. Another astonishing common feature that is a direct corollary from (4.21) is the correlation of $\mathcal{F}_{\alpha,\lambda}$ and $\mathcal{H}_{\alpha,\lambda}$ by the so-called *fundamental entropy-information relation* in case that $\Omega = \mathbb{R}$. This relation allows to study the long-time behaviour of solutions to (4.1) in a graceful way, and even to prove that the stationary solutions of (4.1) are identically equal to the ones of (4.20). We are going to discuss the fundamental entropy-information relation and its consequences more deeply in Section 4.3.

4.2.2. Structure-preservation of the numerical schemes.

4.2.2.a. Ansatz space and discrete entropy/information functionals. The entropies $\mathcal{H}_{\alpha,\lambda}$ and $\mathcal{F}_{\alpha,\lambda}$ as defined in (4.19) and (4.4) are functionals on $\mathcal{P}_2^r(\Omega)$. If we first consider the zero-confinement case $\lambda = 0$, one can derive in analogy to Chapter 3 the discretization in (4.9) of $\mathcal{H}_{\alpha,0}$ just by restriction to the finite-dimensional submanifold $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ of $\mathcal{P}_2^r(\Omega)$. Thus using φ_α and f_α from (4.9) and (4.19), a change of variables $x = \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, and the definition (2.18) of the $\vec{\mathrm{x}}$-dependent vectors $\vec{\mathrm{z}}$, one attains

$$\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}) = \mathcal{H}_{\alpha,0}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]) = \int_\Omega \varphi_\alpha\big(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\big)\,\mathrm{d}x = \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} f_\alpha(z_\kappa).$$

Note that this is perfectly compatible with (4.9). Obviously, one cannot derive the discrete information functional $\mathbf{F}_{\alpha,0}$ in the same way, since $\mathcal{F}_{\alpha,0}$ is not defined on $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$. So instead of restriction, we mimic property (4.21) that is

$$\mathbf{F}_{\alpha,0}(\vec{\mathrm{x}}) = \langle \nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}), \nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}})\rangle_{\boldsymbol{\xi}} \tag{4.22}$$

for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. Using furthermore the calculation in (2.29) one gains the explizit representation of the gradient $\partial_{\vec{\mathrm{x}}}\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}})$,

$$\partial_{\vec{\mathrm{x}}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}) = \Theta_\alpha\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^{\alpha+\frac12}\,\frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}, \tag{4.23}$$

remember Example 2.3 and (2.30) within, where we defined $\mathbf{e}_k$ as the kth canonical unit vector with the convention $\mathbf{e}_0 = \mathbf{e}_K = 0$ in case of bounded Ω. In analogy, one can write for the discretized information functional

$$\mathbf{F}_{\alpha,0}(\vec{\mathrm{x}}) = \|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}})\|_{\boldsymbol{\xi}}^2 = \Theta_\alpha^2\delta \sum_{k\in\mathbb{I}_K}\left(\frac{z_{k+\frac12}^{\alpha+\frac12} - z_{k-\frac12}^{\alpha+\frac12}}{\delta}\right)^2.$$

In the case of positive confinement $\lambda > 0$, we note that the drift potential $u \mapsto \int_\Omega |x|^2 u(x)\,\mathrm{d}x$ fulfills an equivalent representation in terms of Lagrangian coordinates that is

$$\mathbf{X} \mapsto \int_{\mathcal{M}} |\mathbf{X}(\xi)|^2\,\mathrm{d}\xi. \tag{4.24}$$

In our setting, the simplest discretization of this functional is hence attained by summing over all values x_k weighted with δ. This yields

$$\mathbf{H}_{\alpha,\lambda}(\vec{x}) = \mathbf{H}_{\alpha,0}(\vec{x}) + \frac{\Lambda_{\alpha,\lambda}}{2}\delta \sum_{k\in\mathbb{I}_K} |x_k|^2 \quad \text{and} \quad \mathbf{F}_{\alpha,\lambda}(\vec{x}) = \mathbf{F}_{\alpha,0}(\vec{x}) + \frac{\lambda}{2}\delta \sum_{k\in\mathbb{I}_K} |x_k|^2$$

as an extension to the case of positive λ, which is nothing else than (4.9) and (4.10).

A first structural property of the above simple discretization is convexity retention from the continuous to the discrete setting:

Lemma 4.5. *The functional $\vec{x} \mapsto \mathbf{H}_{\alpha,\lambda}$ is $\Lambda_{\alpha,\lambda}$-convex, i.e.*

$$\mathbf{H}_{\alpha,\lambda}\big((1-s)\vec{x} + s\vec{y}\big) \leqslant (1-s)\mathbf{H}_{\alpha,\lambda}(\vec{x}) + s\mathbf{H}_{\alpha,\lambda}(\vec{y}) - \frac{\Lambda_{\alpha,\lambda}}{2}(1-s)s\delta \sum_{k\in\mathbb{I}_K} |x_k - y_k|^2, \tag{4.25}$$

for any $\vec{x}, \vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$ and $s \in (0,1)$.

Proof. The statement in (4.25) is essentially a corollary of Lemma 3.8 replacing W_2 by $\delta\mathbb{I}$, and due to the $\Lambda_{\alpha,\lambda}$-convexity of $\vec{x} \mapsto \frac{\Lambda_{\alpha,\lambda}}{2}\delta \sum_{k\in\mathbb{I}_K} |x_k|^2$. □

4.2.2.b. Interpretation of the scheme as a discrete Wasserstein gradient flow. Starting from the discretized information functional $\mathbf{F}_{\alpha,\lambda}$ we approximate the spatially discrete gradient flow equation

$$\partial_t \vec{x} = -\nabla_{\boldsymbol{\xi}} \mathbf{F}_{\alpha,\lambda}(\vec{x}) \tag{4.26}$$

also in time, using minimizing movements. Remember the temporal decomposition of $[0, +\infty)$ given by

$$\{0 = t_0 < t_1 < \ldots < t_n < \ldots\}, \quad \text{where} \quad t_n := \sum_{j=1}^{n} \tau_j,$$

using time step sizes $\boldsymbol{\tau} := (\tau_1, \tau_2, \ldots)$ with $\tau_n \leqslant \tau$ and $\tau > 0$. For each $\vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$, introduce the *Yosida-regularized information functional* $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\cdot,\cdot,\vec{y}) : [0,\tau] \times \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ by

$$\mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \vec{x}, \vec{y}) = \frac{1}{2\sigma}\|\vec{x} - \vec{y}\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,\lambda}(\vec{x}). \tag{4.27}$$

A fully discrete approximation $\vec{x}_\Delta = (\vec{x}_\Delta^0, \vec{x}_\Delta^1, \ldots)$ of (4.26) is now defined inductively from a given initial datum $\vec{x}_\Delta^0$ by choosing each $\vec{x}_\Delta^n$ as a global minimizer of $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\tau_n, \cdot, \vec{x}_\Delta^{n-1})$. Below, we prove that such a minimizer always exists (see Proposition 4.6).

In practice, one wishes to define $\vec{x}_\Delta^n$ as — preferably unique — solution to the Euler-Lagrange equations associated to $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\tau_n, \cdot, \vec{x}_\Delta^{n-1})$, which leads to the implicit Euler time stepping:

$$\frac{\vec{x} - \vec{x}_\Delta^{n-1}}{\tau_n} = -\nabla_{\boldsymbol{\xi}} \mathbf{F}_{\alpha,\lambda}(\vec{x}). \tag{4.28}$$

Using the explicit representation of $\partial_{\vec{x}} \mathbf{F}_{\alpha,\lambda}$, it is immediately seen that (4.28) is indeed the same as (4.8). Equivalence of (4.28) and the minimization problem is guaranteed at least for sufficiently small $\tau > 0$, as the following proposition shows.

Proposition 4.6. *For each discretization* Δ *and every initial condition* $\vec{x}^0 \in \mathfrak{x}_{\boldsymbol{\xi}}$*, the sequence of equations* (4.28) *can be solved inductively. Moreover, if* $\tau > 0$ *is sufficiently small with respect to* δ *and* $\mathbf{F}_{\alpha,\lambda}(\vec{x}^0)$*, then each equation* (4.28) *possesses a unique solution with* $\mathbf{F}_{\alpha,\lambda}(\vec{x}) \leqslant \mathbf{F}_{\alpha,\lambda}(\vec{x}^0)$*, and that solution is the unique global minimizer of* $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\tau_n, \cdot, \vec{x}_{\Delta}^{n-1})$.

The proof of this proposition is a consequence of the following rather technical lemma.

Lemma 4.7. *Fix a spatial discretization* $\boldsymbol{\xi}$ *and a bound* $C > 0$*. Then for every* $\vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$ *with* $\mathbf{F}_{\alpha,\lambda}(\vec{y}) \leqslant C$*, the following are true:*

- *For each* $\sigma > 0$*, the function* $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \cdot, \vec{y})$ *possesses at least one global minimizer* $\vec{x}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$ *which satisfies the system of Euler-Lagrange equations*
$$\frac{\vec{x}^* - \vec{y}}{\sigma} = -\nabla_{\boldsymbol{\xi}} \mathbf{F}_{\alpha,\lambda}(\vec{x}^*).$$
- *There exists a* $\tau_C > 0$ *independent of* $\vec{y}$ *such that for each* $\sigma \in (0, \tau_C)$*, the global minimizer* $\vec{x}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$ *is strict and unique, and it is the only critical point of* $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \cdot, \vec{y})$ *with* $\mathbf{F}_{\alpha,\lambda}(\vec{x}) \leqslant C$.

Proof. Fix $\vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$ with $\mathbf{F}_{\alpha,\lambda}(\vec{y}) \leqslant C$, and define the nonempty (since it contains $\vec{y}$) sublevel set $A_C := \big(\mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \cdot, \vec{y})\big)^{-1}([0, C]) \subset \mathfrak{x}_{\boldsymbol{\xi}}$. If Ω is bounded, it is clear that any $\vec{x} \in A_C$ lies in the interval $[a, b]$. So if $\Omega = \mathbb{R}$, then any $\vec{x} \in A_C$ satisfies $\|\vec{y} - \vec{x}\|_{\boldsymbol{\xi}} \leqslant \sqrt{2\sigma C}$ due to $\mathbf{F}_{\alpha,\lambda} \geqslant 0$. This implies that

$$y_0 - \sqrt{\frac{2\sigma C}{\delta}} \leqslant x_0 < x_K \leqslant y_K + \sqrt{\frac{2\sigma C}{\delta}}. \tag{4.29}$$

Hence, there is an interval $[-L, L]$, such that all components of an arbitrary $\vec{x} \in A_C$ lie in $[-L, L]$, independent of the boundedness of Ω.

Let $\vec{z} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{x}]$, and observe that $z_\kappa \geqslant \delta/(2L)$ for each $z \in \mathbb{I}_K^{1/2}$. From here, it follows further that

$$z_\kappa^{\alpha+\frac{1}{2}} - \left(\frac{\delta}{2L}\right)^{\alpha+\frac{1}{2}} \leqslant \sum_{k \in \mathbb{I}_K} |z_{k+\frac{1}{2}}^{\alpha+\frac{1}{2}} - z_{k-\frac{1}{2}}^{\alpha+\frac{1}{2}}| \leqslant \left(\sum_{k \in \mathbb{I}_K} \delta\right)^{\frac{1}{2}} \left(\delta \sum_{k \in \mathbb{I}_K} \left(\frac{z_{k+\frac{1}{2}}^{\alpha+\frac{1}{2}} - z_{k-\frac{1}{2}}^{\alpha+\frac{1}{2}}}{\delta}\right)^2\right)^{\frac{1}{2}} \tag{4.30}$$

This implies that the differences $x_{\kappa+\frac{1}{2}} - x_{\kappa-\frac{1}{2}} = \delta/z_\kappa$ have a uniform positive lower bound on A_C. In combination with (4.29) it follows that A_C is a compact subset in the interior of $\mathfrak{x}_{\boldsymbol{\xi}}$. Consequently, the continuous function $\mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \cdot, \vec{y})$ attains a global minimum at $\vec{x}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$. Since $\vec{x}^* \in A_C$ lies in the interior of $\vec{x}$, it satisfies $\partial_{\vec{x}} \mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \vec{x}^*, \vec{y}) = 0$, which is the system of Euler-Lagrange equations. This proves the first claim.

Since $\mathbf{F}_{\alpha,\lambda} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ is smooth, its restriction to the compact set A_C is λ_C-convex with some $\lambda_C \in \mathbb{R}$, i.e., $\partial_{\vec{x}}^2 \mathbf{F}_{\alpha,\lambda}(\vec{x}) \geqslant \lambda_C \mathbb{I} \in \mathbb{R}^{\aleph \times \aleph}$ for all $\vec{x} \in A_C$. Independently of $\vec{y}$, we have that

$$\partial_{\vec{x}}^2 \mathbf{F}_{\Delta}^{\alpha,\lambda}(\sigma, \vec{x}, \vec{y}) = \partial_{\vec{x}}^2 \mathbf{F}_{\alpha,\lambda}(\vec{x}) + \frac{\delta}{\sigma} \mathbb{I},$$

which means that $\vec{x} \mapsto \mathbf{F}_\Delta^{\alpha,\lambda}(\sigma, \vec{x}, \vec{y})$ is strictly convex on A_C if

$$0 < \sigma < \tau_C := \frac{\delta}{(-\lambda_C)}.$$

Consequently, each such $\mathbf{F}_\Delta^{\alpha,\lambda}(\sigma, \cdot, \vec{y})$ has at most one critical point $\vec{x}^*$ in the interior of A_C, and this $\vec{x}^*$ is necessarily a strict global minimizer. □

Lemma 4.8. *If $\Omega = (a, b)$ is bounded, then*

$$(z_\kappa^n)^{\alpha+\frac{1}{2}} \leqslant M^{1-1/q} \left(\delta \sum_{k \in \mathbb{I}_K} \left(\frac{z_{k+\frac{1}{2}}^{\alpha+\frac{1}{2}} - z_{k-\frac{1}{2}}^{\alpha+\frac{1}{2}}}{\delta} \right)^q \right)^{1/q} + \left(\frac{M}{b-a} \right)^{\alpha+\frac{1}{2}} \tag{4.31}$$

for any $n \in \mathbb{N}$, any $\kappa \in \mathbb{I}_K^{1/2}$ and $q \geqslant 1$. Consequently

$$(z_\kappa^n)^{\alpha+\frac{1}{2}} \leqslant \Theta_\alpha^{-1/2} \big(M \mathbf{F}_{\alpha,0}(\vec{x}_\Delta^n) \big)^1 2 + \left(\frac{M}{b-a} \right)^{\alpha+\frac{1}{2}} \quad \textit{for all } \kappa \in \mathbb{I}_K^{1/2}. \tag{4.32}$$

Proof. In case of a bounded domain, any component of $\vec{x}_\Delta^n$ lies in $[a, b]$, one can hence interchange $2L$ by $(b - a)$ in (4.30) from the previous proof. The estimate in (4.31) is then attained by a simple modification of the estimate in (4.30). The second claim (4.32) immediately follows by (4.31) for $q = 2$ and the definition of $\mathbf{F}_{\alpha,0}$. □

4.3. Analysis of the long-time behaviour and equilibria for $\Omega = \mathbb{R}$

Henceforth, let $\Omega = \mathbb{R}$ for the rest of the chapter. In the following, we will analyze the long-time behaviour in the discrete setting and will especially prove Theorem 4.1, Theorem 4.2, and Theorem 4.3.

As already shown in [**MMS09**], a key-ingredient for the analysis of the equations‘ equilibria and long-time behaviour is the correlation of $\mathcal{F}_{\alpha,\lambda}$ and $\mathcal{H}_{\alpha,\lambda}$ by the so-called *fundamental entropy-information relation*: For any $u \in \mathcal{P}_2^r(\Omega)$ with $\mathcal{H}_{\alpha,\lambda}(u) < \infty$, one obtains

$$\mathcal{F}_{\alpha,\lambda}(u) = |\operatorname{grad}_{\mathcal{W}_2} \mathcal{H}_{\alpha,\lambda}|^2 + (2\alpha - 1)\Lambda_{\alpha,\lambda}\mathcal{H}_{\alpha,\lambda}(u), \quad \text{for any } \lambda \geqslant 0, \tag{4.33}$$

see [**MMS09**, Corollary 2.3]. In addition, a typical property of diffusion processes like (4.1) or (4.20) with positive confinement $\lambda, \Lambda_{\alpha,\lambda} > 0$ is the convergence towards unique stationary solutions u^∞ and v^∞, respectively, independent of the choice of initial data. It is maybe one of the most surprising facts that both equations (4.1) and (4.20) share the same steady state, i.e. the stationary solutions u^∞ and v^∞ are identical. Those stationary states are solutions of the elliptic equations

$$-\partial_{xx}\big(\mathrm{P}(u)\big) + \Lambda_{\alpha,\lambda}\partial_x(xu) = 0, \tag{4.34}$$

with $\mathrm{P}(s) := \Theta_\alpha s^{\alpha+1/2}$, and have the form of Barenblatt profils or Gaussians, respectively, see definition (4.12) and (4.13). This was first observed by Denzler and McCann in [**DM08**], and further studied in [**MMS09**] using the Wasserstein gradient flow structure of both equations and their remarkable relation via (4.21).

As a further conclusion of our natural discretization, we get a *discrete fundamental entropy-information relation* analogously to the continuous one in (4.33).

Corollary 4.9. *For any* $\lambda \geqslant 0$ *and every* $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$ *with* $\mathbf{H}_{\alpha,0}(\vec{x}) < \infty$*, we have*

$$\begin{aligned} \mathbf{F}_{\alpha,\lambda}(\vec{x}) &= \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 + (2\alpha - 1)\Lambda_{\alpha,\lambda}\mathbf{H}_{\alpha,\lambda}(\vec{x}) \quad \text{for } \alpha \in (\tfrac{1}{2}, 1] \quad \text{and} \\ \mathbf{F}_{1/2,\lambda}(\vec{x}) &= \left\|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{1/2,\lambda}(\vec{x})\right\|_{\boldsymbol{\xi}}^2 + \Lambda_{1/2,\lambda} \qquad\qquad \text{for } \alpha = \tfrac{1}{2}. \end{aligned} \tag{4.35}$$

Remark 4.10. *At first glance, it seems that there is a discontinuity of* $\alpha \mapsto \mathbf{F}_{\alpha,\lambda}$ *at* $\alpha = \frac{1}{2}$*, but this is a fallacy. For* $\alpha > \frac{1}{2}$*, the second term on the right-hand side of* (4.35) *is explicitly given by*

$$\begin{aligned} (2\alpha - 1)\Lambda_{\alpha,\lambda}\mathbf{H}_{\alpha,\lambda}(\vec{x}) &= (2\alpha - 1)\Lambda_{\alpha,\lambda} \left(\Theta_\alpha \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} \frac{z_\kappa^{\alpha-1/2}}{\alpha - 1/2} + \frac{\Lambda_{\alpha,\lambda}}{2} \|\vec{x}\|_{\boldsymbol{\xi}}^2 \right) \\ &= 2\Lambda_{\alpha,\lambda}\Theta_\alpha \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha-1/2} + (2\alpha - 1)\frac{\Lambda_{\alpha,\lambda}}{2} \|\vec{x}\|_{\boldsymbol{\xi}}^2 . \end{aligned}$$

For $\alpha \downarrow \frac{1}{2}$*, one gets* $\Lambda_{\alpha,\lambda} \to \Lambda_{1/2,\lambda}$*,* $\Theta_\alpha \to \frac{1}{2}$ *and especially* $\delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha-1/2} \to M = 1$*. The drift-term vanishes since* $(2\alpha - 1) \to 0$*.*

Proof of Corollary 4.9. Let us first assume $\alpha \in (\frac{1}{2}, 1]$. A straight-forward calculation using the definition of $\|.\|_{\boldsymbol{\xi}}$, $\nabla_{\boldsymbol{\xi}}$ and $\partial_{\vec{x}}\mathbf{H}_{\alpha,\lambda}$ in (4.23) yields

$$\begin{aligned} \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 &= \delta^{-1} \langle \partial_{\vec{x}}\mathbf{H}_{\alpha,\lambda}(\vec{x}), \partial_{\vec{x}}\mathbf{H}_{\alpha,\lambda}(\vec{x}) \rangle \\ &= \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,0}(\vec{x})\|_{\boldsymbol{\xi}}^2 - 2\Theta_\alpha \Lambda_{\alpha,\lambda} \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha - \frac{1}{2}} + \Lambda_{\alpha,\lambda}^2 \delta \sum_{k \in \mathbb{I}_K} |x_k|^2. \end{aligned} \tag{4.36}$$

Here we used the explicit representation of $\partial_{\vec{x}}\mathbf{H}_{\alpha,\lambda}(\vec{x})$, see (4.23),

$$\partial_{\vec{x}}\mathbf{H}_{\alpha,\lambda}(\vec{x}) = \Theta_\alpha \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha+\frac{1}{2}} \frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta} + \Lambda_{\alpha,\lambda} \delta \sum_{k \in \mathbb{I}_K} x_k \mathbf{e}_k,$$

and especially the definition of (2.18), which yields

$$\begin{aligned} \delta^{-1} \left\langle \Theta_\alpha \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha+\frac{1}{2}} \frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta}, \Lambda_{\alpha,\lambda} \delta \sum_{k \in \mathbb{I}_K} x_k \mathbf{e}_k \right\rangle &= \Theta_\alpha \Lambda_{\alpha,\lambda} \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha+\frac{1}{2}} \frac{x_{\kappa-\frac{1}{2}} - x_{\kappa+\frac{1}{2}}}{\delta} \\ &= -\Theta_\alpha \Lambda_{\alpha,\lambda} \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^{\alpha-\frac{1}{2}} \end{aligned}$$

Since $\alpha \neq \frac{1}{2}$, we can write $2\Theta_\alpha = (2\alpha - 1)\frac{\Theta_\alpha}{\alpha - 1/2}$. Further note that the relation $\Lambda_{\alpha,\lambda} = \sqrt{\lambda/(2\alpha + 1)}$ yields

$$\Lambda_{\alpha,\lambda}^2 = \frac{\lambda}{2\alpha + 1} = \frac{\lambda}{2}\left(\frac{1}{\alpha + 1/2}\right) = \frac{\lambda}{2}\left(1 - \frac{\alpha - 1/2}{\alpha + 1/2}\right) = \frac{\lambda}{2}\left(1 - \frac{2\alpha - 1}{2\alpha + 1}\right).$$

Using this information and the definition of $\mathcal{H}_{\alpha,0}$, we proceed in the above calculations by

$$\begin{aligned}\|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 &= \mathbf{F}_{\alpha,0}(\vec{x}) - (2\alpha-1)\Lambda_{\alpha,\lambda}\mathbf{H}_{\alpha,0}(\vec{x}) + \frac{\lambda}{2}\left(1-\frac{2\alpha-1}{2\alpha+1}\right)\delta\sum_{k\in\mathbb{I}_K}|x_k|^2 \\ &= \mathbf{F}_{\alpha,0}(\vec{x}) - (2\alpha-1)\Lambda_{\alpha,\lambda}\mathbf{H}_{\alpha,0}(\vec{x}) + \frac{\lambda}{2}\delta\sum_{k\in\mathbb{I}_K}|x_k|^2 - (2\alpha-1)\frac{\Lambda_{\alpha,\lambda}^2}{2}\delta\sum_{k\in\mathbb{I}_K}|x_k|^2 \\ &= \mathbf{F}_{\alpha,\lambda}(\vec{x}) - (2\alpha-1)\Lambda_{\alpha,\lambda}\mathbf{H}_{\alpha,\lambda}(\vec{x}).\end{aligned}$$

In case of $\alpha = \frac{1}{2}$, we see that $\Theta_{1/2} = \frac{1}{2}$, and $\Lambda_{1/2,\lambda} = \sqrt{\lambda/2}$. We hence conclude in (4.36) that

$$\|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{1/2,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 = \|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{1/2,0}(\vec{x})\|_{\boldsymbol{\xi}}^2 - \Lambda_{1/2,\lambda}\delta\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^0 + \frac{\lambda}{2}\delta\sum_{k\in\mathbb{I}_K}|x_k|^2 = \mathbf{F}_{\alpha,\lambda}(\vec{x}) - \Lambda_{1/2,\lambda}.$$

□

For the following reason, the above representation of $\mathbf{F}_{\alpha,\lambda}$ is indeed a little miracle: From a naive point of view, one would ideally hope to gain a discrete counterpart of the fundamental entropy-information relation (4.33), if one takes the one-to-one discretization of the L^2-Wasserstein distance, which is (in the language of Lagrangian vectors) realized by $\vec{x} \mapsto \langle\vec{x}, \mathrm{W}_2\vec{x}\rangle$ with W_2 from (2.21) instead of our simpler choice $\vec{x} \mapsto \|\vec{x}\|_{\boldsymbol{\xi}}$. Indeed, with this ansatz, the above proof would fail at the moment at which one tries to calculate the scalar product of $\partial_{\vec{x}}\mathbf{H}_{\alpha,0}$ and $\partial_{\vec{x}}\langle\vec{x}, \mathrm{W}_2\vec{x}\rangle = 2\mathrm{W}_2\vec{x}$. This is why our discretization of the L^2-Wasserstein distance by the norm $\|\cdot\|_{\boldsymbol{\xi}}$ seems to be the right choice, if one is interested in a structure-preserving discretization.

Let us proceed in the analysis of the schemes's long-time behaviour. For this purpose, we are going to prove first the existence of minimizers of $\mathbf{H}_{\alpha,\lambda}$:

Lemma 4.11. *For each $\alpha \in [\frac{1}{2}, 1]$, the functional $\mathbf{H}_{\alpha,\lambda}$ admits a unique minimizer $\vec{x}_{\boldsymbol{\xi}}^{\min} \in \mathfrak{x}_{\boldsymbol{\xi}}$. If we further assume $\Lambda_{\alpha,\lambda} > 0$, then*

$$\frac{\Lambda_{\alpha,\lambda}}{2}\|\vec{x} - \vec{x}_{\boldsymbol{\xi}}^{\min}\|_{\boldsymbol{\xi}}^2 \leqslant \mathbf{H}_{\alpha,\lambda}(\vec{x}) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min}) \leqslant \frac{1}{2\Lambda_{\alpha,\lambda}}\|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 \tag{4.37}$$

for any $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$

Proof. To prove that the convexity of $\mathbf{H}_{\alpha,\lambda}$, see (4.25), implies the existence of a minimizer of $\mathbf{H}_{\alpha,\lambda}$ we first have to guarantee that $\vec{x} \mapsto \mathbf{H}_{\alpha,\lambda}(\vec{x})$ is bounded from below. Since this is trivially valid for $\alpha > 1/2$, we consider $\alpha = 1/2$ and refer the result in Lemma A.7, which eventually shows that

$$\mathbf{H}_{1/2,\lambda}(\vec{x}) \geqslant -\frac{2\sqrt{\pi}}{e}\left(M + \|\vec{x}\|_{\boldsymbol{\xi}}^2\right)^{1/2} + \frac{\lambda}{2}\|\vec{x}\|_{\boldsymbol{\xi}}^2 \geqslant -\frac{2\sqrt{\pi}}{e}\left(\sqrt{M} + \|\vec{x}\|_{\boldsymbol{\xi}}\right) + \frac{\lambda}{2}\|\vec{x}\|_{\boldsymbol{\xi}}^2.$$

One can hence find two constants $c_\lambda > 0$ and $d_\lambda > 0$ depending on λ, such that $\mathbf{H}_{1/2,\lambda}(\vec{x}) \geqslant c_\lambda\|\vec{x}\|_{\boldsymbol{\xi}}^2 - d_\lambda$, which further shows that $\mathbf{H}_{\alpha,\lambda}$ are bounded from below at least by $-d_\lambda$ for all $\alpha \in (\frac{1}{2}, 1]$. Further take $C > 0$ such that $A_C := \mathbf{H}_{\alpha,\lambda}^{-1}([-d_\lambda, C])$ is not empty, then

$$\|\vec{x}\|_\infty \leqslant \frac{\|\vec{x}\|_{\boldsymbol{\xi}}}{\delta} \leqslant \sqrt{\frac{2}{\lambda\delta}(C + d_\lambda)}.$$

Hence, there is an interval $[-L, L]$, such that all components of A_c lie in $[-L, L]$. From this point on, one can proceed as in Proposition 3.9 to show that $\mathbf{H}_{\alpha,\lambda}$ has a unique minimizer.

Deviding (4.25) by $s > 0$ and passing to the limit as $s \downarrow 0$ yields

$$\mathbf{H}_{\alpha,\lambda}(\vec{x}) - \mathbf{H}_{\alpha,\lambda}(\vec{y}) \leqslant \langle \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}), \vec{x} - \vec{y} \rangle_{\boldsymbol{\xi}} - \frac{\Lambda_{\alpha,\lambda}}{2} \|\vec{x} - \vec{y}\|_{\boldsymbol{\xi}}^2 .$$

The second inequality of (4.37) now follows from Young's inequality $|pq| \leqslant \varepsilon |p|^2 + (2\varepsilon)^{-1}\frac{1}{2}|q|^2$ with $\varepsilon = (2\delta\Lambda_{\alpha,\lambda})^{-1}$, and even holds true for arbitrary $\vec{y} \in \mathfrak{x}_{\boldsymbol{\xi}}$.

To get the first inequaltiy of (4.37), we set $\vec{x} = \vec{x}_{\boldsymbol{\xi}}^{\min}$ and again devide (4.25) by $s > 0$, then

$$\frac{\mathbf{H}_{\alpha,\lambda}\big((1-s)\vec{x}_{\boldsymbol{\xi}}^{\min} + s\vec{y}\big) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})}{s} \leqslant \mathbf{H}_{\alpha,\lambda}(\vec{y}) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min}) - \frac{\Lambda_{\alpha,\lambda}}{2}(1-s) \left\|\vec{x}_{\boldsymbol{\xi}}^{\min} - \vec{y}\right\|_{\boldsymbol{\xi}}^2 ,$$

where the left-hand side is obviously nonnegative for any $s > 0$. Since $s > 0$ was arbitrary, the statement is proven. ☐

Corollary 4.12. *The unique minimizer* $\vec{x}_{\boldsymbol{\xi}}^{\min} \in \mathfrak{x}_{\boldsymbol{\xi}}$ *of* $\mathbf{H}_{\alpha,\lambda}$ *is a minimizer of* $\mathbf{F}_{\alpha,\lambda}$. *Furthermore, one has*

$$\mathbf{F}_{\alpha,\lambda}(\vec{x}) - \mathbf{F}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min}) \leqslant \frac{2\alpha+1}{2} \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 \tag{4.38}$$

for any $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$

Proof. Equality (4.35) and $2\alpha - 1 \geqslant 0$ shows that $\vec{x} \mapsto \mathbf{F}_{\alpha,\lambda}(\vec{x})$ is minimal, if one has that $\|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}} = 0$ and $\mathbf{H}_{\alpha,\lambda}(\vec{x})$ is minimal. This is the case for $\vec{x} = \vec{x}_{\boldsymbol{\xi}}^{\min}$. The representation in (4.35) further implies

$$\begin{aligned} &\mathbf{F}_{\alpha,\lambda}(\vec{x}) - \mathbf{F}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min}) \\ &= \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 - \left\|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})\right\|_{\boldsymbol{\xi}}^2 + (2\alpha-1)\Lambda_{\alpha,\lambda}\big(\mathbf{H}_{\alpha,\lambda}(\vec{x}) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})\big) \\ &= \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 + (2\alpha-1)\Lambda_{\alpha,\lambda}\big(\mathbf{H}_{\alpha,\lambda}(\vec{x}) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})\big) \leqslant \left(1 + \frac{2\alpha-1}{2}\right) \|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x})\|_{\boldsymbol{\xi}}^2 , \end{aligned}$$

where we used (4.37) in the last step. ☐

4.3.1. Entropy dissipation – the case of positive confinement $\boldsymbol{\lambda} > \mathbf{0}$. In this section, we pursue the discrete rate of decay towards discrete equilibria and try to verify the statements in Theorem 4.1 to that effect. That is why we assume henceforth $\lambda > 0$.

Lemma 4.13. *A solution* $\vec{x}_\Delta$ *to the discrete minizing movement scheme* (4.11) *dissipates the entropies* $\mathbf{H}_{\alpha,\lambda}$ *and* $\mathbf{F}_{\alpha,\lambda}$ *at least exponentially, i.e.*

$$\big(1 + 2\tau_n\lambda\big)\left(\mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) - \mathbf{H}_{\alpha,\lambda}^{\min}\right) \leqslant \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^{n-1}) - \mathbf{H}_{\alpha,\lambda}^{\min} \quad \textit{and} \tag{4.39}$$

$$\big(1 + 2\tau_n\lambda\big)\left(\mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n) - \mathbf{F}_{\alpha,\lambda}^{\min}\right) \leqslant \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^{n-1}) - \mathbf{F}_{\alpha,\lambda}^{\min} \tag{4.40}$$

for any time step $n \geqslant 1$.

Proof. Due to (4.35), the gradient of the information functional $\mathbf{F}_{\alpha,\lambda}$ is given by

$$\partial_{\vec{x}} \mathbf{F}_{\alpha,\lambda}(\vec{x}) = 2\delta^{-1}(\partial_{\vec{x}} \mathbf{H}_{\alpha,\lambda}(\vec{x}))^T \partial_{\vec{x}}^2 \mathbf{H}_{\alpha,\lambda}(\vec{x}) + (2\alpha-1)\Lambda_{\alpha,\lambda} \partial_{\vec{x}} \mathbf{H}_{\alpha,\lambda}(\vec{x}),$$

which yields in combination with the $\Lambda_{\alpha,\lambda}$-convexity of $\mathbf{H}_{\alpha,\lambda}$ and (4.28)

$$\begin{aligned}
&\mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^{n-1}) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \\
\geqslant &\tau_n \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n), \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \\
\geqslant &2\tau_n \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n), \partial_{\vec{x}}^2 \mathbf{H}_{\alpha,\lambda}(\vec{x}) \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} + \tau_n(2\alpha-1)\Lambda_{\alpha,\lambda} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 \\
\geqslant &2\tau_n \Lambda_{\alpha,\lambda} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 + \tau_n(2\alpha-1)\Lambda_{\alpha,\lambda} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 \geqslant \tau_n(2\alpha+1)\Lambda_{\alpha,\lambda} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 .
\end{aligned} \tag{4.41}$$

Using inequality (4.37), we conclude that

$$\left(1 + 2\tau_n(2\alpha+1)\Lambda_{\alpha,\lambda}^2\right) \left(\mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min}) \right) \leqslant \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^{n-1}) - \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})$$

for any $n \in \mathbb{N}$. Since $(2\alpha+1)\Lambda_{\alpha,\lambda}^2 = \lambda$, this shows (4.39).

To prove (4.40), we proceed as follows: First introduce for $\sigma > 0$ the vector $\vec{x}_\sigma \in \mathfrak{x}_{\boldsymbol{\xi}}$ as the unique minimizer of

$$\vec{y} \mapsto \frac{1}{2\sigma} \left\| \vec{y} - \vec{x}_\Delta^n \right\|_{\boldsymbol{\xi}}^2 + \mathbf{H}_{\alpha,\lambda}(\vec{y}),$$

which is further a solution to the system of Euler-Lagrange equations, hence

$$\frac{\vec{x}_\sigma - \vec{x}_\Delta^n}{\sigma} = -\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\sigma).$$

This especially induces by passing to the limit as $\sigma \downarrow 0$ that

$$\lim_{\sigma \downarrow 0} \frac{\vec{x}_\sigma - \vec{x}_\Delta^n}{\sigma} = -\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n). \tag{4.42}$$

Furthermore, note that $\vec{x}_\Delta^n$ is a minimizer of $\vec{x} \mapsto \mathbf{F}_\Delta^{\alpha,\lambda}(\tau_n, \vec{x}, \vec{x}_\Delta^{n-1})$ by definition of $\vec{x}_\Delta$ as a solution to the numerical scheme. This implies in particular that

$$\frac{1}{2\tau_n} \left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n) \leqslant \frac{1}{2\tau_n} \left\| \vec{x}_\sigma - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,\lambda}(\vec{x}_\sigma),$$

and therefore

$$\begin{aligned}
\mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n) - \mathbf{F}_{\alpha,\lambda}(\vec{x}_\sigma) &\leqslant \frac{1}{2\tau_n} \left(\left\| \vec{x}_\sigma - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 - \left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}^2 \right) \\
&\leqslant \frac{1}{2\tau_n} \left\| \vec{x}_\sigma - \vec{x}_\Delta^n \right\|_{\boldsymbol{\xi}} \left(\left\| \vec{x}_\sigma - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}} + \left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}} \right).
\end{aligned}$$

We now devide both side by σ and pass to the limit as $\sigma \downarrow 0$, then we get

$$\left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n), \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \leqslant \frac{1}{\tau_n} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}} \left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}, \tag{4.43}$$

due to (4.42). Furthermore, we have seen in (4.41), among other estimates, that

$$\tau_n(2\alpha+1)\Lambda_{\alpha,\lambda} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 \leqslant \tau_n \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n), \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\rangle_{\boldsymbol{\xi}}.$$

This yields in combination with (4.43)

$$\tau_n(2\alpha+1)\Lambda_{\alpha,\lambda} \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 \leqslant \left\| \nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n) \right\|_{\boldsymbol{\xi}} \left\| \vec{x}_\Delta^n - \vec{x}_\Delta^{n-1} \right\|_{\boldsymbol{\xi}}.$$

As a consequence, we get two types of inequalities, namely

$$\begin{aligned} \tau_n\sqrt{(2\alpha+1)\lambda}\,\|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n)\|_{\boldsymbol{\xi}} &\leqslant \left\|\vec{\mathrm{x}}_\Delta^n-\vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}} \quad \text{and} \\ 2\tau_n^2\lambda\big(\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n)-\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})\big) &\leqslant \left\|\vec{\mathrm{x}}_\Delta^n-\vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2, \end{aligned} \tag{4.44}$$

where we used $\Lambda_{\alpha,\lambda}=\sqrt{\lambda/(2\alpha+1)}$ and (4.38). To get the desired estimate, fix $\vec{\mathrm{x}}_\Delta^{n-1}$ and denote now by $\vec{\mathrm{x}}_\sigma^n$ a minimizer of

$$\vec{\mathrm{y}}\mapsto\frac{1}{2\sigma}\left\|\vec{\mathrm{y}}-\vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2+\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{y}})$$

for $\sigma\in(0,\tau_n]$. Then $\vec{\mathrm{x}}_\sigma^n$ connects $\vec{\mathrm{x}}_\Delta^{n-1}$ and $\vec{\mathrm{x}}_\Delta^n$ and the monotonicity of $\sigma\mapsto\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\sigma^n)$ and (4.44) yields for any $\sigma\in(0,\tau]$

$$\begin{aligned} 2\sigma^2\lambda\big(\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n)-\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})\big) &\leqslant 2\tau_n^2\lambda\big(\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\sigma^n)-\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})\big) \\ &\leqslant \left\|\vec{\mathrm{x}}_\sigma^n-\vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2. \end{aligned} \tag{4.45}$$

Now apply (A.3) from Lemma A.5, which induces in this special case

$$\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n)+\frac{\left\|\vec{\mathrm{x}}_\Delta^n-\vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2}{2\tau_n}+\int_0^{\tau_n}\frac{\left\|\vec{\mathrm{x}}_\sigma^n-\vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2}{2\sigma^2}\,\mathrm{d}\sigma=\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^{n-1}).$$

Inserting (4.45) in the above equation then finally yields

$$(1+2\tau_n\lambda)\left(\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n)-\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})\right)\leqslant\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^{n-1})-\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min}),$$

and the claim is proven. □

Remark 4.14. *In the continuous situation, the analogue proofs of* (4.39) *and* (4.40) *require a deeper understanding of variational techniques. An essential tool in this context is the* flow interchange lemma*, see for instance [**MMS09**, Theorem 3.2]. Although one can easily proof a discrete counterpart of the flow interchange lemma, it is not essential in the above proof, since the smoothness of* $\vec{\mathrm{x}}\mapsto\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}})$ *allows an explict calculation of its gradient and hessian.*

Lemma 4.13 paves the way for the exponential decay rates of Theorem 4.1. Effectively, (4.14) and (4.15) are just applications of the following version of the discrete Gronwall lemma: Assume $(c_n)_{n=0}^\infty$ and $(y_n)_{n=0}^\infty$ to be sequences with values in $[0,+\infty)$, satisfying $(1+c_n)y_n\leqslant y_{n-1}$ for any $n\in\mathbb{N}$, then

$$y_n\leqslant y_0e^{-\sum_{k=0}^{n-1}\frac{c_k}{1+c_k}}\quad\text{for any } n\in\mathbb{N}.$$

This statement can be easily proven by induction. Furthermore, inequality (4.16) is then a corollary of (4.14) and a Csiszar-Kullback inequality, see [**CJM⁺01**, Theorem 30].

4.3.2. Convergence towards Barenblatt profiles and Gaussians. Let us again assume $\lambda>0$. As already mentioned, the stationary solutions u^∞ and v^∞ of (4.1) and (4.20), respecively, are identical. Those stationary states have the form of Barenblatt profils or Gaussians, respectively,

$$\mathrm{b}_{\alpha,\lambda} = \left(\mathsf{a} - \mathsf{b}|x|^2\right)_+^{1/(\alpha-1/2)}, \quad \mathsf{b} = \frac{\alpha - 1/2}{\sqrt{2\alpha}}\Lambda_{\alpha,\lambda} \quad \text{for } \alpha > 1/2 \text{ and}$$
$$\mathrm{b}_{1/2,\lambda} = \mathsf{a}e^{-\Lambda_{1/2,\lambda}|x|^2} \quad \text{for } \alpha = 1/2,$$

where $\mathsf{a} \in \mathbb{R}$ is chosen to conserve unit mass.

To prove the statement of Theorem 4.2, we are going to show that the sequence of functionals $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda} : \mathcal{P}_2^r(\Omega) \to (-\infty, +\infty]$ given by

$$\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u) := \begin{cases} \mathcal{H}_{\alpha,\lambda}(u) & \text{for } u \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega), \\ +\infty & \text{for } u \notin \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega) \end{cases}$$

Γ-congerves towards $\mathcal{H}_{\alpha,\lambda}$. More detailed, for any $u \in \mathcal{P}_2^r(\Omega)$ the following points are satisfied:

(i) $\liminf_{\delta\to 0} \mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u_{\boldsymbol{\xi}}) \geqslant \mathcal{H}_{\alpha,\lambda}(u)$ for any sequence $u_{\boldsymbol{\xi}}$ with $\lim_{\delta\to 0} \mathcal{W}_2(u_{\boldsymbol{\xi}}, u) = 0$.

(ii) There exists a *recovery sequence* $u_{\boldsymbol{\xi}}$ of u, i.e. $\limsup_{\delta\to 0} \mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u_{\boldsymbol{\xi}}) \leqslant \mathcal{H}_{\alpha,\lambda}(u)$ and $\lim_{\delta\to 0} \mathcal{W}_2(u_{\boldsymbol{\xi}}, u) = 0$.

The Γ-convergence of $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}$ towards $\mathcal{H}_{\alpha,\lambda}$ is a powerful property, since it implies convergence of the sequence of minimizers $u^{\min}_{\boldsymbol{\xi}} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}]$ towards $\mathrm{b}_{\alpha,\lambda}$ or $\mathrm{b}_{1/2,\lambda}$, repsectively, with respect to the L^2-Wasserstein distance, see [**Bra02**]. To conclude even strong convergence of $u^{\min}_{\boldsymbol{\xi}}$ at least in $L^p(\Omega)$ for arbitrary $p \geqslant 1$, we proceed similarly as in [**MO14a**, Proposition 18]. To understand this, recall that the definition of the total variation of a function $f \in L^1(\Omega)$ in (1.14) that is

$$\mathrm{TV}[f] = \sup\left\{ \int_\Omega f(x)\varphi'(x)\,\mathrm{d}x \;\middle|\; \varphi \in \mathrm{Lip}(\Omega) \text{ with compact support}, \sup_{x\in\Omega} |\varphi(x)| \leqslant 1 \right\}. \tag{4.46}$$

If f is a piecewise constant function with compact support $[x_0, x_K]$, taking values $f_{k-\frac12}$ on intervals $(x_{k-1}, x_k]$, then the integral in (4.46) amounts to

$$\int_\Omega f(x)\varphi'(x)\,\mathrm{d}x = \sum_{k=1}^{K} \left[f(x)\varphi(x)\right]_{x=x_{k-1}+0}^{x_k-0} = \sum_{k=1}^{K-1} (f_{k-\frac12} - f_{k+\frac12})\varphi(x_k) + f_{\frac12}\varphi(x_0) - f_{K-\frac12}\varphi(x_K).$$

Consequently, for such f, the supremum in (4.46) equals

$$\mathrm{TV}[f] = \sum_{k=1}^{K-1} |f_{k+\frac12} - f_{k-\frac12}| + |f_{\frac12}| + |f_{K-\frac12}| \tag{4.47}$$

and is attained for every $\varphi \in \mathrm{Lip}(\Omega)$ with values $\varphi(x_k) = \mathrm{sgn}(f_k - f_{k+1})$ at $k = 1, \ldots, K-1$, $\varphi(x_0) = \mathrm{sgn}(f_{\frac12})$ and $\varphi(x_K) = -\mathrm{sgn}(f_{K-\frac12})$.

Lemma 4.15. *For any $\alpha \in [\frac12, 1]$, assume $\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ to be the unique minimizer of $\mathbf{H}_{\alpha,\lambda}$ and declare the sequence of functions $u^{\min}_{\boldsymbol{\xi}} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}]$. Then*

$$u^{\min}_{\boldsymbol{\xi}} \longrightarrow \mathrm{b}_{\alpha,\lambda}, \text{ strongly in } L^p(\Omega) \text{ for any } p \geqslant 1 \tag{4.48}$$

as $\delta \to 0$.

Proof. We will first prove the Γ-convergence of $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}$ towards $\mathcal{H}_{\alpha,\lambda}$. The first requirement (i) is a conclusion of the lower semi-continuity of $\mathcal{H}_{\alpha,\lambda}$.

For the second point (ii), we fix $u \in \mathcal{P}_2^r(\Omega)$ and assume $\mathrm{X} : \mathcal{M} \to [-\infty, +\infty]$ to be the Lagrangian map of u. If there exists an bounded interval $I \subseteq \Omega$ such that the whole mass of u is concentrated in I, i.e. $\int_I u \,\mathrm{d}x = M$, then one can introduce an interpolation $u_{\boldsymbol{\xi}}$ of u analogously to Lemma 3.24 by pointwise evaluation of the pseudo-inverse distribution function X, such that (ii) holds true. So let us assume that there is no such interval, hence $\int_{\mathcal{K}} u \,\mathrm{d}x < M$ for any compact subset $\mathcal{K} \subseteq \Omega$, and further assume without loss of generality that the center of mass is at $x = 0$, i.e. $\int_{-\infty}^0 u(x)\,\mathrm{d}x = M/2$. Then one can find for any $\varepsilon > 0$ a compact set of the form $\mathcal{K} = [L_1, L_2]$ with $L_1 < 0 < L_2$, and an integer $K \in \mathbb{N}$, such that

$$\int_{\Omega\setminus\mathcal{K}} |x|^2 u(x)\,\mathrm{d}x < \varepsilon, \quad \text{and} \quad \int_{-\infty}^{L_1} u(x)\,\mathrm{d}x = \int_{L_2}^{+\infty} u(x)\,\mathrm{d}x = \delta := MK^{-1} \tag{4.49}$$

The first statement is valid due to the boundedness of the second momentum of u, and the last one is satisfied since one can choose $K \in \mathbb{N}$ arbitrarily large. An immediate consequence of the above choises is that $2\delta L^2 < \varepsilon$ for $L = \max\{|L_1|, |L_2|\}$ due to

$$2(L_1^2 + L_2^2)\delta = L_1^2 \int_{-\infty}^{L_1} u(x)\,\mathrm{d}x + L_2^2 \int_{L_2}^{+\infty} u(x)\,\mathrm{d}x \leqslant \int_{\Omega\setminus\mathcal{K}} |x|^2 u(x)\,\mathrm{d}x < \varepsilon.$$

Using $\delta = MK^{-1}$ we define an equidistant decomposition $\boldsymbol{\xi}$ of the mass domain $\mathcal{M}$. We furthermore declare $x_0 = -2L$, $x_K = 2L$ and $x_k = \mathrm{X}(\xi_k)$ for any $k = 1, \ldots, K-1$ and introduce the locally constant density $u_{\boldsymbol{\xi}} \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ that corresponds to the Lagrangian map $\mathrm{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$. This procedure defines a sequence of densities $u_{\boldsymbol{\xi}}$, since $\varepsilon > 0$ was arbitrary, and we are going to prove that $u_{\boldsymbol{\xi}}$ is the right choice for the recovery sequence. To prove the convergence in the L^2-Wasserstein distance, we fix $\varepsilon > 0$. Then the last property of u in (4.49) yields especially that $x_1 = L_1$ and $x_{K-1} = L_2$ Furthermore, since X and $\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ are monotonically increasing, one obtains for any $\xi \in [\xi_1, \xi_{K-1}]$ that

$$|\mathrm{X}(\xi) - \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}](\xi)| \leqslant \big(\mathrm{X}(\xi_k) - \mathrm{X}(\xi_{k-1})\big) \leqslant 2L, \text{ with } \xi \in [\xi_{k-1}, \xi_k], k = 2, \ldots, K-1.$$

Therefore

$$\|\mathrm{X} - \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\|^2_{L^2([\xi_1,\xi_{K-1}])} \leqslant 2\delta L \sum_{k=2}^{K-1} \big(\mathrm{X}(\xi_k) - \mathrm{X}(\xi_{k-1})\big) \leqslant 2\delta L^2 < \varepsilon, \tag{4.50}$$

where we used $x_1 = L_1$ and $x_{K-1} = L_2$. As a next step, we note that $|x_1|, |x_{K-1}| \leqslant L$ and $|x_0| = |x_K| = 2L$, which yields

$$\begin{aligned}
\|\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\|^2_{L^2(\mathcal{M}\setminus[\xi_1,\xi_{K-1}])} &= \int_{[x_0,x_K]\setminus[x_1,x_{K-1}]} |x|^2 u_{\boldsymbol{\xi}}(x)\,\mathrm{d}x \\
&= \frac{\delta}{x_K - x_{K-1}} \int_{x_{K-1}}^{x_K} |x|^2\,\mathrm{d}x + \frac{\delta}{x_1 - x_0} \int_{x_0}^{x_1} |x|^2\,\mathrm{d}x \\
&\leqslant \frac{2\delta}{3}\left(x_K^2 + x_{K-1}^2 + x_1^2 + x_0^2\right) \leqslant \frac{40}{3}\delta L^2 < 7\varepsilon,
\end{aligned} \tag{4.51}$$

where we used the elementary equality $(a^3 - b^3) = (a-b)(a^2 + b^2 + ab)$. Combining (4.49), (4.50), and (4.51), and the fact that $\mathrm{X}(\mathcal{M}\backslash[\xi_1, \xi_{K-1}]) = \Omega\backslash\mathcal{K}$, we finally conclude

$$\begin{aligned}\mathcal{W}_2(u, u_{\boldsymbol{\xi}}) &= \|\mathrm{X} - \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\|_{L^2(\mathcal{M})} \leqslant \|\mathrm{X} - \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\|_{L^2([\xi_1,\xi_{K-1}])} + \|\mathrm{X} - \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\|_{L^2(\mathcal{M}\backslash[\xi_1,\xi_{K-1}])} \\ &\leqslant \sqrt{\varepsilon} + \|\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]\|_{L^2(\mathcal{M}\backslash[\xi_1,\xi_{K-1}])} + \|\mathrm{X}\|_{L^2(\mathcal{M}\backslash[\xi_1,\xi_{K-1}])} \\ &\leqslant \sqrt{\varepsilon} + \sqrt{7\varepsilon} + \left(\int_{\Omega\backslash\mathcal{K}} |x|^2 u(x)\,\mathrm{d}x\right)^{1/2} < 4\sqrt{\varepsilon}.\end{aligned}$$

This shows $u_{\boldsymbol{\xi}} \to u$ in L^2-Wasserstein as $\delta \to 0$. The second point in *(ii)* easily follows by using Jensen's inequality,

$$\begin{aligned}\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u_{\boldsymbol{\xi}}) = \mathcal{H}_{\alpha,\lambda}(u_{\boldsymbol{\xi}}) &= \sum_{\kappa\in\mathbb{I}_K^{1/2}} \int_{x_{\kappa-\frac12}}^{x_{\kappa+\frac12}} \varphi_\alpha\left(\frac{\delta}{x_{\kappa+\frac12} - x_{\kappa-\frac12}}\right) \mathrm{d}x \\ &= \sum_{\kappa\in\mathbb{I}_K^{1/2}} (x_{\kappa+\frac12} - x_{\kappa-\frac12})\varphi_\alpha\left(\frac{1}{x_{\kappa+\frac12} - x_{\kappa-\frac12}} \int_{x_{\kappa-\frac12}}^{x_{\kappa+\frac12}} u(s)\,\mathrm{d}s\right) \\ &\leqslant \sum_{\kappa\in\mathbb{I}_K^{1/2}} \int_{x_{\kappa-\frac12}}^{x_{\kappa+\frac12}} \varphi_\alpha\big(u(s)\big)\,\mathrm{d}s = \int_{x_0}^{x_K} \varphi_\alpha\big(u(s)\big)\,\mathrm{d}s.\end{aligned}$$

Taking the limes superior on both sides proves $\limsup_{\delta\to0} \mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u_{\boldsymbol{\xi}}) \leqslant \mathcal{H}_{\alpha,\lambda}(u)$. Since $\mathcal{H}_{\alpha,\lambda}$ is lower semi-continuous, we especially obtain $\lim_{\delta\to0} \mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u_{\boldsymbol{\xi}}) = \mathbf{H}_{\alpha,\lambda}(u)$.

To conclude the convergence of $u^{\min}_{\boldsymbol{\xi}}$ towards $\mathrm{b}_{\alpha,\lambda}$ with respect to $\mathcal{W}_2$ and the convergence of $\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}})$ towards $\mathcal{H}_{\alpha,\lambda}(\mathrm{b}_{\alpha,\lambda})$, we invoke [**Bra02**, Theorem 1.21]. Therefore note that $\inf_{u\in\mathcal{P}_2^r(\Omega)} \mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}(u) = \mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}})$ by definition of $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}$, hence the minimum of $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}$ is $u^{\min}_{\boldsymbol{\xi}}$. Furthermore, each functional $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}$ has precompact sublevels which is a consequence of $\lambda > 0$ and Prokhorov's Theorem, see for instance [**AGS05**, Theorem 5.1.3]. Since $\mathcal{H}^{\boldsymbol{\xi}}_{\alpha,\lambda}$ Γ-converges towards $\mathcal{H}_{\alpha,\lambda}$, all requirements for [**Bra02**, Theorem 1.21] are satisfied.

Let us finally prove (4.48). The convergence of $\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}})$ to $\mathcal{H}_{\alpha,\lambda}(\mathrm{b}_{\alpha,\lambda})$ yields on the one hand the uniform boundedness of $\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}})$ with respect to the spatial discretization parameter δ, and on the other hand the uniform boundedness of $\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}})$, which is a conclusion of (4.35) and $\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}) = 0$. One can now proceed analogously to the proof of Proposition 3.13 to verify that the term $\mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}})$ is an upper bound on the total variation of $\mathrm{P}(u^{\min}_{\boldsymbol{\xi}})$ with $\mathrm{P}(s) := \Theta_\alpha s^{\alpha+1/2}$. Take any arbitrary $\vec{\mathrm{y}} \in \mathbb{R}^{K+1}$ with $\|\vec{\mathrm{y}}\|_\infty \leqslant 1$. Then

$$\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}), \vec{\mathrm{y}}\right\rangle_{\boldsymbol{\xi}} = \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,\lambda}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}), \vec{\mathrm{y}}\right\rangle_{\boldsymbol{\xi}} - \Lambda_{\alpha,\lambda}\left\langle \vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}, \vec{\mathrm{y}}\right\rangle_{\boldsymbol{\xi}}, \tag{4.52}$$

and the left-hand side can be reformulated, using (4.23),

$$\begin{aligned}\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}^{\min}_{\boldsymbol{\xi}}), \vec{\mathrm{y}}\right\rangle_{\boldsymbol{\xi}} &= \sum_{\kappa\in\mathbb{I}_K^{1/2}} \mathrm{P}(z_\kappa)(y_{\kappa-\frac12} - y_{\kappa+\frac12}) \\ &= \sum_{k\in\mathbb{I}_K^+} \big(\mathrm{P}(z_{k+\frac12}) - \mathrm{P}(z_{k-\frac12})\big)y_k + \mathrm{P}(z_{\frac12})y_0 - \mathrm{P}(z_{K-\frac12})y_K.\end{aligned}$$

Respecting that $\|\vec{y}\|_{\boldsymbol{\xi}} \leqslant M\|\vec{y}\|_\infty$ we can take the supremum over all $\vec{y}$ with $\|\vec{y}\|_\infty \leqslant 1$ in (4.52). Then the Cauchy-Schwarz inequality and the representation of TV $[\cdot]$ in (4.47) yields

$$\mathrm{TV}\left[\mathrm{P}(u_{\boldsymbol{\xi}}^{\min})\right] \leqslant M \left\|\nabla_{\boldsymbol{\xi}} \mathbf{H}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})\right\|_{\boldsymbol{\xi}} + \Lambda_{\alpha,\lambda} M \left\|\vec{x}_{\boldsymbol{\xi}}^{\min}\right\|_{\boldsymbol{\xi}},$$

which is uniformly bounded from above due to (4.35) and the uniform boundedness of $\mathbf{F}_{\alpha,\lambda}(\vec{x}_{\boldsymbol{\xi}}^{\min})$. This proves the uniform boundedness of TV $\left[\mathrm{P}(u_{\boldsymbol{\xi}}^{\min})\right]$. Further note that the superlinear growth of $s \mapsto \mathrm{P}(s)$ especially yields that $u \mapsto \mathrm{P}(u)$ is $L^p(\Omega)$-continuously invertible for any $p \geqslant 1$, which can be shown by adapting the prove of Lemma 3.18. Together with [**Giu84**, Proposition 1.19], we conclude (4.48) ☐

4.3.3. Entropy dissipation – the case of zero confinement $\boldsymbol{\lambda = 0}$. We will now consider equation (4.1) in case of vanishing confinement $\lambda = 0$, hence

$$\partial_t u = -\partial_x\big(u\partial_x(u^{\alpha-1}\partial_{xx}u^\alpha)\big) \quad \text{for } (t,x) \in (0,+\infty)\times\Omega, \tag{4.53}$$

and $u(0) = u^0$ for arbitrary initial density $u^0 \in \mathcal{P}_2^r(\Omega)$. From the continuous theory, it is known that solutions to (4.53) or (4.20) with $\Lambda_{\alpha,\lambda} = 0$ branches out over the whole set of real numbers $\Omega = \mathbb{R}$, hence converges towards zero at almost every point. This matter of fact makes rigorous analysis of the long-time behaviour of solutions to (4.53) more difficult as in the case of positive confinement. However, the unperturbed functionals $\mathcal{H}_{\alpha,0}$ and $\mathcal{F}_{\alpha,0}$ satisfy the scaling property, see again [**MMS09**],

$$\mathcal{H}_{\alpha,0}(\mathfrak{d}_r u) = r^{-(2\alpha-1)/2}\mathcal{H}_{\alpha,0}(u) \quad \text{and} \quad \mathcal{F}_{\alpha,0}(\mathfrak{d}_r u) = r^{-(2\alpha+1)}\mathcal{F}_{\alpha,0}(u), \tag{4.54}$$

for any $r > 0$ and $\mathfrak{d}_r u(x) := r^{-1}u(r^{-1}x)$ with $u \in \mathcal{P}_2^r(\Omega)$. Due to this, it is possible to find weak solutions to a rescaled version of (4.53) by solving problem (4.1) with $\lambda = 1$. More precisely, the following lemma is satisfied, see for instance [**MMS09**, Lemma 5.4]:

Lemma 4.16. *A function $u \in L^2_{\mathrm{loc}}((0,+\infty); W^{2,2}(\Omega))$ is a weak solution to* (4.1) *with $\lambda = 1$, if and only if*

$$w(t,\cdot) = \mathfrak{d}_{R(t)}u(\log(R(t)),\cdot), \quad \textit{with} \quad R(t) := \big(1 + (2\alpha+3)t\big)^{1/(2\alpha+3)} \tag{4.55}$$

is a weak solution to (4.53).

A consequence of the above lemma is that one can describe how a solution w to (4.53) vanishes asymptotically as $t \to \infty$, although the gained information is not very strong and useful: In fact, the first observation (without studying local asymptotics in more detail) is, that w decays to zero with the same rate as the rescaled (time-dependent) Barenblatt-profile $\mathrm{b}^*_{\alpha,0}$ defined by $\mathrm{b}^*_{\alpha,0}(t,\cdot) := \mathfrak{d}_{R(t)}\mathrm{b}_{\alpha,1}$, with $R(t)$ of (4.55). It therefore exists a constant $C > 0$ depending only on $\mathcal{H}_{\alpha,0}(w^0) = \mathcal{H}_{\alpha,0}(u^0)$ with

$$\|w(t,\cdot) - \mathrm{b}^*_{\alpha,0}(t,\cdot)\|_{L^1(\Omega)} \leqslant CR(t)^{-1}, \tag{4.56}$$

for any $t > 0$. In [**MMS09**], this behaviour was described using weak solutions constructed by minimizing movements. We will adopt this methods to derive a discrete analogue of (4.56) for our discrete solutions $\vec{x}_\Delta$ of (4.27).

First of all, we reformulate the scaling operator $\mathfrak{d}_r$ for fixed $r > 0$ in the setting of monotonically increasing vectors $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. Since $\mathfrak{d}_r u(x) := r^{-1}u(r^{-1}\cdot)$ for arbitrary density in $\mathcal{P}_2^r(\Omega)$, the same can be done for $u_{\boldsymbol{\xi}} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, hence

$$\mathfrak{d}_r u_{\boldsymbol{\xi}}(x) = \sum_{k=1}^{K} \frac{r^{-1}\delta}{x_k - x_{k-1}} \mathbf{1}_{(x_{\kappa-\frac{1}{2}}, x_{\kappa+\frac{1}{2}}]}(r^{-1}x) = \sum_{k=1}^{K} \frac{\delta}{rx_k - rx_{k-1}} \mathbf{1}_{(rx_{\kappa-\frac{1}{2}}, rx_{\kappa+\frac{1}{2}}]}(x) = \mathbf{u}_{\boldsymbol{\xi}}[r\vec{\mathrm{x}}](x)$$

for any $x \in \Omega$. The natural extension of $\mathfrak{d}_r$ to the set $\mathfrak{x}_{\boldsymbol{\xi}}$ is hence

$$\mathfrak{d}_r\vec{\mathrm{x}} := r\vec{\mathrm{x}}, \quad \text{with corresponding} \quad \mathfrak{d}_r\vec{\mathrm{z}} = \mathbf{z}_{\boldsymbol{\xi}}[\mathfrak{d}_r\vec{\mathrm{x}}] = r^{-1}\vec{\mathrm{z}}.$$

As a consequence of this definition, we note that a discrete scaling property for $\mathbf{H}_{\alpha,0}$ and $\mathbf{F}_{\alpha,0}$ is valid, i.e. for any $r > 0$ and $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$,

$$\mathbf{H}_{\alpha,0}(\mathfrak{d}_r\vec{\mathrm{x}}) = r^{-(2\alpha-1)/2}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}) \quad \text{and} \quad \mathbf{F}_{\alpha,0}(\mathfrak{d}_r\vec{\mathrm{x}}) = r^{-(2\alpha+1)}\mathcal{F}_{\alpha,0}(\vec{\mathrm{x}}). \tag{4.57}$$

The first equality is fulfilled due to $\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}}) = \mathcal{H}_{\alpha,0}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}])$ and the scaling property (4.54) of the continuous entropy functions. The analogue claim for $\mathbf{F}_{\alpha,0}$ in (4.57) follows by inserting $\mathfrak{d}_r\vec{\mathrm{x}}$ into $\partial_{\vec{\mathrm{x}}}\mathbf{H}_{\alpha,0}$ and using $\mathfrak{d}_r\vec{\mathrm{z}} = r^{-1}\vec{\mathrm{z}}$, then

$$\partial_{\vec{\mathrm{x}}}\mathbf{H}_{\alpha,0}(\mathfrak{d}_r\vec{\mathrm{x}}) = \Theta_\alpha\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} \left(\mathfrak{d}_r\vec{\mathrm{z}}_\kappa\right)^{\alpha+\frac{1}{2}} \frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta} = r^{-(\alpha+1/2)}\partial_{\vec{\mathrm{x}}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}})$$

$$\Longrightarrow \mathbf{F}_{\alpha,0}(\mathfrak{d}_r\vec{\mathrm{x}}) = \|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\mathfrak{d}_r\vec{\mathrm{x}})\|_{\boldsymbol{\xi}}^2 = r^{-(2\alpha+1)}\,\|\nabla_{\boldsymbol{\xi}}\mathbf{H}_{\alpha,0}(\vec{\mathrm{x}})\|_{\boldsymbol{\xi}}^2 = r^{-(2\alpha+1)}\mathbf{F}_{\alpha,0}(\vec{\mathrm{x}}).$$

This scaling properties can now be used to build a bridge between solutions of discrete minimizing movement schemes with $\lambda = 0$ and those with positive confinement. The following Lemma is based on the proof of Theorem [**MMS09**, Theorem 5.6], but nevertheless, it is an impressive example for the powerful structure-preservation of the numerical scheme.

Lemma 4.17. *Assume $\vec{\mathrm{x}}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$ and fix $\tau > 0$ and $R > S > 0$. Then $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ is a minimizer of*

$$\vec{\mathrm{y}} \mapsto \mathbf{F}_\Delta^{\alpha,\lambda}(\tau, \vec{\mathrm{y}}, \vec{\mathrm{x}}^*) = \frac{1}{2\tau}\|\vec{\mathrm{y}} - \vec{\mathrm{x}}^*\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,0}(\vec{\mathrm{y}}) + \frac{\lambda}{2}\|\vec{\mathrm{y}}\|_{\boldsymbol{\xi}}^2, \tag{4.58}$$

if and only if $\mathfrak{d}_R\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ minimizes the functional

$$\vec{\mathrm{w}} \mapsto \mathbf{F}_\Delta^{\alpha,\hat{\lambda}}(\hat{\tau}, \vec{\mathrm{w}}, \mathfrak{d}_S\vec{\mathrm{x}}^*) = \frac{1}{2\hat{\tau}}\|\vec{\mathrm{w}} - \mathfrak{d}_S\vec{\mathrm{x}}^*\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,0}(\vec{\mathrm{w}}) + \frac{\hat{\lambda}}{2}\|\vec{\mathrm{w}}\|_{\boldsymbol{\xi}}^2, \quad \textit{with}$$
$$\hat{\tau} = \tau S R^{2\alpha+2}, \quad \hat{\lambda} = \frac{S(1+\lambda\tau) - R}{\hat{\tau}R}. \tag{4.59}$$

Proof. To simplify the proof, we first show that we can assume $S = 1$ without loss of generality, which is because of the following calculation: If for $R > S > 0$ the vector $\mathfrak{d}_R\vec{\mathrm{x}}$ minimizes (4.59), then the linearity of $\|\cdot\|_{\boldsymbol{\xi}}$ and (4.57) yield

$$\begin{aligned}\mathbf{F}_{\Delta}^{\alpha,\widehat{\lambda}}(\widehat{\tau},\mathfrak{d}_R\vec{x},\mathfrak{d}_S\vec{x}^*) &= \frac{S^2}{2\widehat{\tau}}\left\|S^{-1}\mathfrak{d}_R\vec{x}-\vec{x}^*\right\|_{\boldsymbol{\xi}}^2 + S^{-2\alpha+1}\mathbf{F}_{\alpha,0}(S^{-1}\mathfrak{d}_R\vec{x}) + S^2\frac{\widehat{\lambda}}{2}\left\|S^{-1}\mathfrak{d}_R\vec{x}\right\|_{\boldsymbol{\xi}}^2 \\ &= S^{-(2\alpha+1)}\left(\frac{1}{2\widehat{\tau}S^{-(2\alpha+3)}}\left\|\mathfrak{d}_{\widetilde{R}}\vec{x}-\vec{x}^*\right\|_{\boldsymbol{\xi}}^2 + \mathbf{F}_{\alpha,0}(\mathfrak{d}_{\widetilde{R}}\vec{x}) + S^{2\alpha+3}\frac{\widehat{\lambda}}{2}\left\|\mathfrak{d}_{\widetilde{R}}\vec{x}\right\|_{\boldsymbol{\xi}}^2\right) \\ &= S^{-(2\alpha+1)}\mathbf{F}_{\Delta}^{\alpha,\widetilde{\lambda}}(\widetilde{\tau},\mathfrak{d}_{\widetilde{R}}\vec{x},\vec{x}^*),\end{aligned}$$

with $\widetilde{R}=\frac{R}{S}>1>0$ and the new constants

$$\widetilde{\tau}=\tau S R^{2\alpha+2}S^{-(2\alpha+3)}=\tau\widetilde{R}^{2\alpha+3} \quad \text{and} \quad \widetilde{\lambda}=S^{2\alpha+3}\frac{(1+\lambda\tau)-R/S}{\widehat{\tau}R/S}=\frac{(1+\lambda\tau)-\widetilde{R}}{\widetilde{\tau}\widetilde{R}},$$

hence $\mathfrak{d}_{\widetilde{R}}\vec{x}$ minimizes $\mathbf{F}_{\Delta}^{\alpha,\widetilde{\lambda}}(\widetilde{\tau},\mathfrak{d}_{\widetilde{R}}\vec{x},\vec{x}^*)$.

So assume $S=1$ and $R>1$ in (4.59) from now on. Further introduce the functional $g:\mathfrak{x}_{\boldsymbol{\xi}}\times\mathbb{R}\to\mathbb{R}$

$$g(\vec{y},r):=\frac{1}{2}\left\|\mathfrak{d}_r\vec{y}-\vec{x}^*\right\|_{\boldsymbol{\xi}}^2 + r\tau\mathcal{F}_{\alpha,0}(\vec{y}) + \frac{r}{2}(1+\lambda\tau-r)\left\|\vec{y}\right\|_{\boldsymbol{\xi}}^2,$$

then by definition

$$\tau^{-1}g(\vec{y},1)=\mathbf{F}_{\Delta}^{\alpha,\lambda}(\tau,\vec{y},\vec{x}^*) \quad \text{and} \quad (\tau R^{2\alpha+2})^{-1}g(\vec{y},R)=\mathbf{F}_{\Delta}^{\alpha,\widehat{\lambda}}(\widehat{\tau},\mathfrak{d}_R\vec{y},\vec{x}^*). \tag{4.60}$$

For fixed $\vec{y}\in\mathfrak{x}_{\boldsymbol{\xi}}$, a straight-forward calculation shows that the derivative of $r\mapsto g(\vec{y},r)$ satisfies

$$\begin{aligned}\partial_r g(\vec{y},r) &= \langle\mathfrak{d}_r\vec{y}-\vec{x}^*,\vec{y}\rangle_{\boldsymbol{\xi}} + \mathcal{F}_{\alpha,0}(\vec{y}) - \frac{r}{2}\left\|\vec{y}\right\|_{\boldsymbol{\xi}}^2 + \frac{1}{2}(1+\lambda\tau-r)\left\|\vec{y}\right\|_{\boldsymbol{\xi}}^2 \\ &= -\langle\vec{x}^*,\vec{y}\rangle_{\boldsymbol{\xi}} + \mathcal{F}_{\alpha,0}(\vec{y}) + \frac{1}{2}(1+\lambda\tau)\left\|\vec{y}\right\|_{\boldsymbol{\xi}}^2 = \frac{1}{2}\left\|\vec{y}-\vec{x}^*\right\|_{\boldsymbol{\xi}}^2 - \frac{1}{2}\left\|\vec{x}^*\right\|_{\boldsymbol{\xi}}^2 + \mathcal{F}_{\alpha,0}(\vec{y}) + \frac{\lambda\tau}{2}\left\|\vec{y}\right\|_{\boldsymbol{\xi}}^2 \\ &= g(\vec{y},1) - \frac{1}{2}\left\|\vec{x}^*\right\|_{\boldsymbol{\xi}}^2.\end{aligned}$$

Hence, if $\vec{x}$ minimizes (4.58), then the same vector minimizes $\vec{y}\mapsto g(\vec{y},1)$ and furthermore $\vec{y}\mapsto\partial_r g(\vec{y},r)$ for any $r>0$. By integration one attains

$$\begin{aligned} & g(\vec{y},r)-g(\vec{y},1)=\int_1^r\partial_s g(\vec{y},s)\,\mathrm{d}s=(r-1)(g(\vec{y},1)-\frac{1}{2}\left\|\vec{x}^*\right\|_{\boldsymbol{\xi}}^2) \\ \Longrightarrow\ & g(\vec{y},r)=rg(\vec{y},1)-(r-1)\frac{1}{2}\left\|\vec{x}^*\right\|_{\boldsymbol{\xi}}^2\end{aligned}$$

for any $r>1$ and $\vec{y}\in\mathfrak{x}_{\boldsymbol{\xi}}$. This means especially that for arbitrary $r>1$, the function $g(\vec{y},r)$ is minimal if and only if $g(\vec{y},1)$ is so. In combination with (4.60) this proves that $\mathfrak{d}_R\vec{x}$ is a minimizer of (4.59). By integration of $\partial_s g(\vec{y},s)$ over $[r^{-1},1]$, $r>1$, one can analogously prove that if $\widehat{\vec{x}}\in\mathfrak{x}_{\boldsymbol{\xi}}$ is a minimizer of (4.59), the rescaled vector $\mathfrak{d}_{R^{-1}}\widehat{\vec{x}}$ has to be a minimizer of (4.58). ☐

Before we prove the claim of Theorem 4.3, let us introduce the rescaled discrete Barenblatt-profile. Define inductively for $n\geqslant 0$

$$S_\tau^0:=1,\quad S_\tau^n=(1+\tau_n)S_\tau^{n-1}. \tag{4.61}$$

Further take the minimizer $\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min} \in \mathfrak{x}_{\boldsymbol{\xi}}$ of the functional $\vec{\mathrm{x}} \mapsto \mathbf{H}_{\alpha,1}(\vec{\mathrm{x}})$. Then denote the scaled vector $\vec{\mathrm{b}}^n_{\Delta,\alpha,0} := \mathfrak{d}_{S^n_\tau}\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min}$ and define its corresponding density function $\mathrm{b}^n_{\Delta,\alpha,0} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{b}}^n_{\Delta,\alpha,0}]$. This function can be interpreted as a self-similar solution of (4.59) with initial density $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min}]$, $\widehat{\lambda} = 0$ and with time steps $\widehat{\tau}_n$ inductively defined by $\widehat{\tau}_n := \tau_n S^{n-1}_\tau (S^n_\tau)^{2\alpha+2}$.

Proof of Theorem 4.3. As already mentioned above, we define a sequence of functions S^n_τ inductively through (4.61) and declare a new partition of the time scale $[0,+\infty)$ by

$$\{0 = \hat{s}_0 < \hat{s}_2 < \ldots < \hat{s}_n < \ldots\}, \quad \text{where } \hat{s}_n := \sum_{k=1}^n \widehat{\tau}_k \text{ and } \widehat{\tau}_k := \tau_k S^{k-1}_\tau (S^k_\tau)^{2\alpha+2}, \tag{4.62}$$

and we write $\widehat{\boldsymbol{\tau}} = (\widehat{\tau}_1, \widehat{\tau}_2, \ldots)$. As a first consequence of the iterative character of the above object, we note that $(1+x) \leqslant e^x$ causes $S^n_\tau \leqslant e^{t_n}$ for any $n \geqslant 0$. Moreover,

$$\hat{s}_n = \sum_{k=1}^n \tau_k S^{k-1}_\tau (S^k_\tau)^{2\alpha+2} = \sum_{k=1}^n \tau_k (1+\tau_k)^{2\alpha+2} (S^{k-1}_\tau)^{2\alpha+3} \leqslant (1+\tau)^{2\alpha+2} \sum_{k=1}^n \tau_k e^{(2\alpha+3)t_{k-1}}.$$

This is an useful observation, insofar as the right-hand side is a lower sum of the integral $(1+\tau)^{2\alpha+2}\int_0^{t_n} e^{(2\alpha+3)s}\,\mathrm{d}s$, hence

$$\begin{aligned} \hat{s}_n &\leqslant (1+\tau)^{2\alpha+2}(2\alpha+3)^{-1}\big[e^{(2\alpha+3)t_n} - 1\big] \\ \Longrightarrow e^{-t_n} &\leqslant \big(1 + a_\tau \hat{s}_n(2\alpha+3)\big)^{-1/(2\alpha+3)}, \end{aligned} \tag{4.63}$$

with $a_\tau = (1+\tau)^{-(2\alpha+2)}$ converging to 1 as $\tau \to 0$. For a given solution $\vec{\mathrm{x}}_\Delta$ of (4.58) with $\lambda = 1$ and fixed discretization $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$, it is not difficult to check that the recursively defined sequence of vectors $\mathfrak{d}_{S^n_\tau}\vec{\mathrm{x}}^n_\Delta$ is a solution to (4.59) for $S = S^{n-1}_\tau$, $R = S^n_\tau$, $\widehat{\lambda} = 0$ and $\widehat{\tau} = \widehat{\tau}_n$ defined in (4.62). Henceforth, we write $\vec{\mathrm{x}}^n_{\widehat{\Delta}} = \mathfrak{d}_{S^n_\tau}\vec{\mathrm{x}}^n_\Delta$ with the discretization $\widehat{\Delta} = (\widehat{\boldsymbol{\tau}}; \boldsymbol{\xi})$. We can hence use the discrete scaling property of $\mathbf{H}_{\alpha,\lambda}$ and invoke (4.39) of Lemma 4.13, then

$$\begin{aligned} &(1+2\tau_n)(S^n_\tau)^{\frac{2\alpha-1}{2}}\big(\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^n_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^n_{\Delta,\alpha,0})\big) \leqslant (S^{n-1}_\tau)^{\frac{2\alpha-1}{2}}\big(\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^{n-1}_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^{n-1}_{\Delta,\alpha,0})\big) \\ \Longrightarrow\ &(1+2\tau_n)(1+\tau_n)^{\frac{2\alpha-1}{2}}\big(\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^n_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^n_{\Delta,\alpha,0})\big) \leqslant \mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^{n-1}_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^{n-1}_{\Delta,\alpha,0}) \\ \Longrightarrow\ &(1+2\tau_n)\big(\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^n_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^n_{\Delta,\alpha,0})\big) \leqslant \mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^{n-1}_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^{n-1}_{\Delta,\alpha,0}), \end{aligned} \tag{4.64}$$

where we used in the last step $(1+\tau_n) > 1$. As before in the proof of (4.14) of Theorem 4.1, this yields for any $n \geqslant 1$

$$\begin{aligned} \mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^n_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{b}}^n_{\Delta,\alpha,0}) &\leqslant \big(\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^0_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})\big)e^{-\frac{2t_n}{1+2\tau}} \\ &\leqslant \big(\mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}^0_{\widehat{\Delta}}) - \mathbf{H}_{\alpha,1}(\vec{\mathrm{x}}_{\boldsymbol{\xi}}^{\min})\big)\big(1 + a_\tau \hat{s}_n(2\alpha+3)\big)^{-\frac{2}{b_\tau(2\alpha+3)}}, \end{aligned}$$

with $b_\tau = 1 + 2\tau$, due to (4.63). Theorem 4.3 is proven, using $\mathrm{b}^n_{\Delta,\alpha,0} = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{b}}_{\Delta,\alpha,0}]$ and a Csiszar-Kullback inequality, see [**CJM**$^+$**01**, Theorem 30]. □

4.4. Numerical results

In view of the next chapter, the implementation of the numerical scheme is explained for both cases $\aleph = K \pm 1$, although the numerical experiments in this chapter are formulated only on $\Omega = \mathbb{R}$, hence $\aleph = K + 1$.

4.4.1. Non-uniform meshes. An equidistant mass grid — as used in the analysis above — leads to a high spatial resolution of regions where the values of u_Δ are large, but provides a very poor one if u_Δ is small. Since we are interested in regions of low density, and especially in the evolution of supports, it is natural to use a *non-equidistant* mass grid with an adapted spatial resolution, like we did in Section 2.2: The mass discretization of $\mathcal{M}$ is determined by a vector $\tilde{\boldsymbol{\xi}} = (\xi_0, \xi_1, \xi_2, \dots, \xi_{K-1}, \xi_K)$, with $0 = \xi_0 < \xi_1 < \cdots < \xi_{K-1} < \xi_K = M$ and we accordingly introduce $\delta_{k-\frac{1}{2}} = \xi_k - \xi_{k-1}$ for all $k = 1, \dots, K$. The piecewise constant density function $u \in \mathcal{P}_{\tilde{\boldsymbol{\xi}}}(\Omega)$ corresponding to a vector $\vec{\mathrm{x}} \in \mathbb{R}^\aleph$ is now given by $u = \mathbf{u}_{\tilde{\boldsymbol{\xi}}}[\vec{\mathrm{x}}]$ with $\vec{z} = \mathbf{z}_{\tilde{\boldsymbol{\xi}}}[\vec{\mathrm{x}}]$ that respects the convention as defined in (2.19), hence $z_{-\frac{1}{2}} = z_{K+\frac{1}{2}} = 0$ if $\aleph = K + 1$, or $z_{-\frac{1}{2}} = z_{\frac{1}{2}}$ and $z_{K+\frac{1}{2}} = z_{K-\frac{1}{2}}$ if $\aleph = K - 1$, respectively. The Wasserstein-like metric (and its corresponding norm) needs to be adapted as well: For this we introduce the diagonal matrix

$$\mathrm{W} \in \mathbb{R}^{\aleph \times \aleph}, \quad \text{with entries} \quad [\mathrm{W}]_{k,k} = \frac{1}{2}(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}),$$

where $k \in \mathbb{I}_K$ or $k \in \mathbb{I}_K^+$, respectively. Here we use the additional convention that

$$\delta_{-\frac{1}{2}} = \delta_{K+\frac{1}{2}} = 0.$$

The scalar product $\langle \cdot, \cdot \rangle_{\tilde{\boldsymbol{\xi}}}$ and its induced norm $\|\cdot\|_{\tilde{\boldsymbol{\xi}}}$ are then adapted in means of Section 2.2.2 using the diagonal matrix W. Hence the metric gradient of a function $f : \mathfrak{x}_{\tilde{\boldsymbol{\xi}}} \to \mathbb{R}$ at $\vec{\mathrm{x}} \in \mathfrak{x}_{\tilde{\boldsymbol{\xi}}}$ is given by $\nabla_{\tilde{\boldsymbol{\xi}}} f(\vec{\mathrm{x}}) = \mathrm{W}^{-1} \partial_{\vec{\mathrm{x}}} f(\vec{\mathrm{x}}) \in \mathbb{R}^\aleph$. Otherwise, we proceed as before just with the difference that $\Delta = (\tilde{\boldsymbol{\xi}}; \boldsymbol{\tau})$: The entropy is discretized by restriction, and the discretized information functional is the self-dissipation of the discretized entropy. Explicitly, the resulting fully discrete gradient flow equation attains the form

$$\frac{\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1}}{\tau_n} = -\nabla_{\tilde{\boldsymbol{\xi}}} \mathbf{F}_{\alpha,\lambda}(\vec{\mathrm{x}}_\Delta^n). \tag{4.65}$$

4.4.2. Implementation. To guarantuee the existence of an initial vector $\vec{\mathrm{x}}_\Delta^0 \in \mathfrak{x}_{\boldsymbol{\xi}}$ in case of $\aleph = K + 1$, which "reaches" any mass point of u^0, i.e. $[x_0^0, x_K^0] = \mathrm{supp}(u^0)$, one has to consider initial density functions u^0 with an interval as compact support. If $\aleph = K - 1$, hence $\Omega = (a, b)$ is bounded, we set $x_0^0 = a$ and $x_K^0 = b$.

In the numerical experiments that follows, our choice for the discretization of the initial condition is to use an equidistant grid $\vec{\mathrm{x}}^0$ with K vertices on Ω, $x_k^0 = x_0 + k(x_K - x_0)/K$, and an accordingly adapted mesh $\boldsymbol{\xi}$ on $\mathcal{M}$, with

$$\xi_k = \int_{x_0^0}^{x_k^0} u^0(y)\, \mathrm{d}y.$$

Starting from the initial condition $\vec{x}_\Delta^0$, the fully discrete solution is calculated inductively by solving the implicit Euler scheme (4.65) for given $\vec{x}_\Delta^{n-1}$. In each time step, a damped Newton iteration is performed, with the solution from the previous time step as initial guess.

4.4.3. Numerical experiments. For the first series of numerical experiments, we consider the initial density function

$$u^0 = \begin{cases} 0.25|\sin(x)| \cdot (0.5 + \mathbf{1}_{x>0}(x)), & x \in [-\pi, \pi], \\ 0, & x \in \mathbb{R}\backslash[-\pi, \pi]. \end{cases} \tag{4.66}$$

We further perform all experiments with $\alpha = 1$.

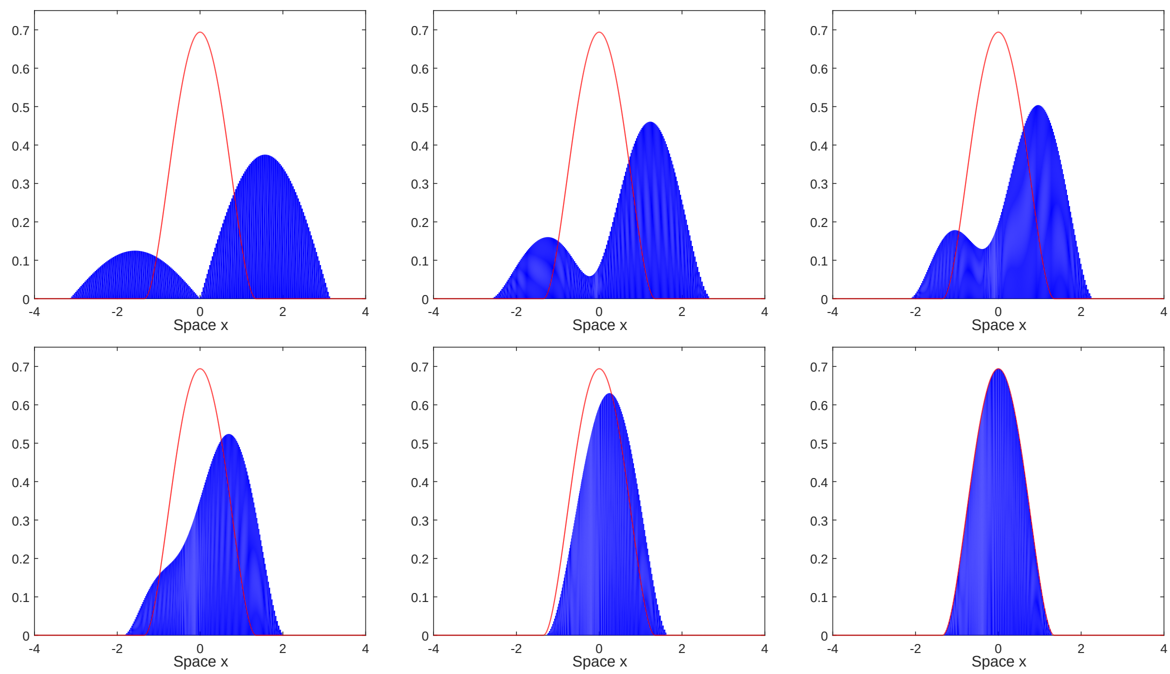


FIGURE 4.1. Evolution of a discrete solution u_Δ, evaluated at different times $t = 0, 0.05, 0.1, 0.15, 0.175, 0.25$ (from top left to bottom right). The red line is the corresponding Barenblatt-profile $\mathrm{b}_{\alpha,\lambda}$.

4.4.3.a. Evolution and exponential decay rates. As a first numerical experiment, we want to analyze the rate of decay in case of positive confinement $\lambda = 5$. For that purpose, consider the initial density function (4.66). Figure 4.1 shows the evolution of the discrete density u_Δ at times $t = 0.05, 0.1, 0.15, 0.175, 0.225$, using $K = 200$. The two initially separated clusters quickly merge, and finally change the shape towards a Barenblatt-profile (red line).

The exponential decay of the entropies $\mathbf{H}_{\alpha,\lambda}$ and $\mathbf{F}_{\alpha,\lambda}$ along the solution can be seen in Figure 4.2/left for $K = 25, 50, 100, 200$, where we observe the evolution for $t \in [0, 0.8]$. Note that we write $H_{\alpha,\lambda}(t) = \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^n)$ and $F_{\alpha,\lambda}(t) = \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^n)$ for $t \in (t_{n-1}, t_n]$, and set $H_{\alpha,\lambda}(0) = \mathbf{H}_{\alpha,\lambda}(\vec{x}_\Delta^0)$ and $F_{\alpha,\lambda}(0) = \mathbf{F}_{\alpha,\lambda}(\vec{x}_\Delta^0)$. As the picture shows, the rate of decay does not really depend on the choice of K, since the curves lie de facto on the top of each other. Furthermore, the curves are

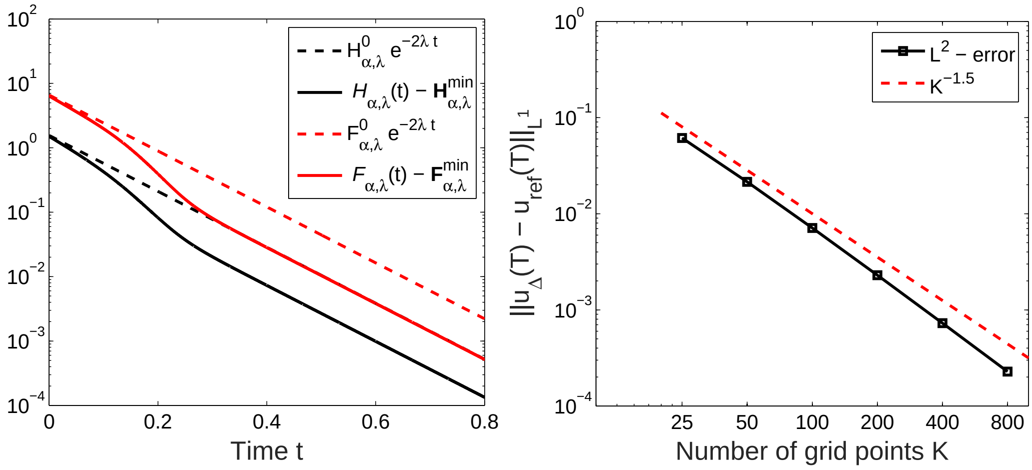


FIGURE 4.2. *Left*: numerically observed decay of $H_{\alpha,\lambda}(t) - \mathbf{H}^{\min}_{\alpha,\lambda}$ and $F_{\alpha,\lambda}(t) - \mathbf{F}^{\min}_{\alpha,\lambda}$ along a time period of $t \in [0, 0.8]$, using $K = 200$, in comparison to the upper bounds $\mathcal{H}^0_{\alpha,\lambda} \exp(-2\lambda t)$ and $\mathcal{F}^0_{\alpha,\lambda} \exp(-2\lambda t)$ with $\mathcal{H}^0_{\alpha,\lambda} := (\mathcal{H}_{\alpha,\lambda}(u^0) - \mathcal{H}_{\alpha,\lambda}(\mathrm{b}_{\alpha,\lambda}))$ and $\mathcal{F}^0_{\alpha,\lambda} := (\mathcal{F}_{\alpha,\lambda}(u^0) - \mathcal{F}_{\alpha,\lambda}(\mathrm{b}_{\alpha,\lambda}))$, respectively. *Right*: convergence of discrete minimizers $u^{\min}_{\boldsymbol{\xi}}$ with a rate of $K^{-1.5}$.

bounded from above by $(\mathcal{H}_{\alpha,\lambda}(u^0) - \mathcal{H}_{\alpha,\lambda}(\mathrm{b}_{\alpha,\lambda})) \exp(-2\lambda t)$ and $(\mathcal{F}_{\alpha,\lambda}(u^0) - \mathcal{F}_{\alpha,\lambda}(\mathrm{b}_{\alpha,\lambda})) \exp(-2\lambda t)$ at any time, respectively, as (4.14) and (4.15) from Theorem 4.1 postulate. One can even recognize that the decay rates are bigger at the beginning, until the moment when u_Δ finishes its "fusion" to one single Barenblatt-like curve. After that, the solution's evolution mainly consists of a transversal shift towards the stationary solution $\mathrm{b}_{\alpha,\lambda}$, which is reflected by a henceforth constant rate of approximately -2λ.

4.4.3.b. Rate of convergence towards equilibrium. Consider again a positive confinement with $\lambda = 5$ and the initial density as given in (4.66). Figure 4.3/right pictures the convergence of $u^{\min}_{\boldsymbol{\xi}}$ towards $\mathrm{b}_{\alpha,\lambda}$. We used several values for the spatial discretization, $K = 25, 50, 100, 200, 400, 800$, and plotted the L^2-error. The observed rate of convergence is $K^{-1.5}$.

4.4.3.c. Self-similar solutions. A very interesting consequence of Section 4.3.3 is, that the existence of self-similiar solutions bequeath from the continuous to the discrete case. In more detail, this means the following: Set $\lambda = 0$ and define for $t \in [0, +\infty)$

$$\mathrm{b}^*_{\alpha,0}(t,\cdot) := \mathfrak{d}_{R(t)} \mathrm{b}_{\alpha,1}, \quad \text{with} \quad R(t) := \big(1 + (2\alpha+3)t\big)^{1/(2\alpha+3)}, \tag{4.67}$$

then $\mathrm{b}^*_{\alpha,0}$ is a solution of the continuous problem (4.53) with $u^0 = \mathrm{b}^*_{\alpha,0}(0,\cdot)$. In the discrete setting, solutions to (4.65) with $\lambda = 0$ are inductively given by an initial vector $\vec{\mathrm{b}}^0_{\Delta,\alpha,0}$ with corresponding density $u^0_\Delta = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{b}}^0_{\Delta,\alpha,0}]$ that approaches $\mathrm{b}^*_{\alpha,0}(0,\cdot)$, and $\vec{\mathrm{b}}^n_{\Delta,\alpha,0} = \mathfrak{d}_{S^n_\tau} \vec{\mathrm{b}}^0_{\Delta,\alpha,0}$ with S^n_τ defined as in (4.61), for further $n \geqslant 1$.

As Figure 4.3 shows, the resulting sequence of densities u_Δ (black lines) approaches the continuous solution $\mathrm{b}^*_{\alpha,0}$ of (4.67) (red lines) astonishingly well, even if the discretization parameters

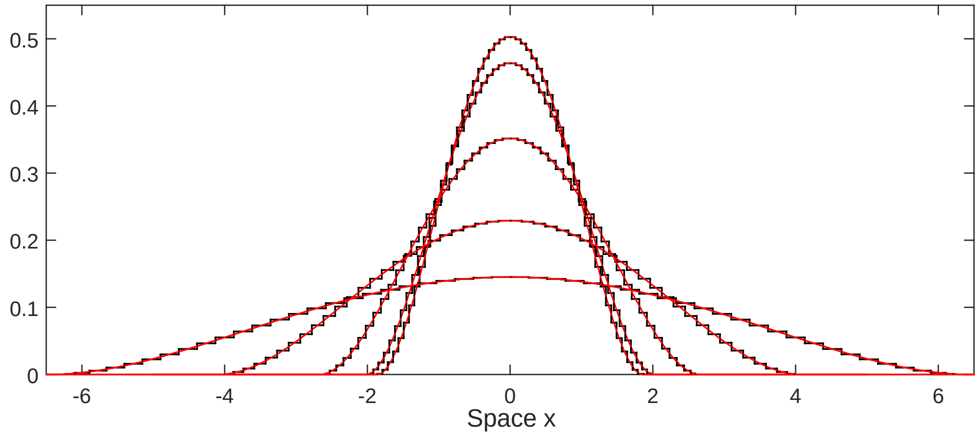


FIGURE 4.3. Snapshots of the densities $\mathrm{b}^*_{\alpha,0}(t,\cdot)$ (red lines) and u_Δ (black lines) for the initial condition $\mathrm{b}^*_{\alpha,0}(0,\cdot)$ at times $t = 0$ and $t = 0.1 \cdot 10^i$, $i = 0, \ldots, 3$, using $K = 50$ grid points and the time step size $\tau = 10^{-3}$.

are choosen quite rough. In this specific case we used $K = 50$ and $\tau = 10^{-3}$. The discrete and continuous solutions are evaluated at times $t = 0, 0.1, 1, 10, 100$.

CHAPTER 5

Proof of Theorem 4.4 — Fourth order DLSS equation

The content of this chapter is joint work with my PhD-supervisor Daniel Matthes. A preprint of the submitted paper can be found online [**MO14b**]. The paper is currently in revision.

5.1. Introduction

In the following chapter, we are going to study the numerical scheme from Chapter 4 for equation (4.1) in the special case that $\alpha = \frac{1}{2}$, $\lambda = 0$, and $\Omega = (a, b)$ is a bounded domain. More precisely, we consider the no-flux boundary problem

$$\partial_t u + \partial_x \left(u \, \partial_x \left(\frac{\partial_{xx}\sqrt{u}}{\sqrt{u}} \right) \right) = 0 \quad \text{for } x \in \Omega \text{ and } t > 0, \tag{5.1}$$

$$\partial_x u = 0, \quad u \, \partial_x \left(\frac{\partial_{xx}\sqrt{u}}{\sqrt{u}} \right) = 0 \quad \text{for } t > 0 \text{ and } x \in \partial\Omega, \tag{5.2}$$

$$u = u^0 \geqslant 0 \quad \text{at } t = 0. \tag{5.3}$$

Equation (5.1) is known as the *DLSS* equation, where the acronym refers to Derrida, Lebowitz, Speer and Spohn. Originally, the four authors derived (5.1) on the half line $(0, +\infty)$ to describe fluctuations of the interface between regions of predominantly positive and negative splins in the anchored Toom model [**DLSS91a**, **DLSS91b**]. This equation later rises from the field of semiconductor physics as a low-temperature, field-free limit of the well-established quantum drift diffusion model, see [**DMR05**, **Jün09**], and hence got more and more of great interest.

In view of the content in Subsection 4.1.1, let us remember that solutions to (5.1) can be interpreted as a L^2-Wasserstein gradient flow in the potential landscape of the so-called *Fisher information*,

$$\mathcal{F}(u) := \mathcal{F}_{1/2,0}(u) = \int_\Omega \left(\partial_x \sqrt{u(x)}\right)^2 \mathrm{d}x.$$

5.1.1. Description of the numerical scheme and main result. For the sake of completeness, let us shortly summarize the main aspects of the numerical scheme decribed in Section 4.1.2 with $\alpha = \frac{1}{2}$, and reformulate the main Theorem 4.4 from the previous chapter.

Fix a spatio-temporal discretization parameter $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$, where $\boldsymbol{\tau}$ consists of varying time step sizes $(\tau_1, \tau_2, \ldots)$ with $\tau_n \in (0, \tau]$, and $\boldsymbol{\xi} = (\xi_0, \ldots, \xi_K)$ provides an equidistant decomposition of the mass domain $\mathcal{M}$ with constant mesh size $\delta = MK^{-1}$. Further remember that $\mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$ is equipped with the discrete metric $\mathrm{d}_{\boldsymbol{\xi}}$ that is induced by the matrix $\mathrm{W} = \delta\mathbb{I} \in \mathbb{R}^{(K-1)\times(K-1)}$, as suggested in Section 2.2.2. Then the numerical scheme from Section 4.1.2 with $\alpha = \frac{1}{2}$ yields at any time step $n = 1, 2, \dots$ a recursively defined vector $\vec{\mathrm{x}}_\Delta^n \in \mathfrak{x}_{\boldsymbol{\xi}}$ that is a solution to

$$\frac{x_k^n - x_k^{n-1}}{\tau_n} = \frac{1}{2\delta}\left[(z_{k+\frac{1}{2}}^n)^2\left(\frac{z_{k+\frac{3}{2}}^n - 2z_{k+\frac{1}{2}}^n + z_{k-\frac{1}{2}}^n}{\delta^2}\right) - (z_{k-\frac{1}{2}}^n)^2\left(\frac{z_{k+\frac{1}{2}}^n - 2z_{k-\frac{1}{2}}^n + z_{k-\frac{3}{2}}^n}{\delta^2}\right)\right], \tag{5.4}$$

where the values $z_{\ell-\frac{1}{2}}^n \geqslant 0$ are defined as in (2.18) with convention (2.19). The problem in (5.4) is well-posed, remember Proposition 4.6, and a solution $\vec{\mathrm{x}}_\Delta^n$ of (5.4) is especially a solution to the implicit Euler time stepping

$$\frac{\vec{\mathrm{x}} - \vec{\mathrm{x}}_\Delta^{n-1}}{\tau_n} = -\nabla_{\boldsymbol{\xi}}\mathbf{F}(\vec{\mathrm{x}}). \tag{5.5}$$

Here we use the simplified notation $\mathbf{F} = \mathbf{F}_{1/2,0}$ for the *discretized Fisher information*, that is defined by the discrete auto-dissipation of the entropy $\mathbf{H}_{1/2,0}$. More precisely, we define the *discretized Boltzmann entropy* $\mathbf{H}$ as the restriction of the *Boltzmann entropy* $\mathcal{H}$,

$$\mathcal{H}(u) := 2\mathcal{H}_{1/2,0}(u) = \int_\Omega u(x)\ln\big(u(x)\big)\,\mathrm{d}x,$$

to the set of locally constant densities, i.e. $\mathbf{H}(\vec{\mathrm{x}}) = \mathcal{H}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}])$ for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. Then $\mathbf{H} = 2\mathbf{H}_{1/2,0}$ and $\mathbf{F}$ has the form

$$\mathbf{F}(\vec{\mathrm{x}}) = \frac{1}{4}\left\|\nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}})\right\|_{\boldsymbol{\xi}}^2 = \frac{\delta}{4}\sum_{\kappa\in\mathbb{I}_K^{1/2}}\left(\frac{z_{\kappa+\frac{1}{2}} - z_{\kappa-\frac{1}{2}}}{\delta}\right)^2.$$

Furthermore, remember the definition of the $K-1$ canonical unit vectors $\mathbf{e}_k \in \mathbb{R}^{K-1}$ in Example 2.3 in case of $\aleph = K-1$, then we obtain for the derivatives of $\mathbf{H}$

$$\partial_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}}) = \delta\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa\frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta} \tag{5.6}$$

$$\partial_{\vec{\mathrm{x}}}^2\mathbf{H}(\vec{\mathrm{x}}) = \delta\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2\left(\frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta}\right)\left(\frac{\mathbf{e}_{\kappa-\frac{1}{2}} - \mathbf{e}_{\kappa+\frac{1}{2}}}{\delta}\right)^T \tag{5.7}$$

and further

$$\nabla_{\boldsymbol{\xi}}\mathbf{F}(\vec{\mathrm{x}}) = \frac{\delta^{-2}}{2}\partial_{\vec{\mathrm{x}}}^2\mathbf{H}(\vec{\mathrm{x}})\partial_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}}) = \frac{1}{2}\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2\left(\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2}\right)\left(\frac{\mathbf{e}_{\kappa+\frac{1}{2}} - \mathbf{e}_{\kappa-\frac{1}{2}}}{\delta}\right). \tag{5.8}$$

The explicit representation of the gradient shows that the implicit Euler stepping in (5.5) equals (5.4).

The aim of this chapter is to verify the following convergence result for solutions of the numerical scheme in case of $\alpha = \frac{1}{2}$, $\lambda = 0$, and the bounded domain $\Omega = (a, b)$, as already stated in Theorem 4.4:

Theorem 5.1. *Let a nonnegative initial condition u^0 with $\mathcal{H}(u^0) < \infty$ be given. Choose initial conditions $\vec{x}^0_\Delta$ such that u^0_Δ converges to u^0 weakly as $\Delta \to 0$, and*

$$\overline{\mathcal{H}} := \sup_\Delta \mathbf{H}(\vec{x}^0_\Delta) < \infty \quad \text{and} \quad \lim_{\Delta\to 0}(\tau+\delta)\mathbf{F}(\vec{x}^0_\Delta) = 0. \tag{5.9}$$

For each Δ, construct a discrete approximation $\vec{x}_\Delta$ according to the procedure described in (4.11) *from Chapter 4 before, i.e. $\vec{x}^0_\Delta$ gives an approximation of the initial datum u^0 and $\vec{x}^n_\Delta$ solves* (5.4) *at any iteration $n \in \mathbb{N}$. Then there exist a subsequence with $\Delta \to 0$ and a limit function $u_* \in C((0,+\infty)\times\Omega)$ such that:*

- *$\{u_\Delta\}_{\boldsymbol{\tau}}$ converges to u_* locally uniformly on $(0,+\infty)\times\Omega$,*
- *$\sqrt{u_*} \in L^2_{\mathrm{loc}}((0,+\infty); H^1(\Omega))$,*
- *u_* satisfies the following weak formulation of* (5.1)*:*

$$\int_0^\infty \int_\Omega \partial_t\varphi\, u_* \,\mathrm{d}x\,\mathrm{d}t + \int_\Omega \varphi(0,x)u^0(x)\,\mathrm{d}x + \int_0^\infty N(u_*,\varphi)\,\mathrm{d}t = 0, \tag{5.10}$$

with

$$N(u,\varphi) := \frac{1}{2}\int_\Omega \partial_{xxx}\varphi\,\partial_x u + 4\partial_{xx}\varphi\left(\partial_x\sqrt{u}\right)^2\mathrm{d}x, \tag{5.11}$$

for every test function $\varphi \in C^\infty([0,+\infty)\times\Omega)$ that is compactly supported in $[0,+\infty)\times\overline{\Omega}$ and satisfies $\partial_x\varphi(t,a) = \partial_x\varphi(t,b) = 0$ for any $t \in [0,+\infty)$.

Remark 5.2.
1. Quality of convergence: *Since $\{u_\Delta\}_{\boldsymbol{\tau}}$ is piecewise constant in space and time, uniform convergence is obviously the best kind of convergence that can be achieved.*
2. Rate of convergence: *Numerical experiments with smooth initial data u^0 show that the rate of convergence is of order $\tau + \delta^2$, see Section 5.4.*
3. Initial condition: *We emphasize that our only hypothesis on u^0 is $\mathcal{H}(u^0) < \infty$, which allows the same general initial conditions as in [**GST09, JM08**]. If $\mathcal{F}(u^0)$ happens to be finite, and also* $\sup_\Delta \mathbf{F}(\vec{x}^0_\Delta) < \infty$, *then the uniform convergence of $\{u_\Delta\}_{\boldsymbol{\tau}}$ holds up to $t = 0$.*
4. No uniqueness: *Since our notion of solution is too weak to apply the uniqueness result from [**Fis13**], we cannot exclude that different subsequences of $\{u_\Delta\}_{\boldsymbol{\tau}}$ converge to different limits.*

The claims of this theorem are proven separately: The first two points about the convergence and the regularity of the limit curve are provided in the Propositions 5.11 and 5.13 from Section 5.2, whereas the validity of the weak formulation is shown in Proposition 5.14, Section 5.3.

In most papers from the literature attending the DLSS equation from a variational point of view, the domain Ω is considered to be $\mathbb{R}$ (or $\mathbb{R}^d$ for a higher-dimensional formulation of (5.1)), see for instance [**MMS09**], hence no boundary conditions appear. Similar Neumann boundary conditions as ours in (5.2) appear in [**GST09**], but instead of $u_x = 0$ the authors state the condition $(\sqrt{u})_x = 0$ on $\partial\Omega$. Therefore we give a short justification why the definition of the weak formulation in Theorem 5.1 suits problem (5.1) with boundary conditions (5.2): Assume therefore $u : [0,+\infty)\times\Omega \to [0,+\infty)$ to be a sufficient smooth solution of (5.10) which satisfies the boundary conditions (5.2). Then for any test function that complies with the requirements in Theorem 5.1, repetetive integration by parts yields

$$\begin{aligned} 2N(u,\varphi) &= \int_\Omega \partial_x u \partial_{xxx}\varphi + 4(\partial_x\sqrt{u})^2\partial_{xx}\varphi \,\mathrm{d}x = \big[\partial_x u\partial_{xx}\varphi\big]_{x=a}^{x=b} + \int_\Omega \big(-\partial_{xx}u + 4(\partial_x\sqrt{u})^2\big)\,\partial_{xx}\varphi\,\mathrm{d}x \\ &\overset{(5.2)}{=} \big[\,\big(-\partial_{xx}u + 4(\partial_x\sqrt{u})^2\big)\,\partial_x\varphi\big]_{x=a}^{x=b} + \int_\Omega \partial_x\,\big(\partial_{xx}u - 4(\partial_x\sqrt{u})^2\big)\,\varphi_x\,\mathrm{d}x \\ &= \big[\partial_x\big(u\partial_{xx}\ln u\big)\varphi\big]_{x=a}^{x=b} - \int_\Omega \partial_{xx}\big(u(\partial_{xx}\ln u)\big)\varphi\,\mathrm{d}x \overset{(5.2)}{=} -\int_\Omega \partial_{xx}\big(u\partial_{xx}\ln u\big)\varphi\,\mathrm{d}x, \end{aligned}$$

where we use the following identity:

$$\partial_x\big(u\partial_{xx}\ln u\big) = 2u\partial_x\left(\frac{\partial_{xx}\sqrt{u}}{\sqrt{u}}\right). \tag{5.12}$$

A further integration by parts with respect to the time derivative then shows that u is a solution to (5.1).

5.1.2. Key estimates. In what follows, we give a formal outline for the derivation of the main a priori estimates on the fully discrete solutions.

In the continuous theory of well-posedness of (5.1), two crucial a priori estimates are provided by the dissipation of the Fisher information $\mathcal{F}$ and the Boltzmann entropy $\mathcal{H}$. Formally, the corresponding estimates are easily derived by an integration by parts:

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(u) = 2\int_\Omega \partial_x\sqrt{u}\,\partial_x\left(\frac{\partial_x\left(u\,\partial_x\left(\frac{\partial_{xx}\sqrt{u}}{\sqrt{u}}\right)\right)}{\sqrt{u}}\right)\mathrm{d}x = 2\int_\Omega u\left[\partial_x\left(\frac{\partial_{xx}\sqrt{u}}{\sqrt{u}}\right)\right]^2\mathrm{d}x \tag{5.13}$$

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(u) = \frac{1}{2}\int_\Omega (\ln u + 1)\,\partial_{xx}(u\,\partial_{xx}\ln u)\,\mathrm{d}x = \frac{1}{2}\int_\Omega u(\partial_{xx}\ln u)^2\,\mathrm{d}x, \tag{5.14}$$

where we again use the identity in (5.12).

In view of our numerical scheme, it turns out that the explicit estimate in (5.13) is useless for our purpose. In fact, we are not able to give a useful meaning to the right-hand side of (5.13) in the discrete setting. The only information from (5.13) that finds a discrete counterpart in the later calculations is that $\mathcal{F}$ is a Lyapunov functional, but this is a trivial conclusion from the gradient flow structure of (5.1). An even stronger implication from the gradient flow structure is, that each solution $t \mapsto u(t)$ is globally Hölder-$\frac{1}{2}$-continuous with respect to $\mathcal{W}_2$, see [**AGS05**]. Fortunately, these properties are inherited to our discretization, remember Section 4.2.2.b from Chapter 4, where we show that solutions to (5.4) are gradient flows of the flow potential $\mathbf{F}$ (which approximates $\mathcal{F}$ in a certain sense) with respect to the particular metric $\mathrm{d}_{\boldsymbol{\xi}}$ on the space of piecewise constant density functions $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$.

Conversely, an interpretation of (5.14) in terms of our discretization is possible. Using Lagrangian coordinates and $\mathrm{Z} = u \circ \mathrm{X}$, the above expression turns into

$$\frac{1}{2}\int_\Omega u(\partial_{xx}\ln u)^2\,\mathrm{d}x = \frac{1}{2}\int_{\mathcal{M}} \mathrm{Z}^2\,(\partial_{\xi\xi}\mathrm{Z})^2\,\mathrm{d}\xi,$$

which we shall eventually work with, see Lemma 5.5. The formulation of an H^2-estimate would require a global $C^{1,1}$-interpolation of the piecewise constant densities u_Δ that respects positivity, which seems impractical. Instead, we settle for a control on the total variation of the first derivative $\partial_x\sqrt{\widehat{u}_\Delta}$ of a simple locally affine interpolation $\widehat{u}_\Delta$, see Proposition 5.8. This TV-control is a perfect replacement for the H^2-estimate in (5.14) and is the source for compactness, see Proposition 5.13.

5.1.3. Spatial interpolations. In the following, we fix a Lagrangian vector $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ and denote its corresponding density $\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ by u and its Lagrangian map $\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ by $\mathbf{X}$. We furthermore write $\vec{\mathrm{z}} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$. Recall that $u \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ is piecewise constant with respect to the (non-uniform) grid $(a, x_1, \ldots, x_{K-1}, b)$. To facilitate the study of convergence of weak derivatives in the forthcoming sections, we introduce also *piecewise affine* interpolations $\widehat{z} : \mathcal{M} \to (0, +\infty)$ and $\widehat{u} : \overline{\Omega} \to (0, +\infty)$.

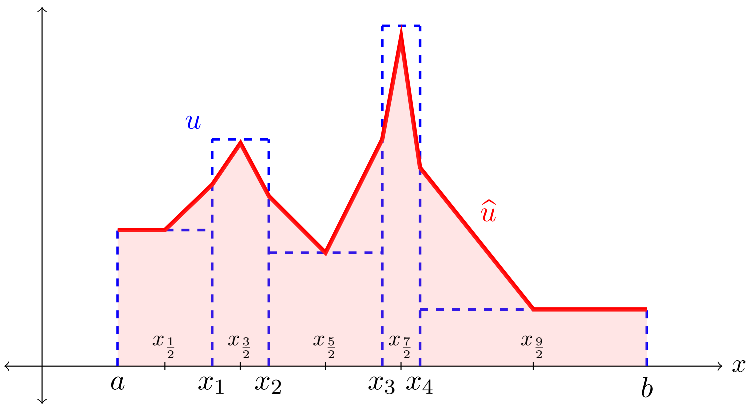


FIGURE 5.1. A density $u \in \mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ (dashed line in blue) with its associated piecewise affine interpolation $\widehat{u}$ (red line).

In addition to $\xi_k = k\delta$ for $k \in \mathbb{I}_K$, introduce the intermediate points $\xi_\kappa = \kappa\delta$ for $\kappa \in \mathbb{I}_K^{1/2}$. Accordingly, introduce the intermediate values for the vectors $\vec{\mathrm{x}}$ and $\vec{\mathrm{z}}$:

$$
\begin{aligned}
x_\kappa &= \frac{1}{2}\left(x_{\kappa+\frac{1}{2}} + x_{\kappa-\frac{1}{2}}\right) \quad \text{for } \kappa \in \mathbb{I}_K^{1/2}, \\
z_k &= \frac{1}{2}\left(z_{k+\frac{1}{2}} + z_{k-\frac{1}{2}}\right) \quad \text{for } k \in \mathbb{I}_K^{+}.
\end{aligned}
\tag{5.15}
$$

Now define

- $\widehat{z} : \mathcal{M} \to \mathbb{R}$ as the piecewise affine interpolation of the values $(z_{\frac{1}{2}}, z_{\frac{3}{2}}, \ldots, z_{K-\frac{1}{2}})$ with respect to the equidistant grid $(\xi_{\frac{1}{2}}, \xi_{\frac{3}{2}}, \ldots, \xi_{K-\frac{1}{2}})$, and
- $\widehat{u} : [a, b] \to \mathbb{R}$ as the piecewise affine function with

$$\widehat{u} \circ \mathbf{X} = \widehat{z}. \tag{5.16}$$

Our convention is that $\widehat{z}(\xi) = z_{\frac{1}{2}}$ for $0 \leqslant \xi \leqslant \delta/2$ and $\widehat{z}(\xi) = z_{K-\frac{1}{2}}$ for $M - \delta/2 \leqslant \xi \leqslant M$, and accordingly $\widehat{u}(x) = z_{\frac{1}{2}}$ for $x \in [a, x_{\frac{1}{2}}]$ and $\widehat{u}(x) = z_{K-\frac{1}{2}}$ for $x \in [x_{K-\frac{1}{2}}, b]$. The definitions have been made such that

$$x_k = \mathbf{X}(\xi_k), \quad z_k = \widehat{z}(\xi_k) = \widehat{u}(x_k) \quad \text{for all } k \in \mathbb{I}_K \cup \mathbb{I}_K^{1/2}. \tag{5.17}$$

Notice that $\widehat{u}$ is piecewise affine with respect to the "double grid" $(a, x_{\frac{1}{2}}, x_1, \ldots, x_{K-\frac{1}{2}} b)$, but in general not with respect to the subgrid $(a, x_1, \ldots, x_{K-1}, b)$. By direct calculation, we obtain

$$\begin{aligned} \partial_x \widehat{u}\big|_{(x_{k-\frac{1}{2}}, x_k)} &= \frac{z_k - z_{k-\frac{1}{2}}}{x_k - x_{k-\frac{1}{2}}} = \frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{x_k - x_{k-1}} = z_{k-\frac{1}{2}} \frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \quad \text{for } k \in \mathbb{I}_K \backslash \{0\}, \\ \partial_x \widehat{u}\big|_{(x_k, x_{k+\frac{1}{2}})} &= \frac{z_{k+\frac{1}{2}} - z_k}{x_{k+\frac{1}{2}} - x_k} = \frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{x_{k-1} - x_k} = z_{k+\frac{1}{2}} \frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \quad \text{for } k \in \mathbb{I}_K \backslash \{K\}. \end{aligned} \tag{5.18}$$

Trivially, we also have that $\partial_x \widehat{u}$ vanishes identically on the intervals $(a, x_{\frac{1}{2}})$ and $(x_{K-\frac{1}{2}}, b)$.

5.1.4. A discrete Sobolev-type estimate. The following inequality plays a key role in our analysis, especially for the control of error terms in the weak formulation later in Section 5.3. Recall the conventions (2.19) that $z_{-\frac{1}{2}} = z_{\frac{1}{2}}$ and $z_{K+\frac{1}{2}} = z_{K-\frac{1}{2}}$.

Lemma 5.3. *For any* $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$,

$$\delta \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right)^4 \leqslant 9\delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^2 \left(\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2} \right)^2. \tag{5.19}$$

Proof. Due to the conventions on $\vec{z}$, one can even sum over all $k \in \mathbb{I}_K$ on the left-hand side of (5.19). By "summation by parts"

$$\begin{aligned} (A) = \delta \sum_{k \in \mathbb{I}_K} \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right)^4 &= \sum_{k \in \mathbb{I}_K} (z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}) \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right)^3 \\ &= - \sum_{k \in \mathbb{I}_K^{1/2}} z_\kappa \left[\left(\frac{z_{\kappa+1} - z_\kappa}{\delta} \right)^3 - \left(\frac{z_\kappa - z_{\kappa-1}}{\delta} \right)^3 \right] \end{aligned}$$

Using the elementary identity $(p^3 - q^3) = (p - q)(p^2 + q^2 + pq)$ for arbitrary real numbers p, q, and Young's inequality, one obtains further

$$\begin{aligned} (A) &= -\delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa \frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2} \times \\ &\quad \times \left[\left(\frac{z_{\kappa+1} - z_\kappa}{\delta} \right)^2 + \left(\frac{z_\kappa - z_{\kappa-1}}{\delta} \right)^2 + \left(\frac{z_{\kappa+1} - z_\kappa}{\delta} \right) \left(\frac{z_\kappa - z_{\kappa-1}}{\delta} \right) \right] \\ &\leqslant \frac{3\delta}{2} \sum_{\kappa \in \mathbb{I}_K^{1/2}} \left| z_\kappa \frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2} \right| \left[\left(\frac{z_{\kappa+1} - z_\kappa}{\delta} \right)^2 + \left(\frac{z_\kappa - z_{\kappa-1}}{\delta} \right)^2 \right] \\ &\leqslant \frac{3}{2} \left(\delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^2 \left[\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2} \right]^2 \right)^{1/2} \left(4\delta \sum_{k \in \mathbb{I}_K} \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right)^4 \right)^{1/2}. \end{aligned}$$

Note that the last sum above is again equal to (A), hence deviding both sides with $(A)^{1/2}$ yields the desired estimate. □

5.2. A priori estimates and compactness

Throughout this section, we consider a sequence $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ of discretization parameters such that $\delta \to 0$ and $\tau \to 0$ in the limit, formally denoted by $\Delta \to 0$. We assume that a fully discrete solution $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}_\Delta^0, \vec{\mathrm{x}}_\Delta^1, \ldots)$ is given for each Δ-mesh, defined by (5.4). The sequences u_Δ, $\widehat{u}_\Delta$, $\widehat{z}_\Delta$ and X_Δ of spatial interpolations are defined from the respective $\vec{\mathrm{x}}_\Delta$ accordingly. For notational simplification, we write the entries of the vectors $\vec{\mathrm{x}}_\Delta^n$ and $\vec{\mathrm{z}}_\Delta^n$ and their intermediate values defined in (5.15) as x_k, x_κ and z_k, z_κ, respectively, whenever there is no ambiguity in the choice of Δ and the time step n.

For the sequence of initial conditions $\vec{\mathrm{x}}_\Delta^0$, we assume that $\widehat{u}_\Delta^0 \to u^0$ weakly in $L^1(\Omega)$, that there is some finite $\overline{\mathcal{H}}$ with

$$\mathbf{H}(\vec{\mathrm{x}}_\Delta^0) \leqslant \overline{\mathcal{H}} \quad \text{for all } \Delta, \tag{5.20}$$

and that

$$(\tau + \delta)\mathbf{F}(\vec{\mathrm{x}}_\Delta^0) \to 0 \quad \text{as } \Delta \to 0. \tag{5.21}$$

5.2.1. Energy and entropy dissipation. The following estimates for the discrete Fisher information $\mathbf{F}$ are immediate conclusions from Lemma 2.4.

Lemma 5.4. *The discrete Fisher information* $\mathbf{F}$ *is monotone, i.e.* $\mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{F}(\vec{\mathrm{x}}_\Delta^{n-1})$, *and furthermore*

$$\left\|\vec{\mathrm{x}}_\Delta^{\overline{n}} - \vec{\mathrm{x}}_\Delta^{\underline{n}}\right\|_{\boldsymbol{\xi}}^2 \leqslant 2\mathbf{F}(\vec{\mathrm{x}}_\Delta^0)\,(t_{\overline{n}} - t_{\underline{n}}) \quad \text{for all } \overline{n} \geqslant \underline{n} \geqslant 0, \tag{5.22}$$

$$\sum_{n=1}^\infty \tau_n \left\| \frac{\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1}}{\tau_n} \right\|_{\boldsymbol{\xi}}^2 = \sum_{n=1}^\infty \tau_n \left\|\nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n)\right\|_{\boldsymbol{\xi}}^2 \leqslant 2\mathbf{F}(\vec{\mathrm{x}}_\Delta^0). \tag{5.23}$$

The key to our convergence analysis is a refined a priori estimate, which follows from the dissipation of the entropy $\mathbf{H}$ along the fully discrete solution.

Lemma 5.5. *The entropy* $\mathbf{H}$ *is monotone, i.e.,* $\mathbf{H}(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{H}(\vec{\mathrm{x}}_\Delta^{n-1})$, *and furthermore*

$$\sum_{n=1}^\infty \tau_n \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} (z_\kappa^n)^2 \left(\frac{z_{\kappa+1}^n - 2z_\kappa^n + z_{\kappa-1}^n}{\delta^2} \right)^2 \leqslant 2\overline{\mathcal{H}}. \tag{5.24}$$

Proof. By convexity of $\mathbf{H}$ and the discrete evolution (5.5), we have

$$\mathbf{H}(\vec{\mathrm{x}}_\Delta^{n-1}) - \mathbf{H}(\vec{\mathrm{x}}_\Delta^n) \geqslant \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{x}}_\Delta^n \right\rangle_{\boldsymbol{\xi}} = \tau_n \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}}$$

for each $n \geqslant 1$. Evaluate the (telescopic) sum with respect to n and use that $\mathbf{H}(\vec{\mathrm{x}}) \geqslant 0$ for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ to obtain

$$\sum_{n=1}^\infty \tau_n \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \leqslant \mathbf{H}(\vec{\mathrm{x}}_\Delta^0).$$

It remains to make the scalar product explicit, using (5.6) and (5.8). For any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ one obtains

$$\begin{aligned}&\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}), \nabla_{\boldsymbol{\xi}}\mathbf{F}(\vec{\mathrm{x}})\rangle_{\boldsymbol{\xi}}\\ =&\frac{\delta}{2}\sum_{\kappa\in\mathbb{I}_K^{1/2},\,k\in\mathbb{I}_K^+} z_\kappa^2\left(\frac{z_{\kappa+1}-2z_\kappa+z_{\kappa-1}}{\delta^2}\right)\left(\frac{z_{k+\frac12}-z_{k-\frac12}}{\delta}\right)\left(\frac{\mathbf{e}_{\kappa+\frac12}-\mathbf{e}_{\kappa-\frac12}}{\delta}\right)^T\mathbf{e}_k\\ =&\frac{\delta}{2}\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2\Big(\frac{z_{\kappa+1}-2z_\kappa+z_{\kappa-1}}{\delta^2}\Big)^2,\end{aligned}$$

where we use that $z_{-\frac12} = z_{\frac12}$ and $z_{K+\frac12} = z_{K-\frac12}$, according to our convention (2.19) in case of $\aleph = K-1$. □

We draw several conclusions from (5.24). The first is an a priori estimate on the ξ-derivative of the affine functions $\widehat{z}_\Delta^n$, that is

$$\sum_{n=1}^{\infty}\tau_n\big\|\partial_\xi\widehat{z}_\Delta^n\big\|_{L^4(\mathcal{M})}^4 \leqslant 18\overline{\mathcal{H}}. \tag{5.25}$$

The estimate is an immediate consequence of (5.19) and (5.24).

Remark 5.6. *Morally, a bound on $\partial_\xi\widehat{z}$ in $L^4(\mathcal{M})$ corresponds to a bound on $\partial_x\sqrt[4]{\widehat{u}}$ in $L^4(\Omega)$.*

The a priori estimate (5.25) is the basis for almost all of the further estimates. For instance, the following control on the oscillation of the z-values at neighboring grid points is a consequence of (5.25).

Lemma 5.7. *One has*

$$\sum_{n=1}^{\infty}\tau_n\delta\sum_{k\in\mathbb{I}_K^+}\bigg[\Big(\frac{z_{k+\frac12}^n}{z_{k-\frac12}^n}-1\Big)^4+\Big(\frac{z_{k-\frac12}^n}{z_{k+\frac12}^n}-1\Big)^4\bigg] \leqslant 36(b-a)^4\overline{\mathcal{H}}. \tag{5.26}$$

Moreover, given $T>0$, then for each $N_{\boldsymbol{\tau}}\in\mathbb{N}$ with $T\leqslant\sum_{n=0}^{N_{\boldsymbol{\tau}}}\tau_n\leqslant(T+1)$, one obtains

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\delta\sum_{k\in\mathbb{I}_K^+}\bigg[\Big(\frac{z_{k+\frac12}^n}{z_{k-\frac12}^n}-1\Big)^2+\Big(\frac{z_{k-\frac12}^n}{z_{k+\frac12}^n}-1\Big)^2\bigg] \leqslant 6\sqrt{2}(b-a)^2(T+1)^{1/2}\overline{\mathcal{H}}^{1/2}\delta^{1/2}. \tag{5.27}$$

Proof. Due to the definition of $\mathbf{z}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, one has that $z_\kappa \geqslant \delta/(b-a)$ for all κ. Consider the first term in the inner summation in (5.26):

$$\delta\sum_{k\in\mathbb{I}_K^+}\Big(\frac{z_{k+\frac12}^n}{z_{k-\frac12}^n}-1\Big)^4 = \delta\sum_{k\in\mathbb{I}_K^+}\Big(\frac{\delta}{z_{k-\frac12}^n}\Big)^4\Big(\frac{z_{k+\frac12}^n-z_{k-\frac12}^n}{\delta}\Big)^4 \leqslant (b-a)^4\|\widehat{z}_\Delta^n\|_{L^4(\Omega)}^4.$$

The same estimate is attained for the second term. The claim (5.26) is now directly deduced from (5.25) above. The proof of the second claim (5.27) is similar, using the Cauchy-Schwarz inequality instead of the modulus estimate:

$$\delta\sum_{k\in\mathbb{I}_K^+}\Big(\frac{z_{k+\frac12}^n}{z_{k-\frac12}^n}-1\Big)^2 = \delta\sum_{k\in\mathbb{I}_K^+}\Big(\frac{\delta}{z_{k-\frac12}^n}\Big)^2\Big(\frac{z_{k+\frac12}^n-z_{k-\frac12}^n}{\delta}\Big)^2 \leqslant \left(\delta\sum_{k\in\mathbb{I}_K^+}\Big(\frac{\delta}{z_{k-\frac12}^n}\Big)^4\right)^{1/2}\|\widehat{z}_\Delta^n\|_{L^4(\Omega)}^2.$$

Use estimate (A.4), sum over $n = 1, \ldots, N_{\boldsymbol{\tau}}$, and apply the Cauchy-Schwarz inequality to this second summation. This yields

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac{1}{2}}^n}{z_{k-\frac{1}{2}}^n} - 1 \right)^2 \leqslant \delta^{1/2} (b-a)^2 \left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \right)^{1/2} \left(\sum_{n=1}^{\infty} \tau_n \| \widehat{z}_\Delta^n \|_{L^4(\Omega)}^4 \right)^{1/2} .$$

Invoking again (5.25) and recalling that $\sum_{n=0}^{N_{\boldsymbol{\tau}}} \tau_n \leqslant (T+1)$, we arrive at (5.27). □

5.2.2. Bound on the total variation. We are now going to prove the main consequence from the entropy dissipation $\mathbf{H}(\vec{x}_\Delta^n) \leqslant \mathbf{H}(\vec{x}_\Delta^0)$, namely a control on the total variation of $\sqrt{\widehat{u}_\Delta^n}$. This estimate is the key ingredient for obtaining strong compactness in Proposition 5.13. For this purpose, recall that an appropriate definition of the total variation of a function $f \in L^1(\Omega)$ is given by (1.15), i.e.

$$\mathrm{TV}\,[f] = \sup \left\{ \sum_{j=1}^{J-1} |f(r_{j+1}) - f(r_j)| \;:\; J \in \mathbb{N},\, a < r_1 < r_2 < \cdots < r_J < b \right\}. \tag{5.28}$$

Proposition 5.8. *One has that*

$$\sum_{n=1}^{\infty} \tau_n \mathrm{TV} \left[\partial_x \sqrt{\widehat{u}_\Delta^n} \right]^2 \leqslant 20(b-a)\overline{\mathcal{H}}. \tag{5.29}$$

Proof. Fix n. Observe that $\sqrt{\widehat{u}_\Delta^n}$ is smooth on Ω except for the points $x_{\frac{1}{2}}, x_1, \ldots, x_{K-\frac{1}{2}}$, with derivatives given by

$$\partial_x \sqrt{\widehat{u}_\Delta^n} = \frac{1}{2\sqrt{\widehat{u}_\Delta^n}} \partial_x \widehat{u}_\Delta^n, \quad \partial_{xx} \sqrt{\widehat{u}_\Delta^n} = -\frac{1}{4\sqrt{\widehat{u}_\Delta^n}^3} \left(\partial_x \widehat{u}_\Delta^n \right)^2 \leqslant 0. \tag{5.30}$$

Therefore, $\partial_x \sqrt{\widetilde{u}_\Delta^n}$ is monotonically decreasing in between the (potential) jump discontinuities at the points $x_{\frac{1}{2}}, x_1, \ldots, x_{K-\frac{1}{2}}$. Furthermore, recall that

$$\partial_x \sqrt{\widehat{u}_\Delta^n}(x) = 0 \quad \text{for all } x \in (a, a+\delta/2) \text{ and all } x \in (b-\delta/2, b). \tag{5.31}$$

It follows that the supremum in (5.28) can be realized (in the limit $\varepsilon \downarrow 0$) for a sequence of just $J = 2(2K-1)$ many points r_j^ε, chosen as follows:

$$r_{2i-1}^\varepsilon = x_{i/2} - \varepsilon \quad \text{and} \quad r_{2i}^\varepsilon = x_{i/2} + \varepsilon, \quad \text{for } i = 1, \ldots, 2K-1.$$

On the one hand,

$$\lim_{\varepsilon \downarrow 0} \left| \partial_x \sqrt{\widehat{u}_\Delta}(r_{2i-1}^\varepsilon) - \partial_x \sqrt{\widehat{u}_\Delta}(r_{2i}^\varepsilon) \right| = \left| \left[\!\left[\partial_x \sqrt{\widehat{u}_\Delta^n} \right]\!\right]_{x_{i/2}} \right|. \tag{5.32}$$

On the other hand, since $\partial_x\sqrt{\widehat{u}^n_\Delta}$ is monotone decreasing in between r^ε_{2i} and r^ε_{2i+1}, and vanishes near the boundary by (5.31), we have that

$$\lim_{\varepsilon\downarrow 0}\sum_{i=1}^{2K-2}\Big(\partial_x\sqrt{\widehat{u}^n_\Delta}(r^\varepsilon_{2i})-\partial_x\sqrt{\widehat{u}^n_\Delta}(r^\varepsilon_{2i+1})\Big)=\lim_{\varepsilon\downarrow 0}\sum_{i=1}^{2K-1}\Big(\partial_x\sqrt{\widehat{u}^n_\Delta}(r^\varepsilon_{2i})-\partial_x\sqrt{\widehat{u}^n_\Delta}(r^\varepsilon_{2i-1})\Big)$$
$$\leqslant\sum_{k\in\mathbb{I}_K^+}\Big|\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_k}\Big|+\sum_{\kappa\in\mathbb{I}_K^{1/2}}\Big|\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_\kappa}\Big|. \tag{5.33}$$

Summarizing (5.32) and (5.33), we obtain the estimate

$$\mathrm{TV}\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\leqslant 2\sum_{k\in\mathbb{I}_K^+}\Big|\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_k}\Big|+2\sum_{\kappa\in\mathbb{I}_K^{1/2}}\Big|\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_\kappa}\Big|. \tag{5.34}$$

Let us omit the index n in the forthcoming calculation. In view of (5.18), we have that

$$\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_k}=\frac{1}{2\sqrt{z_k}}\frac{(z_{k-\frac12}-z_{k+\frac12})^2}{\delta}\quad\text{for } k\in\mathbb{I}_K^+,$$
$$\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_\kappa}=\frac{1}{2}\sqrt{z_\kappa}\,\frac{z_{\kappa+1}-2z_\kappa+z_{\kappa-1}}{\delta}\quad\text{for } \kappa\in\mathbb{I}_K^{1/2}.$$

Accordingly, using that $1/z_k\leqslant(1/z_{k+\frac12}+1/z_{k-\frac12})/2$ by the arithmetic-harmonic mean inequality,

$$\sum_{k\in\mathbb{I}_K^+}\Big|\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_k}\Big|=\frac{\delta}{2}\sum_{k\in\mathbb{I}_K^+}\frac{(z_{k-\frac12}-z_{k+\frac12})^2}{\delta^2}\cdot\frac{1}{\sqrt{z_k}}$$
$$\leqslant\frac12\left(\delta\sum_{k\in\mathbb{I}_K^+}\left[\frac{z_{k-\frac12}-z_{k+\frac12}}{\delta}\right]^4\right)^{1/2}\left(\sum_{k\in\mathbb{I}_K^+}\frac{\delta}{z_k}\right)^{1/2}=\frac12\|\partial_\xi\widehat{z}^n_\Delta\|^2_{L^4(\Omega)}(b-a)^{1/2}, \tag{5.35}$$

and also

$$\sum_{\kappa\in\mathbb{I}_K^{1/2}}\Big|\Big[\!\Big[\partial_x\sqrt{\widehat{u}^n_\Delta}\Big]\!\Big]_{x_\kappa}\Big|=\frac{\delta}{2}\sum_{\kappa\in\mathbb{I}_K^{1/2}}z_\kappa\left|\frac{z_{\kappa+1}-2z_\kappa+z_{\kappa-1}}{\delta^2}\right|\cdot\frac{1}{\sqrt{z_\kappa}}$$
$$\leqslant\frac12\left(\delta\sum_{\kappa\in\mathbb{I}_K^{1/2}}z_\kappa^2\left[\frac{z_{\kappa+1}-2z_\kappa+z_{\kappa-1}}{\delta^2}\right]^2\right)^{1/2}(b-a)^{1/2}. \tag{5.36}$$

Combine (5.35) with the $L^4(\mathcal{M})$-bound from (5.25), and (5.36) with the entropy dissipation inequality (5.24). Finally insert this into (5.34) to obtain the claim (5.29). □

5.2.3. Convergence of time interpolants. Recall that we require the a priori bound (5.20) on the initial entropy, but only (5.21) on the initial Fisher information. This estimate improves over time.

Lemma 5.9. *For every $n \geqslant 1$, one has that*

$$\mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \leqslant 3\overline{\alpha}_1 \left(\frac{M}{2}\overline{\mathcal{H}}\right)^{1/2} (n\underline{\tau})^{-1/2}, \tag{5.37}$$

where $\overline{\alpha}_1$ is defined in (2.11)*. Consequently, $\{\mathbf{F}(\vec{\mathrm{x}}_\Delta)\}_{\boldsymbol{\tau}}(t)$ is bounded for each $t > 0$, uniformly in Δ.*

Proof. Since $\mathbf{F}(\vec{\mathrm{x}}_\Delta^n)$ is monotonically decreasing in n (for fixed Δ), it follows that

$$\begin{aligned}
\mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \leqslant \frac{1}{n}\sum_{j=1}^n \mathbf{F}(\vec{\mathrm{x}}_\Delta^j) &= \frac{1}{2n}\sum_{j=1}^n \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^j - z_{k-\frac12}^j}{\delta}\right)^2 \\
&\leqslant \frac{1}{2n\underline{\tau}} \left(\sum_{j=1}^n \tau_j \delta \sum_{k\in\mathbb{I}_K^+} 1\right)^{1/2} \left(\sum_{j=1}^\infty \tau_j \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^j - z_{k-\frac12}^j}{\delta}\right)^4\right)^{1/2} \\
&\leqslant \frac{1}{2n\underline{\tau}} (n\tau M)^{1/2} (18\overline{\mathcal{H}})^{1/2} = 3\overline{\alpha}_1 \left(\frac{M}{2}\overline{\mathcal{H}}\right)^{1/2} (n\underline{\tau})^{-1/2},
\end{aligned}$$

where we used in the last step that $\tau/\underline{\tau} < \overline{\alpha}_1$, see (2.11). □

The above estimate yields a Δ-uniform bound on $\{\mathbf{F}(\vec{\mathrm{x}}_\Delta)\}_{\boldsymbol{\tau}}(t)$ for any $t > 0$, but remember that $\{\mathbf{F}(\vec{\mathrm{x}}_\Delta)\}_{\boldsymbol{\tau}}(0)$ can even diverge for $\delta \to 0$. This is why one cannot expect uniform convergence on time intervals including the value $t = 0$ in the convergence results below. In the following, we denote by $[\underline{t}, \overline{t}] \subseteq (0, +\infty)$ a time intervals with $0 < \underline{t} < \overline{t} < \infty$.

Lemma 5.10. *We have that, for each $[\underline{t}, \overline{t}] \subseteq (0, +\infty)$,*

$$\sup_{t\in[\underline{t},\overline{t}]} \|\partial_x \{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\Omega)} < \infty, \tag{5.38}$$

$$\sup_{t\in[\underline{t},\overline{t}]} \|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - \{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)} \longrightarrow 0, \;\; \textit{as } \Delta \to 0 \tag{5.39}$$

$$\sup_{t\in[\underline{t},\overline{t}]} \|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)} < \infty. \tag{5.40}$$

Moreover, the functions $\{u_\Delta\}_{\boldsymbol{\tau}}$ and $\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}$ are uniformly bounded on $[\underline{t}, \overline{t}] \times \Omega$.

Proof. For each $n \in \mathbb{N}$,

$$\begin{aligned}
\|\partial_x \hat{u}_\Delta^n\|_{L^2(\Omega)}^2 &= \sum_{k\in\mathbb{I}_K^+} \left[(x_{k+\frac12}^n - x_k^n)\Big(\frac{z_{k+\frac12}^n - z_k^n}{x_{k+\frac12}^n - x_k^n}\Big)^2 + (x_k^n - x_{k-\frac12}^n)\Big(\frac{z_k^n - z_{k-\frac12}^n}{x_k^n - x_{k-\frac12}^n}\Big)^2 \right] \\
&\leqslant \delta \sum_{k\in\mathbb{I}_K^+} \frac{z_{k+\frac12}^n + z_{k-\frac12}^n}{2} \Big(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\Big)^2 \leqslant \mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \max_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^n.
\end{aligned}$$

Now combine this with the estimates (5.37) from above and (4.32) from the previous chapter to obtain (5.38). Estimate (5.39) follows directly from the elementary observation that

$$\sup_{x\in\Omega} |u_\Delta^n(x) - \hat{u}_\Delta^n(x)|^2 \leqslant \max_{k\in\mathbb{I}_K^+} \big|z_{k+\frac12}^n - z_{k-\frac12}^n\big|^2 \leqslant \delta\mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \leqslant \delta\mathbf{F}(\vec{\mathrm{x}}_\Delta^0),$$

and an application of (5.21). Finally, (5.40) is a consequence of (5.38) and (5.39). First, note that

$$\|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} \leqslant \|\{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} + \|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - \{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} \leqslant M + \delta\mathbf{F}(\vec{\mathrm{x}}_\Delta^0)$$

is uniformly bounded. Now apply the interpolation inequality

$$\|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)} \leqslant C\|\partial_x\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\Omega)}^{2/3}\|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)}^{1/3}$$

to obtain the bound in (5.40). □

Proposition 5.11. *There exists a function $u_* : (0,+\infty)\times\Omega \to [0,+\infty)$ with*

$$u_* \in C^{1/2}_{\mathrm{loc}}((0,+\infty);\mathcal{P}_2^r(\Omega)) \cap L^\infty_{\mathrm{loc}}((0,+\infty);H^1(\Omega)), \tag{5.41}$$

and there exists a subsequence of Δ (still denoted by Δ), such that, for every $[\underline{t},\overline{t}] \subseteq (0,+\infty)$, the following are true:

$$\{u_\Delta\}_{\boldsymbol{\tau}}(t) \longrightarrow u_*(t) \quad \textit{in } \mathcal{P}_2^r(\Omega), \textit{ uniformly with respect to } t\in[\underline{t},\overline{t}], \tag{5.42}$$

$$\{u_\Delta\}_{\boldsymbol{\tau}}, \{\hat{u}_\Delta\}_{\boldsymbol{\tau}} \longrightarrow u_* \quad \textit{uniformly on } [\underline{t},\overline{t}]\times\Omega. \tag{5.43}$$

Proof. Fix $[\underline{t},\overline{t}] \subseteq (0,+\infty)$. From the discrete energy inequality (5.22), the bound on the Fisher information in Lemma 5.9, and the equivalence (2.27) of $\mathrm{d}_{\boldsymbol{\xi}}$ with the usual L^2-Wasserstein distance $\mathcal{W}_2$, one can proceed analogously to the proof of Proposition 2.5 to conclude the existence of a subsequence of $\{u_\Delta\}_{\boldsymbol{\tau}}$ that converges to a limit curve $u_{\underline{t}} \in C^{1/2}([\underline{t},\overline{t}];\mathcal{P}_2^r(\Omega))$ at least uniformly with respect to $t\in[\underline{t},\overline{t}]$. Clearly, the previous argument applies to every choice of $\underline{t}>0$. Using a diagonal argument, one constructs a limit u_* defined on all $(0,+\infty)$, such that $u_{\underline{t}}$ is the restriction of u_* to $[\underline{t},\infty)$. Note especially that in addition to the weak convergence in (5.42), one obtains that $\{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}(t)$ converges to $\mathrm{X}_*(t)$ in $L^2(\mathcal{M})$, uniformly with respect to $t\in[\underline{t},\overline{t}]$, where $\mathrm{X}_* \in C^{1/2}_{\mathrm{loc}}((0,+\infty);L^2(\mathcal{M}))$ is the Lagrangian map of u_*. The reason for this is once again (2.27).

For proving (5.43), it suffices to show that $\{\hat{u}_\Delta\}_{\boldsymbol{\tau}} \to u_*$ uniformly on $[\underline{t},\overline{t}]\times\Omega$: Indeed, (5.39) implies that if $\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}$ converges uniformly to some limit, so does $\{u_\Delta\}_{\boldsymbol{\tau}}$. As an intermediate step towards proving uniform convergence of $\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}$, we show that

$$\hat{u}_\Delta(t) \longrightarrow u_*(t) \quad \text{in } L^2(\Omega), \text{ uniformly in } t\in[\underline{t},\overline{t}]. \tag{5.44}$$

For $t\in[\underline{t},\overline{t}]$, we expand the L^2-norm as follows:

$$\begin{aligned}\|\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - u_*(t)\|_{L^2(\Omega)}^2 = &\int_\Omega \Big[\big(\{\hat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\big)\{u_\Delta\}_{\boldsymbol{\tau}}\Big](t,x)\,\mathrm{d}x \\ &+ \int_\Omega \Big[\big(\{\hat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\big)\big(\{\hat{u}_\Delta\}_{\boldsymbol{\tau}} - \{u_\Delta\}_{\boldsymbol{\tau}}\big)\Big](t,x)\,\mathrm{d}x \\ &- \int_\Omega \Big[\big(\{\hat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\big)u_*\Big](t,x)\,\mathrm{d}x.\end{aligned}$$

On the one hand, observe that

$$\sup_{t\in[\underline{t},\overline{t}]}\int_\Omega \Big[\big(\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\big)\big(\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} - \{u_\Delta\}_{\boldsymbol{\tau}}\big)\Big](t,x)\,\mathrm{d}x$$
$$\leqslant \sup_{t\in[\underline{t},\overline{t}]}\Big(\big(\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)} + \|u_*(t)\|_{L^\infty(\Omega)}\big)\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - \{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)}\Big)$$

which converges to zero as $\Delta \to 0$, using the conclusions from Lemma 5.10. On the other hand, we can use property (2.4) to write

$$\int_\Omega \Big[\big(\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\big)\{u_\Delta\}_{\boldsymbol{\tau}}\Big](t,x)\,\mathrm{d}x - \int_\Omega \Big[\big(\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\big)u_*\Big](t,x)\,\mathrm{d}x$$
$$= \int_{\mathcal{M}} \Big[\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\Big]\big(t,\{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}(t,x)\big)\,\mathrm{d}\xi - \int_{\mathcal{M}} \Big[\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} - u_*\Big]\big(t,\mathrm{X}_*(t,\xi)\big)\,\mathrm{d}\xi.$$

We regroup terms under the integrals and use the triangle inequality. For the first term, we obtain

$$\sup_{t\in[\underline{t},\overline{t}]}\left|\int_{\mathcal{M}}\big(\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}\big(t,\{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}(t,\xi)\big) - \{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}\big(t,\mathrm{X}_*(t,\xi)\big)\big)\,\mathrm{d}\xi\right|$$
$$\leqslant \sup_{t\in[\underline{t},\overline{t}]}\int_{\mathcal{M}}\int_{\mathrm{X}_*(t,\xi)}^{\{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}(t,\xi)} |\partial_x\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}|(t,y)\,\mathrm{d}y\,\mathrm{d}\xi$$
$$\leqslant \sup_{t\in[\underline{t},\overline{t}]}\int_{\mathcal{M}} \|\partial_x\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}\|_{L^2(\Omega)}|\mathrm{X}_* - \{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}|(t,\xi)^{1/2}\,\mathrm{d}\xi$$
$$\leqslant \sup_{t\in[\underline{t},\overline{t}]}\Big(\|\partial_x\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\Omega)}\|\mathrm{X}_*(t) - \{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\mathcal{M})}^{1/4}\Big).$$

A similar reasoning applies to the integral involving u_* in place of $\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}$. Together, this proves (5.44), and it further proves that $u_* \in L^\infty([\underline{t},\overline{t}];H^1(\Omega))$, since the uniform bound on $\widehat{u}_\Delta$ from (5.38) is inherited by the limit.

Now the Gagliardo-Nirenberg inequality (A.1) provides the estimate

$$\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - u_*(t)\|_{C^{1/6}(\Omega)} \leqslant C\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - u_*(t)\|_{H^1(\Omega)}^{2/3}\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - u_*(t)\|_{L^2(\Omega)}^{1/3}. \tag{5.45}$$

Combining the convergence in $L^2(\Omega)$ by (5.44) with the boundedness in $H^1(\Omega)$ from (5.38), it readily follows that $\widehat{u}_\Delta(t) \to u_*(t)$ in $C^{1/6}(\Omega)$, uniformly in $t \in [\underline{t},\overline{t}]$. This clearly implies that $\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} \to u_*$ uniformly on $[\underline{t},\overline{t}] \times \Omega$. □

Remark 5.12. *In view of the above convergence proof, notice that we just used the convergence of $\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}$ towards $\{u_\Delta\}_{\boldsymbol{\tau}}$ in $L^1(\Omega)$ uniformly with respect to time $t \in [\underline{t},\overline{t}]$, instead of the stronger result in* (5.39)*.*

Proposition 5.13. *Under the hypotheses and with the notations of Proposition 5.11, we have that $\sqrt{u_*} \in L^2((0,+\infty);H^1(\Omega))$, and*

$$\Big\{\sqrt{\widehat{u}_\Delta}\Big\}_{\boldsymbol{\tau}} \longrightarrow \sqrt{u_*} \quad \textit{strongly in } L^2([\underline{t},\overline{t}];H^1(\Omega)) \tag{5.46}$$

for any $[\underline{t},\overline{t}] \subseteq (0,+\infty)$ as $\Delta \to 0$.

Notice that $\partial_x\sqrt{u_*} \in L^2([0,\bar{t}] \times \Omega)$ for each $\bar{t} > 0$, but strong convergence takes place only on each $[\underline{t}, \bar{t}] \times \Omega$.

Proof of Proposition 5.13. Fix $[\underline{t}, \bar{t}] \subseteq (0, +\infty)$. We are going to prove that for any Δ and $n \in \mathbb{N}$,

$$\left\|\partial_x\sqrt{\widehat{u}_\Delta^n}\right\|_{L^2(\Omega)}^2 \leqslant 2\left\|\sqrt{\widehat{u}_\Delta^n}\right\|_{L^\infty(\Omega)} \mathrm{TV}\left[\partial_x\sqrt{\widehat{u}_\Delta^n}\right] \tag{5.47}$$

is satisfied. To this end, remember that $\sqrt{\widehat{u}_\Delta^n}$ is differentiable on any interval $(x_{\kappa-\frac{1}{2}}, x_\kappa]$ for $\kappa \in \mathbb{I}_K^+ \cup \mathbb{I}_K^{1/2} \cup \{K\}$, and that $\partial_x\sqrt{\widehat{u}_\Delta^n}$ is monotonically decreasing due to (5.30). This implies together with the fundamental theorem of calculus that

$$\int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} |\partial_{xx}\sqrt{\widehat{u}_\Delta^n}| = -\int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} \partial_{xx}\sqrt{\widehat{u}_\Delta^n} = \lim_{x\downarrow x_{\kappa-\frac{1}{2}}} \partial_x\sqrt{\widehat{u}_\Delta^n}(x) - \lim_{x\uparrow x_\kappa} \partial_x\sqrt{\widehat{u}_\Delta^n}(x)$$

for any $\kappa \in \mathbb{I}_K^+ \cup \mathbb{I}_K^{1/2} \cup \{K\}$. Further, recall that $\partial_x\sqrt{\widehat{u}_\Delta^n}(x) = 0$ for all $x \in (a, a+\delta/2)$ and all $x \in (b-\delta/2, b)$. Therefore,

$$\begin{aligned}\sum_{\kappa\in\mathbb{I}_K^+\cup\mathbb{I}_K^{1/2}\cup\{K\}} \int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} \sqrt{\widehat{u}_\Delta^n}\partial_{xx}\sqrt{\widehat{u}_\Delta^n}\,\mathrm{d}x &\leqslant \left\|\sqrt{\widehat{u}_\Delta^n}\right\|_{L^\infty(\Omega)} \sum_{\kappa\in\mathbb{I}_K^+\cup\mathbb{I}_K^{1/2}\cup\{K\}} \int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} |\partial_{xx}\sqrt{\widehat{u}_\Delta^n}|\,\mathrm{d}x \\ &\leqslant \left\|\sqrt{\widehat{u}_\Delta^n}\right\|_{L^\infty(\Omega)} \mathrm{TV}\left[\partial_x\sqrt{\widehat{u}_\Delta^n}\right].\end{aligned} \tag{5.48}$$

By integration by parts and a rearrangement of the terms one obtains together with (5.48) that

$$\begin{aligned}\left\|\partial_x\sqrt{\widehat{u}_\Delta^n}\right\|_{L^2(\Omega)}^2 &= \sum_{\kappa\in\mathbb{I}_K^+\cup\mathbb{I}_K^{1/2}\cup\{K\}} \int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} \partial_x\sqrt{\widehat{u}_\Delta^n}\partial_x\sqrt{\widehat{u}_\Delta^n}\,\mathrm{d}x \\ &= \sum_{\kappa\in\mathbb{I}_K^+\cup\mathbb{I}_K^{1/2}\cup\{K\}} \left[\left[\sqrt{\widehat{u}_\Delta^n}(x)\partial_x\sqrt{\widehat{u}_\Delta^n}(x)\right]_{x=x_{\kappa-\frac{1}{2}}+0}^{x=x_\kappa-0} - \int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} \sqrt{\widehat{u}_\Delta^n}\partial_{xx}\sqrt{\widehat{u}_\Delta^n}\,\mathrm{d}x\right] \\ &\leqslant 2\left\|\sqrt{\widehat{u}_\Delta^n}\right\|_{L^\infty(\Omega)} \mathrm{TV}\left[\partial_x\sqrt{\widehat{u}_\Delta^n}\right].\end{aligned}$$

This shows (5.47). Take further two arbitrary discretizations Δ_1, Δ_2 and apply the above result to the difference $\left\{\sqrt{\widehat{u}_{\Delta_1}}\right\}_{\boldsymbol{\tau}} - \left\{\sqrt{\widehat{u}_{\Delta_2}}\right\}_{\boldsymbol{\tau}}$. Using that $\mathrm{TV}[f-g] \leqslant \mathrm{TV}[f] + \mathrm{TV}[g]$ we obtain by integration with respect to time that

$$\begin{aligned}&\int_{\underline{t}}^{\bar{t}} \left\|\partial_x\left\{\sqrt{\widehat{u}_{\Delta_1}}\right\}_{\boldsymbol{\tau}} - \partial_x\left\{\sqrt{\widehat{u}_{\Delta_2}}\right\}_{\boldsymbol{\tau}}\right\|_{L^2(\Omega)}^2 \mathrm{d}t \\ &\leqslant (\bar{t}-\underline{t})^{1/2} \sup_{t\in[\underline{t},\bar{t}]} \left\|\left\{\sqrt{\widehat{u}_{\Delta_1}}\right\}_{\boldsymbol{\tau}} - \left\{\sqrt{\widehat{u}_{\Delta_2}}\right\}_{\boldsymbol{\tau}}\right\|_{L^\infty(\Omega)} \times \\ &\qquad \times \left(2\int_{\underline{t}}^{\bar{t}} \mathrm{TV}\left[\partial_x\left\{\sqrt{\widehat{u}_{\Delta_1}}\right\}_{\boldsymbol{\tau}}\right]^2 + \mathrm{TV}\left[\partial_x\left\{\sqrt{\widehat{u}_{\Delta_2}}\right\}_{\boldsymbol{\tau}}\right]^2 \mathrm{d}t\right)^{1/2}.\end{aligned}$$

This shows that $\{\sqrt{\hat{u}_\Delta}\}_{\boldsymbol{\tau}}$ is a Cauchy-sequence in $L^2([\underline{t},\overline{t}];H^1(\Omega))$, remember (5.29) and especially (5.39), and its limit has to coincide with $\sqrt{u_*}$ in the sense of distributions, due to the uniform convergence of $\{\sqrt{\hat{u}_\Delta}\}_{\boldsymbol{\tau}}$ to $\sqrt{u_*}$ on $[\underline{t},\overline{t}]\times\Omega$. □

5.3. Weak formulation of the limit equation

To close the proof of Theorem 5.1, we are going to verify that the limit curve u_* obtained in Proposition 5.11 is indeed a weak solution to (5.1) with no-flux boundary conditions (5.2). The idea for this is the same as in Section 3.4 from Chapter 3 before:

(1) We first show the validity of a discrete weak formulation for $\{u_\Delta\}_{\boldsymbol{\tau}}$, using a discrete flow interchange estimate.
(2) Using the results from Proposition 5.13, we pass to the limit in the discrete weak formulation.

From now on, $\vec{\mathrm{x}}_\Delta=(\vec{\mathrm{x}}_\Delta^0,\vec{\mathrm{x}}_\Delta^1,\ldots)$ with its derived functions u_Δ, $\hat{u}_\Delta$, X_Δ is a (sub)sequence for which the convergence results stated in Proposition 5.11 and Proposition 5.13 are satisfied. We continue to assume (5.20) and (5.21). The goal of this section is to prove the following.

Proposition 5.14. *For every $\rho\in C^\infty(\Omega)$ with $\rho'(a)=\rho'(b)=0$, and for every $\eta\in C_c^\infty([0,+\infty))$, the limit curve u_* satisfies*

$$\int_0^\infty \eta'(t)\left(\int_\Omega \rho(x)u_*(t,x)\,\mathrm{d}x\right)\mathrm{d}t+\eta(0)\int_\Omega \rho(x)u^0(x)\,\mathrm{d}x+\int_0^\infty \eta(t)N(u_*,\rho)\,\mathrm{d}t=0, \tag{5.49}$$

where the highly nonlinear term N from (5.11) *is given by*

$$N(u,\rho)=\frac{1}{2}\int_\Omega \left[\rho'''(x)\partial_x u(t,x)+4\rho''(x)\big(\partial_x\sqrt{u}(t,x)\big)^2\right]\mathrm{d}x. \tag{5.50}$$

Note especially that the weak formulation (5.10) is equivalent to (5.49). Simply observe that any $\varphi\in C^\infty([0,+\infty)\times\Omega)$ that has a compact support in $[0,+\infty)\times\overline{\Omega}$ and satisfies $\partial_x\varphi(t,a)=\partial_x\varphi(t,b)=0$ for any $t\in[0,+\infty)$, can be approximated by linear combinations of products $\eta(t)\rho(x)$ with functions $\eta\in C^\infty([0,+\infty))$ and $\rho\in C^\infty(\Omega)$, which satisfies the requirements formulated in Proposition 5.14.

For definiteness, fix a spatial test function $\rho\in C^\infty(\Omega)$ with $\rho'(a)=\rho'(b)=0$, and a temporal test function $\eta\in C_c^\infty([0,+\infty))$ with $\operatorname{supp}\eta\subseteq[0,T)$ for a suitable $T>0$. Denote again by $N_{\boldsymbol{\tau}}\in\mathbb{N}$ an integer with $\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\in(T,T+1)$. Let $\varpi>0$ be chosen such that

$$\|\rho\|_{C^4(\Omega)}\leqslant\varpi\quad\text{and}\quad\|\eta\|_{C^1([0,+\infty))}\leqslant\varpi. \tag{5.51}$$

For convenience, we assume $\delta<1$ and $\tau<1$. In the estimates that follow, the non-explicity constants possibly depend on Ω, T, ϖ, and $\overline{\mathcal{H}}$, but not on Δ.

Lemma 5.15 (discrete weak formulation). *A solution to the numerical scheme satisfies*

$$\sum_{n=1}^{\infty}\tau_n\eta(t_{n-1})\left|\int_{\mathcal{M}}\frac{\rho(\mathbf{X}_\Delta^n)-\rho(\mathbf{X}_\Delta^{n-1})}{\tau_n}\,\mathrm{d}\xi-\big\langle\nabla_{\boldsymbol{\xi}}\mathbf{F}(\vec{\mathrm{x}}_\Delta^n),\rho'(\vec{\mathrm{x}}_\Delta^n)\big\rangle_{\boldsymbol{\xi}}\right|\leqslant C\big(\tau\mathbf{F}(\vec{\mathrm{x}}_\Delta^0)+(\delta\mathbf{F}(\vec{\mathrm{x}}_\Delta^0))^{1/2}\big), \tag{5.52}$$

where we use the short-hand notation $\rho'(\vec{x}) := (\rho'(x_1), \dots, \rho'(x_{K-1}))$ *for any* $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$.

Proof. A Taylor expansion of the term in the inner integral yields

$$\frac{\rho(\mathbf{X}_\Delta^n) - \rho(\mathbf{X}_\Delta^{n-1})}{\tau_n} = \rho'(\mathbf{X}_\Delta^n)\left(\frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n}\right) + \frac{\tau_n}{2}\rho''(\widetilde{\mathbf{X}})\left(\frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n}\right)^2, \tag{5.53}$$

where $\widetilde{\mathbf{X}}$ symbolizes suitable intermediate values in $\mathcal{M}$. We analyze the first term on the right-hand side of (5.53): Using the representation (2.16) of X_Δ in terms of hat functions θ_k, we can write its integral as follows,

$$\int_{\mathcal{M}} \rho'(\mathbf{X}_\Delta^n)\left(\frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n}\right) \mathrm{d}\xi = \sum_{k \in \mathbb{I}_K^+} \left(\frac{x_k^n - x_k^{n-1}}{\tau_n}\right) \int_{\xi_{k-1}}^{\xi_{k+1}} \rho'(\mathbf{X}_\Delta^n)\theta_k \,\mathrm{d}\xi. \tag{5.54}$$

Moreover, since

$$\int_{\xi_{k-1}}^{\xi_{k+1}} \theta_k(\xi)\,\mathrm{d}\xi = \delta, \tag{5.55}$$

the validity of the system of Euler-Lagrange equations (5.5) yields that

$$-\left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} = \left\langle \rho'(\vec{x}_\Delta^n), \frac{\vec{x}_\Delta^n - \vec{x}_\Delta^{n-1}}{\tau_n}\right\rangle_{\boldsymbol{\xi}} = \sum_{k \in \mathbb{I}_K^+} \left(\frac{x_k^n - x_k^{n-1}}{\tau_n}\right) \int_{\xi_{k-1}}^{\xi_{k+1}} \rho(x_k^n)\theta_k(\xi)\,\mathrm{d}\xi. \tag{5.56}$$

Finally, observing that

$$|\mathbf{X}_\Delta^n(\xi) - x_k^n| \leqslant (x_{k+1}^n - x_{k-1}^n) \quad \text{for each } \xi \in (\xi_{k-1}, \xi_{k+1}),$$

we can estimate the difference of the terms in (5.54) and (5.56) making use of the bound (5.51) on ρ as follows:

$$\begin{aligned} &\left| \int_{\mathcal{M}} \rho'(\mathbf{X}_\Delta^n)\left(\frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n}\right) \mathrm{d}\xi - \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{x}_\Delta^n), \rho'(\vec{x}_\Delta^n)\right\rangle_{\boldsymbol{\xi}} \right| \\ &\leqslant \sum_{k \in \mathbb{I}_K^+} \left|\frac{x_k^n - x_k^{n-1}}{\tau_n}\right| \int_{\xi_{k-1}}^{\xi_{k+1}} \left|\rho'(\mathbf{X}_\Delta^n(\xi)) - \rho'(x_k^n)\right| \theta_k(\xi)\,\mathrm{d}\xi \\ &\leqslant \varpi\delta \sum_{k \in \mathbb{I}_K^+} \left|\frac{x_k^n - x_k^{n-1}}{\tau_n}\right| (x_{k+1}^n - x_{k-1}^n). \end{aligned} \tag{5.57}$$

Combining (5.53) and (5.57), the claim is proven due to

$$
\begin{aligned}
&\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left(\left|\eta(t_{n-1})\right| \left| \int_{\mathcal{M}} \frac{\rho(\mathbf{X}_\Delta^n) - \rho(\mathbf{X}_\Delta^{n-1})}{\tau_n} \,\mathrm{d}\xi - \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \right| \right) \\
\leqslant & \varpi \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left(\left| \int_{\mathcal{M}} \rho'(\mathbf{X}_\Delta^n) \left(\frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n} \right) \mathrm{d}\xi - \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \right| \right. \\
&+ \left. \frac{\varpi \tau_n}{2} \int_{\mathcal{M}} \left(\frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n} \right)^2 (\xi) \,\mathrm{d}\xi \right) \\
\leqslant & \varpi^2 \left(\sum_{n=1}^{\infty} \tau_n \delta \sum_{k \in \mathbb{I}_K^+} \left(\frac{x_k^n - x_k^{n-1}}{\tau_n} \right)^2 \right)^{1/2} \left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k \in \mathbb{I}_K^+} (x_{k+1}^n - x_{k-1}^n)^2 \right)^{1/2} \\
&+ \frac{\varpi^2 \tau}{2} \sum_{n=1}^{\infty} \tau_n \left\| \frac{\mathbf{X}_\Delta^n - \mathbf{X}_\Delta^{n-1}}{\tau_n} \right\|_{L^2(\mathcal{M})}^2 \\
\leqslant & \varpi^2 \big(2(b-a)^2 T \big)^{1/2} (\delta \mathbf{F}(\vec{\mathrm{x}}_\Delta^0))^{1/2} + \varpi^2 (\tau \mathbf{F}(\vec{\mathrm{x}}_\Delta^0)),
\end{aligned}
$$

where we used the energy estimate (5.23) and the bound (A.4) in the last step. □

In what follows, we are going to prove that the weak formulation (5.49) is indeed the limit of the discrete weak formulation from Lemma 5.15, as $\Delta \to 0$. The two main steps for this identification are to establish the following estimates, respectively:

$$
\begin{aligned}
\mathrm{e}_{1,\Delta} := \Bigg| \int_0^T & \left(\eta'(t) \int_\Omega \rho(x) \{u_\Delta\}_{\boldsymbol{\tau}}(t,x) \,\mathrm{d}x + \eta(t) \left\{ \left\langle \rho'(\vec{\mathrm{x}}_\Delta), \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta) \right\rangle_{\boldsymbol{\xi}} \right\}_{\boldsymbol{\tau}}(t) \right) \mathrm{d}t \\
& + \eta(0) \int_\Omega \rho(x) u_\Delta^0(x) \,\mathrm{d}x \Bigg| \leqslant C\big((\delta \mathbf{F}(\vec{\mathrm{x}}_\Delta^0))^{1/2} + (\tau \mathbf{F}(\vec{\mathrm{x}}_\Delta^0)) \big),
\end{aligned} \tag{5.58}
$$

and

$$
\begin{aligned}
\mathrm{e}_{2,\Delta} := \Bigg| \int_0^T \eta(t) & \left(\frac{1}{2} \int_\Omega \left[\rho'''(x) \partial_x \{\hat{u}_\Delta\}_{\boldsymbol{\tau}}(t,x) + 4\rho''(x) \partial_x \left\{ \sqrt{\hat{u}_\Delta} \right\}_{\boldsymbol{\tau}}(t,x)^2 \right] \mathrm{d}x \right. \\
& \left. - \left\{ \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \right\}_{\boldsymbol{\tau}}(t) \right) \mathrm{d}t \Bigg| \leqslant C\delta^{1/4}.
\end{aligned} \tag{5.59}
$$

We proceed by proving (5.58) and (5.59). At the end of this section, it is shown how the claim (5.49) follows from (5.58) and (5.59) on basis of the convergence for $\{u_\Delta\}_{\boldsymbol{\tau}}$ obtained previously.

The first estimate in (5.58) is a consequence of Lemma 5.15:

Proof of (5.58)**.** Using that $\eta(t_n) = 0$ for any $n \geqslant N_{\boldsymbol{\tau}}$, we obtain after "summation by parts":

$$
\begin{aligned}
-\int_0^T \eta'(t) \left(\int_\Omega \rho(x) \left\{u_\Delta\right\}_{\boldsymbol{\tau}}(t,x)\, \mathrm{d}x \right) \mathrm{d}t &= -\sum_{n=1}^{N_{\boldsymbol{\tau}}} \left(\int_{t_{n-1}}^{t_n} \eta'(t)\, \mathrm{d}t \int_\Omega \rho(x) \bar{u}_\Delta^n(x)\, \mathrm{d}x \right) \\
&= -\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left(\frac{\eta(t_n) - \eta(t_{n-1})}{\tau_n} \int_{\mathcal{M}} \rho \circ \mathrm{X}_\Delta^n(\xi)\, \mathrm{d}\xi \right) \qquad (5.60) \\
&= \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left(\eta(t_{n-1}) \int_{\mathcal{M}} \frac{\rho \circ \mathbf{X}_\Delta^n(\xi) - \rho \circ \mathbf{X}_\Delta^{n-1}(\xi)}{\tau_n}\, \mathrm{d}\xi \right) + \eta(0) \int_{\mathcal{M}} \rho \circ \mathrm{X}_\Delta^0(\xi)\, \mathrm{d}\xi.
\end{aligned}
$$

Finally observe that

$$
\begin{aligned}
R &:= \left| \int_0^T \eta(t) \left\{ \left\langle \rho'(\vec{\mathrm{x}}_\Delta), \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta) \right\rangle_{\boldsymbol{\xi}} \right\}_{\boldsymbol{\tau}}(t)\, \mathrm{d}t - \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \eta(t_{n-1}) \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \right| \\
&\leqslant \left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left| \frac{1}{\tau_n} \int_{t_{n-1}}^{t_n} \eta(t)\, \mathrm{d}t - \eta(t_{n-1}) \right|^2 \right)^{1/2} \left(\sum_{n=1}^{\infty} \tau_n \varpi^2 \left\| \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n) \right\|_{\boldsymbol{\xi}}^2 \right)^{1/2} \\
&\leqslant \big((T+1) \varpi^2 \tau^2 \big)^{1/2} (2\varpi^2 \mathbf{F}(\vec{\mathrm{x}}_\Delta^0))^{1/2} = C' \mathbf{F}(\vec{\mathrm{x}}_\Delta^0)^{1/2} \tau,
\end{aligned}
$$

using the energy estimate (5.23). We conclude that

$$
\begin{aligned}
\mathrm{e}_{1,\Delta} &\overset{(5.60)}{\leqslant} R + \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left(\left| \eta(t_{n-1}) \right| \left| \int_{\mathcal{M}} \frac{\rho \circ \mathbf{X}_\Delta^n(\xi) - \rho \circ \mathbf{X}_\Delta^{n-1}(\xi)}{\tau_n}\, \mathrm{d}\xi - \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \right| \right) \\
&\leqslant C' \tau \mathbf{F}(\vec{\mathrm{x}}_\Delta^0)^{1/2} + C \big(\tau \mathbf{F}(\vec{\mathrm{x}}_\Delta^0) + (\delta \mathbf{F}(\vec{\mathrm{x}}_\Delta^0))^{1/2} \big),
\end{aligned}
$$

where we used (5.52). □

The proof of (5.59) is treated essentially in 2 steps. In the first one we rewrite the term $\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \rangle_{\boldsymbol{\xi}}$ (see Lemma 5.16) and use Taylor expansions to identify it with the corresponding integral terms of (5.50) up to some additional error terms, see Lemmata 5.17-5.19. Then we use the strong compactness result of Proposition 5.13 to pass to the limit as $\Delta \to 0$ in the second step.

Lemma 5.16. *With the short-hand notation $\rho'(\vec{\mathrm{x}}) = (\rho'(x_1), \ldots, \rho'(x_{K-1}))$ for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$, one has that*

$$
-2 \left\langle \nabla_{\boldsymbol{\xi}} \mathbf{F}(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} = A_1^n - A_2^n + A_3^n + A_4^n, \qquad (5.61)
$$

where

$$A_1^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right)^2 \left(\frac{z^n_{k+\frac12} + z^n_{k-\frac12}}{2}\right) \left(\frac{\rho'(x^n_{k+1}) - \rho'(x^n_{k-1})}{\delta}\right),$$

$$A_2^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right)^2 \left(\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2z^n_{k+\frac12}z^n_{k-\frac12}}\right) \rho''(x^n_k),$$

$$A_3^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right) \left(\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2}\right) \left(\frac{\rho'(x^n_{k+1}) - \rho'(x^n_k) - (x^n_{k+1} - x^n_k)\rho''(x^n_k)}{\delta^2}\right),$$

$$A_4^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right) \left(\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2}\right) \left(\frac{\rho'(x^n_{k-1}) - \rho'(x^n_k) - (x^n_{k-1} - x^n_k)\rho''(x^n_k)}{\delta^2}\right).$$

Proof. Fix some time index $n \in \mathbb{N}$ (omitted in the calculations below). Recall the representation of $\nabla_{\boldsymbol{\xi}}\mathbf{F}$ from (5.8). By a "summation by parts", it follows that

$$-2\left\langle \nabla_{\vec{\mathrm{x}}}\mathbf{F}(\vec{\mathrm{x}}_\Delta), \rho'(\vec{\mathrm{x}}_\Delta)\right\rangle_{\boldsymbol{\xi}} = -\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} \frac{1}{\delta}\left(\frac{z_{\kappa+1} - z_\kappa}{\delta} - \frac{z_\kappa - z_{\kappa-1}}{\delta}\right) z_\kappa^2 \left(\frac{\rho'(x_{\kappa+\frac12}) - \rho'(x_{\kappa-\frac12})}{\delta}\right)$$
$$= \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right) \frac{1}{\delta}\left(z^2_{k+\frac12}\frac{\rho'(x_{k+1}) - \rho'(x_k)}{\delta} - z^2_{k-\frac12}\frac{\rho'(x_k) - \rho'(x_{k-1})}{\delta}\right).$$

Using the elementary identity (for arbitrary numbers $p_\pm$ and $q_\pm$)

$$p_+q_+ - p_-q_- = \frac{p_+ + p_-}{2}(q_+ - q_-) + (p_+ - p_-)\frac{q_+ + q_-}{2},$$

we further obtain

$$-2\left\langle \nabla_{\vec{\mathrm{x}}}\mathbf{F}(\vec{\mathrm{x}}_\Delta), \rho'(\vec{\mathrm{x}}_\Delta)\right\rangle_{\boldsymbol{\xi}}$$
$$= \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right) \left(\frac{z^2_{k+\frac12} - z^2_{k-\frac12}}{2\delta}\right) \left(\frac{\rho'(x_{k+1}) - \rho'(x_{k-1})}{\delta}\right) \tag{5.62}$$
$$+ \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right) \left(\frac{z^2_{k+\frac12} + z^2_{k-\frac12}}{2}\right) \left(\frac{\rho'(x_{k+1}) - 2\rho'(x_k) + \rho'(x_{k-1})}{\delta^2}\right). \tag{5.63}$$

The sum in (5.62) equals A_1^n. In order to see that the sum in (5.63) equals $-A_2^n + A_3^n + A_4^n$, simply observe that the identity

$$\frac{x_{k+1} - x_k}{\delta} + \frac{x_{k-1} - x_k}{\delta} = \frac{1}{z_{k+\frac12}} - \frac{1}{z_{k-\frac12}} = -\frac{z_{k+\frac12} - z_{k-\frac12}}{z_{k+\frac12}z_{k-\frac12}},$$

makes the coefficient of $\rho''(x_k)$ vanish. □

Lemma 5.17. *There is a constant $C_1 > 0$ expressible in Ω, T, B and $\overline{\mathcal{H}}$ such that*

$$R_1 := \sum_{n=1}^{N_\tau} \tau_n \Big| A_1^n - 2\int_{\mathcal{M}} \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \Big| \leqslant C_1 \delta^{1/4}.$$

Proof. First, observe that by definition of $\widehat{z}_\Delta^n$,

$$\int_{\mathcal{M}} \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi = \sum_{k\in\mathbb{I}_K^+} \Big(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\Big)^2 \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi,$$

and therefore, by Hölder's inequality,

$$R_1 \leqslant R_{1a}^{1/2} R_{1b}^{1/2}, \tag{5.64}$$

with, recalling (5.25),

$$R_{1a} = \sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \Big(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\Big)^4 \leqslant \sum_{n=1}^{\infty} \tau_n \|\widehat{z}_\Delta^n\|_{L^4(\Omega)}^4 \leqslant 9\overline{\mathcal{H}}, \tag{5.65}$$

$$R_{1b} = \sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \Big[\frac{z_{k+\frac12}^n + z_{k-\frac12}^n}{2} \frac{\rho'(x_{k+1}^n) - \rho'(x_{k-1}^n)}{\delta} - \frac{2}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho'' \circ \mathrm{X}_\Delta^n\,\mathrm{d}\xi\Big]^2. \tag{5.66}$$

To simplify R_{1b}, let us fix n (omitted in the following), and introduce $\tilde{x}_k^+ \in [x_k, x_{k+1}]$ and $\tilde{x}_k^- \in [x_{k-1}, x_k]$ such that

$$\begin{aligned}\frac{\rho'(x_{k+1}) - \rho'(x_{k-1})}{\delta} &= \frac{\rho'(x_{k+1}) - \rho'(x_k)}{\delta} + \frac{\rho'(x_k) - \rho'(x_{k-1})}{\delta} \\ &= \rho''(\tilde{x}_k^+)\frac{x_{k+1} - x_k}{\delta} + \rho''(\tilde{x}_k^+)\frac{x_{k+1} - x_k}{\delta} = \frac{\rho''(\tilde{x}_k^+)}{z_{k+\frac12}} + \frac{\rho''(\tilde{x}_k^-)}{z_{k-\frac12}}.\end{aligned}$$

For each $k \in \mathbb{I}_K^+$, we have that — recalling (5.55) —

$$\begin{aligned}&\frac{z_{k+\frac12} + z_{k-\frac12}}{2}\Big(\frac{\rho''(\tilde{x}_k^+)}{z_{k+\frac12}} + \frac{\rho''(\tilde{x}_k^-)}{z_{k-\frac12}}\Big) - \frac{2}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho'' \circ \mathrm{X}_\Delta\,\mathrm{d}\xi \\ &= \frac12\Big[\Big(\frac{z_{k-\frac12}}{z_{k+\frac12}} + 1\Big)\rho''(\tilde{x}_k^+) + \Big(\frac{z_{k+\frac12}}{z_{k-\frac12}} + 1\Big)\rho''(\tilde{x}_k^-)\Big] - \frac{2}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho'' \circ \mathrm{X}_\Delta\,\mathrm{d}\xi \\ &= \frac12\Big[\Big(\frac{z_{k-\frac12}}{z_{k+\frac12}} - 1\Big)\rho''(\tilde{x}_k^+) + \Big(\frac{z_{k+\frac12}}{z_{k-\frac12}} - 1\Big)\rho''(\tilde{x}_k^-)\Big] \\ &\quad - \frac{2}{\delta}\int_{\xi_k}^{\xi_{k+\frac12}} \big[\rho'' \circ \mathrm{X}_\Delta - \rho''(\tilde{x}_k^+)\big]\,\mathrm{d}\xi - \frac{2}{\delta}\int_{\xi_{k-\frac12}}^{\xi_k} \big[\rho'' \circ \mathrm{X}_\Delta - \rho''(\tilde{x}_k^-)\big]\,\mathrm{d}\xi.\end{aligned}$$

Since $\tilde{x}_k^+$ lies in $[x_k, x_{k+1}]$ and $\mathrm{X}_\Delta(\xi) \in [x_k, x_{k+\frac12}]$ for each $\xi \in [\xi_k, \xi_{k+\frac12}]$, one obtains that $|\mathrm{X}_\Delta(\xi) - \tilde{x}_k^+| \leqslant x_{k+1} - x_k$, and therefore

$$\frac{2}{\delta}\int_{\xi_k}^{\xi_{k+\frac12}} \big|\rho'' \circ \mathrm{X}_\Delta(\xi) - \rho''(\tilde{x}_k^+)\big|\,\mathrm{d}\xi \leqslant 2\varpi(x_{k+1} - x_k). \tag{5.67}$$

A similar estimate is satisfied for the other integral. Thus

$$R_{1b} \leqslant \varpi^2 \sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \Big[\Big(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1\Big)^2 + \Big(\frac{z^n_{k+\frac12}}{z^n_{k-\frac12}} - 1\Big)^2 + 2(x^n_{k+1} - x^n_{k-1})^2\Big].$$

Recalling the estimates (5.27) and (A.4), we further conclude that

$$R_{1b} \leqslant \varpi^2\big(6(b-a)^2(\overline{\mathcal{H}}(T+1)\delta)^{1/2} + 4T(b-a)^2\delta\big), \tag{5.68}$$

remember $\sum_{n=1}^{N_\tau}\tau_n \in (T, T+1)$. In combination with (5.64) and (5.65), this proves the claim. □

Lemma 5.18. *There is a constant $C_2 > 0$ expressible in Ω, T, ϖ and $\overline{\mathcal{H}}$ such that*

$$R_2 := \sum_{n=1}^{N_\tau} \tau_n \Big| A_2^n - \int_{\mathcal{M}} \partial_\xi \hat{z}^n_\Delta(\xi)^2 \rho'' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi \Big| \leqslant C_2 \delta^{1/4}.$$

Proof. The proof is almost identical to (and even easier than) the one for Lemma 5.17 above. Again, we have a decomposition of the form

$$R_2 \leqslant R_{2a}^{1/2} R_{2b}^{1/2},$$

where R_{2a} equals R_{1a} from (5.65), and

$$R_{2b} = \sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \Big[\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2 z^n_{k+\frac12} z^n_{k-\frac12}} \rho''(x^n_k) - \frac{1}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho'' \circ \mathrm{X}^n_\Delta \,\mathrm{d}\xi \Big]^2.$$

By writing

$$\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2 z^n_{k+\frac12} z^n_{k-\frac12}} = \frac12\Big(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1\Big) + \frac12\Big(\frac{z^n_{k+\frac12}}{z^n_{k-\frac12}} - 1\Big) + 1,$$

and observing — in analogy to (5.67) — that

$$\frac{1}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \big|\rho'' \circ \mathrm{X}_\Delta(\xi) - \rho''(x_k)\big|\,\mathrm{d}\xi \leqslant \varpi(x_{k+\frac12} - x_{k-\frac12}),$$

we obtain the same bound on R_{2b} as the one on R_{1b} from (5.68). □

Lemma 5.19. *There is a constant $C_3 > 0$ expressible in Ω, T, ϖ and $\overline{\mathcal{H}}$ such that*

$$R_3 := \sum_{n=1}^{N_\tau} \tau_n \Big| A_3^n - \frac12 \int_{\mathcal{M}} \partial_\xi \hat{z}^n_\Delta(\xi) \rho''' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi \Big| \leqslant C_3 \delta^{1/4}.$$

Proof. Arguing like in the previous proofs, we first deduce — now by means of Hölder's inequality instead of the Cauchy-Schwarz inequality — that

$$R_3 \leqslant R_{3a}^{1/4} R_{3b}^{3/4},$$

where $R_{3a} = R_{1a}$, and

$$R_{3b} = \sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \left| \left(\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2} \right) \left(\frac{\rho'(x^n_{k+1}) - \rho'(x^n_k) - (x^n_{k+1} - x^n_k)\rho''(x^n_k)}{\delta^2} \right) - \frac{1}{2\delta} \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho''' \circ \mathrm{X}^n_\Delta \,\mathrm{d}\xi \right|^{4/3}.$$

Introduce intermediate values $\tilde{x}^+_k$ such that

$$\rho'(x^n_{k+1}) - \rho'(x^n_k) - (x^n_{k+1} - x^n_k)\rho''(x^n_k) = \frac12 (x^n_{k+1} - x^n_k)^2 \rho'''(\tilde{x}^+_k) = \frac{\delta^2}{2(z^n_{k+\frac12})^2}\rho'''(\tilde{x}^+_k).$$

Thus we have that

$$\begin{aligned}
&\left(\frac{(z^n_{k+\frac12})^2 + (z^n_{k-\frac12})^2}{2} \right) \left(\frac{\rho'(x^n_{k+1}) - \rho'(x^n_k) - (x^n_{k+1} - x^n_k)\rho''(x^n_k)}{\delta^2} \right) - \frac{1}{2\delta} \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho''' \circ \mathrm{X}^n_\Delta \,\mathrm{d}\xi \\
&= \frac14 \left(\left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} \right)^2 + 1 \right) \rho'''(\tilde{x}^+_k) - \frac{1}{2\delta} \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho''' \circ \mathrm{X}^n_\Delta \,\mathrm{d}\xi \\
&= \frac14 \left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} + 1 \right) \left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1 \right) \rho'''(\tilde{x}^+_k) - \frac{1}{2\delta} \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \left[\rho''' \circ \mathrm{X}^n_\Delta - \rho'''(\tilde{x}^+_k) \right] \mathrm{d}\xi.
\end{aligned}$$

By the analogue of (5.67), it follows further that

$$\begin{aligned}
R_{3b} &\leqslant 2\varpi^{4/3} \sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \left[\left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} + 1 \right)^{4/3} \left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1 \right)^{4/3} + (x^n_{k+1} - x^n_{k-1})^{4/3} \right] \\
&\leqslant 2\varpi^{4/3} \left(\sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} + 1 \right)^4 \right)^{1/3} \left(\sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1 \right)^2 \right)^{2/3} \\
&\quad + 2\varpi^{4/3}(T+1)(b-a)^{4/3}\delta,
\end{aligned}$$

where we used (A.4). At this point, the estimates (5.26) and (5.27) are used to control the first and the second sum, respectively. □

Along the same lines, one proves the analogous estimate for A_4 in place of A_3. It remains to identify the integral expressions inside R_1 to R_3 with those in the weak formulation (5.49).

Lemma 5.20. *One has that*

$$\int_{\mathcal{M}} \partial_\xi \hat{z}^n_\Delta(\xi) \rho''' \circ \mathrm{X}^n_\Delta(\xi) \,\mathrm{d}\xi = \int_\Omega \partial_x \hat{u}^n_\Delta(x) \rho'''(x) \,\mathrm{d}x, \tag{5.69}$$

$$R_5 := \sum_{n=1}^{N_\tau} \tau_n \left| \int_{\mathcal{M}} \partial_\xi \hat{z}^n_\Delta(\xi)^2 \rho'' \circ \mathrm{X}^n_\Delta(\xi) \,\mathrm{d}\xi - 4 \int_\Omega \left(\partial_x \sqrt{\hat{u}^n_\Delta} \right)^2 (x) \rho''(x) \,\mathrm{d}x \right| \leqslant C_5 \delta^{1/4}. \tag{5.70}$$

Proof. The starting point is relation (5.16) that is

$$\widehat{z}^n_\Delta(\xi) = \widehat{u}^n_\Delta \circ \mathbf{X}^n_\Delta(\xi) \tag{5.71}$$

for all $\xi \in \mathcal{M}$. Both sides of this equation are Lipschitz continuous in ξ, and are differentiable except possibly at $\xi_{\frac{1}{2}}, \xi_1, \ldots, \xi_{K-\frac{1}{2}}$. At points ξ of differentiability, we have that

$$\partial_\xi \widehat{z}^n_\Delta(\xi) = \partial_x \widehat{u}^n_\Delta \circ \mathbf{X}^n_\Delta(\xi) \partial_\xi \mathbf{X}^n_\Delta(\xi).$$

Substitute this expression for $\partial_\xi \widehat{z}^n_\Delta(\xi)$ into the left-hand side of (5.69), and perform a change of variables $x = \mathbf{X}^n_\Delta(\xi)$ to obtain the integral on the right.

Next, take the square root in (5.71) before differentiation, then calculate the square and divide by $\partial_\xi \mathbf{X}^n_\Delta(\xi)$ afterwards. This series of calculations ends in

$$\frac{\partial_\xi \widehat{z}^n_\Delta(\xi)^2}{4\widehat{z}^n_\Delta(\xi)\partial_\xi \mathbf{X}^n_\Delta(\xi)} = \big(\partial_x \sqrt{\widehat{u}^n_\Delta}\big)^2 \circ \mathbf{X}^n_\Delta(\xi)\partial_\xi \mathbf{X}^n_\Delta(\xi).$$

Performing the same change of variables as before, this proves that

$$\int_{\mathcal{M}} \frac{\partial_\xi \widehat{z}^n_\Delta(\xi)^2}{\widehat{z}^n_\Delta(\xi)\partial_\xi \mathbf{X}^n_\Delta(\xi)} \rho'' \circ \mathbf{X}^n_\Delta(\xi)\,\mathrm{d}\xi = 4\int_\Omega \Big(\partial_x \sqrt{\widehat{u}^n_\Delta}\Big)^2 (x)\rho''(x)\,\mathrm{d}x. \tag{5.72}$$

It remains to estimate the difference between the ξ-integrals in (5.70) and in (5.72), respectively. To this end, observe that for each $\xi \in (\xi_k, \xi_{k+\frac{1}{2}})$ with some $k \in \mathbb{I}^+_K$, one has $\partial_\xi \mathbf{X}^n_\Delta(\xi) = 1/z^n_{k+\frac{1}{2}}$ and $\widehat{z}_\Delta(\xi) \in [z_{k-\frac{1}{2}}, z_{k+\frac{1}{2}}]$. Hence, for those ξ,

$$\left|1 - \frac{1}{\widehat{z}^n_\Delta(\xi)\partial_\xi \mathbf{X}^n_\Delta(\xi)}\right| \leqslant \left|1 - \frac{z^n_{k+\frac{1}{2}}}{z^n_{k-\frac{1}{2}}}\right|.$$

If instead $\xi \in (\xi_{k-\frac{1}{2}}, \xi_k)$, then this estimate is satisfied with the roles of $z^n_{k+\frac{1}{2}}$ and $z^n_{k-\frac{1}{2}}$ interchanged. Consequently, using once again (5.25) and (5.27),

$$\begin{aligned}
&\sum_{n=1}^{N_\tau} \tau_n \left| \int_{\mathcal{M}} \partial_\xi \widehat{z}^n_\Delta(\xi)^2 \rho'' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi - \int_{\mathcal{M}} \frac{\partial_\xi \widehat{z}^n_\Delta(\xi)^2}{\widehat{z}^n_\Delta(\xi)\partial_\xi \mathbf{X}^n_\Delta(\xi)} \rho'' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi \right| \\
&\leqslant \varpi \sum_{n=1}^{N_\tau} \tau_n \int_{\mathcal{M}} \partial_\xi \widehat{z}^n_\Delta(\xi)^2 \left|1 - \frac{1}{\widehat{z}^n_\Delta(\xi)\partial_\xi \mathbf{X}^n_\Delta(\xi)}\right| \mathrm{d}\xi \\
&\leqslant \varpi \left(\sum_{n=1}^{\infty} \tau_n \|\partial_\xi \widehat{z}^n_\Delta\|^4_{L^4(\Omega)}\right)^{1/2} \left(\sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k\in\mathbb{I}^+_K} \left[\left(1 - \frac{z^n_{k+\frac{1}{2}}}{z^n_{k-\frac{1}{2}}}\right)^2 + \left(1 - \frac{z^n_{k+\frac{1}{2}}}{z^n_{k-\frac{1}{2}}}\right)^2\right]\right)^{1/2} \\
&\leqslant 3\overline{\mathcal{H}}^{1/2}\big(6(b-a)^2 T^{1/2}\overline{\mathcal{H}}^{1/2}\delta^{1/2}\big)^{1/2},
\end{aligned}$$

since $\sum_{n=1}^{N_\tau} \tau_n \leqslant T + 1$ by hypothesis. This shows (5.70). ☐

Proof of (5.59)**.** Combining the discrete weak formulation (5.61), the change of variables formula (5.69) and (5.70), and the definitions of R_1 to R_5, it follows that

$$\mathrm{e}_{2,\Delta} \leqslant \varpi R_5 + \varpi \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left| \frac{1}{2} \int_{\mathcal{M}} \left[\partial_\xi \widehat{z}_\Delta^n \rho''' \circ \mathbf{X}_\Delta^n(\xi) + \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathbf{X}_\Delta^n(\xi) \right] \mathrm{d}\xi - \sum_{i=1}^{5} A_i \right|$$
$$\leqslant \varpi \sum_{i=1}^{5} R_i \leqslant \varpi \sum_{i=1}^{5} C_i \delta^{1/4}.$$

This implies the desired inequality (5.59). □

We are now going to finish the proof of this section's main result, Proposition 5.14. Unfortunately, one can not just apply the convergence results from Proposition 5.11 and Proposition 5.13 "straight-forward", since they are mostly stated for arbitrary, but compact time intervals $[\underline{t}, \overline{t}] \subseteq (0, +\infty)$. To assure the convergence results for the respective time integrals over $(0, T)$, repetitive applications of Vitali's Theorem are needed.

Proof of Proposition 5.14. Owing to (5.58) and (5.59), we know that

$$\left| \int_0^T \eta'(t) \int_\Omega \rho(x) \{u_\Delta\}_{\boldsymbol{\tau}}(t,x)\,\mathrm{d}x\,\mathrm{d}t + \eta(0) \int_\Omega \rho(x) u_\Delta^0(x)\,\mathrm{d}x \right.$$
$$\left. + \int_0^T \eta(t) \frac{1}{2} \int_\Omega \left[\rho'''(x) \partial_x \{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t,x) + 4\rho''(x) \partial_x \left\{ \sqrt{\widehat{u}_\Delta} \right\}_{\boldsymbol{\tau}}(t,x)^2 \right] \mathrm{d}x\,\mathrm{d}t \right|$$
$$\leqslant \mathrm{e}_{1,\Delta} + \mathrm{e}_{2,\Delta} \leqslant C\big((\tau \mathbf{F}(\vec{\mathrm{x}}_\Delta^0)) + (\delta \mathbf{F}(\vec{\mathrm{x}}_\Delta^0))^{1/2} + \delta^{1/4} \big).$$

By our assumption (5.21) on $\mathbf{F}(\vec{\mathrm{x}}_\Delta^0)$, the expression on the right-hand side vanishes as $\Delta \to 0$. To obtain (5.49) in the limit $\Delta \to 0$, we still need to show the convergence of the integrals to their respective limits.

A technical tool is the observation that, for each $p \in [1, 4]$,

$$Q_p := \sup_\Delta \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} (z_\kappa^n)^p < \infty,$$

thanks to the estimates (4.31) and (5.25). For the first integral, we use that $\{u_\Delta\}_{\boldsymbol{\tau}}$ converges to u_* with respect to $\mathcal{W}_2$, locally uniformly on arbitrary $[\underline{t}, \overline{t}] \subseteq (0, +\infty)$. Thus clearly

$$\int_\Omega \rho(x) \{u_\Delta\}_{\boldsymbol{\tau}}(t,x)\,\mathrm{d}x \longrightarrow \int_\Omega \rho(x) u_*(t,x)\,\mathrm{d}x$$

for each $t \in (0, T)$. In order to pass to the limit with the time integral, we apply Vitali's Theorem. To this end, observe that

$$\int_0^T \left| \eta'(t) \int_\Omega \rho(x) \{u_\Delta\}_{\boldsymbol{\tau}}(t,x)\,\mathrm{d}x \right|^2 \mathrm{d}t \leqslant \varpi^2 (b-a) \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \int_\Omega u_\Delta^n(x)^2\,\mathrm{d}x$$
$$= \varpi^2 (b-a) \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^n \leqslant Q_1 \varpi^2 (b-a).$$

Next, using the strong convergence from (5.46), it follows that

$$\partial_x \left\{\widehat{u}_\Delta\right\}_{\boldsymbol{\tau}} = 2\left\{\sqrt{\widehat{u}_\Delta}\right\}_{\boldsymbol{\tau}} \partial_x\sqrt{\widehat{u}_\Delta} \longrightarrow 2\sqrt{u_*}\partial_x\sqrt{u_*} = \partial_x u_*$$

strongly in $L^1(\Omega)$ for almost every $t \in (0,T)$. Again, we apply Vitali's Theorem to conclude convergence of the time integral, on grounds of the following estimate:

$$\int_0^T \left|\eta(t)\int_\Omega \rho'''(x)\partial_x\left\{\widehat{u}_\Delta\right\}_{\boldsymbol{\tau}} \,\mathrm{d}x\right|^2 \mathrm{d}t \leqslant \varpi^2(b-a)\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\int_\Omega \left(\partial_x\widehat{u}_\Delta^n(x)\right)^2\mathrm{d}x$$

$$= \varpi^2(b-a)\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\delta\sum_{k\in\mathbb{I}_K^+}\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)^2\left(\frac{z^n_{k+\frac12}+z^n_{k-\frac12}}{2}\right)$$

$$\leqslant \varpi^2(b-a)\left(\sum_{n=1}^{\infty}\tau_n\sum_{k\in\mathbb{I}_K^+}\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)^4\right)^{1/2}\left(\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\delta\sum_{\kappa\in\mathbb{I}_K^{1/2}}(z^n_\kappa)^2\right)^{1/2} \leqslant 9\overline{\mathcal{H}}^{1/2}Q_2^{1/2}\varpi^2(b-a),$$

where we used (5.25). Finally, the strong convergence (5.46) also implies that

$$\left(\partial_x\left\{\widehat{u}_\Delta\right\}_{\boldsymbol{\tau}}\right)^2 \longrightarrow \left(\partial_x\sqrt{u_*}\right)^2$$

strongly in $L^1(\Omega)$, for almost every $t \in (0,T)$. One more time, we invoke Vitali's Theorem, using that

$$\int_0^T \left|\eta(t)\int_\Omega \rho''(x)\partial_x\left\{\sqrt{\widehat{u}_\Delta}\right\}^2_{\boldsymbol{\tau}}(t,x)\,\mathrm{d}x\right|^2\mathrm{d}t \leqslant \varpi^2\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\int_\Omega\left(\partial_x\sqrt{\widehat{u}^n_\Delta}\right)^4(x)\,\mathrm{d}x$$

$$\leqslant \frac12\varpi^2\sum_{n=1}^{N_{\boldsymbol{\tau}}}\tau_n\delta\sum_{k\in\mathbb{I}_K^+}\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)^2\left[\left(1-\frac{z^n_{k+\frac12}}{z^n_{k-\frac12}}\right)^2+\left(1-\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}}\right)^2\right].$$

$$\leqslant \varpi^2\left(\sum_{n=1}^{\infty}\tau_n\delta\sum_{k\in\mathbb{I}_K^+}\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)^4\right)^{1/2}\left(\sum_{n=1}^{\infty}\tau_n\delta\sum_{k\in\mathbb{I}_K^+}\left[\left(1-\frac{z^n_{k+\frac12}}{z^n_{k-\frac12}}\right)^4+\left(1-\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}}\right)^4\right]\right)^{1/2}.$$

The two terms in the last line are uniformly controlled in view of (5.25) and (5.27), respectively.

□

5.4. Numerical results

We fix $\Omega = (0,1)$ for all experiments described below, hence $\aleph = K-1$.

As in the numerical investigations of the previous chapter, we are going to use non-uniform meshes for our numerical experiments in order to make our discretization more flexible. The choice of non-uniform meshes, of initial grids $\vec{\mathrm{x}}^0_\Delta$ and the scheme's implementation are hence analogue to Section 4.4.1 and 4.4.2.

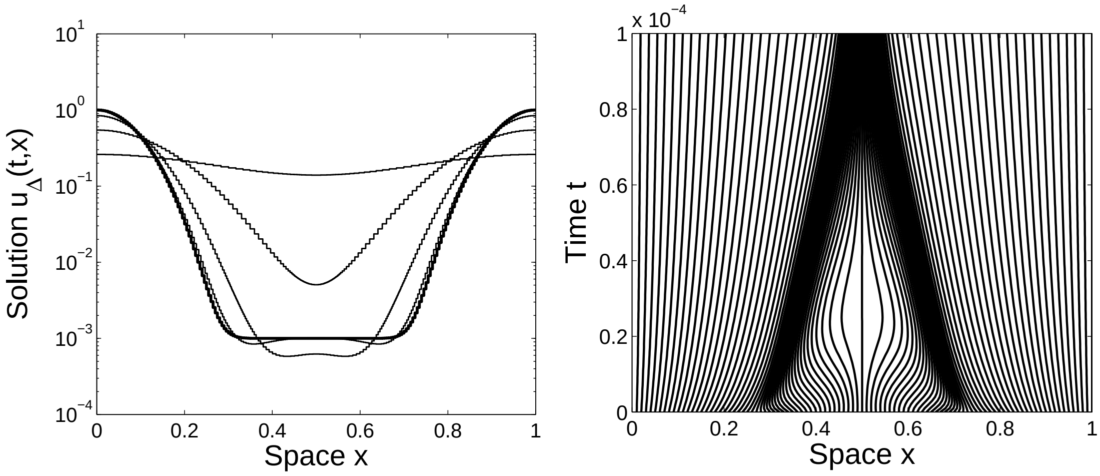


FIGURE 5.2. *Left:* snapshots of the densities u_Δ for the initial condition (5.73) at times $t = 0$ and $t = 10^i$, $i = -6, \dots, -3$, using $K = 200$ grid points and the time step size $\tau = 10^{-6}$. *Right:* associated particle trajectories.

5.4.1. Numerical experiments. Our main experiments are carried out using the by now classical test case from [**BLS94**] that is

$$u^0(x) = \epsilon + \cos^{16}(\pi x) \tag{5.73}$$

with $\epsilon = 10^{-3}$.

5.4.1.a. Evolution of discrete solution. Figure 5.2 provides a qualitative picture of the evolution with initial condition u^0: The plot on the left shows the density function u_Δ at several instances in time, the plot on the right visualizes the motion of the mesh points $\{x_k\}_{\boldsymbol{\tau}}$ associated to the Lagrangian maps X_Δ in continuous time. It is clearly seen that the initial density has a very flat minimum (which is degenerated of order 16) at $x = 1/2$, which bifurcates into two sharper minima at later times, and eventually becomes one single minimum again. This behaviour underlines that no comparison principles are valid for the DLSS equation. Both figures have been generated using $K = 200$ spatial grid points and constant time step sizes $\tau_n \equiv \tau = 10^{-6}$.

5.4.1.b. Reference solution. To measure the quality of our numerical scheme, we compare all our numerical results with those of the scheme described in [**DMM10**], which is fully variational as well, but uses different ansatz functions for the Lagrangian maps. Even without a rigorous result on uniqueness of weak solutions, it seems reasonable to expect that both schemes should approximate the same solution. A technical issue with the comparison of our solution to the reference solution is that both use a different way for the reconstruction of the density from the Lagrangian map. This difference camouflages the true approximation error in the plain L^2-differences. For a fair comparison, we calculate the L^2-difference of the linear interpolations of the values for the density with respect to the nodes of the Lagrangian maps.

5.4.1.c. Fixed τ. In a first series of experiments, we study the decay of the L^2-error under refinement of the spatial discretization. For this purpose, we fix a time decomposition with

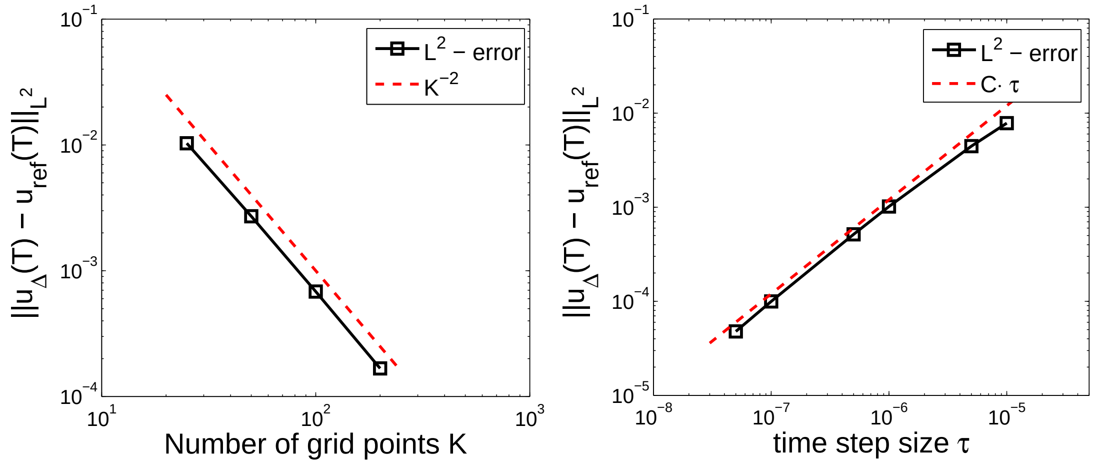


FIGURE 5.3. Numerical error analysis for u^0 from (5.73). *Left:* fixed time step size $\tau = 10^{-8}$ and $K = 25, 50, 100, 200$ spatial grid points. The L^2-errors are evaluated at $T = 5 \cdot 10^{-6}$. *Right:* fixed $K = 800$ using $\tau = 10^{-5}, 5 \cdot 10^{-6}, 10^{-6}, 5 \cdot 10^{-7}, 10^{-7}, 5 \cdot 10^{-8}$. The error is evaluated at $T = 10^{-5}$.

constant time step sizes $\tau_n \equiv \tau = 10^{-8}$ and vary the number of spatial grid points, using $K = 25, 50, 100, 200$. Figure 5.3/left shows the corresponding L^2-error between the solution to our scheme and the reference solution, evaluated at time $T = 10^{-5}$. It is clearly seen that the error decays with an almost perfect rate of $\delta^2 \propto K^{-2}$.

5.4.1.d. Fixed K. For the second series of experiments, we keep the spatial discretization parameter $K = 800$ fixed and run our scheme with the time step sizes $\tau = 10^{-5}, 5 \cdot 10^{-6}, 10^{-6}, 5 \cdot 10^{-7}, 10^{-7}, 5 \cdot 10^{-8}$, respectively, where the time decompositions $\boldsymbol{\tau}$ are always chosen to have constant time step sizes $\tau_n \equiv \tau$. The corresponding L^2-error at $T = 10^{-5}$ is plotted in Figure 5.3/right. It is proportional to τ.

5.4.1.e. Discontinuous initial data. One of the conclusions of Theorem 5.1 is that the discrete approximations u_Δ converge also for (a large class of) non-regular initial data u^0. For illustration of this feature, we consider the discontinuous initial density function

$$u^0_{\mathrm{discont}} = \begin{cases} 1 & \text{for } x \in [0, \frac{1}{3}] \cup [\frac{2}{3}, 1], \\ 10^{-3} & \text{for } x \in (\frac{1}{3}, \frac{2}{3}) \end{cases} \tag{5.74}$$

instead of u^0 from (5.73). According to our hypothesis (5.9), we need to use a sufficiently high spatial and temporal resolution. In practice, this is done in an adaptive way: The K points of the initial grid $\vec{\mathrm{x}}^0_\Delta$ are not placed equidistantly, but with a higher refinement around the points of discontinuity; the applied time steps τ_n are extremely small (down to 10^{-13}) during the initial phase of the evolution, and get larger (up to 10^{-9}) at later times.

Figure 5.4 provides a qualitative picture of the fully discrete evolution for $K = 200$ grid points: Snapshots of the discrete density function u_Δ are shown on the left, corresponding snapshots of the logarithmic density are shown on the right. Note that within a very short time,

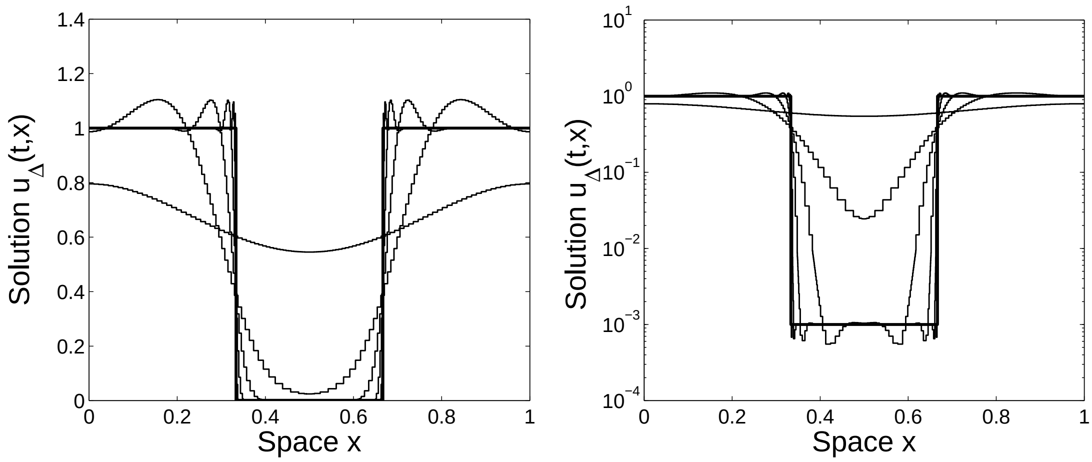


FIGURE 5.4. Snapshots of the densities u_Δ for the initial condition (5.74) at times $t = 0$ and $t = 10^i$, $i = -13, -11, \dots, -5, -3$, using $K = 200$ grid points with linear (left) and logarithmic (right) scaling.

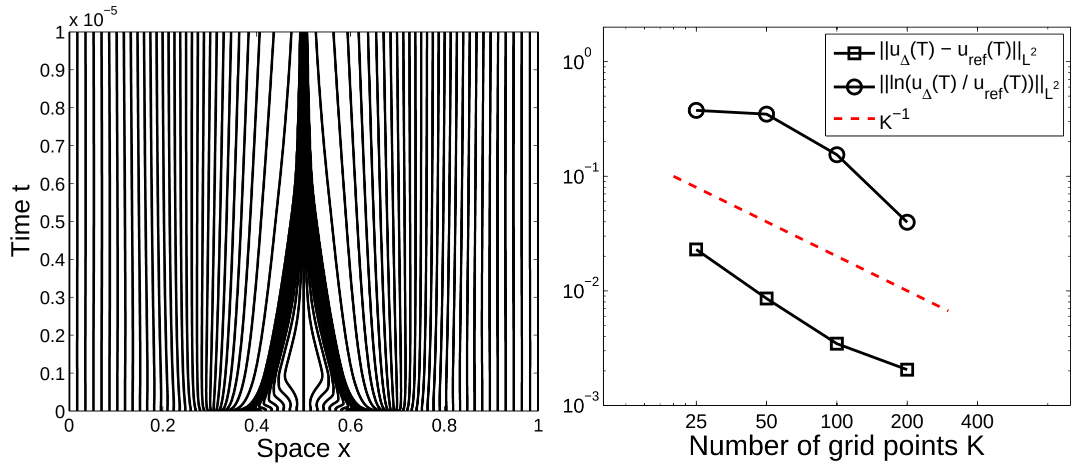


FIGURE 5.5. *Left:* associated particle trajectories of u_Δ using the initial condition (5.74). *Right:* Numerical error analysis for u^0_{discont} from (5.74) with fixed τ and $K = 25, 50, 100, 200$ spatial grid points. The L^2-errors are evaluated at $T = 10^{-8}$.

peaks of relatively high amplitude are generated near the points where u^0 is discontinuous. The associated Lagrangian maps are visualized in Figure 5.5/left. Notice the fast motion of the grid points near the discontinuities.

To estimate the rate of convergence, we performed a series of experiments using $K = 25, 50, 100$ and 200 spatial grid points. For comparison, we calculated a highly refined solution of the following semi-implicit reference scheme,

$$\frac{u^n_{\text{ref}} - u^{n-1}_{\text{ref}}}{\tau_n} = -\Delta_2\big(u^{n-1}_{\text{ref}} \Delta_2 \ln(u^n_{\text{ref}})\big),$$

where Δ_2 is the standard central difference operator Δ_2. We use $K = 800$ spatial grid point for the reference scheme. An adaptive choice of the time steps τ_n needs to be made in order to avoid that the reference solution u_{ref} breaks down because of loss of positivity. The L^2-differences of the densities and of their logarithms have been evaluated at $T = 10^{-8}$, see Figure 5.5/right. As expected, the rate of convergence is no longer quadratic in $\delta \propto K^{-1}$; instead, the error decays approximately linearly.

CHAPTER 6

The thin film equation — an alternative approach

The content of this chapter is joint work with my PhD-supervisor Daniel Matthes and is submitted. An online version of the paper is unfortunately not available so far.

6.1. Introduction

In this last chapter about the numerical treatment of evolution equations in one spatial dimension, we are going to study an alternative numerical approach to the one defined in Chapter 4 for equation (4.1) in the special case that $\alpha = 1$ and $\lambda = 0$, but with an additional, more general potential term. We further assume $\Omega = (a, b)$ to be a bounded domain in this chapter. More precisely, we consider the no-flux boundary problem

$$\partial_t u = -\partial_x\big(u\partial_{xxx}u\big) + \partial_x\big(V_x u\big) \quad \text{for } t > 0 \text{ and } x \in \Omega, \tag{6.1}$$

$$\partial_x u = 0, \quad u(\partial_{xxx}u - V_x) = 0 \quad \text{for } t > 0 \text{ and } x \in \partial\Omega, \tag{6.2}$$

$$u = u^0 \geqslant 0 \quad \text{at } t = 0. \tag{6.3}$$

The initial density is assumed to be integrable with total mass $M > 0$, which is fixed for the rest of this chapter. We further assume that the potential $V \in C^2(\Omega)$ is nonnegative with bounded second derivative,

$$V \geqslant 0, \quad \Lambda := \sup_{x\in\overline{\Omega}} |V_{xx}(x)| < \infty, \tag{6.4}$$

a typical choice being $V(x) = \frac{\Lambda}{2}x^2$.

6.1.1. Gradient flow structure. The gradient flow structure of (6.1) is quite the same as the one of equation (4.1) with $\alpha = 1$ explained in Section 4.1.1, except for the drift-term: It is well known that (6.1) can be written as a gradient flow in the energy landscape of the following (modified) *Dirichlet functional*,

$$\mathcal{D}^V(u) = \mathcal{D}(u) + \mathcal{V}(u), \quad \text{with} \quad \mathcal{D}(u) = \frac{1}{2}\int_\Omega \big(\partial_x u\big)^2 \,\mathrm{d}x \quad \text{and} \quad \mathcal{V}(u) = \int_\Omega V(x)u(x)\,\mathrm{d}x, \tag{6.5}$$

with respect to the L^2-Wasserstein distance [**GO01**]. Using $\mathcal{D}^V$ for $\mathcal{E}$ in (2.6) (which corresponds to $h(x, r, p) = \frac{1}{2}|p|^2 + V(x)r$), then the induced velocity field for the continuity equation (2.7) is given by

$$\mathbf{v}(u) = \partial_{xxx}u - V_x.$$

In analogy to the calculations in Section 4.1.1 of Chapter 4, the Hele-Shaw equation (6.1) can be expressed in terms of X — remember that we denote by X the pseudo-inverse distribution function of u — by

$$\partial_t \mathrm{X} = \frac{2}{3}\partial_\xi\big(\mathrm{Z}^{\frac{5}{2}}\partial_{\xi\xi}\mathrm{Z}^{\frac{3}{2}}\big) + V_x(\mathrm{X}), \quad \text{where} \quad \mathrm{Z}(t,\xi) := \frac{1}{\partial_\xi \mathrm{X}(t,\xi)} = u\big(t, \mathrm{X}(t,\xi)\big), \tag{6.6}$$

which further equals the L^2-gradient flow along the functional

$$\mathcal{D}^V(u \circ \mathrm{X}) = \frac{1}{2\alpha}\int_{\mathcal{M}} \left[\partial_\xi\left(\frac{1}{\partial_\xi \mathrm{X}}\right)\right]^2 \frac{1}{\partial_\xi \mathrm{X}}\,\mathrm{d}\xi + \int_{\mathcal{M}} V(\mathrm{X})\,\mathrm{d}\xi.$$

Since we are looking for an easy discretization of (6.6), it is advisable to reformulate the right-hand side to get rid of the non-integer exponents. Elementary manipulations show that equation (6.6) is equivalent to

$$\partial_t \mathrm{X} = \partial_\xi\left(\frac{1}{2}\mathrm{Z}^3\partial_{\xi\xi}\mathrm{Z} + \frac{1}{4}\mathrm{Z}^2\partial_{\xi\xi}\big(\mathrm{Z}^2\big)\right) + V_x(\mathrm{X}). \tag{6.7}$$

Note at this point that there are infinitely many equivalent ways to rewrite the right-hand side of equation (6.6), and in view of the numerical scheme described in the next section, there are accordingly infinitely many (non-equivalent!) central finite-difference discretizations. The right choice of the representation of (6.6) strongly depends on the desired objective. The convergence result which we are going to derive in this chapter only applies to the particular finite-difference discretizations of (6.6), see (6.8), since only for that one, we obtain "the right" Lyapunov functionals that provide the a priori estimates for the discrete-to-continuous limit. The discretization of (6.7) in (4.8) from Chapter 4 allows an adequate analysis of the schemes long-time behaviour, due to the interpretation of the discretized Dirichlet functional as the auto-dissipation of the respective discrete entropy.

6.1.2. Description of the numerical scheme. As in the previous chapters, we define a numerical scheme for (6.1) as a standard finite element discretization of (6.7) using local linear spline interpolants. By the right choice for the discretization $\mathbf{D}^V$ of the perturbed Dirichlet functional $\mathcal{D}^V$, we are going to show later in Section 4.2.2.b, that the attained numerical scheme equals a natural restriction of a L^2-Wasserstein gradient flow in the potential landscape of $\mathbf{D}^V$.

Let us fix a spatio-temporal discretization parameter $\Delta = (\boldsymbol{\tau}; \boldsymbol{\xi})$ in the following way: Given $\tau > 0$, introduce varying time step sizes $\boldsymbol{\tau} = (\tau_1, \tau_2, \dots)$ with $\tau_n \in (0, \tau]$, and define a time decomposition $(t_n)_{n=0}^\infty$ of $[0, +\infty)$ as in (2.10). As spatial discretization we fix $K \in \mathbb{N}$ and introduce an equidistant spatial decomposition of the mass domain $\mathcal{M}$, so one gets $\boldsymbol{\xi} = (\xi_0, \dots, \xi_K)$ with $\xi_k = k\delta$ for any $k = 0, \dots, K$ and the k-independent mesh size $\delta = MK^{-1}$. We further fix the discrete metric $\mathrm{d}_{\boldsymbol{\xi}}$ on $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$ that is induced by the matrix $\mathrm{W} = \delta\mathbb{I} \in \mathbb{R}^{(K-1)\times(K-1)}$, remember that $\Omega = (a, b)$ is assumed to be bounded, hence $\aleph = K - 1$. That especially induces

$$\langle \vec{\mathrm{v}}, \vec{\mathrm{w}}\rangle_{\boldsymbol{\xi}} = \delta\,\langle \vec{\mathrm{v}}, \vec{\mathrm{w}}\rangle \quad \text{and} \quad \|\vec{\mathrm{v}}\|_{\boldsymbol{\xi}} = \sqrt{\delta\,\langle \vec{\mathrm{v}}, \vec{\mathrm{v}}\rangle}$$

for any $\vec{\mathrm{v}}, \vec{\mathrm{w}} \in \mathbb{R}^{K-1}$. Furthermore, we introduce the central first and second order finite difference operators $\mathrm{D}^1_{\boldsymbol{\xi}}$ and $\mathrm{D}^2_{\boldsymbol{\xi}}$ in analogy to (4.7), see Chapter 4.

Numerical scheme. *Fix a discretization parameter $\Delta = (\boldsymbol{\tau};\boldsymbol{\xi})$. Then the numerical scheme for* (6.1) *is defined as follows:*

(1) *For $n = 0$, fix an initial Lagrangian vector $\vec{\mathrm{x}}_\Delta^0 := (x_1^0,\dots,x_{K-1}^0) \in \mathfrak{x}_{\boldsymbol{\xi}}$ with the usual convention $x_0^0 = a$ and $x_K^0 = b$.*

(2) *For $n \geqslant 1$, recursively define Lagrangian vectors $\vec{\mathrm{x}}_\Delta^n \in \mathfrak{x}_{\boldsymbol{\xi}}$ as solutions to the system consisting of $K-1$ equations*

$$\frac{x_k^n - x_k^{n-1}}{\tau_n} = \mathrm{D}_{\boldsymbol{\xi}}^1\left[\frac{1}{2}(\vec{\mathrm{z}}^n)^3\,\mathrm{D}_{\boldsymbol{\xi}}^2[\vec{\mathrm{z}}^n] + \frac{1}{4}(\vec{\mathrm{z}}^n)^2\,\mathrm{D}_{\boldsymbol{\xi}}^2[(\vec{\mathrm{z}}^n)^2]\right]_k + V_x(x_k), \tag{6.8}$$

where the values $z_{\ell-\frac{1}{2}}^n \geqslant 0$ are defined as in (2.18) *with convention* (2.19). *We later show in Proposition 6.5 that the solvability of the system* (6.8) *is guaranteed.*

From now on we denote a solution to the above scheme by $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}_\Delta^0, \vec{\mathrm{x}}_\Delta^1, \dots)$ and its corresponding sequence of densities by $u_\Delta = (u_\Delta^0, u_\Delta^1, \dots)$, where the components $\vec{\mathrm{x}}_\Delta^n$ and u_Δ^n correlate through the map $\mathbf{u}_{\boldsymbol{\xi}} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathcal{P}_{2,\boldsymbol{\xi}}^r(\Omega)$. Moreover, we introduce for any integer $n \in \mathbb{N}_0$ piecewise affine interpolations $\widehat{u}_\Delta^n : \overline{\Omega} \to (0,+\infty)$ and $\widehat{z}_\Delta^n : \mathcal{M} \to (0,+\infty)$ of u_Δ^n and $u_\Delta^n \circ \mathbf{X}_\Delta^n$, respectively, in analogy to Section 5.1.3 of Chapter 5. The associate sequences are then denoted by $\widehat{u}_\Delta = (\widehat{u}_\Delta^0, \widehat{u}_\Delta^1, \dots)$ and $\widehat{z}_\Delta = (\widehat{z}_\Delta^0, \widehat{z}_\Delta^1, \dots)$, respectively.

6.1.3. Main results. For the statement of our first result, fix a discretization parameter $\Delta = (\boldsymbol{\tau};\boldsymbol{\xi})$. On monotone vectors $\vec{\mathrm{x}} \in \mathbb{R}^{K+1}$ with $\vec{\mathrm{z}} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, introduce the functionals

$$\mathbf{H}(\vec{\mathrm{x}}) := \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} \log(z_\kappa), \qquad \mathbf{D}^V(\vec{\mathrm{x}}) := \frac{\delta}{2}\sum_{k\in\mathbb{I}_K^+} \frac{z_{k+\frac{1}{2}} + z_{k-\frac{1}{2}}}{2}\left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta}\right)^2 + \sum_{k\in\mathbb{I}_K} V_x(x_k),$$

which are discrete replacements for the Boltzmann entropy and the modified Dirichlet energy functionals, respectively.

Theorem 6.1. *From any initial vector $\vec{\mathrm{x}}_\Delta^0 \in \mathfrak{x}_{\boldsymbol{\xi}}$, a sequence of Lagrangian vectors $\vec{\mathrm{x}}_\Delta^n$ satisfying* (6.8) *can be constructed by inductively defining $\vec{\mathrm{x}}_\Delta^n$ as a global minimizer of*

$$\vec{\mathrm{x}} \mapsto \frac{1}{2\tau_n}\left\|\vec{\mathrm{x}} - \vec{\mathrm{x}}_\Delta^{n-1}\right\|_{\boldsymbol{\xi}}^2 + \mathbf{D}^V(\vec{\mathrm{x}}). \tag{6.9}$$

This sequence of vectors $\vec{\mathrm{x}}_\Delta^n$ dissipates both the Boltzmann entropy and the discrete Dirichlet energy in the sense that

$$\mathbf{H}(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{H}(\vec{\mathrm{x}}_\Delta^{n-1}) + \tau_n \Lambda M \qquad \text{and} \qquad \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^{n-1}).$$

To state our main result about convergence, recall the definition (2.14) of the time interpolant. Further, Δ symbolizes a whole sequence of mesh parameters from now on, and we write $\Delta \to 0$ to indicate that $\tau \to 0$ and $\delta \to 0$ simultaneously.

Theorem 6.2. *Let a nonnegative initial condition $u^0 \in H^1(\Omega)$ of finite second moment be given. Choose initial approximations $\vec{\mathrm{x}}_\Delta^0$ such that $u_\Delta^0 = \mathbf{u}[\vec{\mathrm{x}}_\Delta^0] \to u^0$ weakly in $H^1(\Omega)$ as $\Delta \to 0$, and*

$$\overline{\mathcal{D}^V} := \sup_\Delta \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^0) < \infty, \quad \overline{\mathcal{H}} := \sup_\Delta \mathbf{H}(\vec{\mathrm{x}}_\Delta^0) < \infty. \tag{6.10}$$

For each Δ*, construct a discrete approximation* $\vec{\mathrm{x}}_\Delta$ *according to the procedure described in Theorem 6.1 above. Then, there are a subsequence with* $\Delta \to 0$ *and a limit density function* $u_* \in C([0,+\infty)\times\Omega)$ *such that:*

- $\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}$ *converges to* u_* *locally uniformly on* $[0,+\infty)\times\Omega$*,*
- $u_* \in L^2_{\mathrm{loc}}([0,+\infty); H^1(\Omega))$*,*
- $u_*(0) = u^0$*,*
- u_* *satisfies the following weak formulation of* (6.1)*:*

$$\int_0^\infty \int_\Omega \partial_t\varphi u_* \,\mathrm{d}t\,\mathrm{d}x + \int_0^\infty N(u_*,\varphi)\,\mathrm{d}t = 0, \tag{6.11}$$

with

$$N(u,\varphi) := \frac{1}{2}\int_\Omega \partial_x u^2 \partial_{xxx}\varphi + 3(\partial_x u)^2\partial_{xx}\varphi\,\mathrm{d}x + \int_\Omega V_x u \partial_x\varphi\,\mathrm{d}x \tag{6.12}$$

for every test function $\varphi \in C^\infty((0,+\infty)\times\Omega)$ *that is compactly supported in* $(0,+\infty)\times\overline{\Omega}$ *and satisfies* $\partial_x\varphi(t,a) = \partial_x\varphi(t,b) = 0$ *for any* $t \in (0,+\infty)$*.*

Remark 6.3. (1) Rate of convergence: *Numerical experiments with smooth initial data* u^0 *show that the rate of convergence is of order* $\tau + \delta^2$*, see Section 6.5.*
(2) No uniqueness: *Since our notion of solution is very weak, we cannot exclude that different subsequences of* $\{u_\Delta\}_{\boldsymbol{\tau}}$ *converge to different limits.*
(3) Initial approximation: *The assumptions in* (6.10) *are not independent: Boundedness of* $\mathbf{D}^V(\vec{\mathrm{x}}^0_\Delta)$ *implies boundedness of* $\mathbf{H}(\vec{\mathrm{x}}^0_\Delta)$ *from above.*

As in the proof of the respective result of Chapter 5 about the DLSS equation, the claims of Theorem (6.2) are proven separately: The first two claims about the convergence and the regularity of the limit curve are provided in the Propositions 6.12 and 6.13 from Section 6.3, whereas the validity of the weak formulation is shown in Proposition 6.14, Section 6.4.

A similar weak formulation for (6.1) was formulated in [**MMS09**], but on the whole space of real numbers, hence no boundary conditions appear. To motivate that (6.11) is a valid choice for a weak formulation to the problem (6.1) with the no-flux boundary conditions in (6.2), let us assume that $u : [0,+\infty)\times\Omega \to [0,+\infty)$ is a sufficiently smooth solution of (6.11) satisfying the boundary conditions (5.2). Furthermore, choose any test function φ that satisfies the requirements in Theorem 6.2, then repetetive integration by parts yields (for simplicity, we assume $V = 0$)

$$\begin{aligned}
N(u,\varphi) &= \frac{1}{2}\int_\Omega \partial_x u^2\,\partial_{xxx}\varphi + 3(\partial_x u)^2\,\partial_{xx}\varphi\,\mathrm{d}x \\
&= \big[2u\partial_x u\partial_{xx}\varphi\big]_{x=a}^{x=b} - \frac{1}{2}\int_\Omega \big(2u\partial_{xx}u - (\partial_x u)^2\big)\,\partial_{xx}\varphi\,\mathrm{d}x \\
&\overset{(6.2)}{=} -\frac{1}{2}\Big[\big(2u\partial_{xx}u - (\partial_x u)^2\big)\,\partial_x\varphi\Big]_{x=a}^{x=b} + \int_\Omega u\partial_{xxx}u\,\partial_x\varphi\,\mathrm{d}x \\
&= \big[u\partial_{xxx}u\,\varphi\big]_{x=a}^{x=b} - \int_\Omega \partial_x(u\partial_{xxx}u)\,\varphi\,\mathrm{d}x \overset{(6.2)}{=} -\int_\Omega \partial_x(u\partial_{xxx}u)\,\varphi\,\mathrm{d}x.
\end{aligned}$$

A further integration by parts with respect to the time derivative then shows that u is a solution to (6.1).

6.1.4. Key estimates. In what follows, we give a very formal outline for the derivation of the main a priori estimates on the fully discrete solutions.

In the continuous theory of well-posedness of (6.1), two main a priori estimates are provided by the dissipation of the (modified) Dirichlet functional $\mathcal{D}^V$ and the Boltzmann entropy $\mathcal{H}$, and the respective estimates are formally derived by an integration by parts (assuming $V = 0$):

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{D}(u) = \int_\Omega \partial_x u\, \partial_{xx}(u\, \partial_{xxx}u)\,\mathrm{d}x = \int_\Omega u\,(\partial_{xxx}u)^2\,\mathrm{d}x, \tag{6.13}$$

$$-\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{H}(u) = \int_\Omega (\log u + 1)\,\partial_x(u\,\partial_{xxx}u)\,\mathrm{d}x = \int_\Omega (\partial_{xx}u)^2\,\mathrm{d}x. \tag{6.14}$$

Notice that energy dissipation does *not* provide $L^2([0,T];H^3(\mathbb{R}))$-regularity, due to the degeneracy.

In view of our numerical scheme, we are going to show in Section 6.2.1 that discrete solutions to (6.8) are gradient flows of the discretized energy $\mathbf{D}^V$ (which approximates $\mathcal{D}^V$ in a certain sense) with respect to the metric $\mathrm{d}_{\boldsymbol{\xi}}$, which is equivalent to the “real” L^2-Wasserstein distance restricted to $\mathcal{P}^r_{2,\boldsymbol{\xi}}(\Omega)$. The corresponding fully discrete energy estimates are collected in Proposition 6.8. Unfortunately, we cannot extract further information from the dissipation of $\mathbf{D}^V$ and a useful interpretation of (6.13) in the discrete setting is missing.

However, by convexity of $\vec{\mathrm{x}} \mapsto \mathbf{H}(\vec{\mathrm{x}})$, we are able to give a meaning to (6.14) in terms of our discretization. Using Lagrangian coordinates and $\mathrm{Z} = u \circ \mathrm{X}$, the above expression turns into

$$\int_\Omega (\partial_{xx}u)^2\,\mathrm{d}x = \frac{1}{4}\int_{\mathcal{M}} \mathrm{Z}\,(\partial_{\xi\xi}\mathrm{Z}^2)^2\,\mathrm{d}\xi,$$

which is, unfortunately, algebraically more difficult to handle than the equivalent functional

$$\int_\Omega u^2\,(\partial xx \log u)^2\,\mathrm{d}x = \int_{\mathcal{M}} \mathrm{Z}^3\,(\partial_{\xi\xi}\mathrm{Z})^2\,\mathrm{d}\xi, \tag{6.15}$$

which we shall eventually work with, see Lemma 6.9. Obviously, piecewise constant densities u_Δ are impractical for the analytical treatment of an H^2-estimate. Therefore we proceed as before in Chapter 5 and study the total variation of the first derivative $\partial_x\widehat{u}_\Delta$, where $\widehat{u}_\Delta$ is a locally affine interpolation of u_Δ. This TV-control is a perfect replacement for the H^2-estimate in (6.14), and is the source for compactness, see Proposition 6.13.

6.2. Discretization in space and time

6.2.0.a. Ansatz space and discrete entropy/information functionals. To derive a suitable discretization of $\mathcal{D}$ and $\mathcal{D}^V$ from (6.5), we use a similar approach to that in Chapter 4. To this end, note that the Dirichlet functional can be written as the dissipation of the *quadratic Renyi entropy* $\mathcal{Q}(u) := \frac{1}{4}\int_\Omega u^2\,\mathrm{d}x$ along the heat flow, which can be motivated by the formal calculation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{Q}(v) = -\frac{1}{2}\int_\Omega v\partial_{xx}\,\mathrm{d}x = \frac{1}{2}\int_\Omega (\partial_x v)^2\,\mathrm{d}x, \tag{6.16}$$

where $\partial_t v = \partial_{xx} v$. That is why we introduce the functionals $\mathbf{H}, \mathbf{Q} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ as restrictions of $\mathcal{H}$ and $\mathcal{Q}$ on $\mathfrak{x}_{\boldsymbol{\xi}}$, i.e.

$$\mathbf{H}(\vec{x}) = \mathcal{H}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}]) = \int_\Omega \mathbf{u}_{\boldsymbol{\xi}}[\vec{x}] \log\big(\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}]\big)\,\mathrm{d}x = \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} \log(z_\kappa),$$

$$\mathbf{Q}(\vec{x}) = \mathcal{Q}(\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}]) = \frac{1}{4}\int_\Omega \big(\mathbf{u}_{\boldsymbol{\xi}}[\vec{x}]\big)^2\,\mathrm{d}x = \frac{\delta}{4} \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa.$$

Using (2.29), we obtain an explicit representation of the gradients,

$$\partial_{\vec{x}}\mathbf{H}(\vec{x}) = \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa \frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}, \qquad \partial_{\vec{x}}\mathbf{Q}(\vec{x}) = \frac{\delta}{4} \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 \frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}, \tag{6.17}$$

and — for later references — also of the Hessians,

$$\begin{aligned}\partial_{\vec{x}}^2\mathbf{H}(\vec{x}) &= \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 \left(\frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}\right)\left(\frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}\right)^T,\\ \partial_{\vec{x}}^2\mathbf{Q}(\vec{x}) &= \frac{\delta}{2} \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}\right)\left(\frac{\mathbf{e}_{\kappa-\frac12} - \mathbf{e}_{\kappa+\frac12}}{\delta}\right)^T.\end{aligned} \tag{6.18}$$

A key property of our simple discretization ansatz is the preservation of convexity of $\vec{x} \mapsto \mathbf{H}(\vec{x})$ and $\vec{x} \mapsto \mathbf{Q}(\vec{x})$, which immediately follows by inspection of the Hessians in (6.18).

Following the discrete analogue to the calculation in (6.16), one attains a discretization for the energy functional $\mathcal{D}$ from (6.5) that is

$$\mathbf{D}(\vec{x}) := \langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{x}), \nabla_{\boldsymbol{\xi}}\mathbf{Q}(\vec{x})\rangle_{\boldsymbol{\xi}} = \frac{\delta}{2} \sum_{k\in\mathbb{I}_K^{1/2}} \frac{z_{\kappa+\frac12} + z_{\kappa-\frac12}}{2}\left(\frac{z_{\kappa+\frac12} - z_{\kappa-\frac12}}{\delta}\right)^2. \tag{6.19}$$

Remark 6.4. *Although this discretization follows the same idea as the one of $\mathcal{F}_{1,0} = \mathcal{D}$ in Chapter 4, that is "discretization by dissipation", it is conceptually different in the sense that the discrete flow along $\mathbf{D}$ dissipates $\mathbf{H} = \mathbf{H}_{1/2,0}$ instead of $\mathbf{H}_{1,0}$, see Lemma 6.9.*

It remains to define a discrete counterpart for the potential $\mathcal{V}$. A change of variables in the definition in (6.5) yields

$$\mathcal{V}(u) = \int_\Omega V(x)u(x)\,\mathrm{d}x = \int_{\mathcal{M}} V(\mathrm{X})\,\mathrm{d}\xi,$$

Thus, a suitable discretization $\mathbf{V}$ of $\mathcal{V}$ is given by

$$\mathbf{V}(\vec{x}) = \delta \sum_{k\in\mathbb{I}_K} V(x_k).$$

In summary, our discretization $\mathbf{D}^V$ of $\mathcal{D}^V$ is

$$\mathbf{D}^V(\vec{x}) = \mathbf{D}(\vec{x}) + \mathbf{V}(\vec{x}) = \langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{x}), \nabla_{\boldsymbol{\xi}}\mathbf{Q}(\vec{x})\rangle_{\boldsymbol{\xi}} + \mathbf{V}(\vec{x}).$$

6.2.1. Interpretation of the scheme as a discrete Wasserstein gradient flow. We want to discretize the spatially discrete gradient flow equation

$$\partial_t \vec{\mathrm{x}} = -\nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}) \tag{6.20}$$

also in time, using minimizing movements. To this end, fix a time step width $\tau > 0$; we combine the spatial and temporal mesh widths in a single discretization parameter $\Delta = (\tau; \boldsymbol{\xi})$. For each $\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}}$, introduce the *Yosida-regularized Dirichlet functional* $\mathbf{D}^V_\Delta(\cdot, \cdot, \vec{\mathrm{y}}) : [0, \tau] \times \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ by

$$\mathbf{D}^V_\Delta(\sigma, \vec{\mathrm{x}}, \vec{\mathrm{y}}) = \frac{1}{2\sigma} \|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|^2_{\boldsymbol{\xi}} + \mathbf{D}^V(\vec{\mathrm{x}}).$$

A fully discrete approximation $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}^0_\Delta, \vec{\mathrm{x}}^1_\Delta, \ldots)$ of (6.20) is now defined inductively from a given initial datum $\vec{\mathrm{x}}^0_\Delta$ by choosing each $\vec{\mathrm{x}}^n_\Delta$ as a global minimizer of $\mathbf{D}^V_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$. Below, we prove that such a minimizer always exists, see Lemma 6.6.

In practice, one wishes to define $\vec{\mathrm{x}}^n_\Delta$ as — preferably unique — solution to the Euler-Lagrange equations associated to $\mathbf{D}^V_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$, which leads to the implicit Euler time stepping:

$$\frac{\vec{\mathrm{x}} - \vec{\mathrm{x}}^{n-1}_\Delta}{\tau_n} = -\nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}) = -\frac{1}{\delta^2}\left(\partial^2_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}}) \cdot \partial_{\vec{\mathrm{x}}}\mathbf{Q}(\vec{\mathrm{x}}) + \partial^2_{\vec{\mathrm{x}}}\mathbf{Q}(\vec{\mathrm{x}}) \cdot \partial_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}})\right) + \nabla_{\boldsymbol{\xi}}\mathbf{V}(\vec{\mathrm{x}}). \tag{6.21}$$

Using (6.17) and (6.18), a straight-forward calculation shows that (6.21) is precisely the numerical scheme (6.8) from the introduction. Equivalence of (6.21) and the minimization problem for $\mathbf{D}^V_\Delta$ is guaranteed at least for sufficiently small $\tau > 0$.

Proposition 6.5. *For each discretization Δ and every initial condition $\vec{\mathrm{x}}^0 \in \mathfrak{x}_{\boldsymbol{\xi}}$, the sequence of equations* (6.21) *can be solved inductively. Moreover, if $\tau > 0$ is sufficiently small with respect to δ and $\mathbf{D}^V(\vec{\mathrm{x}}^0)$, then each equation* (6.21) *possesses a unique solution with $\mathbf{D}^V(\vec{\mathrm{x}}) \leqslant \mathbf{D}(\vec{\mathrm{x}}^0)$, and that solution is the unique global minimizer of $\mathbf{D}^V_\Delta(\tau_n, \cdot, \vec{\mathrm{x}}^{n-1}_\Delta)$.*

The proof of this proposition is a consequence of the following rather technical lemma.

Lemma 6.6. *Fix a spatial discretization parameter $\boldsymbol{\xi}$ and let $C > 0$. Then for every $\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ with $\mathbf{D}^V(\vec{\mathrm{y}}) \leqslant C$, the following points are fulfilled:*

- *For each $\sigma > 0$, the function $\mathbf{D}^V_\Delta(\sigma, \cdot, \vec{\mathrm{y}})$ possesses at least one global minimizer $\vec{\mathrm{x}}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$ which satisfies the system of Euler-Lagrange equations*

$$\frac{\vec{\mathrm{x}}^* - \vec{\mathrm{y}}}{\sigma} = -\nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}^*).$$

- *There exists a $\tau_C > 0$ independent of $\vec{\mathrm{y}}$ such that for each $\sigma \in (0, \tau_C)$, the global minimizer $\vec{\mathrm{x}}^* \in \mathfrak{x}_{\boldsymbol{\xi}}$ is strict, unique, and the only critical point of $\mathbf{D}^V_\Delta(\sigma, \cdot, \vec{\mathrm{y}})$ with $\mathbf{D}^V(\vec{\mathrm{x}}) \leqslant C$.*

Proof. Fix $\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ with $\mathbf{D}^V(\vec{\mathrm{y}}) \leqslant C$, and define the nonempty (since it contains $\vec{\mathrm{y}}$) sublevel set $A_C := \left(\mathbf{D}^V_\Delta(\sigma, \cdot, \vec{\mathrm{y}})\right)^{-1}([0, C]) \subseteq \mathfrak{x}_{\boldsymbol{\xi}}$. From here, one can proceed analogously to the proof of Lemma 4.7, if one can guarantee that the differences $x_{\kappa+\frac{1}{2}} - x_{\kappa-\frac{1}{2}} = \delta/z_\kappa$ have a uniform positive lower bound on A_C, for any $\vec{\mathrm{x}} \in A_C$. For this purpose, observe that $z_\kappa \geqslant \delta/(b-a)$ for each $z \in \mathbb{I}_K^{1/2}$ and arbitrary $\vec{z} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{x}]$, hence

$$\begin{aligned} z_\kappa - \frac{\delta}{b-a} &\leqslant \sum_{k\in\mathbb{I}_K^+} |z_{k+\frac12} - z_{k-\frac12}| \\ &\leqslant \left(\sum_{k\in\mathbb{I}_K^+} \frac{\delta}{z_{k+\frac12} + z_{k-\frac12}}\right)^{\frac12} \left(\delta \sum_{k\in\mathbb{I}_K^+} (z_{k+\frac12} + z_{k-\frac12}) \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right)^2\right)^{\frac12} \\ &\leqslant \big(2(b-a)\big)^{1/2} \mathbf{D}^V(\vec{x})^{1/2} \leqslant (4(b-a)C)^{1/2}, \end{aligned}$$

where we used (A.4). This shows the desired lower bound on $x_{\kappa+\frac12} - x_{\kappa-\frac12} = \delta/z_\kappa$. □

6.2.2. A discrete Sobolev-type estimate. The following inequality plays a key role in our analysis. Recall the definition of the intermediate value $z_k = \frac12(z_{k+\frac12} + z_{k-\frac12})$ and the conventions $z_{-\frac12} = z_{\frac12}$ and $z_{K+\frac12} = z_{K-\frac12}$ from (2.19).

Lemma 6.7. *For any* $\vec{x} \in \mathfrak{x}_{\boldsymbol{\xi}}$,

$$\delta \sum_{k\in\mathbb{I}_K^+} z_k \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right)^4 \leqslant \frac94 \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2}\right)^2. \tag{6.22}$$

Proof. Due to the conventions on $\vec{z}$, one can even sum up over all $k \in \mathbb{I}_K$ on the left-hand side of (6.22). By "summation by parts"

$$\begin{aligned} (A) = \delta \sum_{k\in\mathbb{I}_K} z_k \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right)^4 &= \delta^{-3} \sum_{k\in\mathbb{I}_K} z_k (z_{k+\frac12} - z_{k-\frac12})^3 (z_{k+\frac12} - z_{k-\frac12}) \\ &= \frac{\delta^{-3}}{2} \sum_{k=1}^K z_{k-\frac12} \Big[(z_{k-\frac12} + z_{k-\frac32})(z_{k-\frac12} - z_{k-\frac32})^3 - (z_{k+\frac12} + z_{k-\frac12})(z_{k+\frac12} - z_{k-\frac12})^3\Big] \\ &= \frac{\delta^{-3}}{2} \sum_{k=1}^K z_{k-\frac12} \Big[(z_{k-\frac32} - z_{k-\frac12})(z_{k-\frac12} - z_{k-\frac32})^3 + (z_{k-\frac12} - z_{k+\frac12})(z_{k+\frac12} - z_{k-\frac12})^3 \\ &\qquad + 2z_{k-\frac12}(z_{k-\frac12} - z_{k-\frac32})^3 - 2z_{k-\frac12}(z_{k+\frac12} - z_{k-\frac12})^3\Big]. \end{aligned}$$

Rearranging terms yields

$$(A) = -(A) - \delta^{-3} \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 \left[(z_\kappa - z_{\kappa-1})^3 - (z_{\kappa+1} - z_\kappa)^3\right]$$

and further using the identity $(p^3 - q^3) = (p-q)(p^2 + q^2 + pq)$ for arbitrary real numbers p, q,

$$\begin{aligned} (A) &= -\frac{\delta^{-3}}{2} \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 \left[(z_\kappa - z_{\kappa-1})^3 - (z_{\kappa+1} - z_\kappa)^3\right] \\ &= -\frac{\delta^{-1}}{2} \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 [\mathrm{D}_{\boldsymbol{\xi}}^2 z]_\kappa \Big[(z_\kappa - z_{\kappa-1})^2 + (z_{\kappa+1} - z_\kappa)^2 + (z_\kappa - z_{\kappa-1})(z_{\kappa+1} - z_\kappa)\Big]. \end{aligned}$$

Invoke Hölder's inequaltiy and the elementary estimate $pq \leqslant \frac{1}{2}(p^2+q^2)$ to conclude that

$$\begin{aligned}
(A) &\leqslant \frac{1}{2}\left(\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 [\mathrm{D}_{\boldsymbol{\xi}}^2 z]_\kappa^2\right)^{\frac{1}{2}} \left(\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa \frac{9}{4}\left[\left(\frac{z_\kappa - z_{\kappa-1}}{\delta}\right)^2 + \left(\frac{z_{\kappa+1}-z_\kappa}{\delta}\right)^2\right]^2\right)^{\frac{1}{2}} \\
&\leqslant \frac{3}{2}\left(\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 [\mathrm{D}_{\boldsymbol{\xi}}^2 z]_\kappa^2\right)^{\frac{1}{2}} \left(\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} \frac{z_\kappa}{2}\left[\left(\frac{z_\kappa - z_{\kappa-1}}{\delta}\right)^4 + \left(\frac{z_{\kappa+1}-z_\kappa}{\delta}\right)^4\right]\right)^{\frac{1}{2}} \\
&= \frac{3}{2}\left(\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 [\mathrm{D}_{\boldsymbol{\xi}}^2 z]_\kappa^2\right)^{\frac{1}{2}} (A)^{\frac{1}{2}},
\end{aligned}$$

where we have used an index shift and the conventions $z_{-\frac{1}{2}} = z_{\frac{1}{2}}$ and $z_{K+\frac{1}{2}} = z_{k-\frac{1}{2}}$ in the last step. □

6.3. A priori estimates and compactness

Throughout this section, we consider a sequence $\Delta = (\boldsymbol{\tau};\boldsymbol{\xi})$ of discretization parameters such that $\delta \to 0$ and $\tau \to 0$ in the limit, formally denoted by $\Delta \to 0$. We assume that a fully discrete solution $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}_\Delta^0, \vec{\mathrm{x}}_\Delta^1, \ldots)$ is given for each Δ-mesh, defined by inductive minimization of the respective $\mathbf{D}_\Delta^V$. The sequences u_Δ, $\widehat{u}_\Delta$, $\widehat{z}_\Delta$ and X_Δ of spatial interpolations are defined from the respective $\vec{\mathrm{x}}_\Delta$ accordingly. For the sequence of initial conditions $\vec{\mathrm{x}}_\Delta^0$, we assume that $\widehat{u}_\Delta^0 \to u^0$ weakly in $L^1(\Omega)$, and that the uniform boundedness of $\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^0)$ and $\mathbf{H}(\vec{\mathrm{x}}_\Delta^0)$ is fulfilled accordingly to (6.10).

6.3.1. Energy and entropy dissipation. The following estimates for the modified discrete Dirichlet functional $\mathbf{D}^V$ are immediate conclusions from Lemma 2.4.

Proposition 6.8. *The discrete Dirichlet functional $\mathbf{D}^V$ is monotone, i.e. $\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^{n-1})$. Furthermore, one has*

$$\left\|\vec{\mathrm{x}}_\Delta^{\overline{n}} - \vec{\mathrm{x}}_\Delta^{\underline{n}}\right\|_{\boldsymbol{\xi}}^2 \leqslant 2\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^0)\,(t_{\overline{n}} - t_{\underline{n}}) \quad \text{for all } \overline{n} \geqslant \underline{n} \geqslant 0, \tag{6.23}$$

$$\sum_{n=1}^{\infty} \tau_n \left\|\frac{\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1}}{\tau_n}\right\|_{\boldsymbol{\xi}}^2 = \sum_{n=1}^{\infty} \tau_n \left\|\nabla_{\boldsymbol{\xi}}\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n)\right\|_{\boldsymbol{\xi}}^2 \leqslant 2\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^0). \tag{6.24}$$

The previous estimates were completely general. The following estimate is very particular for the problem at hand. For convenience, assume that $\tau < 1$ in the following.

Lemma 6.9. *One has that $\mathbf{H}$ satisfies $\mathbf{H}(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{H}(\vec{\mathrm{x}}_\Delta^{n-1}) + \tau_n \Lambda M$. Moreover, for arbitrary $T > 0$ and each $N_{\boldsymbol{\tau}} \in \mathbb{N}$ with $\sum_{n=0}^{N_{\boldsymbol{\tau}}} \tau_n \in (T, T+1)$,*

$$\sum_{n=0}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} (z_\kappa^n)^3 \left(\frac{z_{\kappa+1}^n - 2z_\kappa^n + z_{\kappa-1}^n}{\delta^2}\right)^2 \leqslant \mathcal{C}_1(T, \overline{\mathcal{H}}) \tag{6.25}$$

is satisfied with the Δ-independent constant $\mathcal{C}_1(t,h) := 4\big(h + \Lambda M(t+1)\big)$.

Proof. Fix $T > 0$. Convexity of $\mathbf{H}$ implies that

$$\mathbf{H}(\vec{\mathrm{x}}_\Delta^{n-1}) - \mathbf{H}(\vec{\mathrm{x}}_\Delta^n) \geqslant \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \vec{\mathrm{x}}_\Delta^{n-1} - \vec{\mathrm{x}}_\Delta^n \right\rangle_{\boldsymbol{\xi}} = \tau_n \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \nabla_{\boldsymbol{\xi}}\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}},$$

for each $n = 1, \ldots, N_{\boldsymbol{\tau}}$. Summation of these inequalities over n yields

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \nabla_{\boldsymbol{\xi}}\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} \leqslant \mathbf{H}(\vec{\mathrm{x}}_\Delta^0) - \mathbf{H}(\vec{\mathrm{x}}_\Delta^{N_{\boldsymbol{\tau}}}). \tag{6.26}$$

To estimate the right-hand side in (6.26), observe that $\mathbf{H}(\vec{\mathrm{x}}_\Delta^0) \leqslant \overline{\mathcal{H}}$ by hypothesis, and that $\mathbf{H}(\vec{\mathrm{x}}_\Delta^{N_{\boldsymbol{\tau}}})$ is bounded from below, see Lemma A.7.

We turn to estimate the left-hand side in (6.26) from below. Recall that $\mathbf{D}^V = \mathbf{D} + \mathbf{V}$. For the component corresponding to $\mathbf{V}$ we find, using (6.17) and (6.4),

$$\begin{aligned}\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}_\Delta^n), \nabla_{\boldsymbol{\xi}}\mathbf{V}(\vec{\mathrm{x}}_\Delta^n) \right\rangle_{\boldsymbol{\xi}} &= \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa \frac{V_x(x_{\kappa-\frac12}) - V_x(x_{\kappa+\frac12})}{\delta} \\ &\geqslant \left(-\sup_{x\in\overline{\Omega}} |V_{xx}(x)|\right) \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} \left| z_\kappa \frac{x_{\kappa-\frac12} - x_{\kappa+\frac12}}{\delta} \right| \geqslant -\Lambda M.\end{aligned}$$

This shows in particular $\mathbf{H}(\vec{\mathrm{x}}_\Delta^n) \leqslant \mathbf{H}(\vec{\mathrm{x}}_\Delta^{n-1}) + \tau_n \Lambda M$ due to (6.26). The component corresponding to $\mathbf{D}$ is more difficult to estimate. Owing to (6.17) and (6.18), we have that

$$\begin{aligned}&4\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{D}(\vec{\mathrm{x}}), \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}) \right\rangle_{\boldsymbol{\xi}} \\ &= 4\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}), \nabla_{\boldsymbol{\xi}}^2\mathbf{Q}(\vec{\mathrm{x}})\nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}) \right\rangle_{\boldsymbol{\xi}} + 4\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{Q}(\vec{\mathrm{x}}), \nabla_{\boldsymbol{\xi}}^2\mathbf{H}(\vec{\mathrm{x}})\nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}) \right\rangle_{\boldsymbol{\xi}} \\ &= 2\delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2}\right)^2 + \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 \left(\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2}\right)\left(\frac{z_{\kappa+1}^2 - 2z_\kappa^2 + z_{\kappa-1}^2}{\delta^2}\right)\end{aligned}$$

for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$. Further estimates are needed to control the second sum from below. Observing that

$$\frac{z_{\kappa+1}^2 - 2z_\kappa^2 + z_{\kappa-1}^2}{\delta^2} = 2z_\kappa \frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2} + \left(\frac{z_{\kappa+1} - z_\kappa}{\delta}\right)^2 + \left(\frac{z_{\kappa-1} - z_\kappa}{\delta}\right)^2$$

and that $2pq \geqslant -\frac32 p^2 - \frac23 q^2$ for arbitrary real numbers p, q, we conclude that

$$\begin{aligned}&4\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{D}(\vec{\mathrm{x}}), \nabla_{\boldsymbol{\xi}}\mathbf{H}(\vec{\mathrm{x}}) \right\rangle_{\boldsymbol{\xi}} \\ &\geqslant \left(4 - \frac32\right) \delta \sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2}\right)^2 - \frac{2\delta}{3} \sum_{\kappa\in\mathbb{I}_K} z_k \left(\frac{z_{k+\frac12} - z_{k-\frac12}}{\delta}\right)^4.\end{aligned}$$

Now set $\vec{\mathrm{x}} = \vec{\mathrm{x}}_\Delta^n$ and apply inequality (6.22). □

6.3.2. Bound on the total variation. The following lemma contains the key estimate to derive compactness of fully discrete solutions in the limit $\Delta \to 0$. Below, we prove that from the entropy dissipation (6.25), we obtain a control on the total variation of $\partial_x \widehat{u}_\Delta^n$.

For this purpose, recall that an appropriate definition of the total variation of a function $f \in L^1(\Omega)$ is given by (1.15), i.e.

$$\mathrm{TV}\,[f] = \sup\left\{\sum_{j=1}^{J-1} |f(r_{j+1}) - f(r_j)| \;:\; J \in \mathbb{N},\, a < r_1 < r_2 < \cdots < r_J < b\right\}. \tag{6.27}$$

Proposition 6.10. *For any $T > 0$ and $N_{\boldsymbol{\tau}} \in \mathbb{N}$ with $\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \in (T, T+1)$, one has that*

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \mathrm{TV}\,[\partial_x \widehat{u}_\Delta^n]^2 \leqslant (b-a)\mathcal{C}_2(T, \overline{\mathcal{H}}), \tag{6.28}$$

with the Δ-independent constant $\mathcal{C}_2(t,h) := \frac{25}{2}\mathcal{C}_1(t,h)$ where $\mathcal{C}_1(t,h)$ is given in Lemma 6.9.

Proof. Fix $n \geqslant 1$. The function $\partial_x \widehat{u}_\Delta^n$ is locally constant on each interval $(x_{k-\frac{1}{2}}^n, x_k^n)$. Therefore, the total variation of $\partial_x \widehat{u}_\Delta^n$ is given by the sum over all jumps at the points of discontinuity,

$$\mathrm{TV}\,[\partial_x \widehat{u}_\Delta^n] = \sum_{k \in \mathbb{I}_K^+} |[\![\partial_x \widehat{u}_\Delta^n]\!]_{x_k}| + \sum_{\kappa \in \mathbb{I}_K^{1/2}} |[\![\partial_x \widehat{u}_\Delta^n]\!]_{x_\kappa}|\,. \tag{6.29}$$

In view of (5.18), one obtains by direct calculation for the derivative of $\widehat{u}_\Delta^n$ that

$$\partial_x \widehat{u}_\Delta^n\big|_{(x_{k-\frac{1}{2}}^n, x_k^n)} = z_{k-\frac{1}{2}}^n \frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta} \quad \text{for } k \in \mathbb{I}_K \backslash \{0\},$$

$$\partial_x \widehat{u}_\Delta^n\big|_{(x_k^n, x_{k+\frac{1}{2}}^n)} = z_{k+\frac{1}{2}}^n \frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta} \quad \text{for } k \in \mathbb{I}_K \backslash \{K\}.$$

Furthermore, $\partial_x \widehat{u}_\Delta^n$ vanishes identically on the intervals $(a, x_{\frac{1}{2}}^n)$ and $(x_{K-\frac{1}{2}}^n, b)$. This implies

$$|[\![\partial_x \widehat{u}_\Delta^n]\!]_{x_k}| = \delta \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^2 \quad \text{for } k \in \mathbb{I}_K^+,$$

$$|[\![\partial_x \widehat{u}_\Delta^n]\!]_{x_\kappa}| = \delta z_\kappa^n \left(\frac{z_{\kappa+1}^n - 2z_\kappa^n + z_{\kappa-1}^n}{\delta^2}\right) \quad \text{for } \kappa \in \mathbb{I}_K^{1/2}.$$

We substitute this into (6.29), use Hölder's inequality, and apply (6.22) to obtain as a consequence of elementary estimates that

$$\begin{aligned}
&\mathrm{TV}\,[\partial_x \widehat{u}_\Delta^n] \\
\leqslant&\delta \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^2 + \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^n \left|[\mathrm{D}_{\boldsymbol{\xi}}^2\, \vec{\mathrm{z}}_\Delta^n]_\kappa\right| \\
\leqslant&\left(\sum_{k \in \mathbb{I}_K^+} \frac{\delta}{z_k^n}\right)^{\frac{1}{2}} \left(\delta \sum_{k \in \mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^4\right)^{\frac{1}{2}} + \left(\sum_{\kappa \in \mathbb{I}_K^{1/2}} \frac{\delta}{z_\kappa^n}\right)^{\frac{1}{2}} \left(\delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} (z_\kappa^n)^3 [\mathrm{D}_{\boldsymbol{\xi}}^2\, \vec{\mathrm{z}}_\Delta^n]_\kappa^2\right)^{\frac{1}{2}} \\
\leqslant&\frac{5}{2}(2(b-a))^{\frac{1}{2}} \left(\delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} (z_\kappa^n)^3 [\mathrm{D}_{\boldsymbol{\xi}}^2\, \vec{\mathrm{z}}_\Delta^n]_\kappa^2\right)^{\frac{1}{2}}.
\end{aligned}$$

We square both sides, multiply by τ_n, and sum over $n = 0, \dots, N_{\boldsymbol{\tau}}$. An application of the entropy dissipation inequality (6.25) yields the desired bound (6.28). □

6.3.3. Convergence of time interpolants. The a priori estimates from the previous subsections implicate a series of results for solutions to the scheme:

Lemma 6.11. *There is a constant $C > 0$ just dependent on $\overline{\mathcal{D}^V}$ and Ω, such that the following estimates are uniformly satisfied as $\Delta \to 0$:*

$$\sup_{t\in[0,+\infty)} \|\partial_x \{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\Omega)} \leqslant C, \tag{6.30}$$

$$\sup_{t\in[0,+\infty)} \|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - \{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} \leqslant C\delta, \tag{6.31}$$

$$\sup_{t\in[0,+\infty)} \|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)} \leqslant C. \tag{6.32}$$

Moreover, the functions $\{u_\Delta\}_{\boldsymbol{\tau}}$ and $\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}$ are uniformly bounded on $[0, +\infty) \times \Omega$.

Proof. For each $n \in \mathbb{N}$,

$$\begin{aligned}
\|\partial_x \widehat{u}_\Delta^n\|_{L^2(\Omega)}^2 &= \sum_{k\in\mathbb{I}_K^+} \left[(x_{k+\frac12}^n - x_k^n)\Big(\frac{z_{k+\frac12}^n - z_k^n}{x_{k+\frac12}^n - x_k^n}\Big)^2 + (x_k^n - x_{k-\frac12}^n)\Big(\frac{z_k^n - z_{k-\frac12}^n}{x_k^n - x_{k-\frac12}^n}\Big)^2 \right] \\
&= \sum_{k\in\mathbb{I}_K^+} \left[\frac{x_{k-1}^n - x_k^n}{2}\Big(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{x_{k-1}^n - x_k^n}\Big)^2 + \frac{x_k^n - x_{k-1}^n}{2}\Big(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{x_k^n - x_{k-1}^n}\Big)^2 \right] \\
&= \delta \sum_{k\in\mathbb{I}_K^+} \frac{z_{k+\frac12}^n + z_{k-\frac12}^n}{2}\Big(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\Big)^2 \leqslant 2\mathbf{D}(\vec{\mathrm{x}}_\Delta^n).
\end{aligned}$$

This shows (6.30). For proving (6.31), we start with the observation that

$$|u_\Delta^n(x) - \widehat{u}_\Delta^n(x)| \leqslant |z_{k+\frac12}^n - z_{k-\frac12}^n| \quad \text{for all } x \in [x_{k-\frac12}^n, x_{k+\frac12}^n],$$

which is a consequence of the definition of the piecewise affine function $\widehat{u}_\Delta^n$. Therefore,

$$\begin{aligned}
\|u_\Delta^n - \widehat{u}_\Delta^n\|_{L^1(\Omega)} &\leqslant \delta \sum_{k\in\mathbb{I}_K^+} \delta \left| \frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta} \right| \leqslant \delta \left(\sum_{k\in\mathbb{I}_K^+} \frac{\delta}{z_k^n} \right)^{1/2} \left(\delta \sum_{k\in\mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta} \right)^2 \right)^{1/2} \\
&\leqslant \delta(2(b-a))^{1/2}\mathbf{D}(\vec{\mathrm{x}}_\Delta^n)^{1/2},
\end{aligned}$$

which shows (6.31). Finally, (6.32) is a consequence of (6.30) and (6.31). First, note that

$$\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} \leqslant \|\{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} + \|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - \{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} \leqslant M + C\delta$$

is uniformly bounded. Now apply the interpolation inequality

$$\|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)} \leqslant C\|\partial_x \{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\Omega)}^{2/3} \|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)}^{1/3}$$

to obtain the uniform bound in (6.32). □

Proposition 6.12. *There exists a function* $u_* : [0, +\infty) \times \Omega \to [0, +\infty)$ *with*

$$u_* \in C^{1/2}_{\mathrm{loc}}([0, +\infty); \mathcal{P}^r_2(\Omega)) \cap L^\infty_{\mathrm{loc}}([0, +\infty); H^1(\Omega)), \tag{6.33}$$

and there exists a subsequence of Δ *(still denoted by* Δ*), such that for every* $[0, T] \subseteq [0, +\infty)$ *with* $T > 0$ *the following assertions hold true:*

$$\{u_\Delta\}_{\boldsymbol{\tau}}(t) \longrightarrow u_*(t) \quad \text{in } \mathcal{P}^r_2(\Omega), \text{ uniformly with respect to } t \in [0, T], \tag{6.34}$$

$$\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} \longrightarrow u_* \quad \text{uniformly on } [0, T] \times \Omega. \tag{6.35}$$

Proof. Fix $T > 0$. The proof of (6.34) is a consequence of Proposition 2.5 and the entropy estimates in (6.23) and (6.24). Note especially that in addition to the weak convergence in (6.34), one has that $\{\mathrm{X}_\Delta\}_{\boldsymbol{\tau}}(t)$ converges to $\mathrm{X}_*(t)$ in $L^2(\mathcal{M})$, uniformly with respect to $t \in [0, T]$, where $\mathrm{X}_* \in C^{1/2}_{\mathrm{loc}}([0, +\infty); L^2(\mathcal{M}))$ is the Lagrangian map of u_*. The reason for this is once again (2.27).

Following the proof of Proposition 5.11 in Chaper 5, we see that the convegence result in (6.35) and the regularity stated in (6.33) for the limit curve u_* can be attained, if the following assumptions are fulfilled:

$$\sup_{t \in [0, +\infty)} \|\partial_x \{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^2(\Omega)} \quad \text{and} \quad \sup_{t \in [0, +\infty)} \|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^\infty(\Omega)},$$

are Δ-uniformly bounded, and

$$\sup_{t \in [0, +\infty)} \|\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}}(t) - \{u_\Delta\}_{\boldsymbol{\tau}}(t)\|_{L^1(\Omega)} \longrightarrow 0$$

as $\Delta \to 0$, see Remark 5.12. Since these requirements coincide with the properties of u_Δ shown in Lemma 6.11, an one-to-one adaption of the proof of Proposition 5.11 completes the proof. ☐

Proposition 6.13. *Under the hypotheses and with the notations of Proposition 6.12, we have that*

$$\{\widehat{u}_\Delta\}_{\boldsymbol{\tau}} \longrightarrow u_* \quad \text{strongly in } L^2([0, T]; H^1(\Omega)) \tag{6.36}$$

for any $T > 0$*, as* $\Delta \to 0$*.*

Proof. Fix $T > 0$. Remember that $\widehat{u}^n_\Delta$ is differentiable with locally constant derivatives on any interval $(x_{\kappa-\frac{1}{2}}, x_\kappa]$ for $\kappa \in \mathbb{I}^+_K \cup \mathbb{I}^{1/2}_K \cup \{K\}$, and it especially fulfills $\partial_x \widehat{u}^n_\Delta(x) = 0$ for all $x \in (a, a + \delta/2)$ and all $x \in (b - \delta/2, b)$. Therefore, integration by parts and a rearrangement of the terms yield

$$\begin{aligned}\|\partial_x \widehat{u}^n_\Delta\|^2_{L^2(\Omega)} &= \sum_{\kappa \in \mathbb{I}^+_K \cup \mathbb{I}^{1/2}_K \cup \{K\}} \int_{x_{\kappa-\frac{1}{2}}}^{x_\kappa} \partial_x \widehat{u}^n_\Delta \partial_x \widehat{u}^n_\Delta \, \mathrm{d}x = \sum_{\kappa \in \mathbb{I}^+_K \cup \mathbb{I}^{1/2}_K \cup \{K\}} \Big[\widehat{u}^n_\Delta(x) \partial_x \widehat{u}^n_\Delta(x)\Big]_{x = x_{\kappa-\frac{1}{2}}+0}^{x = x_\kappa - 0} \\ &\leqslant \|\widehat{u}^n_\Delta\|_{L^\infty(\Omega)} \, \mathrm{TV}\left[\partial_x \widehat{u}^n_\Delta\right].\end{aligned}$$

Take further two arbitrary discretizations Δ_1, Δ_2 and apply the above result to the difference $\{\widehat{u}_{\Delta_1}\}_{\boldsymbol{\tau}} - \{\widehat{u}_{\Delta_2}\}_{\boldsymbol{\tau}}$. Using that $\mathrm{TV}[f - g] \leqslant \mathrm{TV}[f] + \mathrm{TV}[g]$ we obtain by integration with respect to time that

$$\int_0^T \|\partial_x \{\hat{u}_{\Delta_1}\}_{\boldsymbol{\tau}} - \partial_x \{\hat{u}_{\Delta_2}\}_{\boldsymbol{\tau}}\|_{L^2(\Omega)}^2 \,\mathrm{d}t$$

$$\leqslant T^{1/2} \sup_{t\in[0,T]} \|\{\hat{u}_{\Delta_1}\}_{\boldsymbol{\tau}} - \{\hat{u}_{\Delta_2}\}_{\boldsymbol{\tau}}\|_{L^\infty(\Omega)} \left(2\int_0^T \mathrm{TV}\left[\partial_x \{\hat{u}_{\Delta_1}\}_{\boldsymbol{\tau}}\right]^2 + \mathrm{TV}\left[\partial_x \{\hat{u}_{\Delta_2}\}_{\boldsymbol{\tau}}\right]^2 \,\mathrm{d}t\right)^{1/2}.$$

This shows that $\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}$ is a Cauchy-sequence in $L^2([0,T];H^1(\Omega))$ — remember (6.28) and especially the convergence result in (6.35) — and its limit has to coincide with u_* in the sense of distributions, due to the uniform convergence of $\{\hat{u}_\Delta\}_{\boldsymbol{\tau}}$ to u_* on $[0,T]\times\Omega$. □

6.4. Weak formulation of the limit equation

To close the proof of Theorem 6.2, we are going to verify that the limit curve u_* obtained in Proposition 6.12 is indeed a weak solution to (6.1) with no-flux boundary conditions (6.2). It seems that following the same strategy as applied in Chapter 3 or Chapter 5 is the right method to attain this aim. Therefore, we are first going to show the validity of a discrete weak formulation for $\{u_\Delta\}_{\boldsymbol{\tau}}$, using a discrete flow interchange estimate. Then the convergence result of Proposition 6.13 suffices to pass to the limit in the discrete weak formulation, which shows that the limit curve u_* satisfies (6.11) from Theorem 6.2.

From now on, $\vec{\mathrm{x}}_\Delta = (\vec{\mathrm{x}}_\Delta^0, \vec{\mathrm{x}}_\Delta^1, \ldots)$ with its derived functions u_Δ, $\hat{u}_\Delta$, X_Δ is a (sub)sequence for which the convergence results stated in Proposition 6.12 and Proposition 6.13 are satisfied. We continue to assume (6.10). The goal of this section is to prove the following:

Proposition 6.14. *For every $\rho \in C^\infty(\Omega)$ with $\rho'(a) = \rho'(b) = 0$, and for every $\eta \in C_c^\infty((0,+\infty))$, the limit curve u_* satisfies*

$$\int_0^\infty \int_\Omega \partial_t \varphi u_* \,\mathrm{d}t\,\mathrm{d}x + \int_0^\infty N(u_*,\varphi)\,\mathrm{d}t = 0, \tag{6.37}$$

where the highly nonlinear term N from (6.12) *is given by*

$$N(u,\rho) = \frac{1}{2}\int_\Omega \partial_x(u^2)\rho''' + 3(\partial_x u)^2\rho''\,\mathrm{d}x + \int_\Omega V_x u\rho'\,\mathrm{d}x. \tag{6.38}$$

Note that the weak formulation (6.11) is equivalent to (6.37). Simply observe that any $\varphi \in C^\infty((0,+\infty)\times\Omega)$ that has a compact support in $(0,+\infty)\times\overline{\Omega}$ and satisfies $\partial_x\varphi(t,a) = \partial_x\varphi(t,b) = 0$ for any $t \in [0,+\infty)$, can be approximated by linear combinations of products $\eta(t)\rho(x)$ with functions $\eta \in C_c^\infty((0,+\infty))$ and $\rho \in C^\infty(\Omega)$, which satisfies the requirements formulated in Proposition 6.14.

For definiteness, fix a spatial test function $\rho \in C^\infty(\Omega)$ with $\rho'(a) = \rho'(b) = 0$, and a temporal test function $\eta \in C_c^\infty((0,+\infty))$ with $\operatorname{supp}\eta \subseteq (0,T)$ for a suitable $T > 0$. Denote again by $N_{\boldsymbol{\tau}} \in \mathbb{N}$ an integer with $\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \in (T, T+1)$. Let $\varpi > 0$ be chosen such that

$$\|\rho\|_{C^4(\Omega)} \leqslant \varpi \quad \text{and} \quad \|\eta\|_{C^1([0,+\infty))} \leqslant \varpi. \tag{6.39}$$

For convenience, we assume $\delta < 1$ and $\tau < 1$. In the estimates that follow, the non-explicity constants possibly depend on Ω, T, ϖ, and $\overline{\mathcal{D}^V}$, but not on Δ.

Lemma 6.15 (discrete weak formulation). *A solution to the numerical scheme satisfies*

$$\sum_{n=1}^{\infty} \tau_n \eta(t_{n-1}) \left| \int_{\mathcal{M}} \frac{\rho(\mathbf{X}_\Delta^n) - \rho(\mathbf{X}_\Delta^{n-1})}{\tau_n} \,\mathrm{d}\xi - \big\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}} \right| \leqslant C\big(\tau + \delta^{1/4}\big), \tag{6.40}$$

where we use the short-hand notation $\rho'(\vec{\mathrm{x}}) := (\rho'(x_1), \ldots, \rho'(x_{K-1}))$ for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$.

Proof. The proof follows the same idea as the one of Lemma 5.15. Here, we additionally use that $\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n)$ is uniformly bounded by $\overline{\mathcal{D}^V}$ for any index $n \in \mathbb{N}_0$, especially for $n = 0$. □

As in the previous Chapter 5, the identification of the weak formulation in (6.37) with the limit of (6.40) is splitted in two main steps: In the first one, we estimate the term that more or less describes the error that is caused by approximating the time derivative in (6.37) with the respective difference quotient in (6.40),

$$\begin{aligned} \mathrm{e}_{1,\Delta} := \left| \int_0^T \left(\eta'(t) \int_\Omega \rho(x) \left\{u_\Delta\right\}_{\boldsymbol{\tau}}(t,x) \,\mathrm{d}x + \eta(t) \left\{ \big\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}} \right\}_{\boldsymbol{\tau}}(t) \right) \mathrm{d}t \right| \\ \leqslant C\big(\tau + \delta^{1/2}\big). \end{aligned} \tag{6.41}$$

Since this temporal approximation does not demand the specific represenation of $\mathbf{D}^V$, one can conveniently adapt the proof of (5.58) from the previous chapter to get the respective result in (6.41), using in addition the energy estimates (6.23) and (6.24).

The second much more challenging step is to prove the error estimate

$$\begin{aligned} \mathrm{e}_{2,\Delta} := \Bigg| \int_0^T \eta(t) \bigg(\frac{1}{2} \int_\Omega \rho'''(x) \partial_x(\{u_\Delta\}_{\boldsymbol{\tau}}^2)(t,x) + 3\rho''(x) \partial_x \left\{u_\Delta\right\}_{\boldsymbol{\tau}}^2(t,x) \,\mathrm{d}x \\ + \int_\Omega V_x(x) \left\{u_\Delta\right\}_{\boldsymbol{\tau}} \rho'(x) \,\mathrm{d}x - \left\{ \big\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}} \right\}_{\boldsymbol{\tau}}(t) \bigg) \mathrm{d}t \Bigg| \leqslant C\delta^{1/4}, \end{aligned} \tag{6.42}$$

which, heuristically spoken, gives a rate of convergence of $\left\{ \big\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}} \right\}_{\boldsymbol{\tau}}$ towards the nonlinear term $N(u_*, \rho)$ from (6.38). The proof of (6.42) is treated essentially in 2 steps. In the first one we rewrite the term $\big\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}}$ (see Lemma 6.16), and use Taylor expansions to identify it with the corresponding integral terms of (6.38) up to some additional error terms, see Lemmata 6.19-6.23. Then we use the strong compactness result of Proposition 6.13 to pass to the limit as $\Delta \to 0$ in the second step.

Lemma 6.16. *With the short-hand notation $\rho'(\vec{\mathrm{x}}) = (\rho'(x_1), \ldots, \rho'(x_{K-1}))$ for any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$, one has that*

$$-\big\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta^n) \big\rangle_{\boldsymbol{\xi}} = A_1^n + A_2^n + A_3^n - A_4^n + A_5^n + A_6^n + A_7^n, \tag{6.43}$$

where

$$A_1^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\right)^2 \left((z_{k+\frac12}^n)^2 + (z_{k-\frac12}^n)^2 + z_{k+\frac12}^n z_{k-\frac12}^n\right)\left(\frac{\rho'(x_{k+1}^n)-\rho'(x_{k-1}^n)}{2\delta}\right),$$

$$A_2^n = \frac{\delta}{4} \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\right)^2 (z_{k+\frac12}^n)^2 \left(\frac{\rho'(x_{k+1}^n)-\rho'(x_k^n)}{\delta}\right),$$

$$A_3^n = \frac{\delta}{4} \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\right)^2 (z_{k-\frac12}^n)^2 \left(\frac{\rho'(x_k^n)-\rho'(x_{k-1}^n)}{\delta}\right),$$

$$A_4^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\right)^2 \left(\frac{(z_{k+\frac12}^n)^3 + (z_{k-\frac12}^n)^3}{2 z_{k+\frac12}^n z_{k-\frac12}^n}\right)\rho''(x_k^n),$$

$$A_5^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\right) \left(\frac{(z_{k+\frac12}^n)^3 + (z_{k-\frac12}^n)^3}{2}\right)\left(\frac{\rho'(x_{k+1}^n)-\rho'(x_k^n)-(x_{k+1}^n-x_k^n)\rho''(x_k^n)}{\delta^2}\right),$$

$$A_6^n = \delta \sum_{k\in\mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta}\right) \left(\frac{(z_{k+\frac12}^n)^3 + (z_{k-\frac12}^n)^3}{2}\right)\left(\frac{\rho'(x_{k-1}^n)-\rho'(x_k^n)-(x_{k-1}^n-x_k^n)\rho''(x_k^n)}{\delta^2}\right),$$

$$A_7^n = \delta \sum_{k\in\mathbb{I}_K^+} V(x_k^n)\rho'(x_k^n).$$

Proof. Fix some time index $n \in \mathbb{N}$ (omitted in the calculations below). Recall the representation of $\nabla_{\boldsymbol{\xi}}\mathbf{D}^V$ as

$$\nabla_{\boldsymbol{\xi}}\mathbf{D}^V(\vec{\mathrm{x}}) = \frac{1}{\delta^2}\left(\partial_{\vec{\mathrm{x}}}^2\mathbf{H}(\vec{\mathrm{x}})\partial_{\vec{\mathrm{x}}}\mathbf{Q}(\vec{\mathrm{x}}) + \partial_{\vec{\mathrm{x}}}^2\mathbf{Q}(\vec{\mathrm{x}})\partial_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}})\right)$$

with corresponding gradients and hessians in (6.17) and (6.18). Multiplication with $\rho'(\vec{\mathrm{x}}_\Delta)$ then yields

$$\begin{aligned}
-\left\langle \nabla_{\boldsymbol{\xi}}\mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta)\right\rangle_{\boldsymbol{\xi}} &= \frac{\delta}{2}\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{z_{\kappa+\frac12} - 2z_\kappa + z_{\kappa-\frac12}}{\delta^2}\right)\left(\frac{\rho'(x_{\kappa+\frac12})-\rho'(x_{\kappa-\frac12})}{\delta}\right)\\
&\quad + \frac{\delta}{4}\sum_{\kappa\in\mathbb{I}_K^{1/2}} z_\kappa^2 \left(\frac{z_{\kappa+\frac12}^2 - 2z_\kappa^2 + z_{\kappa-\frac12}^2}{\delta^2}\right)\left(\frac{\rho'(x_{\kappa+\frac12})-\rho'(x_{\kappa-\frac12})}{\delta}\right)\\
&\quad + \delta\sum_{k\in\mathbb{I}_K^+} V(x_k)\rho'(x_k).
\end{aligned}$$

Observing that

$$\frac{z_{\kappa+1}^2 - 2z_\kappa^2 + z_{\kappa-1}^2}{\delta^2} = 2z_\kappa \frac{z_{\kappa+1} - 2z_\kappa + z_{\kappa-1}}{\delta^2} + \left(\frac{z_{\kappa+1}-z_\kappa}{\delta}\right)^2 + \left(\frac{z_{\kappa-1}-z_\kappa}{\delta}\right)^2,$$

we further obtain that

$$-\left\langle \nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n), \rho'(\vec{\mathrm{x}}_\Delta) \right\rangle_{\boldsymbol{\xi}} = \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{z_{\kappa+\frac{1}{2}} - 2z_\kappa + z_{\kappa-\frac{1}{2}}}{\delta^2} \right) \left(\frac{\rho'(x_{\kappa+\frac{1}{2}}) - \rho'(x_{\kappa-\frac{1}{2}})}{\delta} \right) + A_2 + A_3 + A_7.$$

It hence remains to show that $(A) = A_1 - A_4 + A_5 + A_6$, where

$$(A) := \delta \sum_{\kappa \in \mathbb{I}_K^{1/2}} z_\kappa^3 \left(\frac{z_{\kappa+\frac{1}{2}} - 2z_\kappa + z_{\kappa-\frac{1}{2}}}{\delta^2} \right) \left(\frac{\rho'(x_{\kappa+\frac{1}{2}}) - \rho'(x_{\kappa-\frac{1}{2}})}{\delta} \right).$$

After "summation by parts" and an application of the elementary equality (for arbitrary numbers $p_\pm$ and $q_\pm$)

$$p_+q_+ - p_-q_- = \frac{p_+ + p_-}{2}(q_+ - q_-) + (p_+ - p_-)\frac{q_+ + q_-}{2},$$

one attains

$$\begin{aligned}
(A) &= \frac{\delta}{2} \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right) \left(\frac{z_{k-\frac{1}{2}}^3 - z_{k+\frac{1}{2}}^3}{\delta} \right) \left(\frac{\rho'(x_{k+1}) - \rho'(x_{k-1})}{\delta} \right) \\
&\quad + \frac{\delta}{2} \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right) \left(\frac{z_{k-\frac{1}{2}}^3 + z_{k+\frac{1}{2}}^3}{\delta} \right) \left(\frac{\rho'(x_{k+1}) - 2\rho'(x_k) + \rho'(x_{k-1})}{\delta} \right) \\
&= A_1 + \frac{\delta}{2} \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{\delta} \right) \left(\frac{z_{k-\frac{1}{2}}^3 + z_{k+\frac{1}{2}}^3}{\delta} \right) \left(\frac{\rho'(x_{k+1}) - 2\rho'(x_k) + \rho'(x_{k-1})}{\delta} \right), \quad (6.44)
\end{aligned}$$

where we additionally used the identity $(p^3 - q^3) = (p-q)(p^2 + q^2 + pq)$ in the last step. In order to see that the last sum in (6.44) equals to $-A_4 + A_5 + A_6$, simply observe that the identity

$$\frac{x_{k+1} - x_k}{\delta} + \frac{x_{k-1} - x_k}{\delta} = \frac{1}{z_{k+\frac{1}{2}}} - \frac{1}{z_{k-\frac{1}{2}}} = -\frac{z_{k+\frac{1}{2}} - z_{k-\frac{1}{2}}}{z_{k+\frac{1}{2}} z_{k-\frac{1}{2}}}$$

makes the coefficient of $\rho''(x_k)$ vanish. □

For the analysis of the terms in (6.43), we need some sophisticated estimates presented in the following two lemmata. The first one gives a control on the oscillation of the z-values at neighboring grid points:

Lemma 6.17. *For any $p, q \in \{1, 2\}$ with $p + q \leqslant 3$ one has that*

$$\sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k \in \mathbb{I}_K^+} z_k^n \left| \frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta} \right|^p \left| \frac{(z_{k\pm\frac{1}{2}}^n)^q}{(z_{k\mp\frac{1}{2}}^n)^q} - 1 \right| \leqslant C\delta^{1/4}. \quad (6.45)$$

Proof. Instead of (6.45), we are going to prove that

$$\sum_{n=1}^{N_\tau} \tau_n \delta \sum_{k \in \mathbb{I}_K^+} z_k^n \left| \frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta} \right|^p \left| \frac{z_{k\pm\frac{1}{2}}^n}{z_{k\mp\frac{1}{2}}^n} - 1 \right|^q \leqslant C\delta^{1/4} \quad (6.46)$$

is satisfied for any $p, q \in \{1, 2\}$ with $p + q \leqslant 3$, which implies (6.45) because of the following considerations: The situation is clear for $q = 1$, thus assume $q = 2$ in (6.45). Then (6.46) is an upper bound on (6.45), due to

$$\frac{(z^n_{k\pm\frac{1}{2}})^2}{(z^n_{k\mp\frac{1}{2}})^2} - 1 = \left(\frac{z^n_{k\pm\frac{1}{2}}}{z^n_{k\mp\frac{1}{2}}} - 1\right)^2 + 2\left(\frac{z^n_{k\pm\frac{1}{2}}}{z^n_{k\mp\frac{1}{2}}} - 1\right)$$

for any $n = 1, \ldots, N_{\boldsymbol{\tau}}$.

To prove (6.46), we first apply Hölder's inequality,

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k \left|\frac{z^n_{k+\frac{1}{2}} - z^n_{k-\frac{1}{2}}}{\delta}\right|^p \left|\frac{z^n_{k\pm\frac{1}{2}}}{z^n_{k\mp\frac{1}{2}}} - 1\right|^q = \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k \left|\frac{z^n_{k+\frac{1}{2}} - z^n_{k-\frac{1}{2}}}{\delta}\right|^{p+q} \left(\frac{\delta}{z^n_{k\mp\frac{1}{2}}}\right)^q$$
$$\leqslant \left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \sum_{k\in\mathbb{I}_K^+} \delta z^n_k \left(\frac{z^n_{k+\frac{1}{2}} - z^n_{k-\frac{1}{2}}}{\delta}\right)^4\right)^{\frac{p+q}{4}} \left(\delta \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \sum_{k\in\mathbb{I}_K^+} z^n_k \left(\frac{\delta}{z^n_{k\pm\frac{1}{2}}}\right)^{\frac{q}{\alpha}}\right)^\alpha, \tag{6.47}$$

with $\alpha = 1 - \frac{p+q}{4}$. The first factor is uniformly bounded due to (6.22) and (6.25). For the second term, we use (6.32) and (A.4) to achieve

$$\delta \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \sum_{k\in\mathbb{I}_K^+} z^n_k \left(\frac{\delta}{z^n_{k\pm\frac{1}{2}}}\right)^{\frac{q}{\alpha}} \leqslant (T+1)\delta(b-a)^{\frac{q}{\alpha}} \| \{\hat{u}\}_{\boldsymbol{\tau}} \|_{L^\infty([0,T]\times\Omega)} \leqslant C(T+1)\delta(b-a)^{\frac{q}{\alpha}},$$

which shows (6.46), due to $\alpha \geqslant \frac{1}{4}$. □

Lemma 6.18. *For any $p \in \{1, 2\}$ one obtains that*

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k \left|\frac{z^n_{k+\frac{1}{2}} - z^n_{k-\frac{1}{2}}}{\delta}\right|^2 (x^n_{k+1} - x^n_{k-1})^p \leqslant C\delta^{1/2}. \tag{6.48}$$

Proof. Appling Hölder's inequality,

$$\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k \left|\frac{z^n_{k+\frac{1}{2}} - z^n_{k-\frac{1}{2}}}{\delta}\right|^2 (x^n_{k+1} - x^n_{k-1})^p$$
$$\leqslant \left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k \left|\frac{z^n_{k+\frac{1}{2}} - z^n_{k-\frac{1}{2}}}{\delta}\right|^4\right)^{1/2} \left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k (x^n_{k+1} - x^n_{k-1})^{2p}\right)^{1/2}.$$

The first sum is uniformly bounded thanks to (6.22) and (6.25), and the second one satisfies

$$\left(\sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \delta \sum_{k\in\mathbb{I}_K^+} z^n_k (x^n_{k+1} - x^n_{k-1})^{2p}\right)^{1/2} \leqslant \delta^{1/2}(T+1)^{1/2} \| \{\hat{u}\}_{\boldsymbol{\tau}} \|^{1/2}_{L^\infty([0,T]\times\Omega)} (b-a)^p,$$

where we used (6.32) and (A.4). □

Lemma 6.19. *There is a constant $C_1 > 0$ expressible in Ω, T, ϖ and $\overline{\mathcal{D}^V}$ such that*

$$R_1 := \sum_{n=1}^{N_\tau} \tau_n \left| A_1^n - 3 \int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi) \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \right| \leqslant C_1 \delta^{1/4}.$$

Proof. Let us introduce the term

$$B_1^n := \delta \sum_{k \in \mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta} \right)^2 \frac{3}{\delta} \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi.$$

First observe that by definition of $\widehat{z}_\Delta^n$,

$$\int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi) \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi = \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta} \right)^2 \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \widehat{z}_\Delta^n(\xi) \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi,$$

hence we get for B_1^n

$$\begin{aligned} &\left| 3 \int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi) \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi - B_1^n \right| \\ \leqslant & 3\varpi \sum_{k \in \mathbb{I}_K^+} \left(\frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta} \right)^2 \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \left| \widehat{z}_\Delta^n(\xi) - z_k \right| \mathrm{d}\xi \leqslant 3\varpi\delta \sum_{k \in \mathbb{I}_K^+} z_k^n \left| \frac{z_{k+\frac12}^n - z_{k-\frac12}^n}{\delta} \right|^2 \left| \frac{z_{k+\frac12}^n}{z_{k-\frac12}^n} - 1 \right|. \end{aligned}$$

This especially implies, due to (6.45) that

$$\sum_{n=1}^{N_\tau} \tau_n \left| B_1^n - 3 \int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi) \partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \right| \leqslant C \delta^{1/4}. \tag{6.49}$$

For simplification of R_1, let us fix n (omitted in the following), and introduce $\tilde{x}_k^+ \in [x_k, x_{k+1}]$ and $\tilde{x}_k^- \in [x_{k-1}, x_k]$ such that

$$\begin{aligned} \frac{\rho'(x_{k+1}) - \rho'(x_{k-1})}{2\delta} &= \frac{\rho'(x_{k+1}) - \rho'(x_k)}{2\delta} + \frac{\rho'(x_k) - \rho'(x_{k-1})}{2\delta} \\ &= \rho''(\tilde{x}_k^+) \frac{x_{k+1} - x_k}{2\delta} + \rho''(\tilde{x}_k^+) \frac{x_{k+1} - x_k}{2\delta} = \frac{1}{2} \left(\frac{\rho''(\tilde{x}_k^+)}{z_{k+\frac12}} + \frac{\rho''(\tilde{x}_k^-)}{z_{k-\frac12}} \right). \end{aligned}$$

Recalling that

$$\int_{\xi_{k-1}}^{\xi_{k+1}} \theta_k(\xi)\,\mathrm{d}\xi = \delta, \tag{6.50}$$

one has for each $k \in \mathbb{I}_K^+$,

$$
\begin{aligned}
(A) :=& \frac{1}{2}\left(z_{k+\frac12}^2 + z_{k-\frac12}^2 + z_{k+\frac12}z_{k-\frac12}\right)\left(\frac{\rho''(\tilde{x}_k^+)}{z_{k+\frac12}} + \frac{\rho''(\tilde{x}_k^-)}{z_{k-\frac12}}\right) - \frac{3}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k \rho'' \circ \mathrm{X}_\Delta \,\mathrm{d}\xi \\
=& \frac{1}{4} z_{k-\frac12}\left(2 + \frac{z_{k-\frac12}}{z_{k+\frac12}}\right)\rho''(\tilde{x}_k^+) + \frac{1}{4} z_{k+\frac12}\left(2 + \frac{z_{k-\frac12}^2}{z_{k+\frac12}^2}\right)\rho''(\tilde{x}_k^+) \\
&+ \frac{1}{4} z_{k+\frac12}\left(2 + \frac{z_{k+\frac12}}{z_{k-\frac12}}\right)\rho''(\tilde{x}_k^-) + \frac{1}{4} z_{k-\frac12}\left(2 + \frac{z_{k+\frac12}^2}{z_{k-\frac12}^2}\right)\rho''(\tilde{x}_k^-) - \frac{3}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k \rho'' \circ \mathrm{X}_\Delta \,\mathrm{d}\xi \\
=& \frac{1}{4}\left[z_{k-\frac12}\left(\frac{z_{k-\frac12}}{z_{k+\frac12}} - 1\right) + z_{k+\frac12}\left(\frac{z_{k-\frac12}^2}{z_{k+\frac12}^2} - 1\right)\right]\rho''(\tilde{x}_k^+) \\
&+ \frac{1}{4}\left[z_{k+\frac12}\left(\frac{z_{k+\frac12}}{z_{k-\frac12}} - 1\right) + z_{k-\frac12}\left(\frac{z_{k+\frac12}^2}{z_{k-\frac12}^2} - 1\right)\right]\rho''(\tilde{x}_k^-) \\
&- \frac{3}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k\big[\rho'' \circ \mathrm{X}_\Delta - \rho''(\tilde{x}_k^+)\big]\,\mathrm{d}\xi - \frac{3}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k\big[\rho'' \circ \mathrm{X}_\Delta - \rho''(\tilde{x}_k^-)\big]\,\mathrm{d}\xi.
\end{aligned}
$$

Applying the trivial identity (for arbitrary numbers p and q)

$$
q\left(\frac{p^2}{q^2} - 1\right) = (p+q)\left(\frac{p}{q} - 1\right),
$$

the above term finally reads as

$$
\begin{aligned}
(A) =& \frac{1}{4}\left[z_{k-\frac12}\left(\frac{z_{k-\frac12}}{z_{k+\frac12}} - 1\right) + 2z_k\left(\frac{z_{k-\frac12}}{z_{k+\frac12}} - 1\right)\right]\rho''(\tilde{x}_k^+) \\
&+ \frac{1}{4}\left[z_{k+\frac12}\left(\frac{z_{k+\frac12}}{z_{k-\frac12}} - 1\right) + 2z_k\left(\frac{z_{k+\frac12}}{z_{k-\frac12}} - 1\right)\right]\rho''(\tilde{x}_k^-) \\
&- \frac{3}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k\big[\rho'' \circ \mathrm{X}_\Delta - \rho''(\tilde{x}_k^+)\big]\,\mathrm{d}\xi - \frac{3}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k\big[\rho'' \circ \mathrm{X}_\Delta - \rho''(\tilde{x}_k^-)\big]\,\mathrm{d}\xi.
\end{aligned}
\tag{6.51}
$$

Since $\tilde{x}_k^+$ lies between the values x_k and x_{k+1}, and $\mathrm{X}_\Delta(\xi) \in [x_k, x_{k+\frac12}]$ for each $\xi \in [\xi_k, \xi_{k+\frac12}]$, we conclude that $|\mathrm{X}_\Delta(\xi) - \tilde{x}_k^+| \leqslant x_{k+1} - x_k$, and therefore

$$
\frac{3}{2\delta}\int_{\xi_k}^{\xi_{k+\frac12}} z_k\big|\rho'' \circ \mathrm{X}_\Delta(\xi) - \rho''(\tilde{x}_k^+)\big|\,\mathrm{d}\xi \leqslant \frac{3}{2}\varpi z_k(x_{k+1} - x_k). \tag{6.52}
$$

A similar estimate is valid for the other integral over $[\xi_{k-\frac{1}{2}}, \xi_k]$ and for the integrals with $\rho''(\tilde{x}_k^-)$. Thus, combining (6.51) and (6.52) with $z_{k\pm\frac{1}{2}}^n \leqslant 2z_k^n$ and the definition of A_1^n, one attains that

$$\begin{aligned} |A_1^n - B_1^n| \leqslant 2\varpi \sum_{k\in\mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^2 \left[\left(\frac{z_{k+\frac{1}{2}}^n}{z_{k-\frac{1}{2}}^n} - 1\right) + \left(\frac{z_{k-\frac{1}{2}}^n}{z_{k+\frac{1}{2}}^n} - 1\right)\right] \\ + 3\varpi \sum_{k\in\mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^2 (x_{k+1}^n - x_{k-1}^n), \end{aligned}$$

and further, applying (6.45) and (6.48),

$$\sum_{n=1}^{N_\tau} \tau_n \, |A_1^n - B_1^n| \leqslant C\delta^{1/4}. \tag{6.53}$$

By triangle inequality, (6.49) and (6.53) provide the claim. □

Along the same lines, one proves the analogous estimate for A_2^n and A_3^n in place of A_1^n:

Lemma 6.20. *There are constants $C_2 > 0$ and $C_3 > 0$ expressible in Ω, T, ϖ and $\overline{\mathcal{D}^V}$ such that*

$$R_2 := \sum_{n=1}^{N_\tau} \tau_n \left| A_2^n - \frac{1}{4}\int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi)\partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \right| \leqslant C_2\delta^{1/4},$$

$$R_3 := \sum_{n=1}^{N_\tau} \tau_n \left| A_3^n - \frac{1}{4}\int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi)\partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \right| \leqslant C_3\delta^{1/4}.$$

Lemma 6.21. *There is a constant $C_4 > 0$ expressible in Ω, T, ϖ and $\overline{\mathcal{D}^V}$ such that*

$$R_4 := \sum_{n=1}^{N_\tau} \tau_n \left| A_4^n - \int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi)\partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \right| \leqslant C_4\delta^{1/4}.$$

Proof. The proof is almost identical to the one for Lemma 6.19 above. As before, we introduce the term

$$B_4^n := \delta \sum_{k\in\mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^2 \frac{1}{\delta}\int_{\xi_{k-\frac{1}{2}}}^{\xi_{k+\frac{1}{2}}} \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi$$

and get due to (6.45), analogously to (6.49), that

$$\sum_{n=1}^{N_\tau} \tau_n \left| B_4^n - \int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi)\partial_\xi \widehat{z}_\Delta^n(\xi)^2 \rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \right| \leqslant C\delta^{1/4}. \tag{6.54}$$

By writing

$$\frac{(z_{k+\frac{1}{2}}^n)^3 + (z_{k-\frac{1}{2}}^n)^3}{2z_{k+\frac{1}{2}}^n z_{k-\frac{1}{2}}^n} = z_k^n\Big(\frac{z_{k-\frac{1}{2}}^n}{z_{k+\frac{1}{2}}^n} - 1\Big) + z_k^n\Big(\frac{z_{k+\frac{1}{2}}^n}{z_{k-\frac{1}{2}}^n} - 1\Big) + z_k^n,$$

one obtains that

$$
\begin{aligned}
&\frac{(z^n_{k+\frac12})^3+(z^n_{k-\frac12})^3}{2z^n_{k+\frac12}z^n_{k-\frac12}}\rho''(x^n_k)-\frac{1}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z_k\rho''\circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi\\
=&z^n_k\Big(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}}-1\Big)+z^n_k\Big(\frac{z^n_{k+\frac12}}{z^n_{k-\frac12}}-1\Big)-\frac{1}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z^n_k\big[\rho''\circ \mathrm{X}^n_\Delta(\xi)-\rho''(x^n_k)\big]\,\mathrm{d}\xi.
\end{aligned}
$$

Observing — in analogy to (6.52) — that

$$
\frac{1}{\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z^n_k\big|\rho''\circ \mathrm{X}^n_\Delta(\xi)-\rho''(x^n_k)\big|\,\mathrm{d}\xi\leqslant \varpi z^n_k(x^n_{k+\frac12}-x^n_{k-\frac12}),
$$

we obtain the same bound on $|A^n_4-B^n_4|$ as before on $|A^n_1-B^n_1|$, i.e.

$$
\begin{aligned}
|A^n_4-B^n_4|\leqslant \varpi\sum_{k\in\mathbb{I}^+_K} z^n_k\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)^2\left[\left(\frac{z^n_{k+\frac12}}{z^n_{k-\frac12}}-1\right)+\left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}}-1\right)\right]\\
+\varpi\sum_{k\in\mathbb{I}^+_K} z^n_k\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)^2(x^n_{k+1}-x^n_{k-1}).
\end{aligned}
$$

Again, applying (6.45) and (6.48), we get

$$
\sum_{n=1}^{N_\tau}\tau_n\,|A^n_4-B^n_4|\leqslant C\delta^{1/4}, \tag{6.55}
$$

and the estimates (6.54) and (6.55) imply the desired bound on R_4. □

Lemma 6.22. *There is a constant $C_5>0$ expressible in Ω, T, ϖ and $\overline{\mathcal{D}^V}$ such that*

$$
R_5:=\sum_{n=1}^{N_\tau}\tau_n\left|A^n_5-\frac12\int_{\mathcal{M}}\widehat{z}^n_\Delta(\xi)\partial_\xi\widehat{z}^n_\Delta(\xi)\rho'''\circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi\right|\leqslant C_5\delta^{1/4}.
$$

Proof. The idea of the proof is the same as in the previous proofs. Let us define similar to B^n_1 the term

$$
B^n_5:=\delta\sum_{k\in\mathbb{I}^+_K} z^n_{k+\frac12}\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)\frac{1}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}}\rho'''\circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi.
$$

Note in particular that we weight the integral here with $z^n_{k+\frac12}$. Then

$$
\begin{aligned}
\left|\frac12\int_{\mathcal{M}}\widehat{z}^n_\Delta(\xi)\partial_\xi\widehat{z}^n_\Delta(\xi)\rho'''\circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi-B^n_5\right|&\leqslant\frac12\varpi\sum_{k\in\mathbb{I}^+_K}\left(\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right)\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}}\big|\widehat{z}^n_\Delta(\xi)-z^n_{k+\frac12}\big|\,\mathrm{d}\xi\\
&\leqslant\frac12\varpi\delta\sum_{k\in\mathbb{I}^+_K} z^n_{k+\frac12}\left|\frac{z^n_{k+\frac12}-z^n_{k-\frac12}}{\delta}\right|\left|\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}}-1\right|,
\end{aligned}
$$

where we used that by definition of $\widehat{z}^n_\Delta$,

$$\int_{\mathcal{M}} \widehat{z}^n_\Delta(\xi)\partial_\xi \widehat{z}^n_\Delta(\xi)\rho''' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi = \sum_{k\in\mathbb{I}_K^+} \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right) \int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} \widehat{z}^n_\Delta(\xi)\rho''' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi.$$

This especially implies, due to (6.45) that

$$\sum_{n=1}^{N_\tau} \tau_n \left| B^n_5 - \frac12 \int_{\mathcal{M}} \widehat{z}^n_\Delta(\xi)\partial_\xi \widehat{z}^n_\Delta(\xi)\rho''' \circ \mathrm{X}^n_\Delta(\xi)\,\mathrm{d}\xi \right| \leqslant C\delta^{1/4}. \tag{6.56}$$

Furthermore, one can introduce intermediate values $\tilde{x}^+_k$ such that

$$\rho'(x^n_{k+1}) - \rho'(x^n_k) - (x^n_{k+1} - x^n_k)\rho''(x^n_k) = \frac12 (x^n_{k+1} - x^n_k)^2 \rho'''(\tilde{x}^+_k) = \frac{\delta^2}{2(z^n_{k+\frac12})^2}\rho'''(\tilde{x}^+_k).$$

Using the identity

$$\left(\frac{(z^n_{k+\frac12})^3 + (z^n_{k-\frac12})^3}{2}\right)\frac{1}{2(z^n_{k+\frac12})^2} = \frac{z^n_{k+\frac12}}{2} + \frac{z^n_{k-\frac12}}{4}\left(\frac{(z^n_{k-\frac12})^2}{(z^n_{k+\frac12})^2} - 1\right) + \frac{z^n_{k+\frac12}}{4}\left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1\right),$$

we thus have — using again (6.50) — that

$$\left(\frac{(z^n_{k+\frac12})^3 + (z^n_{k-\frac12})^3}{2}\right)\left(\frac{\rho'(x^n_{k+1}) - \rho'(x^n_k) - (x^n_{k+1} - x^n_k)\rho''(x^n_k)}{\delta^2}\right) - \frac{1}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z^n_k \rho''' \circ \mathrm{X}^n_\Delta\,\mathrm{d}\xi$$
$$= \frac{z^n_{k-\frac12}}{4}\left(\frac{(z^n_{k-\frac12})^2}{(z^n_{k+\frac12})^2} - 1\right) + \frac{z^n_{k+\frac12}}{4}\left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1\right) - \frac{1}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z^n_{k+\frac12}\big[\rho''' \circ \mathrm{X}^n_\Delta - \rho'''(\tilde{x}^+_k)\big]\,\mathrm{d}\xi.$$

Observing — in analogy to (6.52) — that

$$\frac{1}{2\delta}\int_{\xi_{k-\frac12}}^{\xi_{k+\frac12}} z^n_k \big|\rho'' \circ \mathrm{X}^n_\Delta(\xi) - \rho''(x^n_k)\big|\,\mathrm{d}\xi \leqslant \frac{\varpi}{2} z^n_{k+\frac12}(x^n_{k+\frac12} - x^n_{k-\frac12}),$$

and $z^n_{k+\frac12} \leqslant 2z^n_k$, we obtain the following bound on $|A^n_5 - B^n_5|$:

$$|A^n_5 - B^n_5| \leqslant \frac{\varpi}{4}\sum_{k\in\mathbb{I}_K^+} z^n_k \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right)\left[\left(\frac{(z^n_{k-\frac12})^2}{(z^n_{k+\frac12})^2} - 1\right) + \left(\frac{z^n_{k-\frac12}}{z^n_{k+\frac12}} - 1\right)\right]$$
$$+ \varpi \sum_{k\in\mathbb{I}_K^+} z^n_k \left(\frac{z^n_{k+\frac12} - z^n_{k-\frac12}}{\delta}\right)(x^n_{k+1} - x^n_{k-1}).$$

Again, applying (6.45) and (6.48), we get

$$\sum_{n=1}^{N_\tau} \tau_n\,|A^n_5 - B^n_5| \leqslant C\delta^{1/4}, \tag{6.57}$$

and the estimates (6.56) and (6.57) imply the desired bound on R_5. □

Arguing like in the previous proof, one shows the analogous estimate for A_6^n in place of A_5^n. It remains to analyze the potential term A_7^n, where we instantaneously identify the ξ-integral with the x-integral:

Lemma 6.23. *There is a constant $C_7 > 0$ expressible in Ω, T and ϖ such that*

$$R_7 := \sum_{n=1}^{N_\tau} \tau_n \left| A_7^n - \int_\Omega V_x(x) u_\Delta^n(x)\,\mathrm{d}x \right| \leqslant C_7\delta.$$

Proof. Since the product $V_x\rho_x$ is a smooth function on the domain Ω, we can invoke the mean-value theorem and find intermediate values $\tilde{x}_k$, such that

$$\begin{aligned}\left|\delta \sum_{k\in\mathbb{I}_K^+} V_x(x_k^n)\rho_x(x_k^n) - \int_{\mathcal{M}} V_x(\mathbf{X}_\Delta^n(\xi))\rho_x(\mathbf{X}_\Delta^n(\xi))\,\mathrm{d}\xi\right| &\leqslant \delta \sum_{k\in\mathbb{I}_K^+} \partial_x\big(V_x\rho_x\big)(\tilde{x}_k)(x_{\kappa+\frac12}^n - x_{\kappa-\frac12}^n)\\ &\leqslant \delta(b-a)\sup_{x\in\Omega}\big|V_x(x)\rho_x(x)\big|.\end{aligned}$$

The claim then follows by a change of variables. □

It remains to identify the integral expressions inside R_1 to R_5 with those in the weak formulation (6.37).

Lemma 6.24. *One has that*

$$\int_{\mathcal{M}} \hat{z}_\Delta^n(\xi)\partial_\xi \hat{z}_\Delta^n(\xi)\rho''' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi = \frac{1}{2}\int_\Omega \partial_x\big(\hat{u}_\Delta^n(x)\big)^2\rho'''(x)\,\mathrm{d}x, \tag{6.58}$$

$$R_8 := \sum_{n=1}^{N_\tau} \tau_n \left| \int_{\mathcal{M}} \hat{z}_\Delta^n(\xi)(\partial_\xi\hat{z}_\Delta^n)^2(\xi)\rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi - \int_\Omega (\partial_x \hat{u}_\Delta^n)^2(x)\rho''(x)\,\mathrm{d}x\right| \leqslant C_8\delta^{1/4} \tag{6.59}$$

for a constant $C_8 > 0$ expressible in Ω, T, ϖ and $\overline{\mathcal{D}^V}$.

Proof. The starting point is the relation (5.16) between the locally affine interpolants $\hat{u}_\Delta^n$ and $\hat{z}_\Delta^n$ that is

$$\hat{z}_\Delta^n(\xi) = \hat{u}_\Delta^n \circ \mathbf{X}_\Delta^n(\xi) \tag{6.60}$$

for all $\xi \in \mathcal{M}$. Both sides of this equation are differentiable at almost every $\xi \in \mathcal{M}$, with

$$\partial_\xi \hat{z}_\Delta^n(\xi) = \partial_x \hat{u}_\Delta^n \circ \mathbf{X}_\Delta^n(\xi)\partial_\xi \mathbf{X}_\Delta^n(\xi).$$

Substitute this expression for $\partial_\xi\hat{z}_\Delta^n(\xi)$ into the left-hand side of (6.58), and perform a change of variables $x = \mathbf{X}_\Delta^n(\xi)$ to obtain the integral on the right.

Next observe that the x-integral in (6.59) can be written as

$$\int_\Omega (\partial_x\hat{u}_\Delta^n)^2(x)\rho''(x)\,\mathrm{d}x = \int_{\mathcal{M}} (\partial_\xi\hat{z}_\Delta^n)^2(\xi)\frac{1}{\partial_\xi \mathbf{X}_\Delta^n}\rho'' \circ \mathbf{X}_\Delta^n(\xi)\,\mathrm{d}\xi, \tag{6.61}$$

using (6.60). It hence remains to estimate the difference between the ξ-integral in (6.59) and (6.61), respectively. To this end, observe that for each $\xi \in (\xi_k, \xi_{k+\frac12})$ with some $k \in \mathbb{I}_K^+$, one has

$\partial_\xi \mathbf{X}_\Delta^n(\xi) = 1/z_{k+\frac{1}{2}}^n$ and $\widehat{z}_\Delta(\xi) \in [z_{k-\frac{1}{2}}, z_{k+\frac{1}{2}}]$. Hence, for those ξ,

$$\left|1 - \frac{1}{\widehat{z}_\Delta^n(\xi)\partial_\xi \mathbf{X}_\Delta^n(\xi)}\right| \leqslant \left|1 - \frac{z_{k+\frac{1}{2}}^n}{z_{k-\frac{1}{2}}^n}\right|.$$

If instead $\xi \in (\xi_{k-\frac{1}{2}}, \xi_k)$, then this estimate is satisfied with the roles of $z_{k+\frac{1}{2}}^n$ and $z_{k-\frac{1}{2}}^n$ interchanged. Consequently,

$$\begin{aligned}
&\left|\int_{\mathcal{M}} (\partial_\xi \widehat{z}_\Delta^n)^2(\xi)\widehat{z}_\Delta^n(\xi)\rho'' \circ \mathbf{X}_\Delta^n(\xi)\,\mathrm{d}\xi - \int_{\mathcal{M}} (\partial_\xi \widehat{z}_\Delta^n)^2(\xi)\frac{1}{\partial_\xi \mathbf{X}_\Delta^n(\xi)}\rho'' \circ \mathbf{X}_\Delta^n(\xi)\,\mathrm{d}\xi\right| \\
\leqslant{}& \varpi \int_{\mathcal{M}} (\partial_\xi \widehat{z}_\Delta^n)^2(\xi)\widehat{z}_\Delta^n(\xi)\left(1 - \frac{1}{\widehat{z}_\Delta^n(\xi)\partial_\xi \mathbf{X}_\Delta^n(\xi)}\right)\mathrm{d}\xi \\
\leqslant{}& \varpi\delta \sum_{k\in\mathbb{I}_K^+} z_k^n \left(\frac{z_{k+\frac{1}{2}}^n - z_{k-\frac{1}{2}}^n}{\delta}\right)^2 \left(\left|\frac{z_{k+\frac{1}{2}}}{z_{k-\frac{1}{2}}} - 1\right| + \left|\frac{z_{k-\frac{1}{2}}}{z_{k+\frac{1}{2}}} - 1\right|\right),
\end{aligned}$$

which is again at least of order $\mathcal{O}(\delta^{\frac{1}{4}})$, as we have seen before in (6.45). □

Proof of (6.42)**.** Combining the discrete weak formulation (6.43), the change of variables formulae (6.58) and (6.59), and the definitions of R_1 to R_8, it follows that

$$\begin{aligned}
\mathrm{e}_{2,\Delta} \leqslant \varpi R_8 + \varpi \sum_{n=1}^{N_{\boldsymbol{\tau}}} \tau_n \Big| &\int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi)\partial_\xi \widehat{z}_\Delta^n(\xi)\rho''' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi + \frac{3}{2}\int_{\mathcal{M}} \widehat{z}_\Delta^n(\xi)(\partial_\xi \widehat{z}_\Delta^n)^2(\xi)\rho'' \circ \mathrm{X}_\Delta^n(\xi)\,\mathrm{d}\xi \\
&+ \int_\Omega V_x(x)\left\{u_\Delta\right\}_{\boldsymbol{\tau}}(x)\rho'(x)\,\mathrm{d}x - \sum_{i=1}^{7} A_i^n\Big| \\
&\leqslant \varpi \sum_{i=1}^{7} R_i^n \leqslant \varpi \sum_{i=1}^{7} C_i \delta^{1/4}.
\end{aligned}$$

This implies the desired inequality (6.42). □

We are now going to finish the proof of this section's main result, Proposition 6.14.

Proof of Proposition 6.14. Owing to (6.41) and (6.42), we know that

$$\begin{aligned}
\Bigg|\int_0^T \eta'(t)\int_\Omega \rho(x)\left\{u_\Delta\right\}_{\boldsymbol{\tau}}(t,x)\,\mathrm{d}x + \eta(t)\frac{1}{2}\int_\Omega &\rho'''(x)\partial_x(\left\{u_\Delta\right\}_{\boldsymbol{\tau}}^2)(t,x) + 3\rho''(x)(\partial_x\left\{u_\Delta\right\}_{\boldsymbol{\tau}})^2(t,x)\,\mathrm{d}x \\
&+ \int_\Omega V_x(x)\left\{u_\Delta\right\}_{\boldsymbol{\tau}}(t,x)\rho'(x)\,\mathrm{d}t\Bigg| \\
&\leqslant \mathrm{e}_{1,\Delta} + \mathrm{e}_{2,\Delta} \leqslant C\big(\tau + \delta^{1/4}\big).
\end{aligned}$$

To obtain (6.37) in the limit $\Delta \to 0$, we still need to show the convergence of the integrals to their respective limits, but this is no challenging task anymore: Note that (6.36) implies

$$\partial_x\left\{u_\Delta\right\}_{\boldsymbol{\tau}} \longrightarrow \partial_x u_* \quad \text{strongly in } L^2([0,T]\times\Omega), \tag{6.62}$$

hence $(\partial_x \{u_\Delta\}_{\boldsymbol{\tau}})^2$ converges to $(\partial_x u_*)^2$ in $L^1([0,T] \times \Omega)$. Furthermore, we have that

$$\partial_x(\{u_\Delta\}_{\boldsymbol{\tau}}^2) = 2\{u_\Delta\}_{\boldsymbol{\tau}} \partial_x \{u_\Delta\}_{\boldsymbol{\tau}} \longrightarrow 2u_* \partial_x(u_*) = \partial_x(u_*^2) \tag{6.63}$$

in $L^2([0,T] \times \Omega)$. Here we used (6.62) and that $\{u_\Delta\}_{\boldsymbol{\tau}}$ converges to u_* uniformly on $[0,T] \times \Omega$ due to (6.35). Hence, (6.62) and (6.63) suffice to pass to the limit in the second integral. Finally remember the weak convergence result in (6.34), $\{u_\Delta\}_{\boldsymbol{\tau}} \to u_*$ in $\mathcal{P}_2^r(\Omega)$ with respect to time, hence the convergence of the first and third integral is assured as well.

□

6.5. Numerical results

We fix $\Omega = (0,1)$ for all experiments described below and furthermore use $V \equiv 0$ for the rest of this section.

As in the numerical investigations of the previous two chapters, we are going to use non-uniform meshes for our numerical experiments in order to make our discretization more flexible. The choice of non-uniform meshes and the implementation of initial grids $\vec{\mathrm{x}}_\Delta^0$ are hence analogue to Section 4.4.1 and 4.4.2. Furthermore, the entropy is discretized by restriction, and the discretized information functional is the dissipation of the discretized Renyi entropy along the discretized heat flow. Explicitly, the resulting fully discrete gradient flow equation attaines the form

$$\frac{\vec{\mathrm{x}}_\Delta^n - \vec{\mathrm{x}}_\Delta^{n-1}}{\tau_n} = -\nabla_{\boldsymbol{\xi}} \mathbf{D}^V(\vec{\mathrm{x}}_\Delta^n) = -\mathrm{W}^{-1}\left(\partial^2_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}}) \cdot \partial_{\vec{\mathrm{x}}}\mathbf{Q}(\vec{\mathrm{x}}) + \partial^2_{\vec{\mathrm{x}}}\mathbf{Q}(\vec{\mathrm{x}}) \cdot \partial_{\vec{\mathrm{x}}}\mathbf{H}(\vec{\mathrm{x}})\right), \tag{6.64}$$

where $\mathrm{W} \in \mathbb{R}^{(K-1)\times(K-1)}$ is the diagonal matrix with entries

$$[\mathrm{W}]_{k,k} = \frac{1}{2}(\delta_{k+\frac{1}{2}} + \delta_{k-\frac{1}{2}}), \quad k = 1, \ldots, K-1.$$

To solve (6.64), a damped Newton scheme in analogy to Section 4.4.1 and 4.4.2 is applied.

6.5.1. Numerical experiments. In a paper of Gruen and Beck [**BG15**], the authors analyzed, among other things, the behaviour of equation (6.1) on the bounded domain $(0,1)$ with Neumann-boundary conditions and the initial datum

$$u^0(x) = (x-0.5)^4 + 10^{-3}, \quad x \in \Omega = (0,1), \quad \text{with mass } M = 0.0135. \tag{6.65}$$

This case is interesting insofar as the observed film seems to rip at time $t = 0.012$.

6.5.1.a. Evolution of discrete solutions. Figure 6.1 shows the evolution of u_Δ for $K = 400$ and $\tau = 10^{-7}$ at times $t = 0, 0.0022, 0.012, 0.04$, the associated particle flow is printed in Figure 6.2/left. It is clearly seen that the strictly positive initial density has a minimum at $x = 1/2$, which bifurcates into two minima at later times, and eventually becomes one single minimum again. As discussed in [**BG15**], the film seems to rip at time $t = 0.012$. At later times, the observed “degeneracy” alleviates and the film moves towards a stationary state, which is a constant function with mass M.

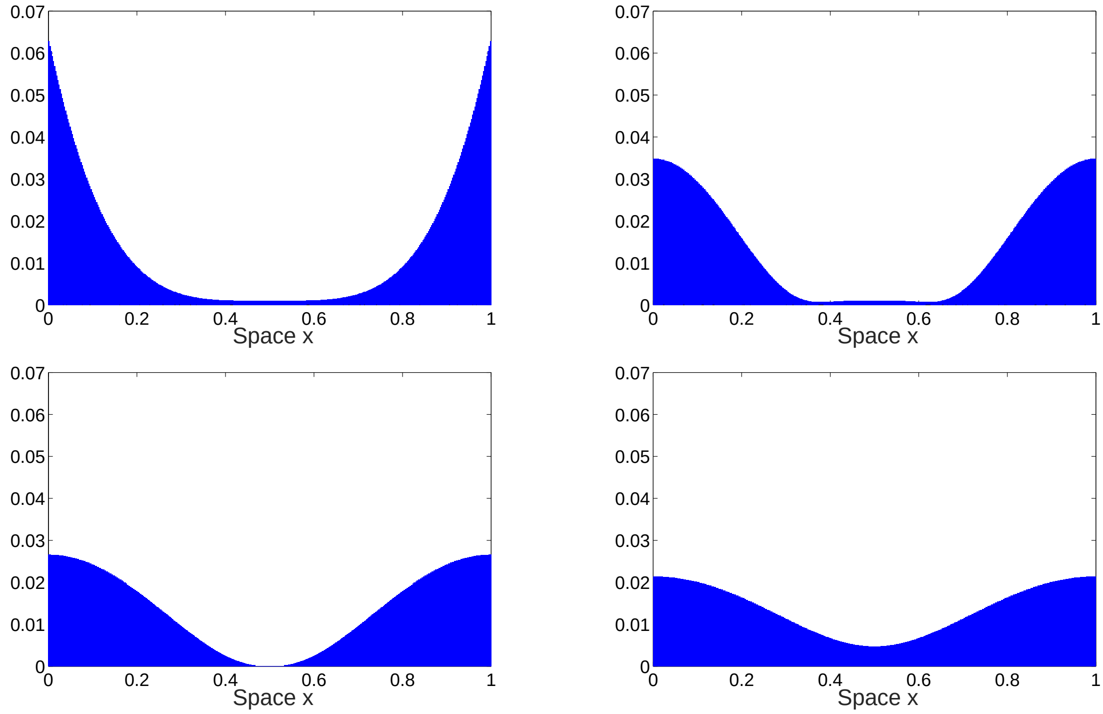


FIGURE 6.1. Evolution of a discrete solution u_Δ, evaluated at different times $t = 0, 0.002, 0.012, 0.04$ (from top left to bottom right)

6.5.1.b. Rate of convergence. For the analysis of the scheme's convergence with initial datum u^0 from (6.65), we compare solutions of the scheme with u_{ref}, which is obtained by solving (6.64) on a much finer grid, which is $\widetilde{\Delta} = (\boldsymbol{\xi}_{\text{ref}}; \boldsymbol{\tau}_{\text{ref}})$. To define $\boldsymbol{\xi}_{\text{ref}}$, we introduce the equidistant grid $x_k = kK_{\text{ref}}^{-1}$ on $\Omega = (0, 1)$, with $k = 0, \dots, K_{\text{ref}}$ and $K_{\text{ref}} = 1600$. Then the entries ξ_k are always chosen, such that

$$\xi_k = \int_{x_0^0}^{x_k^0} u^0(y)\,\mathrm{d}y,$$

for any $k = 0, \dots, K_{\text{ref}}$. For the temporal discretization, we use $\boldsymbol{\tau}_{\text{ref}}$ with constant time step sizes $\tau_n \equiv 5 \cdot 10^{-8}$.

To verify the scheme's convergence at least numerically, we study the decay of the L^p-errors, $p \in \{1, 2, +\infty\}$, under refinement of the spatial discretization. For this purpose, we fix a time decomposition with constant time step sizes $\tau_n \equiv \tau = 10^{-7}$ and vary the number of spatial grid points, using $K = 25, 50, 100, 200, 400$. Figure 6.2/right shows the corresponding L^p-errors between the solution to our scheme and the reference solution u_{ref}, evaluated at time $T = 10^{-4}$. Here, a time decomposition $\boldsymbol{\tau}_{\text{ref}}$ with constant time step sizes $\tau_n \equiv 5 \cdot 10^{-8}$ is used for the reference solution. It is clearly seen that the errors decay with an almost perfect rate of $\delta^2 \propto K^{-2}$.

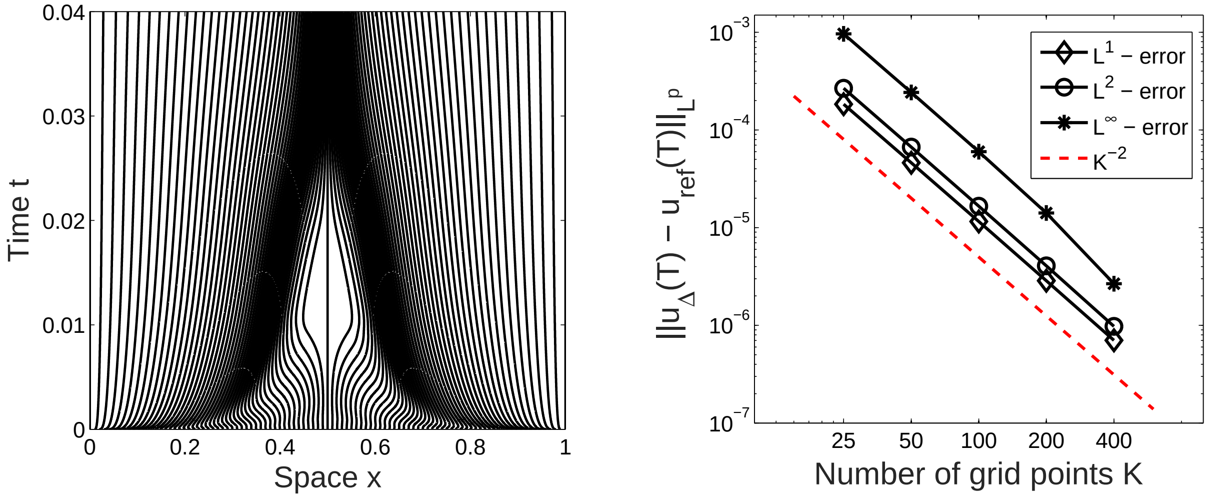


FIGURE 6.2. *Left*: associated particle flow of u_Δ for initial datum (5.73). *Right*: rate of convergence, using $K = 25, 50, 100, 200, 400$ and $\tau = 10^{-7}$. The errors are evaluated at time $t = 10^{-4}$.

Part 2

Two-dimensional case

Compared to the one-dimensional case discussed in the first part of this thesis, the degree of difficulty of the L^2-Wasserstein distance's analysis instantaneously increases as soon as one considers higher dimensions, unfortunately. The existence of solutions to the Kantorovich optimal transportation problem, (1.1), is well studied and several proofs are available, see for instance the content of Chapter 2 of [**Vil03**] for a duality-based proof. But the lack of an easy and practical representation of the L^2-Wasserstein distance between two arbitrary densities — similar to the one in Lemma 2.1 for one spatial dimension — seems to be the bottleneck for a convenient numerical investigation of L^2-Wasserstein gradient flows.

In the forthcoming chapter we describe a discretization of L^2-Wasserstein gradient flows for a family of second order evolution equations on the basis of the following fundamental result: For any densities $u, v \in \mathcal{P}_2^r(\Omega)$ the *optimal transportation map* pushing u to v is provided by the gradient of a convex function. More precisely, there exists a transportation map $\nabla\varphi$ that is the unique gradient (i.e. uniquely determined at almost every $x \in \Omega \subseteq \mathbb{R}^2$) of a convex function such that $v = (\nabla\varphi)_\# u$ and

$$\mathcal{W}_2(u, v) = \int_\Omega |x - \nabla\varphi(x)|^2 u(x)\,\mathrm{d}x.$$

A proof of this statement can be found for instance in [**Vil03**, Theorem 2.12]. The optimal transportation map $\nabla\varphi$ is also called the *Brenier map*, which is due to Brenier's achievements in the field of optimal transportation, see in particular his work [**Bre91**] or Chapter 3 in [**Vil03**] about *Brenier's polar factorization theorem*.

Motivated by the above characterization of the L^2-Wasserstein distance, we choose again a Lagrangian formulation of the considered L^2-Wasserstein gradient flows to derive a numerical scheme. The underlying idea for our approach is the following: Fix a finite-dimensional set of gradients of convex functions, which forms a set of "potential" optimal transportation maps. Then we solve recursively the minimizing movement scheme (1.12) restricted to the subset of density functions that can be reached by pushing the minimizer of the previous time step through an arbitrary optimal transportation map from the fixed finite-dimensional set. A particular property of the gained scheme is the consecutive change of the set of density functions, which is used for solving the minimization problem, in each time step. This sounds impractical for numerical implementations at the first glance, but as we are going to figure out in the following, the Lagrangian reformulation of the minimizing movement scheme constitutes an appropriate and convenient formulation for a numerical treatment.

CHAPTER 7

Second order drift-diffusion equation

This chapter provides joint work in progress with Oliver Junge and my PhD-supervisor Daniel Matthes.

7.1. Introduction

In this chapter, we propose and study a fully variational numerical scheme of the following second order equation with no-flux boundary condition on the spatial domain $\Omega = (0,1)^2$:

$$\partial_t u = \Delta \mathrm{P}\big(u\big) + \mathrm{div}(u\nabla V) \quad \text{for } t > 0 \text{ and } x \in \Omega, \tag{7.1}$$

$$\langle \nabla \mathrm{P}(u) + u\nabla V, \vec{n}\rangle = 0 \quad \text{for } t > 0 \text{ and } x \in \partial\Omega, \tag{7.2}$$

$$u = u^0 > 0 \quad \text{at } t = 0. \tag{7.3}$$

Here, $\vec{n}(x)$ denotes the outward normal vector at $x \in \partial\Omega$. The strictly positive initial density u^0 is assumed to be in $L^1(\Omega)$ with unit mass $M = 1$. The drift potential $V : \overline{\Omega} \to \mathbb{R}$ is assumed to be at least in $C^2(\Omega)$, and $\mathrm{P} : [0,+\infty) \to \mathbb{R}$ is a nonnegative and monotonically increasing function that satisfies the following assumptions:

- One can find a strictly convex function $\phi : [0,+\infty) \to \mathbb{R}$ with $\phi(0) = 0$, such that
$$\mathrm{P}(r) = r\phi'(r) - \phi(r). \tag{7.4}$$
- $r \mapsto \mathrm{P}(r)$ is linear or has superlinear growth, such that
$$r \mapsto r^{-1/2}\mathrm{P}(r) \quad \text{is non-decreasing for } r \in (0,+\infty). \tag{7.5}$$

Common examples for second order equations that have the above form in (7.1) are the *heat equation* ($\mathrm{P}(u) = u$ and usually with $V = 0$) or *porous medium equations* with slow diffusion ($\mathrm{P}(u) = u^m$ with $m > 1$).

Under the given regulartiy assumptions, there are many possibilities to design appropriate numerical schemes for (7.1), for instance by using finite elements/volume methods or finite differences. The following approach is special insofar as it makes use of the equations underlying gradient flow structure, which paves the way to derive a scheme that inherits several structural properties of solutions to (7.1) by construction, for instance preservation of mass and positivity, and dissipation of the entropy.

In what follows, we give a brief introduction to the equation's gradient flow structure. For the more intrested reader, we especially refer to [**AGS05**, **ALS06**, **ESG05**, **Vil03**].

7.1.1. Gradient flow structure. We summarize some basic facts about the variational formulation of (7.1). The divergence form in combination with the no-flux boundary condition implies the conservation of mass and we shall consider $M = 1$ from now on. Similar to Chapter 3 we consider an entropy functional $\mathcal{E}$ given by

$$\mathcal{E}(u) = \int_\Omega \phi(u(x))\,\mathrm{d}x + \int_\Omega u(x)V(x)\,\mathrm{d}x \tag{7.6}$$

for $u \in \mathcal{P}_2^r(\Omega)$. Using the entropy, equation (7.1) can be reformulated in terms of the continuity equation

$$\partial_t u + \operatorname{div}(u\mathbf{v}(u)) = 0, \tag{7.7}$$

where the velocity field $\mathbf{v}(u)$ is given by the gradient of the first variational derivative of $\mathcal{E}$ evaluated at u, i.e.

$$\mathbf{v}(u) = -\nabla\left(\frac{\delta\mathcal{E}(u)}{\delta u}\right) = -\nabla\left(\phi'(u) + V\right) = -\left(\frac{\nabla \mathrm{P}(u)}{u} + \nabla V\right). \tag{7.8}$$

Using the representation of equation (7.1) in (7.7), the no-flux boundary condition then reads as

$$\langle \mathbf{v}(u(t,x)), \vec{n}(x)\rangle = 0 \tag{7.9}$$

for $(t,x) \in (0,+\infty) \times \partial\Omega$.

As we have already mentioned in the one-dimensional situation in Chapter 3, the functional $\mathcal{E}$ is λ-convex along geodesics in $\mathcal{W}_2$ [**McC97**], where $\lambda \in \mathbb{R}$ is chosen such that

$$\mathrm{D}^2 V \geqslant \lambda\mathbb{I}. \tag{7.10}$$

Here, $\mathbb{I} \in \mathbb{R}^{2\times 2}$ denotes the identity matrix and $\mathrm{D}^2 V$ is the hessian of V. The λ-convexity of $\mathcal{E}$ is a powerful ingredient in several analytical applications, which is why we aim to inherit this feature to our numerical scheme.

7.1.2. The gradient flow in Lagrangian coordinates. It is a well-known fact that the L^2-Wasserstein gradient flow turns into a L^2-gradient flow for

$$\mathbf{T} \mapsto \mathcal{E}(\mathbf{T}_\# w) = \int_\Omega \psi\left(\frac{\det \mathrm{D}\,\mathbf{T}(x)}{w(x)}\right) w(x)\,\mathrm{d}x + \int_\Omega V\big(\mathbf{T}(x)\big)w(x)\,\mathrm{d}x \tag{7.11}$$

with $\psi(s) := s\phi(s^{-1})$. Here we used the explicit representation of the push-forward $\mathbf{T}_\# w$ of a density $w \in \mathcal{P}_2^r(\Omega)$ through a transportation map $\mathbf{T} : \Omega \to \Omega$ as given in (1.19). This special relation was first observed by Evans, Gangbo and Savin [**ESG05**] and then further analyzed by Ambrosio, Lisini and Savaré [**ALS06**]. A simple formal argument indicates (we refer to [**ALS06**] for a proper proof of the following assumption) that the L^2-gradient flow along the functional $\mathbf{T} \mapsto \mathcal{E}(\mathbf{T}_\# u^0)$ is a solution to the "ordinary differential equation"

$$\begin{aligned} \partial_t \mathbf{T} &= \mathbf{v}(u) \circ \mathbf{T} \quad \text{for } (t,x) \in (0,+\infty) \times \Omega, \\ \mathbf{T}(0,x) &= x \quad \text{for } x \in \Omega, \end{aligned} \tag{7.12}$$

when u solves (7.1). Using (7.8), the right-hand side in (7.12) attains the explicit form

$$\mathbf{v}(u) \circ \mathbf{T} = \mathrm{P}'(u \circ \mathbf{T})\left[\frac{\nabla u}{u}\right] \circ \mathbf{T} + \big[\nabla V\big] \circ \mathbf{T}.$$

Equation (7.12) means in particular that a solution u to the continuity equation (7.7) with the velocity field in (7.8) has an one-to-one connection to a transportation map $\mathbf{T}$ that solves (7.12).

7.1.3. Description of the numerical scheme. Throughout this section, we fix a time step size τ that induces a temporal decomposition of $[0, +\infty)$ by

$$\{0 = t_0 < t_1 < \ldots < t_n < \ldots\}, \quad \text{where} \quad t_n := n\tau.$$

Unlike the notation used in the first part of this thesis, we denote by τ the temporal decomposition parameter, which in particular shall emphasize the usage of a *uniform* decomposition of the time line.

The derivation of our numerical scheme for (7.1) is once more based on a specific discretization of the minimizing movement scheme, which works in the situation at hand as follows: Given a time step $\tau > 0$, one defines inductively — starting from $u_\tau^0 = u^0$ — approximations u_τ^n of $u(n\tau, \cdot)$ as minimizers in $\mathcal{P}_2^r(\Omega)$ of the "penalized entropy functional" $\mathcal{E}_\tau(\cdot, u_\tau^{n-1})$, given for $n \in \mathbb{N}$ by

$$u_\tau^n = \operatorname*{argmin}_{v \in \mathcal{P}_2^r(\Omega)} \mathcal{E}_\tau(v, u_\tau^{n-1}), \qquad \text{with} \qquad \mathcal{E}_\tau(v, u) := \frac{1}{2\tau}\mathcal{W}_2(v, u) + \mathcal{E}(v). \tag{7.13}$$

To obtain a full spatio-temporal discretization of (7.1) we first introduce a spatio-temporal discretization parameter $\Delta = (\tau; K)$, where $K \in \mathbb{N}$ and τ is chosen as above. The idea is again to perform the minimization in (7.13) on a Δ-dependent discrete submanifold of $\mathcal{P}_2^r(\Omega)$. Compared to the one-dimensional case the situation becomes more delicate in higher dimensions, since an explicit formula of the L^2-Wasserstein disctance between two arbitrary densities $u, v \in \mathcal{P}_2^r(\Omega)$ is *not* available. To circumvent this problem, remember that Monge's optimal transportation problem for two arbitrary densities $u, v \in \mathcal{P}_2^r(\Omega)$ admits a solution that is always a gradient of a certain potential function, i.e. $v = \mathfrak{t}_\# u$ with $\mathfrak{t} \in \mathfrak{X}$, where

$$\begin{aligned} \mathfrak{t} \in \mathfrak{X} \quad :\Longleftrightarrow \quad & \mathfrak{t} = \nabla\varphi : \Omega \to \Omega, \text{ with a convex function } \varphi \text{ that is} \\ & \text{almost every differentiable with } \det(\mathrm{D}^2 \varphi) > 0 \text{ for almost every } x \in \Omega. \end{aligned} \tag{7.14}$$

Note that the condition $\det(\mathrm{D}^2 \varphi) > 0$ for almost every $x \in \Omega$ basically guarantees that $v = \mathfrak{t}_\# u$ with $\mathfrak{t} = \nabla\varphi$ is a regular density, see [**AGS05**, Lemma 5.5.3]. This motivates the following derivation of a fully discrete numerical scheme for (7.1): Instead of solving (7.13) restricted to a fixed time-independent discrete submanifold of $\mathcal{P}_2^r(\Omega)$ (as we did in one spatial dimension), we restrict the set of admissible optimal transports $\mathfrak{X}$ to a finite-dimensional subset $\mathfrak{X}_K$ dependent on the spatial discretization parameter $K \in \mathbb{N}$, fix $n \in \mathbb{N}$, and minimize $v \mapsto \mathcal{E}_\tau(v, u_\Delta^{n-1})$ over all densities $v \in \mathcal{P}_{2,K}^{r,n}(\Omega)$. Here, $\mathcal{P}_{2,K}^{r,n}(\Omega)$ is an iteratively defined submanifold of $\mathcal{P}_2^r(\Omega)$, which contains all densities $v \in \mathcal{P}_2^r(\Omega)$ that can be reached by the pair $(u_\Delta^{n-1}, \mathfrak{t})$ constituted by the solution u_Δ^{n-1} of the previous time step $(n-1)$ and an optimal transportation map $\mathfrak{t} \in \mathfrak{X}_K$, i.e.

$$\begin{aligned} &\mathcal{P}_{2,K}^{r,1}(\Omega) := \left\{v = \mathfrak{t}_\# u_\Delta^0 : \ \mathfrak{t} \in \mathfrak{X}_K\right\} \quad \text{and} \\ &\mathcal{P}_{2,K}^{r,n}(\Omega) := \left\{v = \mathfrak{t}_\# u_\Delta^{n-1} : \ \mathfrak{t} \in \mathfrak{X}_K \text{ and } u_\Delta^{n-1} \text{ solves (7.13) restricted to } \mathcal{P}_{2,K}^{r,n-1}(\Omega)\right\} \end{aligned} \tag{7.15}$$

for $n > 1$. There are infinitely many admissible choices for $\mathfrak{X}_K$, for instance one can choose locally affine or quadratic spline interpolations of transportation maps in $\mathfrak{X}$. In this thesis we use a Fourier-ansatz that is

$$\mathfrak{X}_K := \left\{ \mathfrak{t} = \mathrm{id} + \sum_{k,l=0}^{K} z_{kl} \nabla \varphi_{kl} : \; z_{kl} \in \mathbb{R}, \text{ such that } \det \mathrm{D}\, \mathfrak{t} > 0 \right\}, \tag{7.16}$$

with

$$\varphi_{kl}(x) := c_{kl} \cos(k\pi x_1)\cos(l\pi x_2) \quad \text{for } x = (x_1, x_2) \in \Omega. \tag{7.17}$$

The coefficients $c_{kl} > 0$ are chosen such that the vectors $\nabla\varphi_{kl}$ have unit $L^2(\Omega)$-norm for $(k,l) \neq (0,0)$, see (7.34) for a proper definition. With this specific choice of $\mathfrak{X}_K$ — we are going to prove in Lemma 7.6 that $\mathfrak{X}_K$ is indeed a finite-dimensional subspace of $\mathfrak{X}$ — the numerical scheme reads as follows:

Numerical scheme. *Fix a spatio-temporal discretization $\Delta = (\tau; K)$ consisting of a time step size $\tau > 0$ and a parameter $K \in \mathbb{N}$. Then*

1. *For $n = 0$, fix an initial density function $u_\Delta^0 = u^0 \in \mathcal{P}_2^r(\Omega)$.*
2. *For $n \geqslant 1$, recursively define densities u_Δ^n as solutions to the minimization problem*

$$u_\Delta^n = \operatorname*{argmin}_{v \in \mathcal{P}_{2,K}^{r,n}(\Omega)} \mathcal{E}_\tau(v, u_\Delta^{n-1}), \tag{7.18}$$

where $\mathcal{P}_{2,K}^{r,n}(\Omega)$ changes with each time iteration as given in (7.15).

The above procedure (1) – (2) yields a sequence of densitiy functions that is going to be denoted by $u_\Delta = (u_\Delta^0, u_\Delta^1, \ldots)$ from now on. Compared to other approaches that exploit the equation's underlying variational structure (for instance [**CM10**,**CW**,**MO14a**,**Osb14**,**MO14b**] and many more), the finite-dimensional submanifold $\mathcal{P}_{2,K}^{r,n}(\Omega)$ does not only depend on the spatial discretization K, but also on the previous evolution of u_Δ^{n-1}. Hence, our set of discrete density functions $\mathcal{P}_{2,K}^{r,n}(\Omega)$ changes with every time step. Further note that our approach guarentees that two consecutively calculated discrete minimizers are always connected by an optimal transportation map, without explicitely solving Monge's optimal transportation problem.

We are going to prove later in Proposition 7.1 that the minimization problem (7.18) possesses a unique solution for our choice of $\mathcal{P}_{2,K}^{r,n}(\Omega)$ under an additional assumption on the integrand of the entropy $\mathcal{E}$.

It is convenient for later purposes to introduce some additional notation. We define the set of indices $\mathcal{I}_K := \{(k,l) \in \mathbb{N}^2 : \|(k,l)\|_\infty \leqslant K\} \backslash \{(0,0)\}$ and write $\vec{z} = (z_{kl})_{(k,l)\in\mathcal{I}_K}$ for a vector $\vec{z} \in \mathbb{R}^{(K+1)^2-1}$ with components $z_{kl} \in \mathbb{R}$. Furthermore, define the map

$$\vec{z} \in \mathbb{R}^{(K+1)^2-1} \;\mapsto\; \mathfrak{t}_K[\vec{z}] := \mathrm{id} + \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\nabla\varphi_{kl} \tag{7.19}$$

with φ_{kl} as in (7.17). Note that we exclude the index $(k,l) = (0,0)$ since φ_{00} is a constant function. Furthermore, we denote by $\partial_{\vec{z}} f(\vec{z})$ the gradient of a function $f : \mathbb{R}^{(K+1)^2-1} \to \mathbb{R}$ with respect to $\vec{z}$, i.e.

$$[\partial_{\vec{z}} f(\vec{z})]_{(k,l)} = \frac{\partial}{\partial z_{kl}} f(\vec{z})$$

for any $(k,l) \in \mathcal{I}_K$. If u_Δ is a solution to the numerical scheme, let us finally introduce for any index $n \in \mathbb{N}_0$ the matrix $W_n \in \mathbb{R}^{((K+1)^2-1)\times((K+1)^2-1)}$ given by

$$[W_n]_{(kl),(hj)} := \int_\Omega \langle \nabla\varphi_{kl}, \nabla\varphi_{hj}\rangle u_\Delta^n \, dx. \tag{7.20}$$

7.1.4. Main results. Let us assume in the following that a spatio-temporal discretization $\Delta = (\tau; K)$ consisting of a time step size $\tau > 0$ and a parameter $K \in \mathbb{N}$ is fixed. We further assume for the rest of this chapter the validity of the following general assumptions on the initial density u^0:

$$u^0 > 0 \quad \text{and} \quad \mathcal{E}(u^0) < +\infty. \tag{7.21}$$

The first result pictures the qualitative poperties of solutions to our numerical scheme:

Proposition 7.1. *Assume that the temporal decomposition parameter satisfies $\tau^{-1} + \lambda > 0$. Furthermore, suppose that the integrand $\phi : [0,+\infty) \to \mathbb{R}$ of the entropy $\mathcal{E}$ satisfies*

$$s^2\phi(1/s) \to +\infty \quad \text{as} \quad s \downarrow 0. \tag{7.22}$$

Then the numerical scheme described in Section 7.1.3 is well-posed. More precisely, the minimization problem (7.18) *possesses a unique solution for any $n \geqslant 1$.*

Moreover, a sequence of solution $u_\Delta = (u_\Delta^0, u_\Delta^1, \ldots)$ to (7.18) *satisfies the following properties:*

- *Conservation of mass and positivity: Any solution u_Δ^n to* (7.18) *lies in $\mathcal{P}_2^r(\Omega)$.*
- *Entropy dissipation: $\mathcal{E}(u_\Delta^n) \leqslant \mathcal{E}(u_\Delta^{n-1})$ for any $n \geqslant 1$.*

Positivity, conservation of mass and dissipation of the entropy are trivial conclusions from the scheme's construction, whereas the statement of well-posedness is a nontrivial claim that follows from Lemma 7.10. Note further that the condition (7.22) on the integrand of $\mathcal{E}$ seems to be of a technical nature, since numerical experiments show that one can apply the scheme for more general choices of ϕ, see Section 7.5.

The next result shows that solutions to the numerical scheme satisfy a discrete Euler-Lagrange equation:

Proposition 7.2. *Under the same requirements as in Proposition 7.1, there exists a unique sequence $\mathfrak{t}_\Delta = (\mathfrak{t}_\Delta^0, \mathfrak{t}_\Delta^1, \ldots)$ of optimal transportation maps $\mathfrak{t}_\Delta^n \in \mathfrak{X}$ and a unique sequence of vectors $\vec{z}_\Delta = (\vec{z}_\Delta^0, \vec{z}_\Delta^1, \ldots)$ with $\vec{z}_\Delta^n \in \mathbb{R}^{(K+1)^2-1}$, such that*

$$\mathfrak{t}_\Delta^n = \mathfrak{t}_K[\vec{z}_\Delta^n], \quad \text{and } \mathfrak{t}_\Delta^n \text{ satisfies} \quad u_\Delta^n = (\mathfrak{t}_\Delta^n \circ \mathfrak{t}_\Delta^{n-1} \circ \ldots \circ \mathfrak{t}_\Delta^0)_\# u^0$$

for any $n \in \mathbb{N}_0$. Moreover, each vector $\vec{z}_\Delta^n$ in $\vec{z}_\Delta$, $n \geqslant 1$, is a solution to the system of discrete Euler-Lagrange equations

$$\frac{1}{\tau} W_{n-1}\vec{z} + \partial_{\vec{z}}\mathcal{E}\left(\left(\mathfrak{t}_K[\vec{z}]\right)_\# u_\Delta^{n-1}\right) = 0. \tag{7.23}$$

The above result shows that solutions u_Δ to the numerical scheme are uniquely related to a sequence of vectors $\vec{\mathrm{z}}_\Delta$ with entries that solve the system of Euler-Lagrange equations (7.23).

One can now ask for stability of the scheme at least in each time iteration. More precisely, we are interested in an error estimate for the difference between an arbitrary vector $\vec{\mathrm{y}} \in \mathbb{R}^{(K+1)^2-1}$ and the "scheme's solution" $\vec{\mathrm{z}}_\Delta^n$ at time step $n \in \mathbb{N}$. This error is expressible in terms of the residuum $\vec{\gamma}^n[\vec{\mathrm{y}}]$ defined by

$$\vec{\gamma}^n[\vec{\mathrm{y}}] := \frac{1}{\tau}\mathrm{W}_{n-1}\vec{\mathrm{y}} + \partial_{\vec{\mathrm{z}}}\mathcal{E}\left(\left(\mathrm{t}_K[\vec{\mathrm{y}}]\right)_\# u_\Delta^{n-1}\right) \tag{7.24}$$

and we can prove the following stability result:

Proposition 7.3. *Assume that u_Δ is a solution to the numerical scheme and $\vec{\mathrm{z}}_\Delta$ is the associated sequence of vectors which solve the system of Euler-Lagrange equations* (7.23) *at any time step $n \in \mathbb{N}$. Then*

$$(1 + 2\lambda\tau)\left\|\mathrm{t}_K[\vec{\mathrm{z}}_\Delta^n] - \mathrm{t}_K[\vec{\mathrm{y}}]\right\|^2_{L^2(\Omega;u_\Delta^{n-1})} \leqslant \tau^2 \left\langle \vec{\gamma}^n[\vec{\mathrm{y}}], \mathrm{W}_{n-1}^{-1}\vec{\gamma}^n[\vec{\mathrm{y}}]\right\rangle,$$

for any $\vec{\mathrm{y}} \in \mathbb{R}^{(K+1)^2-1}$, where $\vec{\gamma}^n[\vec{\mathrm{y}}]$ is defined as in (7.24)*.*

Unfortunatelly, we can *not* prove that discrete solutions to the scheme converge towards solutions to (7.1), so far. However, note that the above stability result in combination with a proof of the scheme's consistency can possibly be used to gain a convergence result.

We finally remark that the numerical scheme and all the above results can be easily extended for higher dimensions $d \geqslant 3$, just by a slight adaptation of the set of Lagrangian maps $\mathfrak{X}_K$ in (7.16), see Remark 7.9.

7.1.5. Related schemes. As we have already mentioned in Chapter 3, the construction of numerical schemes for (7.1) as a solution of discrete Wasserstein gradient flows with Lagrangian representation is not new in the literature. Especially in one spatial dimension, studies on Lagrangian schemes for (7.1) that are familiar to our ansatz are popular, take for instance [**AB13**, **BCHR99**, **GT06a**, **KW99**, **MS85**, **MO14a**, **Roe04**, **WW10**].

Based on the reformulation of (7.1) in terms of evolving diffeomorphisms [**ESG05**], Carrillo and Moll [**CM10**] derived a Lagrangian discretization of aggregation equations in two space dimensions. Another approach on basis of the gradient flow structure of (7.1) in dimension two was formulated by Burger et al [**BCW10**], using the hydrodynamical formulation of the Wasserstein distance [**BB00**] instead of the Lagrangian approach. However, there are unfortunately no analytical results concerning convergence or qualitative properties available for the numerical schemes in the aforementioned works. We are indeed just aware of one paper about the second order equation (7.1), the work [**BCMO14**] by Benamou, Carlier, Mérigot and Oudet, in which a proof of convergence for the scheme therein is given: Similar to our approximation, the authors define recursively a sequence of optimal transportation maps that is gained by minimizing the perturbed entropy functional in terms of Lagrangian coordinates. The main difference to our scheme is that the minimum is taken over a set consisting of Legendre-Fenchel transforms, which makes an implementation of the scheme more sophisticated.

7.2. Discretization in space and time

Before we discuss the properties of our approach in Subsection 7.2.2 and its connection to the minimizing movement scheme in Subsection 7.2.3 in more detail, we want to study the Lagrangian formulations of the L^2-Wasserstein distance and the entropy $\mathcal{E}$.

7.2.1. Lagrangian coordinates. Since we are interested in a Lagrangian description of equation (7.1), it is necessary to specify the relation between densities in $\mathcal{P}_2^r(\Omega)$ and transportation maps $\mathbf{T}$ on Ω. This link is provided by the push-forward operator as defined in (1.18). In case of differentiable and bijective maps $\mathbf{T} : \Omega \to \Omega$, equation (1.18) allows an explicit representation as

$$\mathbf{T}_\# w = \frac{w}{\det \mathrm{D}\,\mathbf{T}} \circ \mathbf{T}^{-1} \quad \text{for almost every } x \in \Omega, \tag{7.25}$$

see also (1.19). So starting from an arbitrary (regular) reference density w, its push-forward $\mathbf{T}_\# w$ through the transportation map $\mathbf{T}$ declares a new density that occurs by transporting mass packages distributed by w from a position $x \in \Omega$ to $\mathbf{T}(x)$.

7.2.1.a. L^2-Wasserstein distance in Lagrangian coordinates. In terms of Lagrangian coordinates, the L^2-Wasserstein disctance between two densities $u, v \in \mathcal{P}_2^r(\Omega)$ is given by

$$\mathcal{W}_2(u,v)^2 = \min\left\{ \int_\Omega \|x - \mathfrak{t}(x)\|_2^2 u(x)\,\mathrm{d}x : \ \mathfrak{t} : \Omega \to \Omega \text{ measurable with } v = \mathfrak{t}_\# u \right\}. \tag{7.26}$$

This minimization problem corresponds to the original formulation of Monge's optimal transportation problem, and possesses a solution— the optimal transportation map or Brenier map connecting u and v — see for instance [**AGS05, Vil03**]. As already mentioned at the beginning of Part 2, there exists in particular a function $\mathfrak{t} : \Omega \to \Omega$ with $v = \mathfrak{t}_\# u$, which is the gradient of a convex potential function $\varphi : \Omega \to \mathbb{R}$, hence $\mathfrak{t} \in \mathfrak{X}$.

Let us assume in the following that $\mathbf{T} : \Omega \to \Omega$ is an arbitrary transportation map and $\mathfrak{t} : \Omega \to \Omega$ is the gradient of a convex function, i.e. $\mathfrak{t} \in \mathfrak{X}$. Then the above considerations provide an explicit characterization of the L^2-Wasserstein distance between the densities $\mathbf{T}_\# u^0$ and $(\mathfrak{t} \circ \mathbf{T})_\# u^0$ in a purely Lagrangian formalism, i.e.

$$\mathbf{d}(\mathfrak{t}, \mathbf{T}) := \|\mathbf{T} - \mathfrak{t} \circ \mathbf{T}\|_{L^2(\Omega, u^0)} = \mathcal{W}_2\big((\mathfrak{t} \circ \mathbf{T})_\# u^0, \mathbf{T}_\# u^0\big), \tag{7.27}$$

where we use the explicit formula in (7.25).

7.2.1.b. The entropy in Lagrangian coordinates. As already mentioned, the entropy $\mathcal{E}$ can be written in terms of Lagrangian coordinates using the push-forward operator,

$$\mathbf{T} \mapsto \mathcal{E}(\mathbf{T}_\# w) = \int_\Omega \psi\left(\frac{\det \mathrm{D}\,\mathbf{T}(x)}{w(x)}\right) w(x)\,\mathrm{d}x + \int_\Omega V\big(\mathbf{T}(x)\big) w(x)\,\mathrm{d}x,$$

where $w \in \mathcal{P}_2^r(\Omega)$ stands for an arbitrary reference density and $\psi(s) = s\phi(s^{-1})$. The function ψ is decreasing, strictly convex and satisfies $\psi(s) \to +\infty$ as $s \downarrow 0$ due to the assumptions on P, remember the calculations in (3.18) and (3.19) from Chapter 3. These properties of ψ are crucial to proof the well-posedness of our numerical scheme. But before we come to this, we want to state a purely Lagrangian formulation of the entropy functional, which reflects the iterative character of the above proceeding: Let $\mathfrak{t}, \mathbf{T} : \Omega \to \Omega$ be two transportation maps, then define

$$\mathbf{E}(\mathfrak{t}, \mathbf{T}) := \mathcal{E}\big((\mathfrak{t} \circ \mathbf{T})_{\#} u^0\big). \tag{7.28}$$

Equipped with this notation, we are going to show that the λ-convexity of $\mathcal{E}$ yields an analogue convexity result for the map $\mathfrak{t} \mapsto \mathbf{E}(\mathfrak{t}, \mathbf{T})$. The preservation of this property is a key ingredient for many results that will follow in the forthcoming sections. To this end, we first show the following claim.

Lemma 7.4. *The function $r \mapsto r^2\phi(r^{-2})$, $r \in (0, +\infty)$, is non-increasing and convex.*

Proof. Set $f(r) = r^2\phi(r^{-2})$, then the first derivative satisfies

$$f'(r) = 2r\phi(r^{-2}) - 2r^{-1}\phi'(r^{-2}) = -2r\big(r^{-2}\phi'(r^{-2}) - \phi(r^{-2})\big) = -2r\mathrm{P}(r^{-2}) \leqslant 0,$$

due to the nonnegativity of P. For the second derivative, we further get

$$f''(r) = -2\mathrm{P}(r^{-2}) + 4r^{-2}\mathrm{P}'(r^{-2}) = 4\big(r^{-2}\mathrm{P}'(r^{-2}) - \frac{1}{2}\mathrm{P}(r^{-2})\big).$$

Hence, convexity of f is equivalent to

$$s\mathrm{P}'(s) \geqslant \frac{1}{2}\mathrm{P}(s),$$

which is further fulfilled owing to (7.5). □

Lemma 7.5. *Let $\mathbf{T} : \Omega \to \Omega$ be an arbitrary transportation map. Then $\mathfrak{t} \mapsto \mathbf{E}(\mathfrak{t}, \mathbf{T})$ is bounded from below, i.e.*

$$\mathbf{E}(\mathfrak{t}, \mathbf{T}) \geqslant M \min_{x \in \Omega} V(x) + \phi(M), \tag{7.29}$$

for any $\mathfrak{t} : \Omega \to \Omega$. Furthermore, the restriction of $\mathfrak{t} \mapsto \mathbf{E}(\mathfrak{t}, \mathbf{T})$ to the set of optimal transportation maps $\mathfrak{X}$ is λ-convex in the following sense: For any $\mathfrak{t}^0, \mathfrak{t}^1 \in \mathfrak{X}$ and $s \in [0, 1]$, one obtains

$$\mathbf{E}\big((1-s)\mathfrak{t}^0 + s\mathfrak{t}^1, \mathbf{T}\big) \leqslant (1-s)\mathbf{E}(\mathfrak{t}^0, \mathbf{T}) + s\mathbf{E}(\mathfrak{t}^1, \mathbf{T}) - \lambda\frac{s(1-s)}{2}\|\mathfrak{t}^0 - \mathfrak{t}^1\|^2_{L^2(\Omega;\mathbf{T}_{\#}u^0)}, \tag{7.30}$$

where λ is defined as in (7.10).

Proof. Let $\mathbf{T} : \Omega \to \Omega$ be fixed. Due to the convexity of $s \mapsto \phi(s)$ the functional $\mathfrak{t} \mapsto \mathbf{E}(\mathfrak{t}, \mathbf{T})$ satisfies,

$$\begin{aligned}\mathbf{E}(\mathfrak{t}, \mathbf{T}) &\geqslant M \min_{x \in \Omega} V(x) + \int_\Omega \phi\big((\mathfrak{t} \circ \mathbf{T})_{\#}u^0\big)\,\mathrm{d}x \geqslant M \min_{x \in \Omega} V(x) + \phi\left(\int_\Omega (\mathfrak{t} \circ \mathbf{T})_{\#}u^0\,\mathrm{d}x\right)\\ &= M \min_{x \in \Omega} V(x) + \phi(M),\end{aligned}$$

where we used Jensen's inequality and (7.25). This shows the boundedness of $\mathfrak{t} \mapsto \mathbf{E}(\mathfrak{t}, \mathbf{T})$ from below.

To prove (7.30), we proceed analogously to the proof of Proposition 9.3.9 in [**AGS05**]: First note that for any $s \in [0, 1]$ and $\mathfrak{t}^0, \mathfrak{t}^1 \in \mathfrak{X}$, the map $\mathfrak{t}_s := (1-s)\mathfrak{t}^0 + s\mathfrak{t}^1$ is the gradient of the convex function $(1-s)\varphi^0 + s\varphi^1$, where $\nabla\varphi^{0,1} = \mathfrak{t}^{0,1}$. Therefore, $\mathfrak{t}_s \in \mathfrak{X}$ for any $s \in [0, 1]$. Since $\mathfrak{t}^{0,1}$ are gradients of convex and almost everywhere differentiable functions such that $\det(\mathrm{D}\,\mathfrak{t}^{0,1}) > 0$

for almost every $x \in \Omega$, $\mathrm{D}\,\mathfrak{t}^{0,1}$ are diagonalizable with strictly positive eigenvalues (by [**AGS05**, Theorem 6.2.7]). Let us further define $\mathfrak{t}_0^1 := \mathfrak{t}^1 \circ (\mathfrak{t}^0)^{-1}$. Then the derivative $\mathrm{D}\,\mathfrak{t}_0^1$ is diagonalizable with strictly positive eigenvalues as well, which induces that the map

$$s \mapsto \det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big)^{\frac{1}{2}} \tag{7.31}$$

is concave on $[0,1]$. For simplification let us first investigate the map $s \mapsto \mathbf{E}(\mathfrak{t}_s, \mathbf{T})$ under the assumption that $V \equiv 0$. Then by a substitution with $(\mathfrak{t}^0 \circ \mathbf{T})^{-1}$,

$$\mathbf{E}(\mathfrak{t}_s, \mathbf{T}) = \int_\Omega \psi\left(\frac{\det \mathrm{D}(\mathfrak{t}_s \circ \mathbf{T})}{u^0}\right) u^0 \,\mathrm{d}x$$

$$= \int_\Omega \psi\left(\det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big) \cdot \left[\frac{\det \mathrm{D}(\mathfrak{t}^0 \circ \mathbf{T})}{u^0}\right] \circ (\mathfrak{t}^0 \circ \mathbf{T})^{-1}\right) \left[\frac{u^0}{\det \mathrm{D}(\mathfrak{t}^0 \circ \mathbf{T})}\right] \circ (\mathfrak{t}^0 \circ \mathbf{T})^{-1} \,\mathrm{d}x,$$

where we used

$$\begin{aligned}\det \mathrm{D}(\mathfrak{t}_s \circ \mathbf{T}) &= \det\big(\mathrm{D}\big[(1-s)\,\mathrm{id} + s\mathfrak{t}_0^1\big] \circ (\mathfrak{t}^0 \circ \mathbf{T})\big)\\ &= \big[\det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big)\big] \circ (\mathfrak{t}^0 \circ \mathbf{T}) \cdot \det \mathrm{D}(\mathfrak{t}^0 \circ \mathbf{T}).\end{aligned}$$

Using $\psi(s) = s\phi(s^{-1})$ and the definition of the push-forward, the function $s \mapsto \mathbf{E}(\mathfrak{t}_s, \mathbf{T})$ can be reformulated as

$$\mathbf{E}(\mathfrak{t}_s, \mathbf{T}) = \int_\Omega \phi\left(\frac{(\mathfrak{t}^0 \circ \mathbf{T})_\# u^0}{\det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big)}\right) \det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big) \,\mathrm{d}x.$$

Notice that for almost every $x \in \Omega$,

$$s \mapsto \phi\left(\frac{(\mathfrak{t}^0 \circ \mathbf{T})_\# u^0}{\det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big)}\right) \det\big((1-s)\mathbb{I} + s\,\mathrm{D}\,\mathfrak{t}_0^1\big)$$

is convex, since it can be interpreted as the composition of the convex and non-increasing map $r \mapsto r^2\phi(r^{-2})$ (Lemma 7.4) with the concave function in (7.31). In case of $V \equiv 0$, we conclude that

$$\mathbf{E}\big((1-s)\mathfrak{t}^0 + s\mathfrak{t}^1, \mathbf{T}\big) \leqslant (1-s)\mathbf{E}(\mathfrak{t}^0, \mathbf{T}) + s\mathbf{E}(\mathfrak{t}^1, \mathbf{T}).$$

If $V \neq 0$, a Taylor expansion yields for $s \in [0,1]$

$$V\big((1-s)x + sy\big) \leqslant (1-s)V(x) + sV(y) - \lambda\frac{(1-s)s}{2}|x-y|^2,$$

which shows (7.30) after integration of the inequality. □

7.2.1.c. The minimizing movement scheme in Lagrangian coordinates. Using the notation from Section 7.2.1.a and Section 7.2.1.b, the minimization problem (7.13) can be reformulated as follows:

Given a time discretization consisting of a time step $\tau > 0$, an initial density function $u^0 \in \mathcal{P}_2^r(\Omega)$, and an initial transport map $\mathbf{T}_\tau^0 = \mathrm{id}$, define inductively a set of transport maps $(\mathbf{T}_\tau^n)_{n=0}^\infty$, such that $\mathbf{T}_\tau^n = \mathfrak{t}_\tau^n \circ \mathbf{T}_\tau^{n-1}$ and $\mathfrak{t}_\tau^n$ solves

$$\mathfrak{t}_\tau^n = \operatorname*{argmin}_{\mathfrak{t} \in \mathfrak{X}} \mathbf{E}_\tau(\mathfrak{t}, \mathbf{T}_\tau^{n-1}), \quad \text{with} \quad \mathbf{E}_\tau(\mathfrak{t}, \mathbf{T}) := \frac{1}{2\tau}\mathbf{d}(\mathfrak{t}, \mathbf{T})^2 + \mathbf{E}(\mathfrak{t}, \mathbf{T}), \tag{7.32}$$

for $n \geqslant 1$.

It is immediately seen that $u_\tau^n = (\mathbf{T}_\tau^n)_\# u^0$ is a solution of (7.13), hence the above procedure is equivalent to the minimizing movement scheme as in Subsection 7.1.3. One can therefore apply standard arguments from the literature (we once again refer to [**AGS05**]) to conclude that the $(\tau^{-1} + \lambda)$-convex functional $\mathfrak{t} \mapsto \mathbf{E}_\tau(\mathfrak{t}, \mathbf{T})$ has a unique minimizer in $\mathfrak{X}$, hence (7.32) is uniquely solvable. Furthermore, each $\mathfrak{t}_\tau^n$ from the sequence of minimizers $(\mathfrak{t}_\tau^1, \mathfrak{t}_\tau^2, \ldots)$ is a solution to

$$\frac{\delta \mathbf{E}_\tau(\mathfrak{t}, \mathbf{T}_\tau^{n-1})}{\delta \mathfrak{t}}[\mathbf{w}] = 0, \quad \text{for any smooth and admissible velocity field } \mathbf{w}. \tag{7.33}$$

In this context we call $\mathbf{w}$ *admissible* for $\mathfrak{t} \in \mathfrak{X}$, if $\mathfrak{t} + \mathbf{w}$ is still a measurable map from Ω onto itself, hence it especially does not cross the boundary $\partial\Omega$.

7.2.2. Properties of the spatial discretization. In this subsection, we want to justify our choice of the finite-dimensional space $\mathfrak{X}_K$ in (7.16) and discuss the resulting consequences and properties for our scheme. To this end, remember that our ansatz functions are of the form

$$\varphi_{kl} \in \mathfrak{B} := \{c_{kl}\cos(k\pi x_1)\cos(l\pi x_2)\}_{k,l=0}^\infty, \quad \text{with} \quad c_{kl} := \begin{cases} \frac{2}{\pi\sqrt{k^2+l^2}}, & (k,l) \neq (0,0), \\ 1, & \text{else.} \end{cases} \tag{7.34}$$

The coefficients $c_{kl} > 0$ are defined in such a way that $\|\nabla\varphi_{kl}\|_{L^2(\Omega)} = 1$. Furthermore, note that $\mathfrak{B}$ is chosen such that any function φ in $\operatorname{span}\mathfrak{B}$ satisfies the linear boundary constraint

$$\langle \nabla\varphi(x), \vec{n}(x)\rangle = 0 \quad \text{for any } x \in \partial\Omega. \tag{7.35}$$

Let us fix $K \in \mathbb{N}$ for the rest of this section and introduce $\mathfrak{B}_K := \{\varphi_{kl} : \|(k,l)\|_\infty \leqslant K\}$. Then the $((K+1)^2 - 1)$-dimensional space $\mathfrak{X}_K$ as defined in (7.16) satisfies

$$\mathfrak{X}_K = \left\{ \mathfrak{t} = \mathrm{id} + \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\nabla\varphi_{kl} : \ \varphi_{kl} \in \mathfrak{B}_K \text{ and } z_{kl} \in \mathbb{R} \text{ such that } \det \mathrm{D}\,\mathfrak{t} > 0 \right\}. \tag{7.36}$$

The condition $\det \mathrm{D}\,\mathfrak{t} > 0$ is equivalent to strict convexity of the corresponding potential functions. We further introduce the set of coefficients $\mathfrak{z}_K$,

$$\mathfrak{z}_K := \left\{ \vec{z} = (z_{kl})_{(k,l)\in\mathcal{I}_K} : \mathrm{id} + \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\nabla\varphi_{kl} \in \mathfrak{X}_K \right\} \subseteq \mathbb{R}^{(K+1)^2-1}.$$

The set $\mathfrak{z}_K$ is closely related to $\mathfrak{X}$ through the map $\mathfrak{t}_K$ defined in (7.19), since any optimal transportation map $\mathfrak{t} \in \mathfrak{X}_K$ can be written as $\mathfrak{t}_K[\vec{z}]$ for a certain vector $\vec{z}$ in $\mathfrak{z}_K$.

The following lemma concludes that $\mathfrak{X}_K$ is indeed an affine subspace of the set of optimal transportation maps $\mathfrak{X}$ from Ω to Ω:

Lemma 7.6. *Any map* $\mathfrak{t}$ *in* $\mathfrak{X}_K$ *is a diffeomorphism mapping* Ω *onto* Ω.

Remark 7.7. *This result is valid for any choice of* $\mathfrak{B}_K$*, as long as functions in* $\mathfrak{B}_K$ *are smooth and satisfy the linear boundary constraint in* (7.35).

Proof of Lemma 7.6. We prove that any $\mathfrak{t} \in \mathfrak{X}_K$ is a bijective map with values in Ω. Fix an arbitrary $\mathfrak{t} \in \mathfrak{X}_K$ given by $\mathfrak{t} = \mathrm{id} + \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\nabla\varphi_{kl}$. Then the strict convexity of the respective potential function yields that $\mathfrak{t}$ is strictly monotone, i.e. there exists a constant $c > 0$ such that

$$\langle \mathfrak{t}(x) - \mathfrak{t}(y), x - y\rangle \geqslant c\|x - y\|_2^2 \tag{7.37}$$

for any $x, y \in \overline{\Omega}$. Further note that the boundary condition $\langle \nabla\varphi, \vec{n}\rangle = 0$ for $\varphi \in \mathfrak{B}$ immediately yields that each corner of Ω, $(0,0), (0,1), (1,0), (1,1)$, is mapped on itself.

Next, we prove that values on the boundary $\partial\Omega$ remain on the boundary. For this we fix two neighbouring vertices, for instance $v_1 = (0,0)$ and $v_2 = (0,1)$. Then each intermediate value in $\{0\} \times [0,1]$ is attained by $\lambda v_1 + (1-\lambda)v_2$ for any $\lambda \in [0,1]$ and satisfies

$$0 = \langle \mathfrak{t}(\lambda v_1 + (1-\lambda)v_2), \vec{n}(\lambda v_1 + (1-\lambda)v_2)\rangle = \left\langle \mathfrak{t}(\lambda v_1 + (1-\lambda)v_2), \begin{pmatrix}-1\\0\end{pmatrix}\right\rangle,$$

hence $\mathfrak{t}(\lambda v_1 + (1-\lambda)v_2) \in \{0\} \times [0,1]$. By the monotonicity of $\mathfrak{t}$ in (7.37) and due to $\mathfrak{t}(v_1) = v_1$ and $\mathfrak{t}(v_2) = v_2$, this shows that the restriction of $\mathfrak{t}$ to $\{0\} \times [0,1]$ is bijective with values in $\{0\} \times [0,1]$. One analogously shows the same statement for the other parts of the boundary.

As a next step, let us assume that there is a value $x \in \Omega$ with $\mathfrak{t}(x) \notin \Omega$. By continuity it easily follows that

$$\mathfrak{t}_\varepsilon := \mathrm{id} + \varepsilon \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\nabla\varphi_{kl}$$

is an element of $\mathfrak{X}_K$ for any $\varepsilon \in [0,1]$ and that there exists a value $\bar{\varepsilon} \in [0,1]$ such that $\mathfrak{t}_{\bar{\varepsilon}}(x) \in \partial\Omega$. Due to the behaviour on the boundary, there further exists a value $y_{\bar{\varepsilon}} \in \partial\Omega$ with $\mathfrak{t}_{\bar{\varepsilon}}(y_{\bar{\varepsilon}}) = \mathfrak{t}_{\bar{\varepsilon}}(x)$, but this contradicts the monotonicity since

$$0 = \langle \mathfrak{t}_{\bar{\varepsilon}}(x) - \mathfrak{t}_{\bar{\varepsilon}}(y_{\bar{\varepsilon}}), x - y_{\bar{\varepsilon}}\rangle \geqslant c\|x - y_{\bar{\varepsilon}}\|_2^2 > 0.$$

This shows that $\mathfrak{t} : \Omega \to \Omega$. Finally note that the injectivity is a consequence of the monotonicity and surjectivity follows from the continuity and the fact that the boundary is mapped onto itself.

□

7.2.2.a. The restriction of $\mathbf{d}$ *and* $\mathbf{E}$ *to* $\mathfrak{X}_K$. The one-to-one identification between optimal transportation maps $\mathfrak{t} \in \mathfrak{X}_K$ and vectors $\vec{z} \in \mathfrak{z}_K$ via the map $\mathfrak{t}_K$ leads to a new representation of the L^2-Wasserstein distance,

$$\mathbf{d}(\mathfrak{t}_K[\vec{z}], \mathbf{T})^2 = \langle \vec{z}, \mathrm{W}_2[\mathbf{T}]\vec{z}\rangle, \quad \text{with} \quad \big[\mathrm{W}_2[\mathbf{T}]\big]_{(kl),(hj)} = \int_\Omega [\langle \nabla\varphi_{kl}, \nabla\varphi_{hj}\rangle] \circ \mathbf{T}\, u^0(x)\,\mathrm{d}x. \tag{7.38}$$

The matrix $\mathrm{W}_2[\mathbf{T}]$ depends on the transport $\mathbf{T}$ and the initial density u^0, unfortunately, but it allows an explicit evaluation of the L^2-Wasserstein disctance between two densities $\mathbf{T}_\# u^0$ and $(\mathfrak{t} \circ \mathbf{T})_\# u^0$ just by calculating a "matrix-vector-matrix"-product. Note in addition, that the definition of $\vec{z} \mapsto \mathfrak{t}_K[\vec{z}]$ implies

$$\begin{aligned}\left\langle \vec{z}^0 - \vec{z}^1, \mathrm{W}_2[\mathbf{T}](\vec{z}^0 - \vec{z}^1) \right\rangle &= \int_\Omega \|\mathfrak{t}_K[\vec{z}^0 - \vec{z}^1] - \mathrm{id}\,\|_2^2 \,\mathbf{T}_\# u^0 \,\mathrm{d}x \\ &= \int_\Omega \|\mathfrak{t}_K[\vec{z}^0] - \mathfrak{t}_K[\vec{z}^1]\|_2^2 \,\mathbf{T}_\# u^0 \,\mathrm{d}x\end{aligned} \tag{7.39}$$

for any $\vec{z}^0, \vec{z}^1 \in \mathfrak{z}_K$.

As the following lemma shows, our discretization even preserves one of the most important properties from the continuous setting, namely λ-convexity of the entropy:

Lemma 7.8. *Let $\mathbf{T} : \Omega \to \Omega$ be an arbitrary transportation map. Then $\vec{z} \mapsto \mathbf{E}(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ is bounded from below by the same bound as $\mathcal{E}$ in* (7.29)*. Furthermore, $\vec{z} \mapsto \mathbf{E}(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ is λ-convex in the following sense: For arbitrary vectors $\vec{z}^0, \vec{z}^1 \in \mathfrak{z}_K$ and $s \in [0,1]$, one obtains*

$$\begin{aligned}&\mathbf{E}\big((1-s)\mathfrak{t}_K[\vec{z}^0] + s\mathfrak{t}_K[\vec{z}^1], \mathbf{T}\big) \\ \leqslant &(1-s)\mathbf{E}(\mathfrak{t}_K[\vec{z}^0], \mathbf{T}) + s\mathbf{E}(\mathfrak{t}_K[\vec{z}^1], \mathbf{T}) - \lambda \frac{s(1-s)}{2} \left\langle \vec{z}^0 - \vec{z}^1, \mathrm{W}_2[\mathbf{T}](\vec{z}^0 - \vec{z}^1) \right\rangle,\end{aligned} \tag{7.40}$$

where λ is defined by (7.10)*.*

Proof. Fix $\mathbf{T} : \Omega \to \Omega$. The boundedness of $\vec{z} \mapsto \mathbf{E}(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ immediately follows from Lemma 7.5 and the definition of $\mathbf{E}$ in (7.28). To prove (7.40), note that the map $\vec{z} \mapsto \mathfrak{t}_K[\vec{z}]$ obviously satisfies $\mathfrak{t}_K[(1-s)\vec{z}^0 + s\vec{z}^1] = (1-s)\mathfrak{t}_K[\vec{z}^0] + s\mathfrak{t}_K[\vec{z}^1]$ for $s \in [0,1]$. Then (7.40) is a consequence of (7.30), see again Lemma 7.5 and (7.39). □

Remark 7.9. *The above ansatz for the spatial discretization is easily adaptable to the higher-dimensional situation $(0,1)^d$, $d \geqslant 2$: It suffices to replace the set of ansatz functions $\mathfrak{B}_K$ by its multi-dimensional counterpart*

$$\mathfrak{B}_K = \left\{ \varphi_\kappa := \Pi_{j=1}^d \tilde{c}_\kappa \cos(\kappa_j \pi x_j) \right\}_{\kappa \in \{0,\dots,K\}^d}$$

with adapted coefficients $\tilde{c}_\kappa$, where $\kappa = (\kappa_1, \dots, \kappa_d)$ are multi-indices with components that satisfy $\kappa_j \in \{0, \dots, K\}$ for $j = 1, \dots, d$. It is easily verified that functions in $\mathfrak{B}_K$ still validate the no-flux boundary condition. Furthermore, the above results (especially Lemma 7.6 and Lemma 7.8) still hold true for the respective multi-dimensional extensions of $\mathfrak{X}_K$ and $\mathfrak{z}_K$, and all results that follow in the subsequent sections can be adapted as well.

7.2.3. The numerical scheme in Lagrangian coordinates. We have already seen in Subsection 7.2.1.c that the minimizing movement scheme (7.13) has an equivalent formulation in terms of Lagrangian coordinates, see (7.32). It turns out that one can easily rewrite our numerical scheme as introduced in Section 7.1.3 in the same way: Instead of minimizing (7.18) over the time-dependent and discrete submanifolds $\mathcal{P}_{2,K}^{r,n}(\Omega)$, we perform the minimization in (7.32) with $\mathfrak{X}$ replaced by $\mathfrak{X}_K$. This yields the following Lagrangian representation of our numerical scheme:

Given a discretization $\Delta = (\tau, K)$ consisting of a time step $\tau > 0$, a spatial discretization K, an initial density function $u^0 \in \mathcal{P}_2^r(\Omega)$, an initial vector $\vec{z}_\Delta^0 = 0 \in \mathfrak{z}_K$ and the initial transport $\mathbf{T}_\Delta^0 = \mathrm{id}$. Then define inductively a sequence of vectors $\vec{z}_\Delta = (\vec{z}_\Delta^0, \vec{z}_\Delta^1, \ldots)$, such that $\vec{z}_\Delta^n$ solves

$$\vec{z}_\Delta^n = \operatorname*{argmin}_{\vec{z} \in \mathfrak{z}_K} \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T}_\Delta^{n-1}) \tag{7.41}$$

for $n \geqslant 1$, and set $\mathbf{T}_\Delta^n = \mathfrak{t}_K[\vec{z}_\Delta^n] \circ \mathbf{T}_\Delta^{n-1}$. Further denote $\mathfrak{t}_\Delta^n = \mathfrak{t}_K[\vec{z}_\Delta^n]$, $u_\Delta^n = (\mathbf{T}_\Delta^n)_\# u^0$, and we write $\vec{z}_\Delta = (\vec{z}_\Delta^0, \vec{z}_\Delta^1, \ldots)$, $\mathfrak{t}_\Delta = (\mathfrak{t}_\Delta^0, \mathfrak{t}_\Delta^1, \ldots)$, $u_\Delta = (u_\Delta^0, u_\Delta^1, \ldots)$ and $\mathbf{T}_\Delta = (\mathbf{T}_\Delta^0, \mathbf{T}_\Delta^1, \ldots)$.

It is easily seen that this formulation is indeed equivalent to the original one in Section 7.1.3. The main difference is, that the Lagrangian representation makes the dependence of $\mathcal{P}_{2,K}^{r,n}(\Omega)$ on the previous solution u_Δ^{n-1} a dependence of $\mathbf{E}_\tau$ on $\mathbf{T}_\Delta^{n-1}$. An immediate advantage of the Lagrangian characterization in (7.41) is that it is much easier to handle for numerical applications, since the set over which one performs the minimization is fixed and does not change with every time iteration.

To show that the numerical scheme is well-posed, one has to guarantee that the minimization problem in (7.41) is solvable. Compared to the analogue problem in Proposition 3.9 in one spatial dimension, the situation becomes more complicated for higher dimensions. The reason for this is that $\mathfrak{t} \mapsto \mathbf{E}(\mathfrak{t}, \mathbf{T})$ can even be bounded from above for transport maps $\mathfrak{t}$ with degenerating determinants if the set where $\det(\mathrm{D}\,\mathfrak{t}(x)) = 0$ is small enough, although the integrand ψ of $\mathbf{E}$ has the property that $\psi(s) \to +\infty$ as $s \downarrow 0$. Nevertheless, we can at least guarantee the existence of a minimizer of $\vec{z} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$, if the integrand of entropies $\mathbf{E}$ increases faster at zeros than s^{-1}:

Lemma 7.10. *Suppose that $w = \mathbf{T}_\# u^0 > 0$ for an arbitrary transportation map $\mathbf{T} : \Omega \to \Omega$ and $\mathcal{E}(w) < C$ for a constant $C > 0$. Further assume $\tau^{-1} + \lambda > 0$. If the integrand of $\mathbf{E}$ satisfies $s\psi(s) \to +\infty$ for $s \downarrow 0$, then the functional $\vec{z} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ has a unique minimizer in $\mathfrak{z}_K$.*

Proof. Using the representation of the L^2-Wasserstein disctance (7.38) in terms of the matrix $\mathrm{W}_2[\mathbf{T}]$, the functional $\vec{z} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ attains the form

$$\begin{aligned}\mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T}) &= \mathbf{E}(\mathfrak{t}[\vec{z}], \mathbf{T}) + \frac{1}{2\tau}\langle \vec{z}, \mathrm{W}_2[\mathbf{T}]\vec{z}\rangle \\ &= \mathbf{E}(\mathfrak{t}[\vec{z}], \mathbf{T}) - \frac{\lambda}{2}\langle \vec{z}, \mathrm{W}_2[\mathbf{T}]\vec{z}\rangle + \frac{1}{2}\big(\tau^{-1} + \lambda\big)\langle \vec{z}, \mathrm{W}_2[\mathbf{T}]\vec{z}\rangle .\end{aligned}$$

Since $\vec{z} \mapsto \mathbf{E}(\mathfrak{t}[\vec{z}], \mathbf{T})$ is λ-convex, see Lemma 7.8, and $\tau^{-1} + \lambda$ is supposed to be strictly positive, one concludes that $\mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ is strictly convex. The boundedness of $\vec{z} \mapsto \mathbf{E}(\mathfrak{t}[\vec{z}], \mathbf{T})$ from below further implies

$$\mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T}) \geqslant \mathbf{E}(\mathfrak{t}[\vec{z}], \mathbf{T}) \geqslant M \min_{x \in \Omega} V(x) + \phi(M).$$

Thus, $\vec{z} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ attains at most one critical point in $\mathfrak{z}_K$. Let further $(\vec{z}^j)_{j=0}^\infty$ be a minimizing sequence $\vec{z}^j$ for $\vec{z} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$ with $\vec{z}^j \in \mathfrak{z}_K$, which converges towards $\inf_{\vec{z} \in \mathfrak{z}_K} \mathbf{E}_\tau(\mathfrak{t}_K[\vec{z}], \mathbf{T})$.

Then there exists an index $J \in \mathbb{N}$, such that all vectors $\vec{z}^j$ with $j > J$ have to satisfy

$$\mathbf{E}_\tau(\mathrm{t}_K[\vec{z}^j], \mathbf{T}) \in \big[M \min_{x\in\Omega} V(x) + \phi(M), C\big].$$

The continuity of the map $\vec{z} \mapsto \mathbf{E}_\tau(\mathrm{t}_K[\vec{z}], \mathbf{T})$ then yields the boundedness of the sequence $\vec{z}^j$ in $\mathbb{R}^{(K+1)^2-1}$, this is why one can find a subsequence that converges to a vector $\vec{z}^* \in \mathbb{R}^{(K+1)^2-1}$ with $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*]) \geqslant 0$. It remains to show that $\vec{z}^*$ is in $\mathfrak{z}_K$, i.e. that $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*]) > 0$.

Remember the definition of $\vec{z} \mapsto \mathrm{t}_K[\vec{z}]$ in (7.19). For any $\vec{z} \in \mathfrak{z}_K$, the derivative of $\mathrm{t}_K[\vec{z}]$ is hence given by

$$\mathrm{D}\,\mathrm{t}_K[\vec{z}] = \mathbb{I} + \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\,\mathrm{D}^2\,\varphi_{kl} \quad \text{with}$$

$$\mathrm{D}^2\,\varphi_{kl} = \begin{pmatrix} \partial_1^2\varphi_{kl} & \partial_{1,2}\varphi_{kl} \\ \partial_{2,1}\varphi_{kl} & \partial_2^2\varphi_{kl} \end{pmatrix} = \frac{2\pi}{\sqrt{k^2+l^2}} \begin{pmatrix} -k^2\cos(k\pi x_1)\cos(l\pi x_2) & kl\sin(k\pi x_1)\sin(l\pi x_2) \\ kl\sin(k\pi x_1)\sin(l\pi x_2) & -l^2\cos(k\pi x_1)\cos(l\pi x_2) \end{pmatrix},$$

and its determinant furthermore satisfies for any $x \in \Omega$

$$\begin{aligned} &\det\big(\mathrm{D}\,\mathrm{t}_K[\vec{z}](x)\big) \\ &= \Bigg(1 - \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\partial_1^2\varphi_{kl}\Bigg)\Bigg(1 - \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\partial_2^2\varphi_{kl}\Bigg) - \Bigg(\sum_{(k,l),(h,j)\in\mathcal{I}_K} z_{kl}z_{hj}\partial_{1,2}\varphi_{kl}\partial_{2,1}\varphi_{hj}\Bigg) \\ &= 1 - \sum_{(k,l)\in\mathcal{I}_K} z_{kl}\,\mathrm{tr}\big(\mathrm{D}^2\,\varphi_{kl}\big) + \frac{1}{2}\sum_{(k,l),(h,j)\in\mathcal{I}_K} z_{kl}z_{hj}\,\mathrm{tr}\big(\mathrm{cof}(\mathrm{D}^2\,\varphi_{kl})\,\mathrm{D}^2\,\varphi_{hj}\big). \end{aligned} \tag{7.42}$$

Here we use the short-hand notations ∂_1 and ∂_2 for the partial derivatives with respect to the first and second spatial component, respectively. Equation (7.42) especially shows that $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}])$ is a trigonometric polynomial. Take again the minimizer $\vec{z}^*$, which satisfies $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*]) \geqslant 0$. So assume $\bar{x} \in \Omega$ to be a point of degenerating determinant, i.e. $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*](\bar{x})) = 0$. Then one can invoke for instance the power series definition of cosines and sines to see that the term in (7.42) has maximal quadratic growth close to the root $\bar{x}$ — in fact one just has to exclude that (7.42) grows linearly at $\bar{x}$, but this can be done since $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*])$ would even attain negative values in this case which would contradict to $\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*]) \geqslant 0$. This is why one can assume the existence of a constant $c > 0$ and a sufficient small radius $\delta > 0$, such that

$$\det\big(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*](x)\big) \leqslant c\|x-\bar{x}\|_2^2 \quad \text{for any } x \in \mathbb{B}_\delta(\bar{x}) = \{x \in \mathbb{R}^2 : \|x-\bar{x}\|_2 < \delta\} \subseteq \Omega.$$

The above inequality can be used to show that the assumed existence of the root $\bar{x} \in \Omega$ contradicts the boundedness of $\mathbf{E}_\tau(\mathrm{t}_K[\vec{z}^*], \mathbf{T})$: Set $w = \mathbf{T}_\# u^0$ and remember that ψ is a convex and decreasing function. One can hence apply Jensen's inequality, which yields with $C_r := \int_{\mathbb{B}_r} w(x)\,\mathrm{d}x$

$$\begin{aligned} C &> M \min_{x\in\Omega} V(x) + \int_{\mathbb{B}_r} \psi\left(\frac{\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*])}{w}\right) w\,\mathrm{d}x \\ &= M \min_{x\in\Omega} V(x) + C_r \int_{\mathbb{B}_r} \psi\left(\frac{\det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*])}{w}\right) \frac{w\,\mathrm{d}x}{C_r} \\ &\geqslant M \min_{x\in\Omega} V(x) + C_r \psi\left(\frac{1}{C_r}\int_{\mathbb{B}_r} \det(\mathrm{D}\,\mathrm{t}_K[\vec{z}^*])\,\mathrm{d}x\right) \end{aligned}$$

for any $r \in (0,\delta)$. Since w is assumed to be strictly positive, one can find a constant $\underline{w} > 0$ with $w \geqslant \underline{w}$, and further $C_r \geqslant \underline{w} r^2 \pi$. Due to the monotonicity of ψ, the above calculation yields for $r \in (0,\delta)$ small enough

$$\begin{aligned} C &> M \min_{x\in\Omega} V(x) + C_r \psi\left(\frac{1}{C_r}\int_{\mathbb{B}_r} \det(\mathrm{D}\,\mathfrak{t}_K[\vec{\mathrm{z}}^*])\,\mathrm{d}x\right) \\ &\geqslant M \min_{x\in\Omega} V(x) + \underline{w} r^2 \pi \psi\left(\frac{2\pi c}{C_r}\int_0^r \sigma^3\,\mathrm{d}\sigma\right) \\ &\geqslant M \min_{x\in\Omega} V(x) + \underline{w} r^2 \pi \psi\left(\frac{\pi c r^4}{2C_r}\right) \geqslant M \min_{x\in\Omega} V(x) + \underline{w} r^2 \pi \psi\left(\frac{c r^2}{2\underline{w}}\right), \end{aligned}$$

where the right-hand side tends to $+\infty$ as $r \to 0$. This proves $\vec{\mathrm{z}}^* \in \mathfrak{z}_K$, which is the unique minimizer of $\vec{\mathrm{z}} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T})$ due to the convexity. □

The above result implies the well-posedness of our numerical scheme.

Proof of Proposition 7.1. The definition of $\psi(s) = s\phi(1/s)$ obviously implies the relation

$$s\psi(s) = s^2\phi(1/s),$$

which shows that the condition $s\psi(s) \to 0$ as $s \downarrow 0$ and (7.22) are equivalent. We have to prove that the scheme in Section 7.1.3 has a unique solution at any time iteration $n \in \mathbb{N}$. Starting with $n = 1$, one can immediately apply Lemma 7.10 due to the strict positivity of u^0 and $\mathcal{E}(u^0) < +\infty$, see (7.21). Hence there exists a unique minimizer $\vec{\mathrm{z}}^1_\Delta \in \mathfrak{z}_K$ of $\vec{\mathrm{z}} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}^0_\Delta)$ with $\mathbf{T}^0_\Delta = \mathrm{id}$, and $u^1_\Delta := (\mathfrak{t}^1_\Delta)_\# u^0$, where $\mathfrak{t}^1_\Delta := \mathfrak{t}_K[\vec{\mathrm{z}}^1_\Delta]$ is the unique minimizer of (7.18). By construction, u^1_Δ satisfies $\mathcal{E}(u^1_\Delta) \leqslant \mathcal{E}(u^0_\Delta)$ with $u^0_\Delta = u^0$, and u^1_Δ is strictly positive since u^1_Δ is the push-forward of the strictly positive density u^0 through the transportation map $\mathfrak{t}^1_\Delta$ with striclty positive determinant $\det(\mathrm{D}\,\mathfrak{t}^1_\Delta)$. Therefore, u^1_Δ satisfies the requirements of Lemma 7.10 and one can proceed as before. This proves by induction the existence of a sequence $u_\Delta = (u^0_\Delta, u^1_\Delta, \ldots)$ of strictly positive densities that solve (7.18) and satisfy $\mathcal{E}(u^n_\Delta) \leqslant \mathcal{E}(u^{n-1}_\Delta)$ for any $n \geqslant 1$. □

Due to the above results, we know that the minimization problem in (7.41) has a unique minimizer in $\mathfrak{z}_K$ at each time step $n \in \mathbb{N}$. From this observation, it is not far to conclude that these minimizers satisfy the discrete Euler-Lagrange equation (7.23).

Proof of Proposition 7.2. Fix $n \in \mathbb{N}$. Remember that $\mathfrak{z}_K$ consists of vectors $\vec{\mathrm{z}}$ in $\mathbb{R}^{(K+1)^2-1}$ that satify $\det(\mathrm{D}\,\mathfrak{t}_K[\vec{\mathrm{z}}]) > 0$. This yields by continuity of $\vec{\mathrm{z}} \mapsto \det(\mathrm{D}\,\mathfrak{t}_K[\vec{\mathrm{z}}])$ that $\mathfrak{z}_K$ is an open subset of $\mathbb{R}^{(K+1)^2-1}$. Thus $\vec{\mathrm{z}}^n_\Delta$ is the root of the derivative of $\vec{\mathrm{z}} \mapsto \mathbf{E}_\tau(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}^{n-1}_\Delta)$, i.e. $\vec{\mathrm{z}}^n_\Delta$ satisfies

$$\frac{1}{\tau}\mathrm{W}_{n-1}\vec{\mathrm{z}}^n_\Delta + \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}^n_\Delta], \mathbf{T}^{n-1}_\Delta) = 0. \tag{7.43}$$

Due to the definition of W_{n-1} in (7.20) and the representation of the L^2-Wasserstein distance (7.38) in terms of Lagrangian maps, we conclude that $\mathrm{W}_{n-1} = \mathrm{W}_2[\mathbf{T}^{n-1}_\Delta]$. Finally note that

$$\mathcal{E}\left(\left(\mathfrak{t}_K[\vec{\mathrm{z}}]\right)_\# u^n_\Delta\right) = \mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}^n_\Delta).$$

Therefore, the equations in (7.23) and (7.43) are identical, which proves the claim. □

Remark 7.11. *The identity* $\mathrm{W}_{n-1} = \mathrm{W}_2[\mathbf{T}_\Delta^{n-1}]$ *provides an alternative representation of the system of Euler-Lagrange equations in* (7.23) *or* (7.43)*, which is the following:*

$$\frac{1}{\tau}\mathrm{W}_{n-1}\vec{\mathrm{z}}_\Delta^n + \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n], \mathbf{T}_\Delta^{n-1}) = \frac{\delta \mathbf{E}_\tau(\mathfrak{t}_\Delta^n, \mathbf{T}_\Delta^{n-1})}{\delta \mathfrak{t}}[\nabla\varphi_{kl}] = 0, \tag{7.44}$$

for all $(k,l) \in \mathcal{I}_K$*. This reflects in particular the variational character of our scheme, since discrete solutions* $\vec{\mathrm{z}}_\Delta^n$ *to* (7.41) *can alternatively be found by variation of* $\mathfrak{t} \mapsto \mathbf{E}_\tau(\mathfrak{t}, \mathbf{T}_\Delta^{n-1})$ *along gradients* $\nabla\varphi_{kl}$ *of functions in* $\mathfrak{B}_K$*.*

7.3. Proof of the scheme's stability

It remains to prove the scheme's stability as formulated in Proposition 7.3. Therefore, take a solution u_Δ to the scheme with associated sequence of vectors $\vec{\mathrm{z}}_\Delta$ which solves the system of Euler-Lagrange equations due to Proposition 7.2. Our aim is to prove that

$$(1 + 2\lambda\tau)\,\|\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n] - \mathfrak{t}_K[\vec{\mathrm{y}}]\|^2_{L^2(\Omega;u_\Delta^{n-1})} \leqslant \tau^2\left\langle \vec{\gamma}^n[\vec{\mathrm{y}}], \mathrm{W}_{n-1}^{-1}\vec{\gamma}^n[\vec{\mathrm{y}}]\right\rangle, \tag{7.45}$$

for any $\vec{\mathrm{y}} \in \mathbb{R}^{(K+1)^2-1}$ and any $n \in \mathbb{N}$, where the residuum $\vec{\gamma}^n[\vec{\mathrm{y}}]$ can be formulated as

$$\vec{\gamma}^n[\vec{\mathrm{y}}] = \frac{1}{\tau}\mathrm{W}_{n-1}\vec{\mathrm{y}} + \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{y}}], \mathbf{T}_\Delta^{n-1}).$$

The proof of (7.45) is essentially based on the preserved λ-convexity of $\vec{\mathrm{z}} \mapsto \mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T})$.

Proof of Proposition 7.3. Fix $n \geqslant 1$ and an arbitrary vector $\vec{\mathrm{y}} \in \mathbb{R}^{(K+1)^2-1}$. To simplify the notation, we write $\vec{\gamma} = \vec{\gamma}^n[\vec{\mathrm{y}}]$ in the following. Let us first conclude from the λ-convexity of the functional $\vec{\mathrm{z}} \mapsto \mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}_\Delta^{n-1})$ in (7.40) that

$$\left\langle \vec{\mathrm{z}} - \vec{\mathrm{y}}, \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}_\Delta^{n-1}) - \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{y}}], \mathbf{T}_\Delta^{n-1})\right\rangle \geqslant \lambda\left\langle \vec{\mathrm{z}} - \vec{\mathrm{y}}, \mathrm{W}_{n-1}(\vec{\mathrm{z}} - \vec{\mathrm{y}})\right\rangle, \tag{7.46}$$

for any $\vec{\mathrm{z}} \in \mathfrak{z}_K$, which is gained by Taylor expansion. Furthermore, $\vec{\mathrm{z}}_\Delta^n$ and $\vec{\mathrm{y}}$ satisfy by definition

$$\frac{1}{\tau}\mathrm{W}_{n-1}\vec{\mathrm{z}}_\Delta^n + \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n], \mathbf{T}_\Delta^{n-1}) = 0 \quad \text{and} \quad \frac{1}{\tau}\mathrm{W}_{n-1}\vec{\mathrm{y}} + \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{y}}], \mathbf{T}_\Delta^{n-1}) = \vec{\gamma}. \tag{7.47}$$

since W_{n-1} is a symmetric and positive definite matrix, one can define uniquely a symmetric and positive definite matrix $\mathrm{W}_{n-1}^{1/2}$ — its square root — such that $\mathrm{W}_{n-1}^{1/2}\mathrm{W}_{n-1}^{1/2} = \mathrm{W}_{n-1}$. Multiply both equations in (7.47) with $\tau\mathrm{W}_{n-1}^{-1/2}$ and take the difference, then

$$\mathrm{W}_{n-1}^{1/2}(\vec{\mathrm{y}} - \vec{\mathrm{z}}_\Delta^n) + \tau\mathrm{W}_{n-1}^{-1/2}\big(\partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{y}}], \mathbf{T}_\Delta^{n-1}) - \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n], \mathbf{T}_\Delta^{n-1})\big) = \tau\mathrm{W}_{n-1}^{-1/2}\vec{\gamma}.$$

Taking the norm on both sides yields the estimate

$$\begin{aligned}\langle \vec{\mathrm{y}} - \vec{\mathrm{z}}_\Delta^n, \mathrm{W}_{n-1}(\vec{\mathrm{y}} - \vec{\mathrm{z}}_\Delta^n)\rangle + 2\tau\left\langle \vec{\mathrm{y}} - \vec{\mathrm{z}}_\Delta^n, \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{y}}], \mathbf{T}_\Delta^{n-1}) - \partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n], \mathbf{T}_\Delta^{n-1})\right\rangle \\ \leqslant \tau^2\left\langle \vec{\gamma}, \mathrm{W}_{n-1}^{-1}\vec{\gamma}\right\rangle.\end{aligned} \tag{7.48}$$

Due to the representation formula of W_{n-1} in (7.38) and (7.39) one attains

$$\langle \vec{\mathrm{y}} - \vec{\mathrm{z}}_\Delta^n, \mathrm{W}_{n-1}(\vec{\mathrm{y}} - \vec{\mathrm{z}}_\Delta^n)\rangle = \int_\Omega \|\mathfrak{t}_K[\vec{\mathrm{y}}] - \mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n]\|_2^2\, u_\Delta^{n-1}\,\mathrm{d}x.$$

Together with the convexity estimate in (7.46), we further conclude with (7.48) that

$$\begin{aligned}&(1+2\lambda\tau)\,\|\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n]-\mathfrak{t}_K[\vec{\mathrm{y}}]\|^2_{L^2(\Omega;u_\Delta^{n-1})}\\ \leqslant&\|\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n]-\mathfrak{t}_K[\vec{\mathrm{y}}]\|^2_{L^2(\Omega;u_\Delta^{n-1})}+2\tau\left\langle\vec{\mathrm{y}}-\vec{\mathrm{z}}_\Delta^n,\partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{y}}],\mathbf{T}_\Delta^{n-1})-\partial_{\vec{\mathrm{z}}}\mathbf{E}(\mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n],\mathbf{T}_\Delta^{n-1})\right\rangle\\ \leqslant&\tau^2\left\langle\vec{\gamma},\mathrm{W}_{n-1}^{-1}\vec{\gamma}\right\rangle,\end{aligned}$$

which proves the assumption. □

7.4. Implementation

The iterative character of our scheme — in form of the minimization procedure (7.41) or the system of Euler-Lagrange equations (7.43) — requires an explicit computation of the terms $\mathfrak{t}\mapsto\mathbf{d}(\mathfrak{t},\mathbf{T}_\Delta^{n-1})$ and $\mathfrak{t}\mapsto\mathbf{E}(\mathfrak{t},\mathbf{T}_\Delta^{n-1})$ at any time iteration $n\geqslant 1$. Unfortunately, those integrals cannot be evaluated explicitly for

$$\mathbf{T}_\Delta^{n-1}=\mathfrak{t}_\Delta^{n-1}\circ\ldots\circ\mathfrak{t}_\Delta^1,$$

which consists of successively iterated discrete optimal transportation maps. It is hence necessary to apply some kind of integral quadrature:

$$\int_\Omega f(x,\rho(x),\mathbf{T}(x),(\mathfrak{t}\circ\mathbf{T})(x))\,\mathrm{d}x\simeq\mathcal{Q}_{\boldsymbol{\zeta}}\big[f(x,\rho,\mathbf{T},\mathfrak{t}\circ\mathbf{T})\big],$$

where

$$\mathcal{Q}_{\boldsymbol{\zeta}}\big[f(x,\rho,\mathbf{T},\mathfrak{t}\circ\mathbf{T})\big]:=\sum_{k,l=1}^{K_{\boldsymbol{\zeta}}}\omega_{kl}f(x_{kl},\rho(x_{kl}),\mathbf{T}(x_{kl}),(\mathfrak{t}\circ\mathbf{T})(x_{kl}))$$

with certain sample points $\boldsymbol{\zeta}=(x_{kl})_{k,l=1}^{K_{\boldsymbol{\zeta}}}$ and weights $(\omega_{kl})_{k,l=1}^{K_{\boldsymbol{\zeta}}}$. In our numerical experiments in Section 7.5, we are going to use an integral quadratures of the following kind:
Take $K_b\in\mathbb{N}$ and decompose $\overline{\Omega}=[0,1]^2$ using $(K_b)^2$-many squares of the same size (quadrilateral decomposition of Ω). Then an approximation of the integral on each square is gained by applying a Gauß quadrature using $(K_s)^2$-many weights per square, hence one has $K_{\boldsymbol{\zeta}}^2=K_b^2\cdot K_s^2$ sample points in total.

Fixing a suitable choice of integral quadrature $\mathcal{Q}_{\boldsymbol{\zeta}}$, one can adopt the formulation of our numerical scheme in (7.41) just by replacing the functions $\mathbf{d}(\mathfrak{t},\mathbf{T})$ and $\mathbf{E}(\mathfrak{t},\mathbf{T})$ from (7.28) and (7.27) with

$$\begin{aligned}\mathbf{d}_{\boldsymbol{\zeta}}(\mathfrak{t},\mathbf{T})&=\big(\mathcal{Q}_{\boldsymbol{\zeta}}\big[|\mathbf{T}-\mathfrak{t}\circ\mathbf{T}|^2u^0\big]\big)^{\frac{1}{2}},\qquad\text{and}\\ \mathbf{E}_{\boldsymbol{\zeta}}(\mathfrak{t},\mathbf{T})&=\mathcal{Q}_{\boldsymbol{\zeta}}\left[\psi\left(\frac{[\det\mathrm{D}(\mathfrak{t})]\circ\mathbf{T}\cdot\det\mathrm{D}\,\mathbf{T}}{u^0}\right)u^0\right].\end{aligned}$$

The resulting procedure then reads as follows:

Given a discretization $\Delta = (\tau, K, \boldsymbol{\zeta})$ consisting of a time step $\tau > 0$, a spatial discretization K and a $\boldsymbol{\zeta}$-dependend integral quadrature, an initial density function $u^0 \in \mathcal{P}_2^r(\Omega)$, and an initial transport map $\mathbf{T}_\Delta^0 = \mathrm{id} \in \mathfrak{X}_K$, define inductively a set of transportation maps $\mathbf{T}_\Delta = (\mathbf{T}_\Delta^0, \mathbf{T}_\Delta^1, \ldots)$, such that $\mathbf{T}_\Delta^n = \mathfrak{t}_\Delta^n \circ \mathbf{T}_\Delta^{n-1}$ and $\mathfrak{t}_\Delta^n$ solves

$$\mathfrak{t}_\Delta^n = \operatorname*{argmin}_{\mathfrak{t}\in\mathfrak{X}_K} \frac{1}{2\tau}\mathbf{d}_{\boldsymbol{\zeta}}^2(\mathfrak{t}, \mathbf{T}_\Delta^{n-1}) + \mathbf{E}_{\boldsymbol{\zeta}}(\mathfrak{t}, \mathbf{T}_\Delta^{n-1}) \tag{7.49}$$

for $n \geqslant 1$. Furthermore, set $u_\Delta^n = (\mathbf{T}_\Delta^n)_\# u^0$.

Of course, the above scheme is equivalently expressible in terms of vectors $\vec{z} \in \mathfrak{z}_K$, analogously to (7.41).

As before, this fully-discrete numerical scheme preserves important structural properties from the continuous minimizing movement scheme in (7.13):

(1) Conservation of mass and positivity: This is a consequence of the choice of $\mathfrak{X}_K$, which is independent of the integral quadrature $\mathcal{Q}_{\boldsymbol{\zeta}}$.
(2) Discrete entropy dissipation: $\mathbf{E}_{\boldsymbol{\zeta}}(\mathfrak{t}_\Delta^n, \mathbf{T}_\Delta^{n-1}) \leqslant \mathbf{E}_{\boldsymbol{\zeta}}(\mathrm{id}, \mathbf{T}_\Delta^{n-1})$ for $n \geqslant 1$.
(3) Convexity: Following the proof of Lemma 7.8, it is clear that the integrand of $\mathbf{E}(\mathfrak{t}, \mathbf{T})$ itself is convex for almost every $x \in \Omega$. This implies the convexity of $\mathfrak{t} \mapsto \mathbf{E}_{\boldsymbol{\zeta}}(\mathfrak{t}, \mathbf{T})$ for arbitrary $\mathbf{T} : \Omega \to \Omega$. Especially the discretized perturbed entropy functional

$$\vec{z} \mapsto \frac{1}{2\tau}\mathbf{d}_{\boldsymbol{\zeta}}(\mathfrak{t}_K[\vec{z}], \mathbf{T}_\Delta^n) + \mathbf{E}_{\boldsymbol{\zeta}}(\mathfrak{t}_K[\vec{z}], \mathbf{T}_\Delta^{n-1}) \tag{7.50}$$

restricted to the convex set $\mathfrak{z}_K$ is λ-convex.
(4) Wasserstein-consistency: Dependent on the quadrature rule, there exists a rate $\alpha > 0$, such that for arbitrary $\mathfrak{t}, \mathbf{T}$

$$\mathbf{d}_{\boldsymbol{\zeta}}(\mathfrak{t}, \mathbf{T}) = \mathcal{W}_2((\mathfrak{t} \circ \mathbf{T})_\# u^0, \mathbf{T}_\# u^0) + \mathcal{O}(\delta_{\boldsymbol{\zeta}}^\alpha)$$

with maximal mesh width $\delta_{\boldsymbol{\zeta}} = \max\{|x_{ij} - x_{i\pm1,j\pm1}| : x_{ij}, x_{i\pm1,j\pm1} \in \boldsymbol{\zeta}\}$.

An iterative implementation of the above scheme (7.49) is now given by proceeding as follows:

- Choose a set of weights and sample points $\boldsymbol{\zeta}$ for an integral quadrature.
- Start with $n = 0$, set $\mathfrak{t}_\Delta^0(s) = \mathbf{T}_\Delta^0(s) = s$, $[\det \mathrm{D}(\mathfrak{t}_\Delta^0 \circ \mathbf{T}_\Delta^0)](s) = 1$ for all $s \in \boldsymbol{\zeta}$ and save the evaluation vector $\mathfrak{S} = \mathbf{T}_\Delta^0(\boldsymbol{\zeta})$ that describes the initial position of the sample points, as well as $\mathfrak{S}_{\det} = [\det \mathrm{D}(\mathfrak{t}_\Delta^0 \circ \mathbf{T}_\Delta^0)](\boldsymbol{\zeta})$.
- Perform the following iteration:
  (1) Set $n = n + 1$
  (2) Calculate $\mathfrak{t}^n \in \mathfrak{X}_K$ by solving the minimization problem in (7.49). For this, calculate the variational derivative as in (7.43) and solve the system of Euler-Lagrange equations.
  (3) Set $\mathfrak{S}_{\det} = [\det \mathrm{D}\,\mathfrak{t}_\Delta^n](\mathfrak{S}) \cdot \mathfrak{S}_{\det}$ and $\mathfrak{S} = \mathfrak{t}^n(\mathfrak{S})$. The set $\mathfrak{S}$ now pictures the temporal evolution of the sample points at time $t = n\tau$.
  (4) Stop if the final time is attained, otherwise go to (1).
- Recover the set of density functions $u_\Delta^n = \left[\frac{u^0}{\det \mathrm{D}\,\mathbf{T}_\Delta^n}\right] \circ (\mathbf{T}_\Delta^n)^{-1}$ for $n \geqslant 1$.

It is ad hoc not clear if one can indeed find a vector in $\mathfrak{z}_K$ that solves the system of Euler-Lagrange equations, since the existence result of Proposition 7.1 (or Lemma 7.10, respectively) is not applicable in the new situation. Numerically, one can solve the system of Euler-Lagrange equations due to the convexity of (7.50) by using Newton's method, but note that it is not possible to guarantee that the gained solution $\mathfrak{t}^n$ lies in $\mathfrak{X}_K$. The reason for this is that one has just a finite number of points — the iteratively transported sample points $\mathbf{T}_\Delta^{n-1}(\boldsymbol{\zeta})$ — for which one can check that $\det(\mathrm{D}\,\mathfrak{t}^n)$ is strictly positive. To circumvent this problem at least in numerical applications, one can define in addition to the set of sample points $\boldsymbol{\zeta}$ a large set of random numbers $\boldsymbol{\zeta}_{\mathrm{rand}}$ with values in Ω. Then one can check the positivitiy of $\det(\mathrm{D}\,\mathfrak{t}^n)$ in each Newton step on the iteratively transported set $\mathbf{T}_\Delta^{n-1}(\boldsymbol{\zeta}_{\mathrm{rand}})$.

7.5. Numerical results

In all experiments below we choose $\mathrm{P}(s) = s^2$. Note that this choice is *not* covered from Proposition 7.1 that guarentees the existence of solutions to the numerical scheme. However, the numerical results indicate that one can neglect the conditions of Proposition 7.1 on P in practical applications.

For the integral approximation as explained in Section 7.4, we always choose $K_b = 2K$ and use a Gauß quadrature with four weights per square, which yields a total number of $K_\zeta^2 = 16K^2$ sample points.

7.5.1. Numerical experiments.

7.5.1.a. Reference solution. To study the evolution of discrete solutions and the numerical convergence, we compare our scheme with functions $u_{\mathrm{ref}} = (u_{\mathrm{ref}}^0, u_{\mathrm{ref}}^1, \ldots)$, where each time step u_{ref}^n, $n \geqslant 1$, is a solution to the standard finite element scheme given by

$$\int_\Omega \frac{u^n - u_{\mathrm{ref}}^{n-1}}{\tau}\,\theta_{kl}\,\mathrm{d}x = \int_\Omega \big\langle \nabla\big(u^n\big)^2, \nabla\theta_{kl}\big\rangle + u^n \left\langle \nabla V, \nabla\theta_{kl}\right\rangle \mathrm{d}x, \quad k,l = 0,\ldots,K_{\mathrm{ref}}. \tag{7.51}$$

We use the ansatz $u = \sum_{k,l=1}^{K_{\mathrm{ref}}-1} u_{kl}\theta_{kl}$, where the functions θ_{kl} are tensor products of locally affine functions $\theta_k : (0,1) \to \mathbb{R}$ that fulfill

$$\theta_k(l \cdot K_{\mathrm{ref}}^{-1}) = \begin{cases} 1 & \text{for } k = l, \\ 0 & \text{for } k \neq l, \end{cases}$$

for any $k = 1, \ldots, K_{\mathrm{ref}} - 1$. In order to satisfy the no-flux boundary condition, we further set

$$\theta_1(x) = 1 \text{ for } x \in (0, K_{\mathrm{ref}}^{-1}) \qquad \text{and} \qquad \theta_{K_{\mathrm{ref}}-1}(x) = 1 \text{ for } x \in (1 - K_{\mathrm{ref}}^{-1}, 1).$$

In all numerical experiments below, we use $K_{\mathrm{ref}} = 400$ and $\tau = 5 \cdot 10^{-4}$.

7.5.1.b. Evolution and decay of the entropy. In the first series of numerical investigations, we consider the positive initial density

$$u^0 = C\left(0.1 + x_1\big(\cos(4\pi x_1) - 1.2\big)\big(\cos(2\pi x_2) - 1\big)\right), \tag{7.52}$$

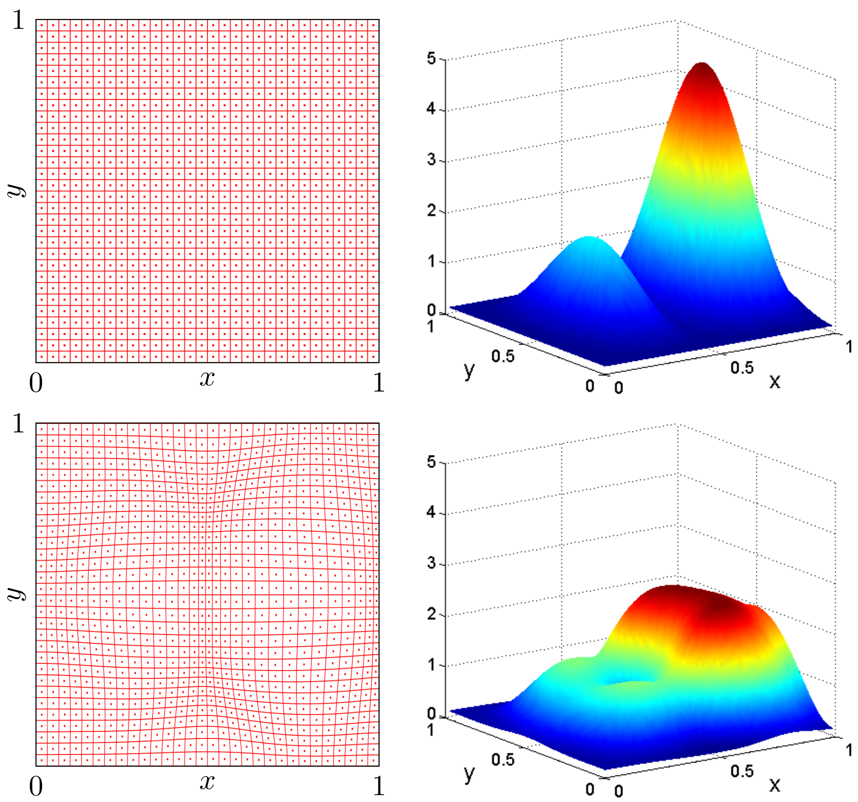
where $C > 0$ is such that u^0 has unit mass, and study the discrete evolution of the numerical scheme with $\mathrm{P}(s) = s^2$ and a "double-well"-like potential that is

$$V(x) = -\lambda\big(\cos(2\pi x_1) - 1\big)\big(\cos(4\pi x_2) - 1\big) \tag{7.53}$$

for $\lambda = 0.75$.

The evolution of the scheme's solution u_Δ and its corresponding transport map $\mathbf{T}_\Delta$ for $K = 32$ is plotted in Figure 7.1. Starting from the initial density that has 2 local maxima, the solution shows a slow diffusion that is typical for a porous medium equation at the very first time iterations, but then a certain "splitting" of the density arises that is caused by the influence of the drift-potential V. Two elevations evolve and move towards the stationary solution with increasing time.

Figure 7.2/right pictures the observed decay of the entropy $\mathcal{E}(u^n_\Delta)$ compared with the one gained by the standard finite element scheme using locally affine ansatz functions. As the figure points out, both curves perfectly lie on top of each other.



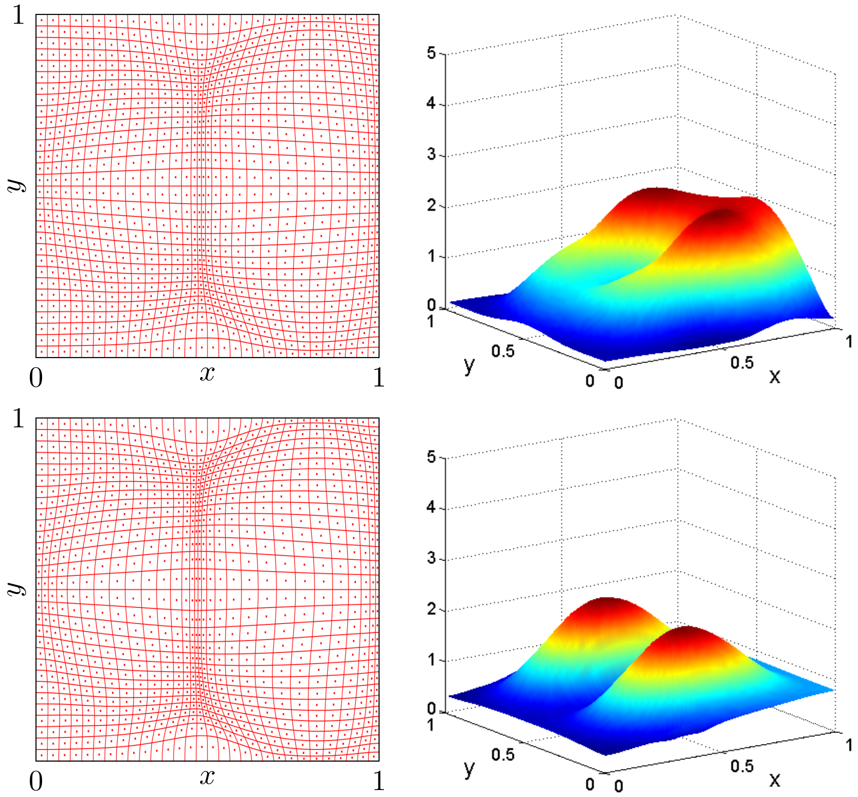


FIGURE 7.1. Evolution of the solution to the initial density (7.52) and its transport maps $\mathbf{T}_\Delta$ at time $t = 0, 2.5 \cdot 10^{-3}, 4 \cdot 10^{-3}$ and $t = 5 \cdot 10^{-2}$

7.5.1.c. Rate of convergence. For the next experiment, we again use the initial datum in (7.52), and fix $V \equiv 0$. To study the convergence of the scheme, we run a series of numerical simulations using the time step width $\tau = 5 \cdot 10^{-4}$ and $K = 4, 8, 12, 16, 20, 24$. The gained numerical solutions u_Δ are compared with the solution u_{ref} of the finite element scheme. To approximate the L^2-norm of the difference $u_\Delta - u_{\text{ref}}$, note that

$$\|u_\Delta^n - u_{\text{ref}}(n\tau, \cdot)\|^2_{L^2(\Omega)} = \int_\Omega \left\| \frac{u^0(x)}{\det \mathrm{D}\,\mathbf{T}_\Delta^n} - u_{\text{ref}}(n\tau, \mathbf{T}_\Delta^n) \right\|_2^2 \det(\mathrm{D}\,\mathbf{T}_\Delta^n)\,\mathrm{d}x,$$

for any $n \in \mathbb{N}$. This norm is numerically approximated by a Gauß quadrature using 400 sample points. Figure 7.2/left shows the obtained L^2-error that is evaluated at $T = 0.01$. The observed rate of convergence behaves approximately like K^{-3}.

7.5.1.d. Convexity. It is a well-known fact from the continuous theory that two solutions u_1 and u_2 of a L^2-Wasserstein gradient flow along a λ-convex entropy functional contract or diverge as

$$\mathcal{W}_2(u_1(t), u_2(t)) \leqslant \mathcal{W}_2(u_1(0), u_2(0))e^{-\lambda t}. \tag{7.54}$$

Since convexity is just locally preserved by our scheme at any time step, see Lemma 7.8, it is ad hoc not clear if (7.54) is valid, and even more, it is not clear how one can compare two numerical

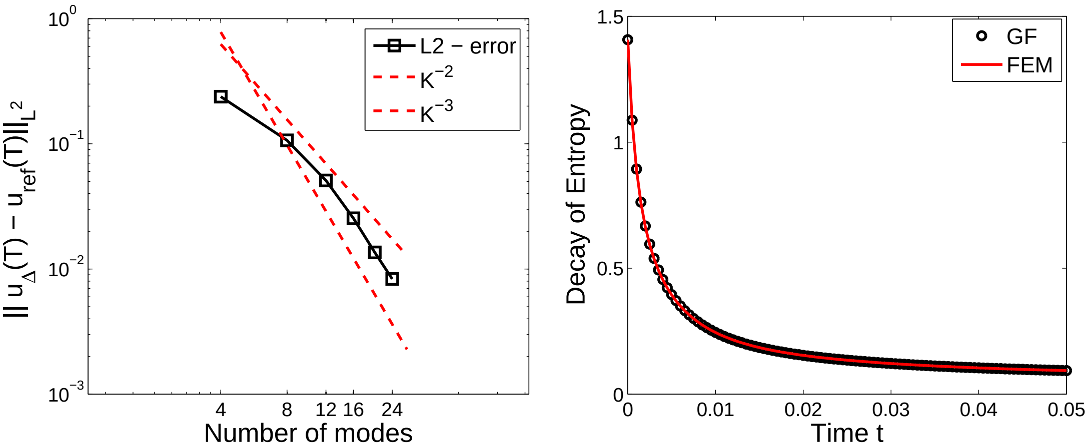


FIGURE 7.2. *Left*: numerically obtained L^2-norm of the differences $u_\Delta - u_{\text{ref}}$ evaluated at final time $T = 0.01$, using $K = 4, 8, 12, 16, 20, 25$. *Right*: observed decay of the entropy.

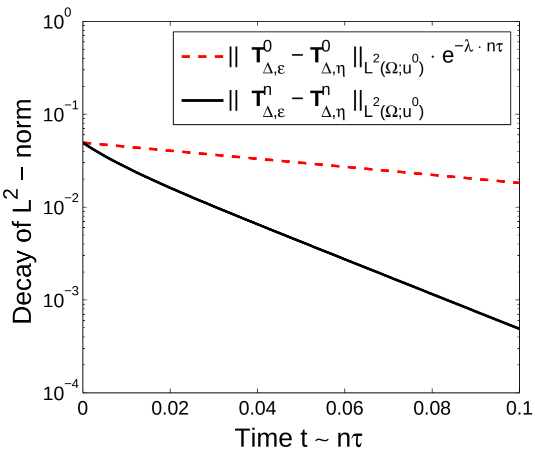


FIGURE 7.3. The exponential decay of $\|\mathbf{T}^n_{\Delta,\vec{\varepsilon}} - \mathbf{T}^n_{\Delta,\vec{\eta}}\|_{L^2(\Omega,u^0)}$ using $K = 12$, $\tau = 10^{-3}$, $n = 0, \ldots, 100$ and the initial densities $u^0_{\Delta,\vec{\varepsilon}}$ and $u^0_{\Delta,\vec{\eta}}$ from (7.55).

solutions with different initial densities. To study (7.54) numerically, we choose $V(x) = \frac{\lambda}{2}\|x\|_2^2$ with $\lambda = 10$ and fix the discretization parameters $K = 12$ and $\tau = 10^{-3}$. Furthermore, we consider $u^0 = 1$ and take two perturbed densities $u^0_{\Delta,\vec{\varepsilon}}$ and $u^0_{\Delta,\vec{\eta}}$, defined by

$$u^0_{\Delta,\vec{\varepsilon}} = \Big(\mathrm{id} + \sum_{(k,l)\in\mathcal{I}_K} \varepsilon_{kl}\nabla\varphi_{kl}\Big)_{\#} u^0 \quad \text{and} \quad u^0_{\Delta,\vec{\eta}} = \Big(\mathrm{id} + \sum_{(k,l)\in\mathcal{I}_K} \eta_{kl}\nabla\varphi_{kl}\Big)_{\#} u^0. \tag{7.55}$$

The vectors $\vec{\varepsilon}$ and $\vec{\eta}$ have entries with random numbers with a maximal absolute value of $1.25 \cdot 10^{-5}$, but in order to enlarge the difference between both densities in (7.55), we randomly add in each vector a single entry that has an absolute value of $5 \cdot 10^{-2}$. However, $\vec{\varepsilon}$ and $\vec{\eta}$ are chosen such that the corresponding transport maps are still gradients of convex functions. We then run the numerical scheme for both perturbed initial densities to get solutions $u_{\Delta,\vec{\varepsilon}}$ and

$u_{\Delta,\vec{\eta}}$. In the semi-logarithmic plot in Figure 7.3, one can see the time evolution of

$$\|\mathbf{T}^n_{\Delta,\vec{\varepsilon}} - \mathbf{T}^n_{\Delta,\vec{\eta}}\|_{L^2(\Omega,u^0)}, \quad n = 0, \ldots, 100, \tag{7.56}$$

which is the best approximation to $\mathcal{W}_2(u^n_{\Delta,\vec{\varepsilon}}, u^n_{\Delta,\vec{\eta}})$ we can accomplish with our method. Similar to the continuous theory, the difference in (7.56) decays exponentially and satisfies the same upper-bound as in (7.54).

CHAPTER 8

Concluding remarks

The last chapter of this thesis is intended to provide some concluding remarks to the presented results and some ideas for possible extensions of the used methods.

Part 1. One-dimensional case. The results for our numerical schemes stated in one spatial dimension are in general satisfiying and confirm the used approximations. For almost all schemes, a proof of convergence is provided and several structural properties from the continuous equations are preserved in the discrete setting.

The usage of piecewise constant density functions for the schemes' derivations has its pros and cons. On the one hand the resulting schemes are easy to implement and the handling with piecewise constant functions makes the analytical investigation of the schemes relatively convenient. But on the other hand a more sophisticated ansatz (for instance using spline interpolants with more regulartiy) would very likely yield to better rates of convergence. Take for example the scheme for the DLSS equations by Düring, Matthes and Pina [**DMM10**], where a locally quadratic spline interpolation is used for the approximation of Lagrangian maps with corresponding continuous and differentiable density functions. Numerical experiments suggest a better rate of convergence for the scheme in [**DMM10**] than for our scheme in Chapter 5. Unfortunately, a proof of convergence for [**DMM10**] is still missing. For this purpose, I once tried to proceed similarly as in Chapter 5 to derive a compactness result for discrete solutions to the scheme in [**DMM10**], which turned out to be a difficult task that I haven't solved yet.

Another point that calls for improvement is the usage of equidistant spatial decompositions in the approaches for fourth order equations. It seems that all analytical results can be adapted to non-equidistant meshes as well without changing the main ideas of proceeding. However, this generalization is absent and could be the content of future considerations.

Part 2. Two-dimensional case. Unfortunately, there are many open questions for our scheme in dimension two: The convergence result in Section 3.6 indicates that the obtained stability result in combination with a consistency result can suffice to show convergence of the scheme in Chapter 7, but a proof of consistency is still missing. Furthermore, it is not clear if one can find useful a priori estimates that yield compactness of discrete solutions. Any effort to exploit the variational structure of our scheme to find appropriate estimates as in the one-dimensional situation in Chapter 3 failed so far, even for other choices of ansatz functions — for instance, we attempted locally affine and quadratic spline interpolations of the Lagrangian maps instead of the Fourier-ansatz presented in this thesis. A part from that, the approximation of solutions to (7.1) starting with discontinuous initial density functions is unconvincing, since strong oscillations occur along points of initial discontinuity because of the Gibbs phenomenon.

But there are also many positive arguments that justify the way of our approximation. Many important structural properties are preserved by construction, for example preservation of mass, dissipation of the entropy and the λ-convexity of the entropy along discrete geodesics. In addition, the preserved variational character of our scheme in Chapter 7 enables an extension to fourth order equations in the same spirit as in Chapter 4 in the one-dimensional case. Take for instance the Boltzmann entropy $\mathcal{H}(u) = \int_\Omega u \log(u)\,\mathrm{d}x$ and define analogously to (7.28) the Lagrangian representation

$$\mathbf{H}(\mathfrak{t}, \mathbf{T}) := \mathcal{H}\big((\mathfrak{t} \circ \mathbf{T})_\# u^0\big)$$

for any density u^0 and transportation maps $\mathfrak{t}, \mathbf{T} : \Omega \to \Omega$ with $\Omega = (0,1)^2$. Then a discrete formulation of the auto-dissipation of the Boltzmann entropy according to the one-dimensional definition in (4.22) would be (using the notation of Chapter 7)

$$\vec{\mathrm{z}} \mapsto \mathbf{F}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}) := \big\langle \partial_{\vec{\mathrm{z}}}\mathbf{H}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}), \mathrm{W}_2[\mathbf{T}]^{-1}\partial_{\vec{\mathrm{z}}}\mathbf{H}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T})\big\rangle,$$

which can be used as a discretization of the Fisher information $\mathcal{F}(u) = \int_\Omega |\nabla\sqrt{u}|^2\,\mathrm{d}x$. Note that this approach of the Fisher information is much easier to implement than for instance a "straight-forward" restriction of $\mathcal{F}$ to $\mathfrak{X}_K$, $\vec{\mathrm{z}} \mapsto \mathcal{F}((\mathfrak{t}_K[\vec{\mathrm{z}}] \circ \mathbf{T})_\# u^0)$. A numerical scheme for the DLSS equation on the domain Ω is then provided by the following recursively defined procedure, where we again use the notation of Chapter 7:

Given a discretization $\Delta = (\tau, K)$ consisting of a time step $\tau > 0$, a spatial discretization K, an initial density function $u^0 \in \mathcal{P}_2^r(\Omega)$, an initial vector $\vec{\mathrm{z}}_\Delta^0 = 0 \in \mathfrak{z}_K$, and the initial transport $\mathbf{T}_\Delta^0 = \mathrm{id}$. Then define inductively a sequence of vectors $\vec{\mathrm{z}}_\Delta = (\vec{\mathrm{z}}_\Delta^0, \vec{\mathrm{z}}_\Delta^1, \ldots)$, such that $\vec{\mathrm{z}}_\Delta^n$ solves

$$\vec{\mathrm{z}}_\Delta^n = \underset{\vec{\mathrm{z}} \in \mathfrak{z}_K}{\operatorname{argmin}}\ \frac{1}{2\tau}\mathbf{d}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}_\Delta^{n-1}) + \mathbf{F}(\mathfrak{t}_K[\vec{\mathrm{z}}], \mathbf{T}_\Delta^{n-1}) \tag{8.1}$$

for $n \geqslant 1$, and set $\mathbf{T}_\Delta^n = \mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n] \circ \mathbf{T}_\Delta^{n-1}$. Further denote $\mathfrak{t}_\Delta^n = \mathfrak{t}_K[\vec{\mathrm{z}}_\Delta^n]$, $u_\Delta^n = (\mathbf{T}_\Delta^n)_\# u^0$, and we write $\vec{\mathrm{z}}_\Delta = (\vec{\mathrm{z}}_\Delta^0, \vec{\mathrm{z}}_\Delta^1, \ldots)$, $\mathfrak{t}_\Delta = (\mathfrak{t}_\Delta^0, \mathfrak{t}_\Delta^1, \ldots)$, $u_\Delta = (u_\Delta^0, u_\Delta^1, \ldots)$ and $\mathbf{T}_\Delta = (\mathbf{T}_\Delta^0, \mathbf{T}_\Delta^1, \ldots)$.

The well-posedness of the above scheme is not studied so far, but initial numerical experiments show that the above minimization procedure seems to be numerically solvable using Newton's method. A first comparison with solutions to the one-dimensional scheme of Chapter 5 furthermore indicates that solutions to the above numerical approximation have the same qualitative behaviour: In Figure 8.1, we plot the evolution to solutions of the scheme in Chapter 5 and to the scheme described in (8.1), using the initial densities

$$\begin{aligned} u_1^0(x) &= C_1(0.3 + \cos^{18}(\pi x)) \quad \text{for } x \in (0,1), \text{ and} \\ u_2^0(x) &= C_2(0.3 + \cos^{18}(\pi x_1) + \cos^{18}(\pi x_2)) \quad \text{for } x = (x_1, x_2) \in (0,1)^2, \end{aligned} \tag{8.2}$$

respectively. The constants $C_1, C_2 > 0$ are chosen such that the initial densities have unit mass. This first experiment motivates that the analysis of the scheme in (8.1) appears to be an interesting issue for future researches.

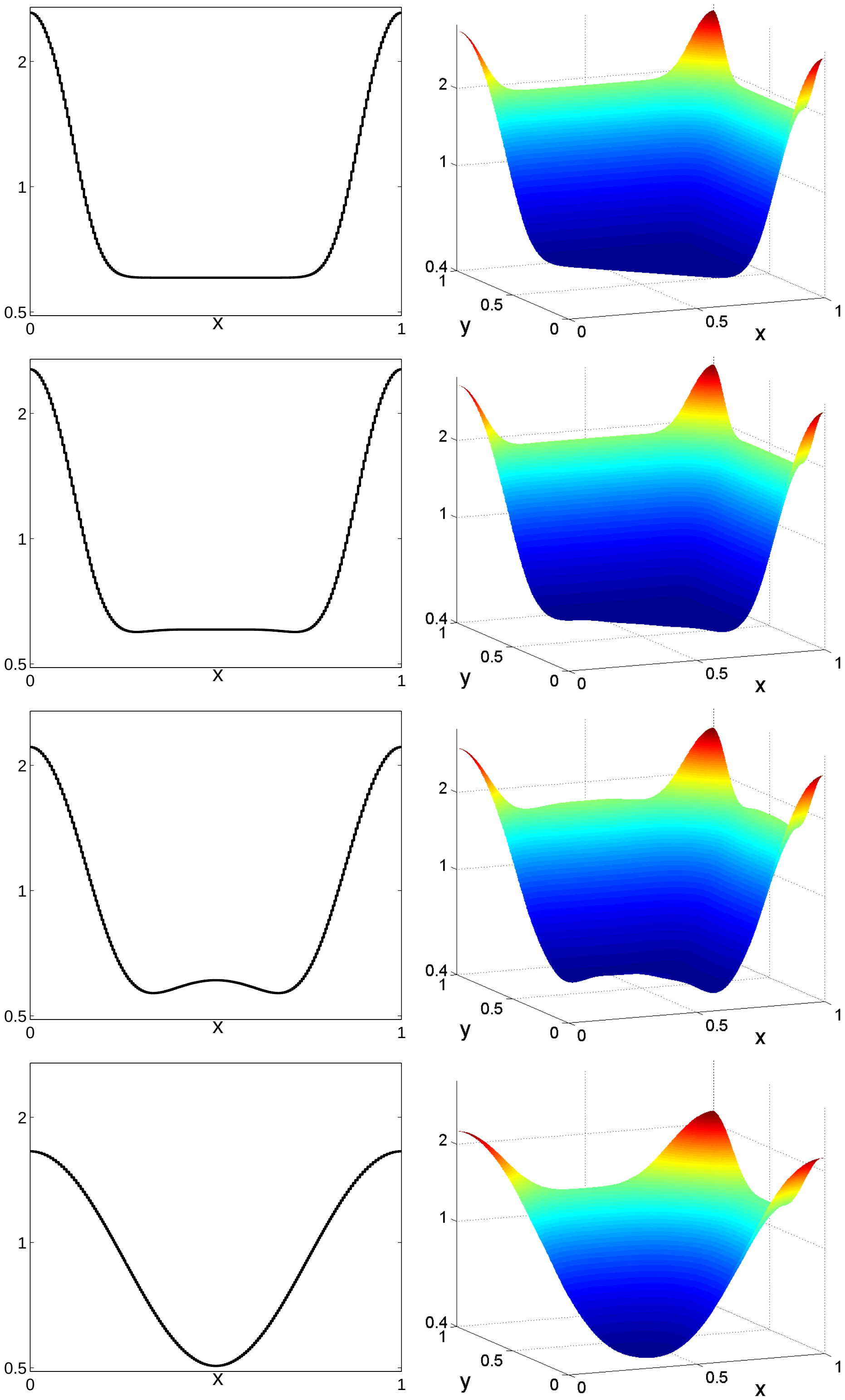


FIGURE 8.1. Solutions to the scheme in Chapter 5 (left) and to the scheme in (8.1) (right) using the initial densities in (8.2) and evaluated at $t = 0, 10^{-6}, 10^{-5}, 10^{-4}$. The plots on the right-hand side are cutted to improve the visibility.

Appendix

A.1. General results from the literature

In this first section of the Appendix, we want to list some useful results from the literature which are crucial for the convergence analysis of our numerical schemes in one spatial dimension.

First of all, we state one of many possible formulations of the well-known Arzelà-Ascoli Theorem.

Theorem A.1 (Arzelà-Ascoli Theorem). *Let $\Omega = (a, b)$ be a bounded interval or $\Omega = \mathbb{R}$. Further let $[\underline{t}, \overline{t}] \subseteq [0, +\infty)$ be a compact time interval, let $\mathcal{K} \subseteq \mathcal{P}_2^r(\Omega)$ be a sequentially compact set with respect to the L^2-Wasserstein distance, and $u_k : [\underline{t}, \overline{t}] \to \mathcal{P}_2^r(\Omega)$ be curves such that*

$$u_k(t) \in \mathcal{K} \quad \text{for any } k \in \mathbb{N},\ t \in [\underline{t}, \overline{t}],$$
$$\mathcal{W}_2(u_k(s), u_k(t)) \leqslant C|t-s|^{1/2} \quad \text{for any } s, t \in [\underline{t}, \overline{t}],\ \text{uniformly in } k.$$

Then there exists a subsequence k' of k and a limit curve $u \in C^{1/2}([\underline{t}, \overline{t}]; \mathcal{P}_2^r(\Omega))$, such that $u_{k'} \to u$ uniformly with respect to $t \in [\underline{t}, \overline{t}]$ as $k' \to \infty$.

Proof. The claim of this theorem is a special case of [**AGS05**, Proposition 3.3.1]. □

The next result is about the convergence of non-increasing functions.

Theorem A.2 (Helly's Theorem). *Suppose $(\varphi_n)_{n=0}^{\infty}$ to be a sequence of non-increasing functions, such that $\varphi_n : [0, T] \to [-\infty, +\infty]$ for any $T > 0$. Then there exist a subsequence $(\varphi_{n'})_{n'=0}^{\infty}$ and a non-increasing function $\varphi : [0, T] \to [-\infty, +\infty]$ such that $\varphi_{n'}(t) \to \varphi(t)$ for any $t \in [0, T]$ as $n' \to \infty$.*

Proof. See [**AGS05**, Lemma 3.3.3] □

Finally, let us formulate the following discrete Gronwall Lemma.

Lemma A.3 (Discrete Gronwall Lemma). *Let $q_n \in [0, +\infty)$, $n = 0, \ldots, N$, such that*

$$q_n \leqslant q_0 + \sum_{k=0}^{n-1} \epsilon_k + \sum_{k=0}^{n-1} L_k q_k \quad \text{for any} \quad n = 1, \ldots, N,$$

where $L_k \in (0, +\infty)$ and $\epsilon_k \in \mathbb{R}$ for $k = 0, \ldots, N-1$. Then

$$q_n \leqslant \big(q_0 + \sum_{k=0}^{n-1} \epsilon_k\big) \exp\big(\sum_{k=0}^{n-1} L_k\big) \quad \text{for any} \quad n = 1, \ldots, N.$$

Proof. A proof of this statement easily follows by induction. □

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A.2. Some technical lemmas for the one-dimensional case

In the last section of the Appendix, some technical results are provided.

Lemma A.4 (Gargliardo-Nirenberg inequality). *For each interval $\Omega \subseteq \mathbb{R}$ and $f \in H^1(\Omega)$, one has that*

$$\|f\|_{C^{1/6}(\Omega)} \leqslant (9/2)^{1/3} \|f\|_{H^1(\Omega)}^{2/3} \|f\|_{L^2(\Omega)}^{1/3}. \tag{A.1}$$

Proof. Assume first that $f \geqslant 0$. Then, for arbitrary $x < y$, $x, y \in \Omega$, the fundamental theorem of calculus and Hölder's inequality imply that

$$\left|f(x)^{3/2} - f(y)^{3/2}\right| \leqslant \frac{3}{2} \int_x^y 1 \cdot f(z)^{1/2} |f'(z)| \,\mathrm{d}z \leqslant \frac{3}{2} |x-y|^{1/4} \|f\|_{L^2(\Omega)}^{1/2} \|f'\|_{L^2(\Omega)}.$$

Since $f \geqslant 0$, we can further estimate

$$|f(x) - f(y)| \leqslant \left|f(x)^{3/2} - f(y)^{3/2}\right|^{2/3} \leqslant (3/2)^{2/3} |x-y|^{1/6} \|f\|_{L^2(\Omega)}^{1/3} \|f\|_{H^1(\Omega)}^{1/3}.$$

This shows (A.1) for nonnegative functions f. A general f can be written in the form $f = f_+ - f_-$, where $f_\pm \geqslant 0$. By the triangle inequality, and since $\|f_\pm\|_{H^1(\Omega)} \leqslant \|f\|_{H^1(\Omega)}$,

$$\|f\|_{C^{1/6}(\Omega)} \leqslant \|f_+\|_{C^{1/6}(\Omega)} + \|f_-\|_{C^{1/6}(\Omega)} \leqslant 2(3/2)^{2/3} \|f\|_{L^2(\Omega)}^{1/3} \|f\|_{H^1(\Omega)}^{1/3}.$$

This proves the claim. □

For the forthcoming lemmata, we use the notation as introduced in Section 2.2 about the spatial discretization. Therefore let us fix in the following a spatial decomposition $\boldsymbol{\xi}$ of the mass domain $\mathcal{M}$ and denote by $\mathfrak{x}_{\boldsymbol{\xi}}$ the set of Lagrangian vectors with entries in Ω, which can be bounded or equal to $\mathbb{R}$. Furthermore, take a norm $\|\cdot\|_{\boldsymbol{\xi}}$ as mentioned in Subsection 2.2.2 which is induced by one of the matrices W_2 or $\delta\mathbb{I}$ (in case of an equidistant mass decomposition), both satisfying (2.24).

Lemma A.5. *Take a functional $\mathbf{E} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ and fix any $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ and $\tau > 0$. Furthermore, assume that*

$$\vec{\mathrm{y}} \mapsto \mathbf{E}_\Delta(\sigma, \vec{\mathrm{y}}, \vec{\mathrm{x}}) \quad \text{with} \quad \mathbf{E}_\Delta(\sigma, \vec{\mathrm{y}}, \vec{\mathrm{x}}) = \frac{1}{2\sigma} \|\vec{\mathrm{y}} - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2 + \mathcal{E}(\vec{\mathrm{y}})$$

attains a (not necessarily unique) minimizer for any $\sigma \in (0, \tau]$, which we denote by $\vec{\mathrm{x}}_\sigma$. Furthermore, denote by

$$|\partial_{\boldsymbol{\xi}} \mathbf{E}| (\vec{\mathrm{x}}) = \limsup_{\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}} : \vec{\mathrm{y}} \to \vec{\mathrm{x}}} \frac{\left(\mathbf{E}(\vec{\mathrm{x}}) - \mathbf{E}(\vec{\mathrm{y}})\right)^+}{\|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}}}$$

the discrete local slope $|\partial_{\boldsymbol{\xi}} \mathbf{E}|$ of $\mathbf{E}$ at $\vec{\mathrm{x}}$.

Then for any $\sigma \in (0, \tau]$, the following points are satisfied:

- Discrete slope estimate: *The discrete local slope $|\partial_{\boldsymbol{\xi}} \mathbf{E}| (\vec{\mathrm{x}})$ fulfills*

$$|\partial_{\boldsymbol{\xi}} \mathbf{E}| (\vec{\mathrm{x}}_\sigma) \leqslant \frac{\|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}}{\sigma}. \tag{A.2}$$

- *The map* $\sigma \to \mathbf{E}_\Delta(\sigma, \vec{\mathrm{x}}_\sigma, \vec{\mathrm{x}})$ *is Lipschitz-continuous and*

$$\frac{\|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2}{2\sigma} + \int_0^\sigma \frac{\|\vec{\mathrm{x}}_r - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2}{2r^2}\,\mathrm{d}r = \mathbf{E}(\vec{\mathrm{x}}) - \mathbf{E}(\vec{\mathrm{x}}_\sigma). \tag{A.3}$$

Proof. The following proof uses the same techniques as applied to Lemma 3.1.3 and Theorem 3.1.4 in [**AGS05**]. By definition of $\vec{\mathrm{x}}_\sigma$ one achieves

$$\begin{aligned}
\mathbf{E}(\vec{\mathrm{x}}_\sigma) - \mathbf{E}(\vec{\mathrm{y}}) &\leqslant \frac{1}{2\sigma}\left(\|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}}^2 - \|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2\right) \\
&= \frac{1}{2\sigma}(\|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}} - \|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}})(\|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}} + \|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}) \\
&\leqslant \frac{1}{2\sigma}\|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}}\left(\|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}} + \|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}\right)
\end{aligned}$$

for any $\vec{\mathrm{y}} \in \mathfrak{x}_{\boldsymbol{\xi}}$, where we used the triangle inequality in the last step. Divide both sides by $\|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}}$, then one attains the desired inequality since

$$|\partial_{\boldsymbol{\xi}}\mathbf{E}|(\vec{\mathrm{x}}_\sigma) \leqslant \limsup_{\vec{\mathrm{y}}\in\mathfrak{x}_{\boldsymbol{\xi}}:\vec{\mathrm{y}}\to\vec{\mathrm{x}}_\sigma} \frac{1}{2\sigma}\left(\|\vec{\mathrm{x}} - \vec{\mathrm{y}}\|_{\boldsymbol{\xi}} + \|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}\right) = \frac{\|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}}{\sigma}.$$

To derive the Lipschitz-continuity of $\sigma \to \mathbf{E}_\Delta(\sigma, \vec{\mathrm{x}}_\sigma, \vec{\mathrm{x}})$, take any two $\sigma_0, \sigma_1 \in (0, \tau]$, $\sigma_0 < \sigma_1$, then $\mathbf{E}_\Delta(\sigma_0, \vec{\mathrm{x}}_{\sigma_0}, \vec{\mathrm{x}}) \leqslant \mathbf{E}_\Delta(\sigma_0, \vec{\mathrm{x}}_{\sigma_1}, \vec{\mathrm{x}})$ yields

$$\mathbf{E}_\Delta(\sigma_0, \vec{\mathrm{x}}_{\sigma_0}, \vec{\mathrm{x}}) - \mathbf{E}_\Delta(\sigma_1, \vec{\mathrm{x}}_{\sigma_1}, \vec{\mathrm{x}}) \leqslant \mathbf{E}_\Delta(\sigma_0, \vec{\mathrm{x}}_{\sigma_1}, \vec{\mathrm{x}}) - \mathbf{E}_\Delta(\sigma_1, \vec{\mathrm{x}}_{\sigma_1}, \vec{\mathrm{x}}) = \frac{\sigma_1 - \sigma_0}{2\sigma_0\sigma_1}\|\vec{\mathrm{x}}_{\sigma_1} - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2.$$

Analogously one gets $\mathbf{E}_\Delta(\sigma_0, \vec{\mathrm{x}}_{\sigma_0}, \vec{\mathrm{x}}) - \mathbf{E}_\Delta(\sigma_1, \vec{\mathrm{x}}_{\sigma_1}, \vec{\mathrm{x}}) \geqslant \frac{\sigma_1-\sigma_0}{2\sigma_0\sigma_1}\|\vec{\mathrm{x}}_{\sigma_0} - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2$ and further

$$\frac{1}{2\sigma_0\sigma_1}\|\vec{\mathrm{x}}_{\sigma_0} - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2 \leqslant \frac{\mathbf{E}_\Delta(\sigma_0, \vec{\mathrm{x}}_{\sigma_0}, \vec{\mathrm{x}}) - \mathbf{E}_\Delta(\sigma_1, \vec{\mathrm{x}}_{\sigma_1}, \vec{\mathrm{x}})}{\sigma_1 - \sigma_0} \leqslant \frac{1}{2\sigma_0\sigma_1}\|\vec{\mathrm{x}}_{\sigma_1} - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2.$$

This yields the local Lipschitz continuity and passing to the limit as $\sigma_0 \uparrow \sigma$ and $\sigma_1 \downarrow \sigma$ for any $\sigma \in (0, \tau]$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}\sigma}\mathbf{E}_\Delta(\sigma, \vec{\mathrm{x}}_\sigma, \vec{\mathrm{x}}) = -\frac{\|\vec{\mathrm{x}}_\sigma - \vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2}{2\sigma^2}.$$

Equation (A.3) then follows by integration. □

Lemma A.6. *For each* $p \geqslant 1$ *and* $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$ *with* $\vec{\mathrm{z}} = \mathbf{z}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$, *one has that*

$$\sum_{\kappa\in\mathbb{I}_K^{1/2}} \left(\frac{\delta}{z_\kappa}\right)^p = \sum_{\kappa\in\mathbb{I}_K^{1/2}} (x_{\kappa+\frac12} - x_{\kappa-\frac12})^p \leqslant (x_K - x_0)^p. \tag{A.4}$$

Proof. The first equality is simply the definition (2.18) of z_κ. Since one has trivially that $x_{\kappa+\frac12} - x_{\kappa-\frac12} \leqslant x_K - x_0$ for each $\kappa \in \mathbb{I}_K^{1/2}$, and since $p - 1 \geqslant 0$, one attains

$$\sum_{\kappa\in\mathbb{I}_K^{1/2}} (x_{\kappa+\frac12} - x_{\kappa-\frac12})^p \leqslant (x_K - x_0)^{p-1} \sum_{\kappa\in\mathbb{I}_K^{1/2}} (x_{\kappa+\frac12} - x_{\kappa-\frac12}) = (x_K - x_0)^p.$$ □

Lemma A.7 (Lower bound on Boltzmann entropy). *For each* $\vec{\mathrm{x}} \in \mathfrak{x}_{\boldsymbol{\xi}}$, *one has that*

$$\mathbf{H}(\vec{\mathrm{x}}) \geqslant -\frac{2\sqrt{\pi}}{e}\left(M + \|\vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2\right)^{1/2},$$

where $\mathbf{H} : \mathfrak{x}_{\boldsymbol{\xi}} \to \mathbb{R}$ *is the restriction of the Boltzmann entropy* $\mathcal{H}(u) = \int_\Omega u \ln(u)\,\mathrm{d}x$ *to* $\mathfrak{x}_{\boldsymbol{\xi}}$*, i.e.*

$$\mathbf{H}(\vec{\mathrm{x}}) = \int_\Omega \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}] \ln(\mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}])\,\mathrm{d}x.$$

Proof. This statement is trivial if $\Omega = (a, b)$ is a bounded domain, due to the convexity of $s \mapsto s\ln(s)$ and Jensen's inequality:

$$\mathcal{H}(u) = (b-a)\int_\Omega u \ln u \frac{\mathrm{d}x}{b-a} \geqslant (b-a)\left(\int_\Omega u\frac{\mathrm{d}x}{b-a}\right)\ln\left(\int_\Omega u\frac{\mathrm{d}x}{b-a}\right) = M\ln\left(\frac{M}{b-a}\right).$$

This especially implies the boundedness of the restriction. Hence let us assume that $\Omega = \mathbb{R}$ and let $u \in \mathcal{P}_2^r(\Omega)$ be a nonnegative density of mass M with finite second moment. Since $-s\log s \leqslant 2e^{-1}s^{1/2}$ for all $s > 0$, one obtains

$$\begin{aligned} -\int_\Omega u\ln u\,\mathrm{d}x &\leqslant \frac{2}{e}\int_\Omega \sqrt{u}\,\mathrm{d}x \\ &\leqslant \frac{2}{e}\left(\int_\Omega \frac{\mathrm{d}x}{1+x^2}\right)^{1/2}\left(\int_\Omega (1+x^2)u\,\mathrm{d}x\right)^{1/2} = \frac{2\sqrt{\pi}}{e}\left(M + \int_\Omega x^2 u\,\mathrm{d}x\right)^{1/2}. \end{aligned}$$

In particular, this inequality is fulfilled for $u = \mathbf{u}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$ with Lagrangian map $\mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]$:

$$-\mathbf{H}(\vec{\mathrm{x}}) \leqslant \frac{2\sqrt{\pi}}{e}\left(M + \int_{\mathcal{M}} \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]^2\,\mathrm{d}\xi\right)^{1/2}.$$

Observing that

$$\int_{\mathcal{M}} \mathbf{X}_{\boldsymbol{\xi}}[\vec{\mathrm{x}}]^2\,\mathrm{d}\xi = \langle \mathrm{W}_2\vec{\mathrm{x}}, \vec{\mathrm{x}}\rangle \leqslant \|\vec{\mathrm{x}}\|_{\boldsymbol{\xi}}^2$$

the claim follows. $\square$

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