Approximation of Traveling Waves by Splitting Methods

Von der KIT-Fakultät für Mathematik des
Karlsruher Instituts für Technologie (KIT)
zur Erlangung des akademischen Grades eines

Doktors der Naturwissenschaften

genehmigte

Dissertation

von

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Tag der mündlichen Prüfung: 30.10.2019

Karlsruhe Institute of Technology

ACKNOWLEDGEMENT

I would like to take this opportunity to express my gratitude to all those people who contributed, directly or indirectly, to this work.

First of all, I want to thank Prof. Dr. Tobias Jahnke. He agreed to take over the supervision of my PhD project at an advanced stage for which I am very grateful. He gave me the opportunity to finish this project and was always there to answer my questions and discuss occurring difficulties.

I am also very grateful to Prof. Dr. Michael Plum for serving as referee. He always had an open door for me and I really enjoyed the inspiring discussions. I also thank Dr. Jens Rottmann-Matthes for giving me the opportunity to work on this project and his support already during my early studies. He introduced me to the interesting field of numerical analysis and in particular he pointed me to operator splitting methods.

In the last eight months I received funding from the Kronmüller-Stipendium. I am very thankful for this funding which gave me the opportunity to finish my PhD project. I also want to thank the CRC 1173 *Wave phenomena: analysis and numerics* for the pleasant surrounding and vibrant research environment it provides and the possibility to present my work in internal workshops and conferences abroad. This work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation – Project-ID 258734477 – SFB 1173).

I also thank our little lunch group and its former members. I very much appreciated all the interesting discussions and non mathematical conversations. I am thankful for the pleasant and supportive working environment provided by the lunch group and my colleagues from my workgroup *Nonlinear Partial Differential Equations*.

I would like to take this opportunity to express my deepest gratitude to Sabine. Without her love, patience and support this thesis would not have been possible. Thank you for sharing your life with me. Finally, I thank my family for their unconditional love and support.

CONTENTS

CHAPTER

ONE

MOTIVATION AND INTRODUCTION

A "*rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed*" – these were the words John Scott Russell used to describe a phenomenon he observed in 1834 as he passed by a canal [Rus45]. This was the first record of a phenomenon which occurs in various forms in different scientific fields: *traveling waves*.

Since then traveling waves became a topic of interest in physics, chemistry and biology and understanding them still presents a challenge in current research, as for example traveling waves occur in optical fibers for data transmission. Traveling waves are special solutions of partial differential equations (PDEs) capturing natural phenomena in mathematical models. For example Russell's observations were described by the Korteweg–de Vries (KdV) equations in 1895. Another nature driven phenomenon is the propagation of a pulse in a nerve axon in animals or humans. Hodgkin and Huxley described in [HH52] a very precise mathematical model of the behavior of the chemical channels by quantitative studies of the excitation of a nerve, a work for which they received the Nobel Prize in 1963. Based on this a simplified model describing the phenomenon how action potentials in neurons are initiated and propagated in animal nerve axons was introduced in [NAY62]. It is determined by the Nagumo equation

$$\partial_t u = \partial_x^2 u + u(1-u)(u-\alpha)$$

with $\alpha \in (0, \frac{1}{2})$. Here ∂_x^2 is a second order differential operator in space and $u(1-u)(u-\alpha)$ is a nonlinear function. PDEs of the form

$$\partial_t u = \partial_x^2 u + f(u), \qquad u : \mathbb{R} \times [0, \infty) \to \mathbb{R} \tag{1.1}$$

for some nonlinear function f are the main subject of this thesis. In particular, we are interested in finding traveling wave solutions of the PDE (1.1), which is – depending on the equation – often a challenging task.

Traveling waves are solutions of (1.1) which can be written as

$$u(x,t) = \bar{u}(x - ct),$$

where $\bar{u} : \mathbb{R} \to \mathbb{R}$ is the profile and $c \in \mathbb{R}$ the speed of the traveling wave. The aim of this thesis is to introduce a numerical scheme which is suitable to approximate traveling wave solutions of (1.1). The usual approach for approximating the profile of a traveling wave is to derive a boundary value problem as follows. If we consider this problem in a co-moving frame by using the new spatial variable $\xi = x - ct$, the solution $u(x,t) = \bar{u}(x - ct) = \bar{u}(\xi)$ becomes a stationary solution of

$$\partial_t u = \partial_x^2 u + f(u) + c\partial_x u$$

and $\bar{u}$ solves the ordinary differential equation (ODE)

$$0 = \partial_x^2 u + f(u) + c\partial_x u.$$

After truncating the whole line $\mathbb{R}$ to a finite interval and applying certain conditions to the boundary, the profile is obtained by solving the resulting boundary value problem (BVP). In order to do this one typically relies on Newton solvers. But it turns out that the initial value for Newton solvers for this problem needs to be sufficiently close to a traveling wave, otherwise the Newton solvers diverge. An approach to obtain suitable initial values is to calculate the evolution equation on long time intervals. Such long-time forward simulations are able to approximate profiles of stable traveling waves as time asymptotic states. We want to take advantage of this and introduce a scheme which is able to efficiently approximate traveling waves without considering the BVP. In contrast to Newton solvers, we want to require as little knowledge as possible of the traveling wave in advance.

In many cases traveling wave solutions leave every bounded domain. As a consequence, long-time forward simulations of traveling waves are a challenging task since in numerical simulations we have to regard finite-space intervals. To deal with this problem, we use a technique called the *method of freezing*. This technique was introduced in [RM00, RKML03, BT04] and further developed in [RM10, Thü05, BOR14]. For this a time dependent spatial shift $\xi = x - \gamma(t)$ of the spatial coordinate in (1.1) is used to go into a co-moving frame. In the ideal case $\gamma(t) = ct$ the traveling wave of (1.1) would be a stationary solution in the new coordinates since $\bar{u}(x-ct) = \bar{u}(\xi)$. As the speed c of the traveling wave is often not known in advance we introduce a time dependent approximation $\mu(t)$. Originating from (1.1) we obtain a system of the form

$$\begin{cases} \partial_t u = \partial_x^2 u + f(u) + \mu \partial_x u, \\ \quad 0 = \Psi(u,\mu), \\ \partial_t \gamma = \mu \end{cases} \tag{1.2}$$

in the co-moving frame. The algebraic constraint $0 = \Psi(u,\mu)$ is called a phase condition in [BT04] and is required to obtain a solution for μ. This system is called a *partial differential algebraic equation* (PDAE).

In this thesis we apply operator splitting methods to the PDAE to approximate its solution in time. We give a short overview of splitting methods in Section 1.4. For a detailed account we refer to the literature [HLW06]. As suggested in [AO17] the strategy is to split (1.2) into a linear PDAE and nonlinear ordinary differential equation (ODE) and solve them consecutively on small time intervals. This yields a method which is able to approximate stationary solutions of the PDAE (1.2). Such stationary solution correspond to traveling wave solutions of (1.1).

There are already results concerning splitting methods for PDAEs as for example in [AO17, EO15, EO16]. The authors are interested in constrained PDEs where the constraint often occurs from boundary conditions. This setting is different from the one considered in this thesis.

The splitting approach allows to use different numerical methods for the subproblems. For the scheme derived in this thesis numerical simulations show quadratic convergence rates for the approximation of the numerical stationary solution obtained by long-time simulations. Corroborated by these results we expect that our numerical scheme is a suitable method to approximate traveling wave solutions. Up to our knowledge, so far there have been no analytical results concerning the approximation of traveling wave solutions by combining the method of freezing and operator splitting methods. In this work we present first analytical results for such a combination which indicate that this approach is indeed suitable to approximate traveling waves.

The main result of this thesis is a convergence result showing that on finite-time intervals the method described above yields arbitrary good approximations to the exact solution (Theorem 2.3.9). This ensures that the scheme is suitable to approximate traveling waves if the initial value of the scheme is far away from the stationary solution.

To prove convergence to a stationary solution one usually relies on the property of *asymptotic stability*. This means that a solution of the PDAE converges to the stationary solution provided we start sufficiently close to the stationary solution. In [Thü05, RM10] the authors analyzed under which conditions asymptotic stability for a stationary solution is given for certain frozen systems. We call the neighborhoods where the evolution of the initial values converges to the stationary solution *stability regions*. In [Thü05, RM10] only the existence of such regions is discussed. So a priori they may be very small. Assume we have an initial value for the Cauchy problem (1.1) not lying in the stability region with an exact solution however converging to a traveling wave. The finite time result of our scheme can then be used to ensure that the solution of our numerical method enters the stability region provided the step size is small enough. With this in mind the convergence result Theorem 2.3.9 is an important step towards a proof that our splitting scheme converges to a traveling wave solution for a large class of initial values, i.e. initial values which can be far away from the traveling wave but with an exact solution converging to it. To achieve this complete result one has to show the existence of asymptotic stability of stationary solutions of the splitting scheme. Such a result is out of scope of this thesis.

The proof of this convergence result, presented in Chapter 2, forms the core of this thesis. Based on this approach we introduce a splitting scheme where we apply the backward and forward Euler method to the linear PDAE and nonlinear ODE in the subproblems of the splitting scheme. This forms the basis for the numerical experiments in Chapter 5. Further we show in Chapter 4 that traveling wave solutions of (1.1) yield fixed points of our numerical scheme, which is validated in the numerical simulations as well.

This thesis is organized as follows. In the remaining chapter we give an introduction to the method of freezing and operator splitting methods. In Chapter 2 we are going to transform the PDAE to a system where we can obtain a solution representation via the variation-of-constants formula. We introduce a splitting approach for this new PDAE by using the exact flows of the subproblems. For this scheme we discuss a convergence proof for finite-time intervals. Finally, we are able to show that polynomials as nonlinearities in (1.1) satisfy the assumptions for the convergence proof. In Chapter 3 we introduce two approaches to get further to a full time discrete version of the splitting scheme. First we discuss an approach where the algebraic constraint is only fulfilled at the beginning of each linear subproblem. The second approach is a full time discrete scheme by using the backward and forward Euler method for the subproblems. In Chapter 4 we show that traveling waves coincide with stationary solutions of the transformed system. Using this we are able to show that traveling wave solutions yield fixed points of our numerical method. In Chapter 5 we validate the analytical results of this thesis by considering the Nagumo equation. In Chapter 6 we present a splitting approach to approximate traveling wave solutions for the Burgers' equation.

Notational Remarks

Throughout this thesis we use the L^2-inner product on the whole line $\mathbb{R}$ given by

$$\langle f, g \rangle := \int_{\mathbb{R}} f(x)g(x)dx.$$

From the beginning of Chapter 2 on we use the abbreviation for the H^s- and L^2-norm on $\mathbb{R}$ given by

$$\|\cdot\|_{H^s} := \|\cdot\|_{H^s(\mathbb{R})}, \qquad \|\cdot\|_{L^2} := \|\cdot\|_{L^2(\mathbb{R})}$$

for $s \in \mathbb{N}_0$.

1.1 Motivation

Many partial differential equations arising from applications in physics, chemistry and biology consist of different parts. A typical PDE is of the form

$$\partial_t u = Au + \partial_x f(u) + g(u) \qquad \text{on } \mathbb{R} \times [0, \infty) \tag{1.3}$$

where A is a linear differential operator and $f, g : \mathbb{R} \to \mathbb{R}$ are nonlinear functions. In certain cases one part of the equation is parabolic while another part is hyperbolic and these parts are nonlinearly coupled. Examples of such hyperbolic-parabolic coupled PDEs are hyperbolic models of chemosensitive movement or reaction-diffusion equations for which not all components diffuse.

One is often interested in special solutions which arise as (time-)asymptotic limits of solutions to the Cauchy problem for (1.3). An important class of such solutions are traveling waves. They describe how mass (or information) travels through the domain. On the basis of this interpretation, it becomes clear that one is often interested not only in the shape but also the velocity of the traveling wave. A precise definition of traveling waves is given in the following

Definition 1.1.1. *Given an evolution equation a* traveling wave $(\bar{u}, \bar{\mu})$ *is a solution of the form*

$$u(x,t) = \bar{u}(x - \bar{\mu}t), \qquad (x \in \mathbb{R}, t \geq 0)$$

for some speed $\bar{\mu} \in \mathbb{R}$ *and some non-constant profile* $\bar{u} : \mathbb{R} \to \mathbb{R}$ *connecting the two asymptotic states*

$$\lim_{x \to -\infty} \bar{u}(x) = u_- \quad \textit{and} \qquad \lim_{x \to +\infty} \bar{u}(x) = u_+.$$

In the phase portrait of a dynamical system the traveling wave is called a heteroclinic orbit if $u_- \neq u_+$, whereas in the case $u_- = u_+$ the traveling wave is referenced as a homoclinic orbit. In the setting of traveling waves we speak of a *traveling front* or a *traveling pulse*, respectively. Note that profiles of traveling waves are independent of the time t. There are many examples of equations yielding traveling waves given in an explicit form. Well known examples of the type of (1.4) are the viscous Burgers' equation, which can be used as a simple model for traffic density, and the Korteweg-de Vries' equation, which was derived to model waves on shallow water surfaces in a canal. They are given by

$$\begin{aligned} \partial_t u &= \partial_x^2 u + u \partial_x u \qquad \text{(Burgers)}, \\ \partial_t u &= \partial_x^3 u + u \partial_x u \qquad \text{(Korteweg-de Vries)}. \end{aligned}$$

Another example, for which the analysis is less complex, is the Nagumo equation

$$\partial_t u = \partial_x^2 u + u(1-u)(u-\alpha)$$

for $0 < \alpha < \frac{1}{2}$. In this case the nonlinearity does not contain any derivatives. For these equations explicit solutions such as traveling waves, pulses, sources and sinks are already known. But in many cases traveling wave solutions cannot be stated by an explicit expression since the profile and the corresponding speed are not known. In this work we are searching for traveling waves $(\bar{u}, \bar{\mu})$ using numerical schemes, more precisely using a long-time forward simulation. Namely, we use operator splitting methods to obtain an approximation of the exact solution of the evolution equation. Forward simulations require that the exact solution converges to a traveling wave for $t \to \infty$. In our discussion of traveling waves we consider PDEs with different kinds of nonlinearities. A class where the nonlinearity does not contain any derivatives is handled in Chapter 2. There we consider the problem from an analytic point of view, whereas in Chapter 5 we validate the results through numerical experiments. Since the Burgers' equation is more complex due to the presence of the spatial derivative in the nonlinearity, this equation is only dealt with numerically in Chapter 6. Before we consider any approach to approximate traveling waves, we introduce an extension of Sobolev spaces. In contrast to $L^2(\mathbb{R})$-functions, functions in this extended space do not have to converge to zero for $x \to \pm\infty$. Thus, we name these spaces Sobolev spaces with constant asymptotics. These function spaces allow a more general solution ansatz than the classical Sobolev spaces with vanishing asymptotics.

1.2 Sobolev Spaces with Constant Asymptotics

Throughout this section, let $s \in \mathbb{N}$. For a subset $\Omega \subseteq \mathbb{R}$ we denote with $H^s(\Omega)$ the Sobolev space $W^{s,2}(\Omega)$, and we set $H^0(\Omega) = L^2(\Omega)$. In most cases we will only consider $\Omega = \mathbb{R}$. Note that if a function v has non-vanishing asymptotics $v(x) \to v_\pm$ for $x \to \pm\infty$ where either $v_+ \neq 0$ or $v_- \neq 0$, then this function cannot lie in a Sobolev space $H^s(\mathbb{R})$, or even $L^2(\mathbb{R})$. Thus, a traveling wave u lying in $H^1(\mathbb{R})$ has to satisfy $u_- = u_+ = 0$ in the Definition 1.1.1. A remedy is to use locally $L^2(\mathbb{R})$-integrable functions and a local version of the Sobolev spaces. We recall the definition from [Alt16, Definition 5.13, p. 150] in a slightly adapted version. For this we introduce the following notation. Let $\Omega \subseteq \mathbb{R}$. We use the abbreviation $D \subset\subset \Omega$ for a relatively compact subset $D \subseteq \mathbb{R}$ with $\overline{D} \subseteq \Omega$.

Definition 1.2.1 ([Alt16])**.** *We define the vector space of* locally $L^2(\mathbb{R})$-integrable *functions by*

$$L^2_{loc}(\mathbb{R}) \coloneqq \{f : \mathbb{R} \to \mathbb{R} \mid f_{|_D} \in L^2(D) \text{ for all } D \subset\subset \mathbb{R}\}$$

and in a similar way we define

$$H^s_{loc}(\mathbb{R}) \coloneqq \{f : \mathbb{R} \to \mathbb{R} \mid f_{|_D} \in H^s(D) \text{ for all } D \subset\subset \mathbb{R}\}$$

for $s \in \mathbb{N}$. We set $H^0_{loc}(\mathbb{R}) = L^2_{loc}(\mathbb{R})$.

However, the typical norms on those spaces cannot be used anymore since the norms are in general not finite. But there exists a metric on $L^2_{\text{loc}}(\mathbb{R})$. Thus, we use another approach. Building on the above definition we construct certain spaces which will help us to transform the PDE such that we can use the classical Sobolev spaces. For this we introduce adapted Sobolev spaces with constant asymptotics, which we will denote by $\mathbb{H}^s_+(\mathbb{R})$, and state some of their basic properties.

Definition 1.2.2. *Let $s \in \mathbb{N}$. We define the Sobolev space with constant asymptotics by*

$$\mathbb{H}^s_+(\mathbb{R}) := H^s_{ca}(\mathbb{R}) + H^s(\mathbb{R})$$

with

$$H^s_{ca}(\mathbb{R}) := \Big\{ f \in H^s_{loc}(\mathbb{R}) \mid \exists\, (q,r,R) \in \mathbb{R}^3, R \geq 1 : \\ f(x) = q \text{ for } x \leq -R,\ f(x) = r \text{ for } x \geq R \Big\}.$$

In a similar way we define

$$L^2_{ca}(\mathbb{R}) := \Big\{ f \in L^2_{loc}(\mathbb{R}) \mid \exists\, (q,r,R) \in \mathbb{R}^3, R \geq 1 : \\ f(x) = q \text{ for } x \leq -R,\ f(x) = r \text{ for } x \geq R \Big\},$$
$$\mathbb{L}^2_+(\mathbb{R}) := L^2_{ca}(\mathbb{R}) + L^2(\mathbb{R}).$$

In particular, we have $H^0_{ca}(\mathbb{R}) := L^2_{ca}(\mathbb{R})$, $\mathbb{H}^0_+(\mathbb{R}) := \mathbb{L}^2_+(\mathbb{R})$.

Some properties we want to show for these spaces rely on the fact stated in the next lemma. For this we denote with $|I|$ the length of an interval $I \subseteq \mathbb{R}$.

Lemma 1.2.3. *There is a constant $c > 0$ such that for every open interval $I \subseteq \mathbb{R}$ with length $|I| \geq 1$ and $f \in H^1(I)$ it holds*

$$\|f\|_{L^\infty(I)} \leq c\,\|f\|_{H^1(I)}\,.$$

Here the constant c is independent of I and f.

Proof. This constant exists due to the continuous Sobolev embedding

$$H^1(I) \hookrightarrow L^\infty(I),$$

which in this form holds true in the one-dimensional case. A proof for the Sobolev embedding is stated in [Bre11, Theorem 8.8, p. 212]. Looking closer to the proof, one sees that the constant c arises as a product of two parts. Only the second depends on the length of the interval. This constant arises from the Extension Theorem [Bre11, Theorem 8.6, p. 209]. A remark following the theorem yields that the constant is bounded above by 8 if $|I| \geq 1$. □

Remark 1.2.4. Note that for small intervals I the constant arising in the Sobolev embedding depends on the length of the interval and tends to ∞ if $|I|$ goes to 0. For this reason we restrict ourselves to the case $|I| \geq 1$. Considering this we require the choice $R \geq 1$ in Definition 1.2.2 even if a priori this is an arbitrary choice and we could work with any positive constant. Since we are interested in situations where the profiles of the traveling waves extend to larger intervals this poses no constraint.

The constant c arising from the Sobolev embedding will occur throughout this section. We state some important properties for Sobolev spaces with constant asymptotics in

Lemma 1.2.5. *Let $s \in \mathbb{N}$ and $I \subseteq \mathbb{R}$ be an open interval with $1 \leq |I| \leq \infty$. In particular the case $I = \mathbb{R}$ is included.*

(i) If $f, g \in H^s(I)$, then $fg \in H^s(I)$. In particular, there is a constant $C(s,c) > 0$, only depending on s and the constant c arising in Lemma 1.2.3, such that

$$\|fg\|_{H^s(I)} \leq C(s,c) \|f\|_{H^s(I)} \|g\|_{H^s(I)} .$$

(ii) If $f, g \in H^s_{ca}(\mathbb{R})$, then $fg \in H^s_{ca}(\mathbb{R})$.

(iii) If $f \in \mathbb{H}^s_+(\mathbb{R})$ and $g \in H^s(\mathbb{R})$, then $fg \in H^s(\mathbb{R})$. In particular, it holds

$$\|fg\|_{H^s(\mathbb{R})} \leq K(f) \|g\|_{H^s(\mathbb{R})} ,$$

where $K(f) = K(f,s,c)$ is a positive constant only depending on f, s and c.

(iv) If $f, g \in \mathbb{H}^s_+(\mathbb{R})$, then $fg \in \mathbb{H}^s_+(\mathbb{R})$.

(v) If $f \in H^s_{ca}(\mathbb{R})$, then $\partial_x^i f \in H^{s-i}(\mathbb{R})$ for every $i = 1, \ldots, s$, where we have $H^0(\mathbb{R}) = L^2(\mathbb{R})$.

Proof. Note that the product rule also holds true for weak derivatives. This can be shown by using the Meyers-Serrin Theorem [Eva10, Section 5.3.2 Theorem 2, p. 251]. The proof of the product rule for Sobolev functions can be found in [Alt16, Theorem 4.25, p. 124]. Thus, if we regard two functions on an interval $I \subseteq \mathbb{R}$ for which the weak derivatives exist, the weak derivative of their product exists as well. Hence, in most cases we only have to verify the boundedness of the norms.

(i) Let $f, g \in H^s(I)$. It follows

$$\begin{aligned}
\|fg\|_{H^s(I)}^2 &= \sum_{j=0}^{s} \left\|\partial_x^j (fg)\right\|_{L^2(I)}^2 \\
&= \sum_{j=0}^{s} \left\| \sum_{k=0}^{j} \binom{j}{k} \left(\partial_x^{j-k} f\right) \left(\partial_x^k g\right) \right\|_{L^2(I)}^2 \\
&\le \sum_{j=0}^{s} \left[\left(\sum_{k=0}^{j-1} \binom{j}{k} \left\|(\partial_x^{j-k} f)(\partial_x^k g)\right\|_{L^2(I)}^2 \right) + \binom{j}{j} \left\|(\partial_x^0 f)(\partial_x^j g)\right\|_{L^2(I)}^2 \right] (j+1) \\
&\le \sum_{j=0}^{s} \left[\left(\sum_{k=0}^{j-1} \binom{j}{k} \left\|\partial_x^{j-k} f\right\|_{L^2(I)}^2 \left\|\partial_x^k g\right\|_{L^\infty(I)}^2 \right) + \|f\|_{L^\infty(I)}^2 \left\|\partial_x^j g\right\|_{L^2(I)}^2 \right] (j+1) \\
&\le \sum_{j=0}^{s} \left[\left(\sum_{k=0}^{j-1} \binom{j}{k} \|f\|_{H^s(I)}^2 c^2 \|g\|_{H^s(I)}^2 \right) + c^2 \|f\|_{H^1(I)}^2 \|g\|_{H^s(I)}^2 \right] (j+1) \\
&\le \sum_{j=0}^{s} \sum_{k=0}^{j} \binom{j}{k} (j+1) c^2 \|f\|_{H^s(I)}^2 \|g\|_{H^s(I)}^2 .
\end{aligned}$$

The second to last inequality follows by Lemma 1.2.3. The statement follows with $C(s,c) := \sqrt{\sum_{j=0}^{s} \sum_{k=0}^{j} \binom{j}{k} (j+1)} c$.

(ii) Let $f, g \in H^s_{\text{ca}}(\mathbb{R})$ and let $(q_f, r_f, R_f), (q_g, r_g, R_g) \in \mathbb{R}^3$ be the corresponding triples according to Definition 1.2.2. Chose $R := \max\{R_f, R_g\}$. It follows that $f(x)g(x) = q_f q_g =: q$ for $x \le -R$ and $f(x)g(x) = r_f r_g =: r$ for $x \ge R$. By the first assertion of the lemma it follows that for every open interval $J \subseteq \mathbb{R}$ the $H^s(J)$-norm can be bounded by

$$\|fg\|_{H^s(J)} \le C(s,c) \|f\|_{H^s(J)} \|g\|_{H^s(J)} .$$

This holds in particular for every finite interval. Hence $fg \in H^s_{\text{loc}}(\mathbb{R})$ by definition since the weak derivative exists as well and we obtain $fg \in H^s_{\text{ca}}(\mathbb{R})$ with (q, r, R) as given above.

(iii) Let $f \in \mathbb{H}^s_+(\mathbb{R})$ and $g \in H^s(\mathbb{R})$. There is $v \in H^s_{\text{ca}}(\mathbb{R})$ and $\psi \in H^s(\mathbb{R})$ such that $f = v + \psi$ and

$$fg = (v + \psi)g = vg + \psi g.$$

Using (i) we know that $\psi g \in H^s(\mathbb{R})$. Let $(q, r, R) \in \mathbb{R}^3$ be the constants from Definition 1.2.2 for $v \in H^s_{\text{ca}}(\mathbb{R})$. To show that vg is an element of $H^s(\mathbb{R})$ we have to prove that the weak derivatives exists and that the $H^s(\mathbb{R})$-norm is bounded. For the boundedness of the norm let $J \coloneqq (-R, R)$. We obtain using (i)

$$\begin{aligned}\sum_{j=0}^{s}\int_{-R}^{R}|\partial_x^j(v(x)g(x))|^2dx &= \|vg\|_{H^s(J)}^2\\ &\leq C(s,c)^2\,\|v\|_{H^s(J)}^2\,\|g\|_{H^s(J)}^2\\ &= \sum_{j=0}^{s}C(s,c)^2\,\|v\|_{H^s(J)}^2\int_{-R}^{R}|\partial_x^j g(x)|^2dx.\end{aligned}$$

Therefore,

$$\begin{aligned}\|vg\|_{H^s(\mathbb{R})}^2 &= \sum_{j=0}^{s}\int_{-\infty}^{\infty}|\partial_x^j(v(x)g(x))|^2dx\\ &= \sum_{j=0}^{s}\left(\int_{-\infty}^{-R}|q\partial_x^j g(x)|^2dx + \int_{-R}^{R}|\partial_x^j(v(x)g(x))|^2dx + \int_{R}^{\infty}|r\partial_x^j g(x)|^2dx\right)\\ &\leq \sum_{j=0}^{s}\Big(q\int_{-\infty}^{-R}|\partial_x^j g(x)|^2dx + \left(C(s,c)^2\,\|v\|_{H^s(J)}^2\right)\int_{-R}^{R}|\partial_x^j g(x)|^2dx\\ &\qquad + r\int_{R}^{\infty}|\partial_x^j g(x)|^2dx\Big)\\ &\leq 3\max\left\{q,r,C(s,c)^2\,\|v\|_{H^s(J)}^2\right\}\sum_{j=0}^{s}\int_{-\infty}^{\infty}|\partial_x^j g(x)|^2dx\\ &= 3\max\left\{q,r,C(s,c)^2\,\|v\|_{H^s(J)}^2\right\}\|g\|_{H^s(\mathbb{R})}^2.\end{aligned}$$

If we set $\kappa(v) \coloneqq \sqrt{3\max\left\{q,r,C(s,c)^2\,\|v\|_{H^s(J)}^2\right\}}$ we obtain

$$\begin{aligned}\|fg\|_{H^s(\mathbb{R})} &= \|vg+\psi g\|_{H^s(\mathbb{R})}\\ &\leq \|vg\|_{H^s(\mathbb{R})} + \|\psi g\|_{H^s(\mathbb{R})}\\ &\leq \kappa(v)\,\|g\|_{H^s(\mathbb{R})} + C(s,c)\,\|\psi\|_{H^s(\mathbb{R})}\,\|g\|_{H^s(\mathbb{R})}\\ &= (\kappa(v)\ + C(s,c)\,\|\psi\|_{H^s(\mathbb{R})})\,\|g\|_{H^s(\mathbb{R})}\\ &= K(f)\,\|g\|_{H^s(\mathbb{R})}\end{aligned}$$

with $K(f) \coloneqq \kappa(v)\ + C(s,c)\,\|\psi\|_{H^s}$, where v, ψ directly depend on f as given above.

The existence of the first weak derivative $\partial_x(fg)$ on $\mathbb{R}$ can be shown as follows. We set $J = [-R-1, R+1] \subseteq \mathbb{R}$, then we denote with $\tilde{v} \in C(J), \tilde{g} \in C(\mathbb{R})$ the unique continuous representative of v and g, respectively. The existence of the unique continuous representative follows by [Bre11, Theorem 8.2, p. 204] with

$$\begin{aligned} v(x) &= \tilde{v}(x) &&\text{a.e. on J,}\\ g(x) &= \tilde{g}(x) &&\text{a.e. on } \mathbb{R}.\end{aligned}$$

The function v is constant on $[-R-1,-R]$ and $[R,R+1]$. By continuity of $\tilde{v}$, we obtain $\tilde{v}(-R) = v(-R) = q$ and $\tilde{v}(R) = v(R) = r$. For the weak derivative we obtain by integration by parts since $\tilde{v}, \tilde{g}$ are continuous and can be evaluated at every point

$$\begin{aligned}
\int_{-\infty}^{\infty} vg\varphi' dx &= \int_{-\infty}^{-R} q\tilde{g}\varphi' dx + \int_{-R}^{R} \tilde{v}\tilde{g}\varphi' dx + \int_{R}^{\infty} r\tilde{g}\varphi' dx \\
&= -\int_{-\infty}^{-R} q\tilde{g}'\varphi dx + q\tilde{g}(-R)\varphi(-R) \\
&\quad - \int_{-R}^{R} (\tilde{v}\tilde{g})'\varphi dx + \tilde{v}(R)\tilde{g}(R)\varphi(R) - \tilde{v}(-R)\tilde{g}(-R)\varphi(-R) \\
&\quad - \int_{R}^{\infty} r\tilde{g}'\varphi dx - r\tilde{g}(R)\varphi(R) \\
&= -\int_{-\infty}^{\infty} h\varphi dx,
\end{aligned}$$

for every test function $\varphi \in C_c^\infty(\mathbb{R})$ with

$$h(x) := \begin{cases} q\tilde{g}'(x) & , x \leq -R \\ (\tilde{v}(x)\tilde{g}(x))' & , -R < x < R \\ r\tilde{g}'(x) & , x \geq R. \end{cases}$$

The other terms vanish since $\tilde{v}(-R) = q, \tilde{v}(R) = r$. The existence of the other weak derivatives follow by (v), which will be proven below.

(iv) Let $f, g \in \mathbb{H}_+^s(\mathbb{R})$ and $f = v + \varphi, g = w + \psi$ with $v, w \in H_{\text{ca}}^s(\mathbb{R})$ and $\varphi, \psi \in H^s(\mathbb{R})$. We have

$$fg = (v+\varphi)(w+\psi) = vw + v\psi + \varphi w + \varphi\psi,$$

where $vw \in H_{\text{ca}}^s(\mathbb{R})$ by (ii) and $v\psi, \varphi w \in H^s(\mathbb{R})$ by (iii) and $\varphi\psi \in H^s(\mathbb{R})$ by (i). This finishes the proof.

(v) Let $f \in H_{\text{ca}}^s(\mathbb{R})$, i.e. by Definition 1.2.2 there is a $R > 0$ such that f takes constant values on the intervals $(-\infty, -R]$ and $[R, \infty)$. We set $J := [-R, R]$. Let $i \in \{1, \ldots, s\}$. It follows

$$\partial_x^i f(x) = 0 \qquad (x \notin J)$$

and thus $\|\partial_x^i f\|_{H^{s-i}(\mathbb{R})} = \|\partial_x^i f\|_{H^{s-i}(J)}$. The proof follows since $f \in H_{\text{loc}}^s(\mathbb{R})$, i.e. $\|\partial_x^i f\|_{H^s(J)} < \infty$ for the relative compact subset $J \subseteq \mathbb{R}$. $\square$

1.3 An Introduction to the Method of Freezing

We are looking at partial differential equations of the type

$$\partial_t u = Au + f(u) \qquad \text{on } \mathbb{R} \times [0, T] \tag{1.4}$$

for some linear differential operator A, some nonlinear function $f : \mathbb{R} \to \mathbb{R}$ and some $T > 0$ with $u : \mathbb{R} \times [0, T] \to \mathbb{R}$. As mentioned before, we propose a numerical scheme to approximate traveling wave solutions for the Cauchy problem (1.4) based on splitting methods. To the best of our knowledge, so far there are only numerical results for such an approach. In this work we present first analytical results. Nevertheless, there are already established methods to approximate traveling wave solutions. In many situations the techniques used are based on Newton solvers for the boundary value problem corresponding to (1.4) as described in the beginning of this thesis. These techniques are for example used for numerical continuation and are a well-established method. A disadvantage of these methods is that the initial data for the Newton solver often has to be very close to a traveling wave. If one is not interested in continuation methods, as continuation is a very special ansatz to find similar solutions, such initial values for the Newton solvers can be obtained by long-time forward simulations of the time-dependent problem (1.4). A forward simulation does not solve the boundary value problem but simulates the solution of the evolution equation in forward time. We exploit this fact and introduce a numerical scheme based on a forward simulation which efficiently approximates a traveling wave. In general, in a forward simulation the problem arises that every traveling wave with non-zero speed leaves the computational domain, which has to be finite for numerical simulations. To overcome this problem we use the *method of freezing*, cf. [BOR14, Thü05, RM10]. The idea behind this technique is that the computational domain or more general the spatial frame should travel with the speed of the traveling wave. In the ideal case this would fix the position of the traveling wave in the new spatial frame. Since the traveling wave we want to approximate is unknown, the speed is typically unknown as well and we have to use an approximation to the speed to fix the spatial frame. Here we rely on an unknown speed $\mu(t)$ varying in time t to capture the behavior that the speed of the traveling wave may change as the profile evolves. Given a general evolution equation $\partial_t u = F(u)$, one uses the ansatz

$$\begin{aligned} u(x,t) &= v(x - \gamma(t), t), \\ \partial_t \gamma(t) &= \mu(t), \end{aligned} \tag{1.5}$$

where $\gamma(t) \in \mathbb{R}$ is the position of the spatial frame at time t. The last equation is given by the physical dependence that the derivative of the position is the speed. Differentiating the first equation with respect to the time t we get

$$(\partial_t u)(x,t) = (\partial_t v)(x-\gamma(t),t) - \partial_t\gamma(t)\cdot(\partial_x v)(x-\gamma(t),t) = F(v(x-\gamma(t),t)).$$

This yields

$$\partial_t v = F(v) + \mu(t)\partial_x v \tag{1.6}$$

in the new coordinates $(\xi,t) = (x-\gamma(t),t)$. This new coordinates are called the *co-moving frame*. As mentioned, the speed $\mu(t)$ in the obtained equation (1.6) is often unknown and to retain well-posedness of the partial differential equation we need an additional condition. As suggested in [BOR14, Section 2.1, p. 105-107] there are two suitable choices which add an algebraic constraint to the PDE. If we apply the ansatz described above to the problem given in (1.4), we obtain the *frozen system*

$$\begin{cases} \partial_t u = Au + f(u) + \mu(t)\partial_x u, \\ \quad 0 = \Psi(u,\mu(t)), \end{cases} \qquad (t \in [0,T]) \tag{1.7}$$

where we denote the solution by u as well such that u corresponds to v in (1.5). This system is now a *partial differential algebraic equation* (PDAE) since the second equation does not involve any derivatives with respect to the time t. The constraint involving the function Ψ is called *phase condition*. This transformation to a PDAE with a suitable phase condition is called the *method of freezing*. The two typical choices for this algebraic constraint are the *orthogonality phase condition* Ψ_{o} and the *fixed phase condition* Ψ_f, which are given by

$$\begin{aligned} \Psi_{\mathrm{o}}(u,\mu) &= \langle \partial_t u, \partial_x u\rangle, \\ \Psi_f(u,\mu) &= \langle \partial_x \hat{u}, u-\hat{u}\rangle, \end{aligned}$$

where $\hat{u}$ is a suitable reference function. In these particular cases the functions Ψ_{o} and Ψ_f do not depend on μ but in general this does not hold. As discussed in [BOR14, Section 2.1, p. 106-107] the function Ψ_o can be obtained by minimizing $\|\partial_t u(t)\|_{L^2}$ at each time t, whereas Ψ_f is derived by requiring that u satisfies

$$\min_{x_0\in\mathbb{R}} \|u(\cdot,t) - \hat{u}(\cdot - x_0)\|_{L^2(\mathbb{R})} = \|u(\cdot,t) - \hat{u}(\cdot)\|_{L^2(\mathbb{R})}.$$

The required properties for the a reference function $\hat{u}$ will be stated below. Even in numerical simulations the orthogonal phase condition leads sometimes to wrong calculations of the speed of the co-moving frame such that the traveling wave leaves the computational domain, cf. Section 6.2. Thus, we restrict ourselves to the fixed phase condition for the rest of this thesis except for Chapter 6.

From now on we denote with $\hat{u}$ a reference function for the fixed phase condition. This function has to be sufficient smooth as we will see later. For the convergence proof we have to state some assumptions on the problem and on the reference function $\hat{u}$, which are not very restrictive for the purpose of approximating traveling waves. These assumptions will be discussed in this section. Note that it is suitable to use a very coarse approximation to the traveling wave as reference function $\hat{u}$, as we will see below. We use the name *reference function*, because this might be the first guess for a traveling wave we are searching for and should be distinguished from the reference solution in numerical simulations in later chapters.

First, we discuss in detail the general assumptions on the traveling wave and reference function and then state them in concise form in Assumption 1.3.1. First of all, given a PDE of the form (1.4) we assume the existence of a traveling wave $(\bar{u}, \bar{\mu})$. This is necessary, since there is no complete existence theory for traveling waves of this PDE with arbitrary nonlinearity f. Moreover, we assume that the asymptotic states $u_\pm$ are known. Depending on the problem, these states can often be derived from the given nonlinearity. Since we are interested in connecting the left asymptotic state u_- and the right asymptotic state u_+, the inequality $\|\partial_x \bar{u}\|_{L^2(\mathbb{R})} > 0$ is satisfied for traveling fronts, i.e. $u_- \neq u_+$. In the case of pulses, $u_- = u_+$, this is satisfied as well if the traveling wave is not trivial, i.e. $\bar{u} \not\equiv \mathit{const}$. Thus, we are searching for a non-trivial traveling wave $(\bar{u}, \bar{\mu})$ such that $\|\partial_x \bar{u}\|_{L^2} > 0$. We fix a reference function for the fixed phase condition denoted by $\hat{u}$ lying in a suitable Hilbert space with the same asymptotic states, i.e.

$$\lim_{x \to \pm\infty} \bar{u}(x) = u_\pm = \lim_{x \to \pm\infty} \hat{u}(x). \tag{1.8}$$

This is fulfilled if there exists a (large) constant $R > 0$ such that

$$\hat{u}(x) = u_\pm \qquad \text{for } x < -R \text{ and } x > R.$$

By this condition $\partial_x \hat{u}$ has compact support, which simplifies integration by parts. These properties are summed up in the space $H^s_{\mathrm{ca}}(\mathbb{R})$ with $s \geq 0$ introduced in Definition 1.2.2. Later we need $\hat{u} \in H^6_{\mathrm{ca}}(\mathbb{R})$. The considerations above also justifies the assumption

$$\langle \partial_x \hat{u}, \partial_x \hat{u} \rangle > 0. \tag{1.9}$$

In addition, we impose that the phase condition satisfies the property

$$\langle \partial_x \hat{u}, \partial_x \bar{u} \rangle > 0$$

for the reference function $\hat{u}$. This assumption expresses that in most segments the reference function follows the behavior of the profile of the traveling wave, i.e. either both functions are increasing or decreasing. All these assumptions are summarized by

Assumption 1.3.1. *We make the following assumption to the traveling wave and to the reference function.*

(i) There exists a non-constant traveling wave $(\bar{u}, \bar{\mu}) \in \mathbb{H}^4_+(\mathbb{R}) \times \mathbb{R}$ *of the PDE* (1.4), *i.e.*

$$\langle \partial_x \bar{u}, \partial_x \bar{u} \rangle > 0.$$

(ii) The reference function $\hat{u} \in H^6_{ca}(\mathbb{R})$ *satisfies*

$$\langle \partial_x \hat{u}, \partial_x \hat{u} \rangle > 0 \quad \textit{and} \quad \langle \partial_x \hat{u}, \partial_x \bar{u} \rangle > 0.$$

In Chapter 4 we will introduce the counterpart of a traveling wave of the original system (1.6) in the setting of the frozen PDAE (1.7), which is called a steady state. We will show that traveling wave solutions of the original problem (1.6) yield steady states of the frozen PDAE (1.7) and vice versa. This was already discussed in a different setting in [Thü05].

The method of freezing can also be used in higher dimensions. It was applied to the two dimensional Burgers' equation in [RM19]. But in the present thesis we restrict ourselves to the one-dimensional case.

It turns out that the fixed phase condition is more robust than the orthogonality phase condition as we will see in Chapter 6, which is also discussed in [BOR14, Section 2.1, p. 105-107]. The orthogonality phase condition has another disadvantage. The ansatz we choose requires a suitable projection to handle the algebraic constraint as we will see in the next chapter. The construction of such a projection is much more complicated in the case of the orthogonality phase condition, since it only contains terms which depend on the solution itself.

1.4 An Introduction to Operator Splitting Methods

In this section we give a short introdution for operator splitting methods or, in short, splitting methods. Splitting methods are a useful technique to approximate solutions $u : \mathbb{R}_+ \to X$ of initial value problems of the form

$$\begin{cases} \partial_t u = A(u) + B(u) \\ u(0) = u_0 \in X. \end{cases} \tag{1.10}$$

Here, $A : \mathcal{D}(A) \to X$ and $B : \mathcal{D}(B) \to X$ are two operators for some Banach space $(X, \|\cdot\|)$. The idea is to split the sum on the right-hand side of the evolution equation into two parts to obtain two simpler initial value problems. Those are given by

$$\begin{cases} \partial_t u = A(u) \\ u(0) = v \in X \end{cases} \tag{1.11}$$

and

$$\begin{cases} \partial_t u = B(u) \\ u(0) = w \in X \end{cases} \tag{1.12}$$

for initial values v and w. We assume the existence of solutions for both problems. Denote with $\Phi_A^t(v)$ the solution operator to the first subproblem at time $t \in \mathbb{R}_+$ and with $\Phi_B^t(w)$ the solution operator to the second subproblem. In many cases, these subproblems prove to be easier to solve than the original problem (1.10). The idea is to iterate the solutions of the problems (1.11) and (1.12) with a given step size $\tau > 0$ to obtain an approximation to a solution of the original problem. We define $t_n = n\tau$ for $n \in \mathbb{N}_0$. The simplest choice to iterate those subproblems is the *Lie-Trotter splitting*, which is given by

$$u_{n+1} = \Phi_B^\tau \circ \Phi_A^\tau(u_n). \qquad (n \in \mathbb{N}_0) \tag{1.13}$$

Here u_{n+1} is supposed to be an approximation to the exact solution u at time t_{n+1}, i.e. $u_{n+1} \approx u(t_{n+1})$. Those approximations typically converge linearly to the exact solution for $\tau \to 0$, this is

$$\|u_n - u(t_n)\| \leq \tau C$$

for some constant $C > 0$. A splitting method that leads to second order convergence under suitable regularity assumptions is the *Strang splitting*,

$$u_{n+1} = \Phi_A^{\tau/2} \circ \Phi_B^\tau \circ \Phi_A^{\tau/2}(u_n). \qquad (n \in \mathbb{N}_0) \tag{1.14}$$

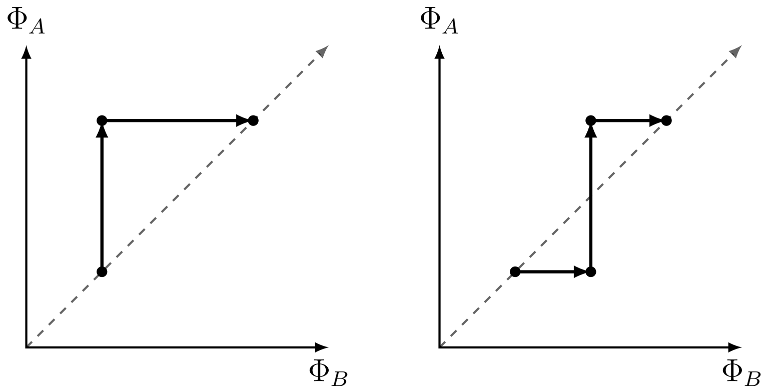

Figure 1.1: Diagram of the Lie-Trotter splitting on the left and the Strang splitting on the right.

For example in [HLR13], the authors show that this scheme is second order convergent for the viscous Burgers' PDE provided the solution is sufficiently regular. Lie and Strang splitting are illustrated by diagrams in Figure 1.1. A step in the vertical direction in Figure 1.1 amounts in solving the Cauchy problem (1.11), whereas a step in the horizontal direction amounts to solve the Cauchy problem (1.12). Only states on the dashed diagonal line might be considered as approximations to solutions to the original problem. We apply the Strang splitting to the frozen PDAE of the viscous Burgers' equation in Chapter 6 and in numerical simulations we see that the resulting method is able to approximate traveling waves of the viscous Burgers' equation.

The basic idea behind splitting methods goes back to the case where A and B are bounded linear operators on X, i.e. $A, B \in L(X,X)$. In this section we define the operator

$$e^Z := \sum_{k=0}^{\infty} \frac{Z^k}{k!}. \qquad (Z \in L(X,X))$$

One can easily show that for $Z_1, Z_2 \in L(X,X)$ the properties

$$\begin{aligned} \partial_t e^{tZ_1} &= Z_1 e^{tZ_1} \\ e^{Z_1+Z_2} &= e^{Z_1} e^{Z_2} \end{aligned}$$

hold true if $Z_1 Z_2 = Z_2 Z_1$, i.e. if Z_1 and Z_2 commute. Thus, if $A, B \in L(X,X)$, then the operators $e^{tA}v$ and $e^{tB}w$ solve the initial value problems (1.11) and (1.12). If in addition the operators A, B commute, the operator $e^{tA}e^{tB}u_0 = e^{t(A+B)}u_0$ solves the Cauchy problem (1.10) and the Lie and Strang splitting yield the exact solution. In most cases the operators do not commute or lack boundedness or linearity. Then a splitting approach can be used to derive approximations to the exact solution. In the special case where the operators are bounded and linear but do not commute one can use the Baker-Campbell-Hausdorff formula to give a representation of the error. In the general case the convergence proofs can be very complicated as in [HLW06] or as in the proof of Theorem 2.3.9.

We outline an important benefit of operator splitting methods. Assume that we want to get numerical approximations for a differential equation with a linear operator A and a nonlinear operator B, e.g.

$$\partial_t u = Au + B(u). \tag{1.15}$$

Applying a splitting approach yields two subproblems

$$\partial_t v = Av, \qquad \partial_t w = B(w),$$

which can be solved using a different method for each problem. The big advantage splitting methods provide is that we can easily combine explicit and implicit schemes to tackle the subproblems. Even the simple case of applying the backward and forward Euler method to the linear and nonlinear subproblems gives an insight to the benefits of the splitting approach.

For the first linear subproblem an implicit scheme might be more suitable in certain cases. If we approximate the linear subproblem with the backward Euler method, one typically only needs to solve one linear system using one LU decomposition. On the other hand, an explicit scheme would require very small step sizes if the subproblem is stiff, which is an often occurring case. If we apply the backward Euler method to the second nonlinear problem, we have to solve the occurring fixed-point equation with Newton's method, including a LU decomposition in every step of the Newton scheme. Therefore, implicit schemes for nonlinear problems require more computational effort and are typically avoided. Moreover, in many cases the nonlinearity does not contain any spatial derivatives and therefore is typically not stiff. By this reason explicit schemes are more suitable for nonlinear problems.

Since we separated the linear and nonlinear part by the splitting approach, we can use a backward Euler method for the linear subproblem and apply a forward Euler method to the nonlinear subproblem. This leads to an efficient scheme to approximate solutions of (1.15). We exploit this advantage in the construction of the splitting approaches in Section 2.2.1 and Chapter 6.

CHAPTER

TWO

DEVELOPING A SPLITTING APPROACH FOR FREEZING WAVES

In this chapter we develop a scheme based on the Lie-Trotter splitting to approximate solutions $(u, \mu) : [0, T] \to \mathbb{H}^1_+(\mathbb{R}) \times \mathbb{R}$ of the PDAE

$$\begin{cases} \partial_t u = Au + f(u) + \mu \partial_x u, \quad u(0) = u_0, \\ \quad 0 = \langle \partial_x \hat{u}, u - \hat{u} \rangle \end{cases} \tag{2.1}$$

obtained by the method of freezing. Here we consider the differential operator

$$\begin{aligned} A : \mathcal{D}(A) = H^2(\mathbb{R}) \subseteq L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ z &\mapsto \partial_x^2 z \end{aligned}$$

and a nonlinear function $f : \mathbb{H}^1_+(\mathbb{R}) \to \mathbb{H}^1_+(\mathbb{R})$. To obtain the splitting scheme, we will first transform the system such that solutions of the new system lie in $H^2(\mathbb{R})$, and we will give the definition of a solution in the new system. For a solution representation of systems of this form we use a variation-of-constants formula of a projected version of the evolution equation. For convenience we will use the following notations for $s \in \mathbb{N}_0$

$$\|\cdot\|_{H^s} \coloneqq \|\cdot\|_{H^s(\mathbb{R})}, \qquad \|\cdot\|_{L^2} \coloneqq \|\cdot\|_{L^2(\mathbb{R})}.$$

The scheme which we develop in this chapter is constructed with the intention to approximate traveling wave solutions occurring as the time-limit $t \to \infty$ of the solution $u(t)$ for suitable initial values u_0.

The main goal of this chapter is to prove convergence on finite-time intervals of the approximations obtained by the new scheme. Note that we prove first order error estimates for a finite-time interval in contrast to the infinite asymptotic $t \to \infty$. Typically, the finite-time estimates are upper bounds of the global error of the form $\tau C e^{cT}$. Those estimates do not allow any statements for $T \to \infty$.

The proceeding of this chapter is as follows. First we are going to transform the PDAE to a system where we can obtain a solution representation via the variation-of-constants formula. We introduce a splitting approach for this new PDAE by using the exact flows of the subproblems. For this scheme we discuss a convergence proof for finite-time intervals. Finally, we are able to show that polynomials as nonlinearities in (2.1) satisfy the assumptions for the convergence proof.

2.1 Solution Representation of the PDAE via Projection

In this section we construct an integral representation of the solution operator of the PDAE, obtained by the method of freezing for the fixed phase condition, i.e. we are searching for a solution u of

$$\begin{cases} \partial_t u = Au + f(u) + \mu \partial_x u, \quad u(0) = u_0, \\ \quad 0 = \langle \partial_x \hat{u}, u - \hat{u} \rangle. \end{cases}$$

This is achieved by applying a variation-of-constants formula in the context of analytic semigroups. It is more challenging to construct a closed solution formula for this system because of the algebraic constraint. Nevertheless, after applying a suited projection to the system, we can use the variation-of-constants formula to represent the solution in an accessible way. First, we need to transform the system such that we are able to apply a projection, i.e. an idempotent endomorphism. Another benefit of the transformation is that the solution of the transformed system lies in $L^2(\mathbb{R})$, i.e. in a normed vector space. Here we restrict the analysis to the method of freezing with the fixed phase condition.

The basic concept for the solution representation is taken from [Thü05], although the setting is quite different: The author applies a linearization at the traveling wave to the frozen system and studies the stability of the traveling wave. In her setting one can use a transformation along the kernel of the resulting linear operator in a straightforward way. In addition, because she is looking at the linearization, one always obtains a linear algebraic constraint. Although we are not using a linearization, it turns out that we are able to transform the right-hand side of the algebraic constraint to a linear operator in a straightforward way and construct a similar solution representation for the PDAE. In addition, the transformation in [Thü05] makes use of the knowledge of a traveling wave in advance. Since she uses this transformation to show certain properties of the traveling wave, this poses no problem. However for the scheme we want to develop this is not the right approach since this scheme is supposed to approximate the traveling wave. Without knowledge of the traveling wave one is in need of an approximation. Here we use the reference function $\hat{u}$ for the transformation, since it can be chosen beforehand.

2.1.1 Transformation of the PDAE

The function spaces $H^s_{\text{ca}}(\mathbb{R})$ and $\mathbb{H}^s_+(\mathbb{R})$ introduced in Section 1.2 are suitable to describe traveling wave solutions. But in contrast to the classical Sobolev spaces $H^s(\mathbb{R})$ there is no straightforward way to use semigroup theory for these function spaces. In particular there is no (easy) way to construct a norm on these spaces as they are subspaces of $L^2_{\text{loc}}(\mathbb{R})$. Thus, we are going to shift the function by the reference function $\hat{u} \in H^6_{\text{ca}}(\mathbb{R})$. In the transformed system we search for solutions in the classical L^2 and Sobolev setting. In addition, this transformation will add a Lagrange multiplier (see for example in [HLW06, Chapter IV.4]) to the equation and transform the right-hand side of the algebraic constraint from an affine linear mapping to a linear one. The original problem in the co-moving frame is given by

$$\begin{cases} \partial_t v = Av + f(v) + \mu \partial_x v, \quad v(0) = v_0 \qquad (x \in \mathbb{R}) \\ \quad 0 = \langle \psi, v - \hat{u} \rangle \end{cases} \tag{2.2}$$

using the fixed phase condition and defining $\psi := \partial_x \hat{u}$.

Definition 2.1.1. *We call a function $z \in L^2(\mathbb{R})$* ***consistent*** *(with the algebraic constraint) if it satisfies the algebraic constraint of the underlying PDAE.*

The transformation of the system is stated in

Lemma 2.1.2. *Let $\hat{u} \in H^{s+2}_{ca}(\mathbb{R})$ with $(u_-, u_+, R) \in \mathbb{R}^3, s \in \mathbb{N}$ and assume that*

$$f : \mathbb{H}^1_+(\mathbb{R}) \to \mathbb{H}^1_+(\mathbb{R}) \quad \textit{satisfies} \quad f(z + \hat{u}) \in H^s(\mathbb{R}) \quad (z \in H^s(\mathbb{R})).$$

In addition, let the initial value $v_0 \in \mathbb{H}^s_+(\mathbb{R})$ be consistent with the algebraic constraint.

Then $v \in \mathbb{H}^s_+(\mathbb{R})$ with (u_-, u_+, R) solves the Cauchy problem

$$\begin{cases} \partial_t v = Av + f(v) + \mu \partial_x v, \quad v(0) = v_0 \qquad (x \in \mathbb{R}) \\ \quad 0 = \langle \psi, v - \hat{u} \rangle \end{cases} \tag{2.3}$$

if and only if $u := v - \hat{u} \in H^s(\mathbb{R})$ *solves*

$$\begin{cases} \partial_t u = Au + g(u) + \mu\partial_x u + \mu\psi, \quad u(0) = v_0 - \hat{u} =: u_0 \qquad (x \in \mathbb{R}) \\ 0 = \langle \psi, u \rangle, \end{cases} \tag{2.4}$$

where

$$\begin{aligned} g : H^1(\mathbb{R}) &\to H^1(\mathbb{R}) \\ u &\mapsto g(u) := f(u + \hat{u}) + \psi' = f(u + \hat{u}) + A\hat{u} \end{aligned} \tag{2.5}$$

is a nonlinear operator.

Note that a necessary condition for $f(z + \hat{u}) \in H^s(\mathbb{R})$ for all $z \in H^s(\mathbb{R})$ is that u_- and u_+ are roots of the nonlinearity f, i.e. $f(u_-) = f(u_+) = 0$. In fact, this condition is also sufficient for polynomial nonlinearities, as we will see later. Although f is a nonlinear function, the transformed nonlinearity g is a nonlinear operator since $\hat{u}$ depends on the spatial variable x. This will be discussed in detail in Section 2.3.3 for polynomial nonlinearities.

Proof. The transformation of the system is given by $u = v - \hat{u}$ ($v = u + \hat{u}$) with $\partial_x \hat{u} = \psi$. We obtain

$$\begin{aligned} \partial_t v = \partial_t u &= Au + A\hat{u} + f(u + \hat{u}) + \mu\partial_x u + \mu\partial_x \hat{u} \\ &= Au + g(u) + \mu\partial_x u + \mu\psi \\ 0 &= \langle \psi, u + \hat{u} - \hat{u} \rangle \\ &= \langle \psi, u \rangle \end{aligned}$$

with the nonlinear function

$$\begin{aligned} g : H^s(\mathbb{R}) &\to H^s(\mathbb{R}) \\ z &\mapsto g(z)(x) = f(z(x) + \hat{u}(x)) + \psi'(x). \end{aligned}$$

Combining the assumptions and Lemma 1.2.5 (v) the property $g(z) \in H^s(\mathbb{R})$ follows for every $z \in H^s(\mathbb{R})$. This shows the equivalence of the systems. It remains to show that $u = v - \hat{u}$ lies in fact in $H^s(\mathbb{R})$. Since $v \in \mathbb{H}^s_+(\mathbb{R})$, there is $a \in H^s_{\text{ca}}(\mathbb{R})$ with (u_+, u_-, R) and $b \in H^s(\mathbb{R})$ such that $v = a + b$. It follows that

$$u = v - \hat{u} = a - \hat{u} + b,$$

where $(a - \hat{u})(x) = 0$ for all $x \leq -R$ and $x \geq R$. Thus, the sum $a - \hat{u} \in H^s_{\text{loc}}(\mathbb{R})$ has compact support and it follows that $a - \hat{u} \in H^s(\mathbb{R})$. As a result u lies in $H^s(\mathbb{R})$. □

Throughout the rest of this chapter, we will only regard the problem in the transformed variable u so that we can use the well-established semigroup theory for Sobolev spaces. But keep in mind that given a problem in the original variables, one has to transform the problem first to check the assumptions stated in the rest of this chapter. In the following we will use the transformed PDAE given as

$$\begin{cases} \partial_t u(t) = Au(t) + g(u(t)) + \mu(t)\partial_x u(t) + \mu(t)\psi, & \quad (2.6a) \\ \qquad 0 = \langle \psi, u(t) \rangle, & (t \in [0,T]) \quad (2.6b) \\ \quad u(0) = u_0 \end{cases}$$

with the Lagrange multiplier $\mu(t)$. The Lagrange multiplier will become important in the next step where we construct a projected PDE equivalent to the system above to which we apply the variation-of-constants formula. Since the map $\xi \mapsto M\langle \psi, \xi \rangle$, where the constant M is given by $M \coloneqq \langle \psi, \psi \rangle^{-1}$, is a left inverse of the mapping $c \mapsto c\psi$ for $c \in \mathbb{R}$, we can easily solve for the unknown speed μ in this equation. We use the orthogonal projector P given in

Definition 2.1.3. *We define the operator*

$$\begin{aligned} P : L^2(\mathbb{R}) &\to \mathcal{R}(P) \subseteq L^2(\mathbb{R}) \\ z &\mapsto z - \psi M \langle \psi, z \rangle \quad \text{with} \quad M \coloneqq \langle \psi, \psi \rangle^{-1} = \|\psi\|_{L^2}^{-2}. \end{aligned}$$

Note that $\langle \psi, \psi \rangle > 0$ by (1.9) from Assumption 1.3.1 on the phase condition. This operator will be used throughout this work without further reference. By the choice of M, the operator P projects along the direction ψ to the subspace where the algebraic constraint is satisfied as stated in

Lemma 2.1.4. *The operator P is a bounded projector with range*

$$\mathcal{R}(P) = \{ z \in L^2(\mathbb{R}) : 0 = \langle \psi, z \rangle \}.$$

In addition for $s \in \mathbb{N}_0$ and $\psi \in H^s$, the operator norm for P as an operator $P : H^s \to H^s$ is bounded by

$$\|P\|_{H^s \leftarrow H^s} \leq 1 + \|\psi\|_{H^s} \|\psi\|_{L^2}^{-1}.$$

Proof. In order to prove

$$\mathcal{R}(P) = \{ v \in L^2(\mathbb{R}) : 0 = \langle \psi, v \rangle \},$$

we only have to show that $\mathcal{R}(P) \subseteq \{v \in L^2(\mathbb{R}) : 0 = \langle \psi, v \rangle\}$. Let $w \in \mathcal{R}(P)$, i.e. there exists $z \in L^2(\mathbb{R})$ such that $Pz = w$. Then we have for the algebraic constraint

$$\begin{aligned}\langle \psi, Pz \rangle &= \langle \psi, z - \psi M \langle \psi, z \rangle \rangle \\ &= \langle \psi, z \rangle - M \langle \psi, \psi \rangle \langle \psi, z \rangle \\ &= 0.\end{aligned}$$

In order to prove that P is a projection, we have to show that $P^2 = P \circ P = P$. By the above calculations it holds $\langle \psi, Pv \rangle = 0$ and hence

$$P^2 v = Pv - \psi M \langle \psi, Pv \rangle = Pv.$$

The bound of the operator norm follows for $s \in \mathbb{N}_0$ and $z \in H^s(\mathbb{R})$ by

$$\begin{aligned}\|Pz\|_{H^s} &\leq \|z\|_{H^s} + M \|\psi\|_{H^s} |\langle \psi, z \rangle| \\ &\leq \|z\|_{H^s} + M \|\psi\|_{H^s} \|\psi\|_{L^2} \|z\|_{L^2} \\ &\leq (1 + M \|\psi\|_{H^s} \|\psi\|_{L^2}) \|z\|_{H^s} \\ &= \left(1 + \|\psi\|_{H^s} \|\psi\|_{L^2}^{-1}\right) \|z\|_{H^s}\end{aligned}$$

using Assumption 1.3.1 (ii). Thus, for the operator norm we have

$$\|P\|_{H^s \leftarrow H^s} \leq 1 + \|\psi\|_{H^s} \|\psi\|_{L^2}^{-1}.$$

□

Remark 2.1.5. Note that the subspace $\mathcal{R}(P) \subseteq L^2(\mathbb{R})$ is the vector space of consistent functions for the PDAE (2.6), cf. Definition 2.1.1.

In addition, we get the projection $P^\perp = (I - P)$ given by

$$\begin{aligned}P^\perp : L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ z &\mapsto \psi M \langle \psi, z \rangle,\end{aligned}$$

where the role of the kernel and image is switched in reference to P.

Lemma 2.1.6. *The operator P is an orthogonal projection, i.e. $\langle Pz, (I-P)z' \rangle = 0$ for all $z, z' \in L^2(\mathbb{R})$, and it holds $\|P\|_{L^2 \leftarrow L^2} = 1$.*

Proof. The projector P is an orthogonal projection, i.e. $\langle Pz, (I-P)z'\rangle = 0$ for $z, z' \in L^2(\mathbb{R})$, since we have

$$\begin{aligned}\langle Pz, z' - Pz'\rangle &= \langle z - \psi M\langle \psi, z\rangle, \psi M\langle \psi, z'\rangle\rangle \\ &= \langle z, \psi M\langle \psi, z'\rangle\rangle - \langle \psi M\langle \psi, z\rangle, \psi M\langle \psi, z'\rangle\rangle \\ &= M\langle z, \psi\rangle\langle \psi, z'\rangle - M\langle \psi, z\rangle\langle \psi, \psi\rangle M\langle \psi, z'\rangle \\ &= 0.\end{aligned}$$

We obtain

$$\begin{aligned}\|z\|_{L^2}^2 &= \langle Pz + (I-P)z, Pz + (I-P)z\rangle \\ &= \|Pz\|_{L^2}^2 + 2\langle Pz, (I-P)z\rangle + \|(I-P)z\|_{L^2}^2 \\ &= \|Pz\|_{L^2}^2 + \|(I-P)z\|_{L^2}^2\end{aligned}$$

and hence

$$\|Pz\|_{L^2} \leq \|z\|_{L^2}.$$

Since for $z \in \mathcal{R}(P)$ we have $Pz = z$, it follows $\|P\|_{L^2} = 1$, which finishes the proof. □

For completeness we give the definition of a solution of the PDAE (2.6). Since we are using the variation-of-constants formula, we use the concept of mild solutions known from semigroup theory. For a differential equation

$$\begin{cases} \partial_t u = Eu + f & \text{on } (0, T], \\ u(0) = u_0 \in X \end{cases} \tag{2.7}$$

on a Hilbert space X with a self-adjoint and dissipative operator E and an inhomogeneity $f \in \mathcal{C}^1\big([0,T], X\big)$ we define

$$u(t) = e^{tE}u_0 + \int_0^t e^{(t-s)E} f(s)ds \in \mathcal{D}(E) \quad \text{for} \quad t > 0,$$

as a (mild) solution of (2.7), where the integral lies in $\mathcal{D}(E)$ for $t > 0$ by [Paz83, Theorem 1.2.4, p. 5]. Although we are not able to apply standard existence theory from semigroup theory as given in [Paz83, EN00], we expect solutions with similar regularity as in this theory. The solution of (2.7) with the given assumptions is unique in $\mathcal{C}\big([0,T], X\big) \cap \mathcal{C}\big((0,T], \mathcal{D}(E)\big) \cap \mathcal{C}^1\big((0,T], X\big)$ as given in [Her12]. Note that, even if the initial value u_0 lies in X, one expects that $e^{tE}u_0 \in \mathcal{D}(E)$ for $t > 0$ by the smoothing property of the semigroup. Note that $e^{t\Lambda}u_0 \in \mathcal{D}(E)$ for $t > 0, u_0 \in X$ also holds true for a sectorial generator Λ of a strongly continuous semigroup.

If one transfers this solution concept to the PDAE (2.6) we obtain a very similar definition of solutions as already stated in [Thü05, Definition 1.11]. We use this definition in a slightly modified version where the evolution equation also holds true at final time. Since we are interested in short time intervals for the splitting scheme, we are not interested in a solution with a maximal existence interval.

Definition 2.1.7. *Let Λ be a sectorial operator in $L^2(\mathbb{R})$ with $\mathcal{D}(\Lambda) = H^2(\mathbb{R}), \psi \in H^1(\mathbb{R})$ and $h : H^1(\mathbb{R}) \times \mathbb{R} \to L^2(\mathbb{R})$. A function $(v, \mu) : [0, S] \to H^1(\mathbb{R}) \times \mathbb{R}$ with $S \in (0, \infty]$ is called a (mild) solution of*

$$\begin{cases} \partial_t v = \Lambda v + h(v, \mu), & \\ \quad 0 = \langle \psi, v \rangle, & (t \in (0, S]) \\ v(0) = v_0 \in H^1(\mathbb{R}) \cap \mathcal{R}(P) & \end{cases} \tag{2.8}$$

in $(0, S]$ if the following conditions hold

(i) $h(v(\cdot), \mu(\cdot)) : [0, S] \to L^2(\mathbb{R})$ *is continuous*

(ii) $v : [0, S] \to H^1(\mathbb{R})$ *is continuous,* $v(t) \in H^2(\mathbb{R})$ *for* $t \in (0, S]$ *and* $v(0) = v_0$

(iii) μ *is continuous in* $[0, S]$

(iv) $\partial_t v(t) \in L^2(\mathbb{R})$ *exists and* $\partial_t v(t) = \Lambda v(t) + h(v(t), \mu(t))$ *for* $t \in (0, S]$

(v) $\langle \psi, v(t) \rangle = 0$ *for all* $t \in [0, S]$.

Note that the evolution equation of the PDAE (2.8) holds only true for $t = 0$ if some further assumptions are fulfilled, cf. Assumption 2.1.27. We give a definition of the solution of the original PDAE (2.2) in a similar way as in [Thü05, Definition 1.12].

Definition 2.1.8. *We call (u, μ) a solution of (2.2) if the difference $(u-\hat{u}, \mu)$ is a solution of (2.6) in the sense of Definition 2.1.7.*

To our knowledge there is no existence or well-posedness theory available for the PDAE (2.2) or PDAE (2.6).

As a next step we analyze the semigroups generated by A in the co-moving frame and combined with the projector P.

2.1.2 Properties of the Projected Generator

We will show that the PDE (2.6a) with constraint (2.6b) is equivalent to a PDE without constraint but with a projected generator. Thus, we will first analyze the projected generators in the following. The first projected generator is given by

$$\begin{aligned} PA : \mathcal{D}(PA) = H^2(\mathbb{R}) \subseteq L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ z &\mapsto P\partial_x^2 z. \end{aligned}$$

In the convergence proof we will fix the speed in front of the advection term gained from the method of freezing and therefore analyze the generator

$$\begin{aligned} B_c : \mathcal{D}(B_c) = H^2(\mathbb{R}) \subseteq L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ z &\mapsto \partial_x^2 z + c\partial_x z \end{aligned} \tag{2.9}$$

and its projected version given by

$$\begin{aligned} PB_c : \mathcal{D}(PB_c) = H^2(\mathbb{R}) \subseteq L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ z &\mapsto P\partial_x^2 z + cP\partial_x z \end{aligned}$$

for a fixed speed $c \in \mathbb{R}$. The generators including the advection term are analyzed in Section 2.1.3. Since projections of generators of semigroups are not very common in the literature, we give a complete overview of the properties of the semigroups in Figure 2.1, and we will give a proof for each property although we do not need all of them for the convergence proof. These properties go back to the following lemma.

Lemma 2.1.9 ([Paz83, Theorem 1.2.2, p. 4])**.** *Let $(T(t))_{t\geq 0}$ be a strongly continuous semigroup of bounded linear operators on $(X, \|\cdot\|)$. There exists constants $\omega \geq 0$ and $\tilde{M} \geq 1$ such that*

$$\|T(t)\| \leq \tilde{M} e^{\omega t} \quad \text{for } 0 \leq t < \infty.$$

Definition 2.1.10. *We call a strongly continuous semigroup $(T(t))_{t\geq 0}$ a contraction semigroup, if $\omega = 0$ and $\tilde{M} = 1$ in the lemma above, i.e. if $\|T(t)\| \leq 1$ for $0 \leq t < \infty$.*

Note that in general the property in Lemma 2.1.9 is not sufficient to show convergence of the splitting scheme as we outline in Remark 2.3.10. In the presence of contraction semigroups it would be possible to prove the convergence in a straightforward way, but the contraction property is not given for the projected generators in the given setting

	analytic	**contractive**	**quasicontractive**
e^{tA}	✓	✓	✓
$e^{t(A+c\partial_x)}$	✓	✓	✓
e^{tPA}	✓	✗	✓
$e^{tP(A+c\partial_x)}$	✓	✗	✓

Figure 2.1: Overview of semigroup properties for the projected generators as well as in the co-moving frame.

as shown below. Even if the proof gets more complicated it turns out that the concept of quasicontractive semigroups is sufficient for the convergence proofs. This property is given in

Definition 2.1.11. *We call a strongly continuous semigroup $(T(t))_{t\geq 0}$ a quasicontractive semigroup, if $\tilde{M} = 1$ in the lemma above, i.e. if $\|T(t)\| \leq e^{\omega t}$ for $0 \leq t < \infty$.*

We note that every contraction semigroup is also quasicontractive by definition with $\omega = 0$. Before we analyze the projected generators, we list some known results of the operator A without the projection. The operator A is the infinitesimal generator of a bounded analytic semigroup $\left(e^{zA}\right)_{z\in\Sigma_\delta\cup\{0\}}$ on $L^2(\mathbb{R})$ as shown in [EN00, Example II.4.10, p. 107]. Here Σ_δ is given by $\Sigma_\delta := \{\lambda \in \mathbb{C} \mid |\arg\lambda| < \delta\} \setminus \{0\}$, where δ is a suitable angle. Thus, the operator A is sectorial and generates a strongly continuous semigroup $\left(e^{tA}\right)_{t\geq 0}$ with $e^{tA}u \in H^2(\mathbb{R})$ for all $u \in L^2(\mathbb{R})$ and $t > 0$ using [EN00, Theorem II.4.6, p. 101]. Its spectrum is given by $(-\infty, 0]$. Note that e^{tA} should be seen as a symbol, because the exponential representation can only be used for uniformly continuous semigroups. The operator A is not bounded on $L^2(\mathbb{R})$ and therefore A is not a generator of a uniformly continuous semigroup, cf. [Paz83, Theorem 1.2, p. 2]. In this work we will often abbreviate the semigroup $\left(e^{tA}\right)_{t\geq 0}$ with the simpler form e^{tA}. The distinguishing between the operator and the semigroup should be clear from the context. In addition, the following lemma holds.

Lemma 2.1.12. *The bound of the semigroup e^{tA} given by*

$$\left\|e^{tA}\right\|_{H^s\leftarrow H^s} \leq 1$$

holds true for $s \in \mathbb{N}_0$. In particular, the operator A generates a contraction semigroup.

Proof. We denote with $\mathcal{H}_t(y) = (4\pi t)^{-1/2} \exp(-\frac{|y|^2}{4t})$ for $y \in \mathbb{R}$ the well-known heat kernel, i.e. $e^{tA}z = \int_{\mathbb{R}} \mathcal{H}_t(y) z(x-y)dy$ for $z \in L^2(\mathbb{R})$. We have for every $k \in \mathbb{N}_0$

$$\partial_x^k e^{tA} z = \partial_x^k (\mathcal{H}_t * z) = \int_{\mathbb{R}} \mathcal{H}_t(y) \partial_x^k z(x-y) dy, \qquad (z \in L^2)$$

for $t > 0$ such that the general Young's inequality yields

$$\left\| \partial_x^k e^{tA} z \right\|_{L^2} \leq \|\mathcal{H}_t\|_{L^1} \left\| \partial_x^k z \right\|_{L^2} = \left\| \partial_x^k z \right\|_{L^2}. \tag{2.10}$$

Note that the L^1-norm of the heat-kernel $\mathcal{H}$ is equal to 1. For $s \in \mathbb{N}_0$ the bound of the operator norm follows by

$$\begin{aligned}
\sup_{\|z\|_{H^s}=1} \left\| e^{tA} z \right\|_{H^s}^2 &= \sup_{\|z\|_{H^s}=1} \sum_{k=0}^{s} \left\| \partial_x^k e^{tA} z \right\|_{L^2}^2 \\
&\overset{(2.10)}{\leq} \sup_{\|z\|_{H^s}=1} \sum_{k=0}^{s} \left\| \partial_x^k z \right\|_{L^2}^2 \\
&= \sup_{\|z\|_{H^s}=1} \|z\|_{H^s}^2 = 1
\end{aligned}$$

for $t > 0$. The case $t = 0$ follows with $e^{0A} = I$. $\square$

We justify the usage of the concept of quasicontractive semigroups by showing that the projected operators PA and $P(A + c\partial_x)$ do, in general, not generate contraction semigroups although A and $A + c\partial_x$ are generators of contraction semigroups. In contrast to the contractive property, the analyticity of the semigroup retains in the projected case as stated in

Lemma 2.1.13. *The projected operator $(PA, \mathcal{D}(A))$ is the infinitesimal generator of an analytic semigroup e^{tPA} on $L^2(\mathbb{R})$ and the quasicontractivity $\left\| e^{tPA} \right\|_{L^2} \leq e^{\omega t}$ for $t \geq 0$ is satisfied with $\omega = \|\psi\|_{L^2}^{-1} \|\psi\|_{H^2}$.*

Before we prove this lemma, we give some theorems from [Paz83, EN00]. For these we need the definition of a relatively bounded operator, which is given in

Definition 2.1.14 ([EN00, Definition III.2.1, p. 169])**.** *Let $E : \mathcal{D}(E) \subseteq X \to X$ be a linear operator on the Banach space $(X, \|\cdot\|)$. An operator $F : \mathcal{D}(F) \subseteq X \to X$ is called (relatively) E-bounded if $\mathcal{D}(E) \subseteq \mathcal{D}(F)$ and if there exist constants $a, b \in \mathbb{R}_+$ such that*

$$\|Fx\| \leq a\|Ex\| + b\|x\| \tag{2.11}$$

for all $x \in \mathcal{D}(E)$. The E-bound of F is

$$a_0 := \inf\{a \geq 0 \mid \text{ there exists } b \in \mathbb{R}_+ \text{ such that } (2.11) \text{ holds}\}.$$

Theorem 2.1.15 ([EN00, Theorem III.2.10]). *Let the operator* $(E, \mathcal{D}(E))$ *generate an analytic semigroup* $T(z)_{z\in\Sigma_\delta\cup\{0\}}$ *on a Banach space* X*. Then there exists a constant* $\alpha > 0$ *such that* $(E + F, \mathcal{D}(E))$ *generates an analytic semigroup for every* E*-bounded operator* F *having* E*-bound* $a_0 < \alpha$*.*

Moreover we use

Theorem 2.1.16 ([EN00, Theorem III.1.3]). *Let* $(E, \mathcal{D}(E))$ *be the generator of a strongly continuous semigroup* $(T(t))_{t\geq 0}$ *on a Banach space* X *satisfying*

$$\|T(t)\| \leq \tilde{M}e^{\tilde{\omega}t} \text{ for all } t \geq 0$$

and some $\tilde{\omega} \in \mathbb{R}, \tilde{M} \geq 1$*. If* $F \in L(X, X)$*, then*

$$C := E + F \quad \text{with} \quad \mathcal{D}(C) := \mathcal{D}(E)$$

generates a strongly continuous semigroup $(S(t))_{t\geq 0}$ *satisfying*

$$\|S(t)\| \leq \tilde{M}e^{(\tilde{\omega}+\tilde{M}\|F\|)t} \text{ for all } t \geq 0.$$

Proof of Lemma 2.1.13. The proof of both properties, the analyticity and quasicontractivity, is done via a perturbation argument of the generator of the analytic contraction semigroup A. For this we calculate

$$\begin{aligned} && A &= (I - P)A + PA, \\ \iff && PA &= A - P^{\perp}A \end{aligned}$$

and consider $-P^{\perp}A$ as a perturbation. This operator is only defined for $z \in \mathcal{D}(A)$ but we extend this operator to $L^2(\mathbb{R})$ by using integration by parts and define

$$\begin{aligned} G : L^2(\mathbb{R}) &\to L^2(\mathbb{R}) \\ z &\mapsto -M\psi\langle\partial_x^2\psi, z\rangle. \end{aligned}$$

In order to prove the analytic property of the semigroup we use Theorem 2.1.15. For the definition of A-bound a_0 see Definition 2.1.14. As we mentioned in the beginning, e^{tA} is an analytic semigroup. Thus, the proof follows directly if G is A-bounded with $a_0 = 0$. The operator G is linear and bounded since

$$\begin{aligned} \|Gz\|_{L^2} &\leq M\|\psi\|_{L^2}|\langle\partial_x^2\psi, z\rangle| \\ &\leq M\|\psi\|_{L^2}\|\psi\|_{H^2}\|z\|_{L^2} \\ &= \|\psi\|_{L^2}^{-1}\|\psi\|_{H^2}\|z\|_{L^2}, \end{aligned}$$

for $z \in H^2(\mathbb{R})$ such that $a = 0$ and $b = \|\psi\|_{L^2}^{-1} \|\psi\|_{H^2}$ in (2.11). This finishes the proof of the analytic semigroup property for PA with Theorem 2.1.15. Since the perturbation G is a linear bounded operator on $L^2(\mathbb{R})$ we use Theorem 2.1.16 with $\tilde{M} = 1, \tilde{\omega} = 0$ (Lemma 2.1.12) to obtain

$$\begin{aligned}\left\|e^{tPA}\right\|_{L^2} &= \left\|e^{t(A+G)}\right\|_{L^2} \\ &\leq e^{\|G\|_{L^2} t} \\ &= e^{(\|\psi\|_{L^2}^{-1}\|\psi\|_{H^2})t}\end{aligned}$$

for $t \geq 0$. Thus, the proof finishes with $\omega := (\|\psi\|_{L^2}^{-1} \|\psi\|_{H^2})$. □

We obtain the following bound of the generator PA on $H^s(\mathbb{R})$.

Corollary 2.1.17. *Let $s \in \mathbb{N}$. The projected operator $(PA, H^{s+2}(\mathbb{R}))$ is the infinitesimal generator of a quasicontractive semigroup e^{tPA} on $H^s(\mathbb{R})$, i.e.*

$$\left\|e^{tPA}\right\|_{H^s \leftarrow H^s} \leq e^{\omega t} \quad \text{for } t \geq 0$$

with

$$\omega = M \|\psi\|_{H^s} \|\psi\|_{H^2}.$$

Proof. The proofs follows by combining Theorem 2.1.16 and Lemma 2.1.12. We have $PA = (I - P^\perp)A$ and the bounded perturbation

$$P^\perp A = M\psi\langle \partial_x^2 \psi, \cdot\rangle.$$

For $z \in H^s(\mathbb{R})$ with $\|z\|_{H^s} = 1$ the boundedness follows by

$$\begin{aligned}\left\|P^\perp A z\right\|_{H^s} &\leq M \|\psi\|_{H^s} \|\psi\|_{H^2} \|z\|_{L^2} \\ &\leq M \|\psi\|_{H^s} \|\psi\|_{H^2}.\end{aligned}$$

Thus, the quasicontractivity follows by Theorem 2.1.16. □

At first sight one might expect that a multiplicative perturbation with an orthogonal projection of a generator may retain important properties of the semigroup. However, it turns out that the contraction property of the semigroup is lost due to the projection of the generator. This surprising fact is stated in

Lemma 2.1.18. *Let $\psi \in H^3(\mathbb{R})$ with compact support and $\psi \not\equiv 0$. Then there exists a $z \in H^2(\mathbb{R})$ and $c \in \mathbb{R}$ such that $z - \partial_x^2 z = c\psi$ and $\|\partial_x z\|_{L^2} = 1$. The operator*

$$\begin{aligned} PA : H^2(\mathbb{R}) &\to \mathcal{R}(P) \subseteq L^2(\mathbb{R}), \\ w &\mapsto PAw = \partial_x^2 w - M\psi\langle\psi, \partial_x^2 w\rangle \end{aligned}$$

*does **not** generate a contraction semigroup if* $1 < \|z\|_{L^2}^2 \|\partial_x^2 z\|_{L^2}^2$.

Note that the last condition is not a strong restriction, in fact, we can easily find a function ψ such that PA does not generate a contraction semigroup. In order to give a proof of the lemma, we have to state the Lumer-Phillips Theorem. For this we need the definition of a dissipative operator in the case of a Banach space.

Definition 2.1.19. *An operator E on a Banach space X is called dissipative if and only if*

$$\|(\lambda - E)x\| \geq \lambda \|x\|$$

holds true for all $\lambda > 0, x \in \mathcal{D}(E)$. If X is a Hilbert space, this is the case if and only if

$$\mathrm{Re}\langle Ex, x\rangle \leq 0.$$

Note that the equivalence to the last property follows by combining [EN00, Proposition 3.23, p. 88] and [EN00, Example 3.25 (i), p. 89].

Theorem 2.1.20 (Lumer-Phillips as in [Paz83, Theorem 1.4.3])**.** *Let E be a linear operator with dense domain $\mathcal{D}(E)$ in X.*

(i) If E is dissipative and there is a $\lambda_0 > 0$ such that the range $\mathcal{R}(\lambda_0 I - E)$ of $\lambda_0 I - E$ is X, then E is the infinitesimal generator of a strongly continuous semigroup of contractions on X.

(ii) If E is the infinitesimal generator of a strongly continuous semigroup of contractions on X then $\mathcal{R}(\lambda I - E) = X$ for all $\lambda > 0$ and E is dissipative. Moreover, for every $x \in D(E)$ and every $x^* \in F(x) := \{x^* | x^* \in X^* \text{ and } \langle x^*, x\rangle = \|x\|^2 = \|x^*\|^2\}$ it holds $\mathrm{Re}\langle Ex, x^*\rangle \leq 0$.

With this prerequisite we give a

Proof of Lemma 2.1.18. A non-dissipative operator cannot generate a contraction semigroup by the Lumer-Phillips theorem. Thus, we show that the generator is not dissipative for some $\psi \in H^3(\mathbb{R})$ with compact support. Since A is a generator of a contraction semigroup, it follows by Lumer-Phillips Theorem 2.1.20 that $\mathcal{R}(\lambda I - A) = L^2(\mathbb{R})$ holds in particular true for $\lambda = 1$. Let $\psi \in H^3(\mathbb{R}) \subseteq L^2(\mathbb{R})$ with compact support. Hence there is a $w \in H^2(\mathbb{R})$ such that $w - \partial_x^2 w = \psi$. Without loss of generality we have $\|\partial_x w\|_{L^2} \neq 0$. We set

$$c := \frac{1}{\|\partial_x w\|_{L^2}} \quad \text{and} \quad z(x) := \begin{cases} cw(x) & \text{for } x \in \operatorname{supp}(\psi) \\ 0 & \text{for } x \notin \operatorname{supp}(\psi) \end{cases}$$

It follows $\|\partial_x z\|_{L^2} = \frac{\|\partial_x w\|_{L^2}}{\|\partial_x w\|_{L^2}} = 1$ and

$$\begin{aligned} z - \partial_x^2 z &= c\left(w - \partial_x^2 w\right) \\ &= c\psi. \end{aligned}$$

The operator PA is not dissipative if

$$\langle PAy, y\rangle > 0 \qquad \text{for one } y \in \mathcal{D}(A). \tag{2.12}$$

We show that this inequality holds true for the function z defined above. We have

$$\langle PAz, z\rangle = \langle \partial_x^2 z, z\rangle - \langle \psi, \psi\rangle^{-1}\langle \psi, z\rangle\langle \psi, \partial_x^2 z\rangle$$

such that the inequality in (2.12) is equivalent to

$$\langle \partial_x^2 z, z\rangle > \langle \psi, \psi\rangle^{-1}\langle \psi, z\rangle\langle \psi, \partial_x^2 z\rangle. \tag{2.13}$$

For the left-hand side we have

$$\langle \partial_x^2 z, z\rangle = -\langle \partial_x z, \partial_x z\rangle = -1$$

by the construction of z and z having compact support. For the right-hand side of (2.13)

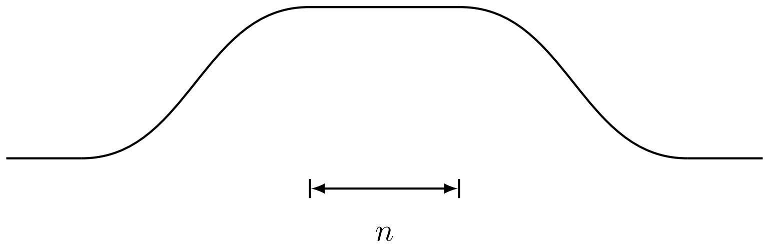

Figure 2.2: Example of a sequence of H^2-functions with the same weak derivatives and growing L^2-norm.

we obtain

$$\begin{aligned}
\langle\psi,\psi\rangle^{-1}\langle\psi,z\rangle\langle\psi,\partial_x^2 z\rangle &= \langle\psi,\psi\rangle^{-1}\langle\tfrac{1}{c}(z-\partial_x^2 z),z\rangle\langle\tfrac{1}{c}(z-\partial_x^2 z),\partial_x^2 z\rangle \\
&= \frac{\frac{1}{c^2}\left(\|z\|_{L^2}^2 - \langle\partial_x^2 z, z\rangle\right)\left(\langle z,\partial_x^2 z\rangle - \|\partial_x^2 z\|_{L^2}^2\right)}{\langle\psi,\psi\rangle} \\
&= -\frac{\frac{1}{c^2}\left(\|z\|_{L^2}^2 + \|\partial_x z\|_{L^2}^2\right)\left(\|\partial_x z\|_{L^2}^2 + \|\partial_x^2 z\|_{L^2}^2\right)}{\frac{1}{c^2}\langle z-\partial_x^2 z, z-\partial_x^2 z\rangle} \\
&= -\frac{\left(1+\|z\|_{L^2}^2\right)\left(1+\|\partial_x^2 z\|_{L^2}^2\right)}{\|z\|_{L^2}^2 - 2\langle z,\partial_x^2 z\rangle + \|\partial_x^2 z\|_{L^2}^2} \\
&= -\frac{\left(1+\|z\|_{L^2}^2\right)\left(1+\|\partial_x^2 z\|_{L^2}^2\right)}{\|z\|_{L^2}^2 + 2\,\|\partial_x z\|_{L^2}^2 + \|\partial_x^2 z\|_{L^2}^2} \\
&= -\frac{\left(1+\|z\|_{L^2}^2\right)\left(1+\|\partial_x^2 z\|_{L^2}^2\right)}{\|z\|_{L^2}^2 + 2 + \|\partial_x^2 z\|_{L^2}^2}.
\end{aligned}$$

We define $a = \|z\|_{L^2}, b = \|\partial_x^2 z\|_{L^2}$ and have with (2.13) and the two calculations above

$$\begin{aligned}
& 1 < \frac{(1+a^2)(1+b^2)}{a^2+b^2+2} \\
\iff \quad & 0 < (1+a^2)(1+b^2) - a^2 - b^2 - 2 \\
& \quad = 1 + a^2 + b^2 + a^2b^2 - a^2 - b^2 - 2 \\
& \quad = a^2b^2 - 1.
\end{aligned}$$

Thus, the operator PA is **not** dissipative if there exists an $z \in H^2(\mathbb{R})$ with the above constructions such that $1 < a^2b^2 = \|z\|_{L^2}^2 \|\partial_x^2 z\|_{L^2}^2$ holds true. It is easy to construct a family of functions $f_n \in H^2(\mathbb{R})$ where $\|\partial_x f_n\|_{L^2}$ and $\|\partial_x^2 f_n\|_{L^2}$ are constant but $\|f_n\|_{L^2}$ tends to infinity for $n \to \infty$, cf. Figure 2.2. Let $n_0 \in \mathbb{N}$ be the index where $1 < \|f_{n_0}\|_{L^2} \|\partial_x^2 f_{n_0}\|_{L^2}$, then the operator PA with $\psi = \|\partial_x f_{n_0}\|_{L^2}^{-1}(f_{n_0} - \partial_x^2 f_{n_0})$ is not dissipative. $\square$

2.1.3 Projected Generators in the Co-Moving Frame

In this section we handle the additional term $\mu(t)\partial_x u$ in the PDAE (2.6) obtained by the method of freezing. An approach to handle this part in the inhomogeneity and therefore in the integral part of a variation-of-constants formula would lead to a reduction of regularity. For this reason, proving the convergence with this approach of the Lie splitting does not seem to be within reach as we will outline in Remark 2.3.11. For the convergence proof we will fix the speed in front of the advection term. We consider this term with a fixed speed $c \in \mathbb{R}$ by $c\partial_x u$ as belonging to the generator of the semigroup. We are therefore interested in the semigroup generated by $B_c = A + c\partial_x$ as defined in (2.9) and the corresponding PDE

$$\begin{cases} \partial_t u = Au + c\partial_x u, \\ u(0) = u_0. \end{cases}$$

Afterwards we regard the projected version of the generator.

In this section we use the following

Theorem 2.1.21 ([EN00, Theorem III.2.7])**.** *Let $(E, \mathcal{D}(E))$ be the generator of a contraction semigroup and assume $(F, \mathcal{D}(F))$ to be a dissipative operator which is E-bounded with E-bound $a_0 < 1$. Then $(E + F, \mathcal{D}(E))$ generates a contraction semigroup.*

We show that B_c generates an analytic contraction semigroup and the projected operator PB_c generates an analytic quasicontractive semigroup as stated in the following lemmas.

Lemma 2.1.22. *The linear operator B_c generates an analytic semigroup e^{tB_c} of contractions on $L^2(\mathbb{R})$.*

Proof. For the case $c = 0$ the analytic semigroup of contractions is given by the semigroup of the heat equation for which we already know that it is an analytic semigroup of contractions on $L^2(\mathbb{R})$. Thus, let c be in $\mathbb{R} \setminus \{0\}$. The equation

$$\begin{cases} \partial_t z = c\partial_x z =: Dz, & t > 0, \\ z(0) = z_0 \in L^2(\mathbb{R}) \end{cases} \tag{2.15}$$

with $D : H^1(\mathbb{R}) \subseteq L^2(\mathbb{R}) \to L^2(\mathbb{R})$ is called the linear transport equation. By using the chain rule, one can show that the translation (semi-)group

$$(\mathrm{e}^{tD} z_0)(x) := z_0(x + ct) \quad \text{for } t, x \in \mathbb{R}$$

is the unique mild solution to (2.15) as a map $L^2(\mathbb{R}) \to L^2(\mathbb{R})$. The (semi-)group properties for the translation (semi-)group on $\mathbb{R}$ and bounded intervals are discussed in [EN00, Section I.4.c and Section II.2.10]. This is in particular done for the Hilbert space $L^2(\mathbb{R})$. The translation operator on $\mathbb{R}$ is obviously an isometry and therefore the operator norm $\left\|e^{tD}\right\|_{L^2}$ is equal to one. Thus, e^{tD} is a contraction semigroup. From the Lumer-Phillips Theorem 2.1.20 we conclude that the operator D is dissipative.

In [EN00, Example III.2.2, p. 169] it is shown that the operator $\partial_x : H^1(\mathbb{R}) \to L^2(\mathbb{R})$ is A-bounded with A-bound $a_0 = 0$, where the operator A is given by $A = \partial_x^2$ with domain $\mathcal{D}(A) = H^2(I)$, $I \subseteq \mathbb{R}$, where the case $I = \mathbb{R}$ is included. The definition of A-boundedness is stated in Definition 2.1.14. Writing down the definition of the A-bound a_0 of the operator ∂_x, cf. (2.11), we see by multiplying the inequality with $|c|$ that the two infima

$$\begin{aligned} a_0 := \inf\{a \geq 0 |\ & \text{there exists } b \in \mathbb{R}_+ \text{ such that} \\ & \|\partial_x z\| \leq a\|Az\| + b\|z\| \text{ holds for all } z \in D(A)\} \\ = \inf\{a \geq 0 |\ & \text{there exists } b \in \mathbb{R}_+ \text{ such that} \\ & \|c\partial_x z\| \leq a|c|\|Az\| + b|c|\|z\| \text{ holds for all } z \in D(A)\} \end{aligned}$$

are equal. Thus, it follows that the A-bound $a_0 = 0$ also holds true for the operator $D = c\partial_x : H^1(\mathbb{R}) \to L^2(\mathbb{R})$.

Summing up, the operator $B_c = A + c\partial_x$ is a pertubation of a generator of a contraction semigroup A by a dissipative operator ∂_x with A-bound $a_0 = 0$ such that we can apply Theorem 2.1.21. This finishes the proof of the contraction semigroup property. The analyticity follows directly by applying Theorem 2.1.15, with the A-bound property derived above. □

Similar to the case of the operator A where the projected operator PA generates a quasicontractive semigroup (Lemma 2.1.13) we can show the following.

Lemma 2.1.23. *The projected operator $(PB_c, \mathcal{D}(B))$ is the infinitesimal generator of an analytic semigroup e^{tPB_c} on $L^2(\mathbb{R})$ and the quasicontractivity $\left\|e^{tPB_c}\right\|_{L^2} \leq e^{\omega t}$ for $t \geq 0$ is satisfied with $\omega = \|\psi\|_{L^2}^{-1} (\|\psi\|_{H^2} + |c| \, \|\psi\|_{H^1})$.*

Proof. This can be proven analogously to Lemma 2.1.13. We again extend the perturbation operator $P^\perp B_c$ to $L^2(\mathbb{R})$ by $P^\perp B_c z = M\psi(\langle \partial_x^2 \psi, z\rangle - c\langle \partial_x \psi, z\rangle)$ for $z \in L^2(\mathbb{R})$. The bound of the perturbation is then given by

$$\begin{aligned}\left\|P^{\perp}B_c z\right\|_{L^2} &= \|\psi\|_{L^2} M|\langle\partial_x^2\psi, z\rangle - c\langle\partial_x\psi, z\rangle| \\ &\leq \|\psi\|_{L^2}^{-1}\left(\|\psi\|_{H^2} + |c|\,\|\psi\|_{H^1}\right)\|z\|_{L^2}\end{aligned}$$

with fixed speed c and $z \in L^2(\mathbb{R})$. In order to prove the quasicontractive property, we obtain the growth constant ω by Theorem 2.1.16. □

Similar to Lemma 2.1.18 we have

Lemma 2.1.24. *Let $\psi \in H^3(\mathbb{R})$ with compact support and $\psi \not\equiv 0$. Then there exists an $z \in H^2(\mathbb{R})$ and $\tilde{c} \in \mathbb{R}$ such that $z - \partial_x^2 z = \tilde{c}\psi$ and $\|\partial_x z\|_{L^2} = 1$. The operator*

$$\begin{aligned}&PB_c : H^2(\mathbb{R}) \to \mathcal{R}(P) \subseteq L^2(\mathbb{R}), \\ &\qquad z \mapsto PB_c v = (\partial_x^2 + c\partial_x)z - M\psi\langle\psi, (\partial_x^2 + c\partial_x)z\rangle\end{aligned}$$

*does **not** generate a contraction semigroup if* $1 < \|z\|_{L^2}^2 \left\|\partial_x^2 z\right\|_{L^2}^2$.

Proof. We argue in the same way as in the proof of Lemma 2.1.18. As before we have $z - \partial_x^2 z = \tilde{c}\psi$ with $z \in H^2(\mathbb{R})$ and z having compact support. The right-hand side of (2.13) differs slightly and we have

$$\langle\psi,\psi\rangle^{-1}\langle\psi, z\rangle\langle\psi, \partial_x^2 z\rangle + c\langle\psi,\psi\rangle^{-1}\langle\psi, z\rangle\langle\psi, \partial_x z\rangle = \langle\psi,\psi\rangle^{-1}\langle\psi, z\rangle\langle\psi, \partial_x^2 z\rangle,$$

since the term

$$\begin{aligned}\langle\tilde{c}\psi, \partial_x z\rangle &= \langle z - \partial_x^2 z, \partial_x z\rangle \\ &= \langle z, \partial_x z\rangle - \langle\partial_x^2 z, \partial_x z\rangle\end{aligned}$$

vanishes. This is due to the fact that z has compact support. We have

$$\langle z, \partial_x z\rangle = -\langle\partial_x z, z\rangle = -\langle z, \partial_x z\rangle$$

using integration by parts and it follows $\langle z, \partial_x z\rangle = 0$ and the second term $\langle\partial_x^2 z, \partial_x z\rangle$ vanishes with the same arguments. With the same arguments as in the proof of Lemma 2.1.18 we obtain that the operator PB_c is **not** dissipative if $1 < \|z\|_{L^2}^2 \left\|\partial_x^2 z\right\|_{L^2}^2$. In this case PB_c does not generate a contraction semigroup. □

Lemma 2.1.25. *Let $s \in \mathbb{N}$. The operator $(B_c, H^{s+2}(\mathbb{R}))$ is the infinitesimal generator of a contraction semigroup e^{tB_c} on $H^s(\mathbb{R})$ and the projected operator $(PB_c, H^{s+2}(\mathbb{R}))$ is the infinitesimal generator of a quasicontractive semigroup e^{tPB_c} on $H^s(\mathbb{R})$, i.e.*

$$\left\|e^{tPB_c}\right\|_{H^s \leftarrow H^s} \leq e^{\omega_c t} \quad \textit{for } t \geq 0$$

with

$$\omega_c = M \left\|\psi\right\|_{H^s} \left\|\psi\right\|_{H^2} (1 + |c|).$$

Proof. The proof of the first part of the lemma is analogous to the proof of Lemma 2.1.22. In the same way one can show that $D = c\partial_x$ is dissipative on $H^s(\mathbb{R})$ as well. To show the A-bound $a_0 = 0$ on $H^s(\mathbb{R})$ we only have to exploit the relative A-bound on $L^2(\mathbb{R})$ $(s+1)$-times. We define

$$\begin{aligned} Y &:= \left\{ a \in \mathbb{R}_+ \;\middle|\; \exists b \in \mathbb{R}_+ : \left\|\partial_x z\right\|_{L^2} \le a \left\|\partial_x^2 z\right\|_{L^2} + b \left\|z\right\|_{L^2} \text{ for all } z \in H^2(\mathbb{R}) \right\}, \\ \overline{Y} &:= \left\{ a \in \mathbb{R}_+ \;\middle|\; \exists b \in \mathbb{R}_+ : \left\|\partial_x z\right\|_{H^s} \le a \left\|\partial_x^2 z\right\|_{H^s} + b \left\|z\right\|_{H^s} \text{ for all } z \in H^{s+2}(\mathbb{R}) \right\}. \end{aligned}$$

We prove that $\inf \overline{Y} = 0$ which proves that the A-bound of ∂_x on $H^s(\mathbb{R})$ is 0. Let $z \in H^{s+2}(\mathbb{R})$. We chose an arbitrary element $a \in Y$. By definition there is $b \in \mathbb{R}_+$ such that $\left\|\partial_x w\right\|_{L^2} \le a \left\|\partial_x^2 w\right\|_{L^2} + b \left\|w\right\|_{L^2}$ for all $w \in H^2(\mathbb{R})$. We have $\partial_x^k z \in H^2(\mathbb{R})$ for $k = 0, \ldots, s$ and obtain with Young's inequality

$$\begin{aligned} \left\|\partial_x z\right\|_{H^s}^2 &= \sum_{k=0}^{s} \left\|\partial_x^k \partial_x z\right\|_{L^2}^2 \\ &= \sum_{k=0}^{s} \left\|\partial_x \partial_x^k z\right\|_{L^2}^2 \\ &= \sum_{k=0}^{s} \left(a \left\|A \partial_x^k z\right\|_{L^2} + b \left\|\partial_x^k z\right\|_{L^2} \right)^2 \\ &= \sum_{k=0}^{s} 2a^2 \left\|\partial_x^k A z\right\|_{L^2}^2 + 2b^2 \left\|\partial_x^k z\right\|_{L^2}^2 \\ &\le \sum_{k=0}^{s} 2a^2 \left\|Az\right\|_{H^s}^2 + 2b^2 \left\|z\right\|_{H^s}^2 \\ &\le 2(s+1)a^2 \left\|Az\right\|_{H^s}^2 + 2(s+1)b^2 \left\|z\right\|_{H^s}^2 . \end{aligned}$$

This yields

$$\left\|\partial_x z\right\|_{H^s} \le \sqrt{2(s+1)}a \left\|Az\right\|_{H^s} + \sqrt{2(s+1)}b \left\|z\right\|_{H^s}$$

hence $\sqrt{2(s+1)}a \in \overline{Y}$. Since $a \ge 0$ was arbitrary, this proves that $\sqrt{2(s+1)}Y \subseteq \overline{Y}$ and therefore

$$0 \le \inf \overline{Y} \le \inf \sqrt{2(s+1)}Y = \sqrt{2(s+1)} \inf Y = 0.$$

So the A-bound of ∂_x on $H^s(\mathbb{R})$ is 0. The A-bound of $c\partial_x$ follows with the same arguments as before. The operator $(A, H^{s+2}(\mathbb{R}))$ is a generator of contractions on $H^s(\mathbb{R})$

by Lemma 2.1.12. It follows that the operator $B_c = A + c\partial_x$ with domain $H^{s+2}(\mathbb{R})$ is a perturbation of a generator of a contraction semigroup on $H^s(\mathbb{R})$ by a dissipative operator with A-bound $a_0 = 0$ such that $(B_c, H^{s+2}(\mathbb{R}))$ generates a contraction semigroup.

The quasicontractive property of the semigroup generated by the projected operator $PB_c = (I - P^\perp)B_c$ follows again with the bounded perturbation

$$P^\perp B_c = M\psi(\langle \partial_x^2 \psi, \cdot\rangle - c\langle \partial_x \psi, \cdot\rangle).$$

For $z \in H^s(\mathbb{R})$ with $\|z\|_{H^s} = 1$ the boundedness follows by

$$\begin{aligned}\left\|P^\perp B_c z\right\|_{H^s} &\leq M \|\psi\|_{H^s} (\|\psi\|_{H^2} \|z\|_{L^2} + |c| \|\psi\|_{H^1} \|z\|_{L^2}) \\ &\leq M \|\psi\|_{H^s} \|\psi\|_{H^2} (1 + |c|).\end{aligned}$$

Thus, the quasicontractivity follows by Theorem 2.1.16.

□

2.1.4 Solution Representation

This subsection deals with two systems of differential equations, namely the transformed system and a system with the projected evolution equation. A main result is that the solutions of these two systems are equivalent in a certain way.

The following lemma is proven in advance with a general inhomogeneity r, which may depend on the solution u and the speed μ. We will use this lemma with different inhomogeneities, which we will choose later. This lemma relies on the definition of a (mild) solution as given in Definition 2.1.7.

Lemma 2.1.26. *Let $S > 0$. Given an inhomogeneity*

$$\begin{aligned} r:\ \mathcal{C}([0,S], H^1(\mathbb{R}) \times \mathbb{R}) &\to \mathcal{C}([0,S], L^2(\mathbb{R})), \\ (u,\mu) &\mapsto r(u,\mu), \end{aligned}$$

the pair (u, μ) is a solution of

$$\begin{cases} \partial_t u = Au + r(u,\mu) + \mu\psi & \qquad (t \in (0,S]) \quad (2.16a) \\ \quad 0 = \langle \psi, u(t)\rangle & \qquad (2.16b) \\ u(0) = u_0, \qquad u_0 \in H^1(\mathbb{R}), \langle \psi, u_0\rangle = 0 \end{cases}$$

on the interval $(0, S]$ *with consistent initial value if and only if* (u, μ) *is a solution on* $(0, S]$ *of the system with the projected PDE*

$$\begin{cases} \partial_t u = P(Au + r(u,\mu)) & (t \in (0,S]) \quad (2.17a) \\ \mu = M\langle \partial_x \psi, \partial_x u\rangle - M\langle \psi, r(u,\mu)\rangle & (t \in [0,S]) \quad (2.17b) \\ u(0) = u_0, \qquad u_0 \in H^1(\mathbb{R}) \cap \mathcal{R}(P) \end{cases}$$

Proof. The proof follows the lines of [Thü05, Lemma 1.17]. Let (u, μ) be a solution on $(0, S]$ of (2.16). To show equation (2.17b), we apply the mapping $\xi \mapsto M\langle \psi, \xi\rangle$ to both sides of (2.16a) and solve for the speed μ which is not included in the function r by

$$\begin{aligned} M\langle \psi, \partial_t u\rangle &= M\langle \psi, Au\rangle + M\langle \psi, r\rangle + \mu, \\ \mu &= M\langle \psi, \partial_t u - Au - r\rangle \end{aligned}$$

for $t \in (0, S]$. Since the algebraic constraint (2.16b) holds for every $t \in [0, S]$ and the time-derivative and the L^2-inner product can be interchanged, the part $\langle \psi, \partial_t u\rangle$ vanishes. We end up with (2.17b) for $t \in (0, S]$. Note that by Definition 2.1.7 (iv) the PDE only holds true for $t \in (0, S]$. But since $\langle \partial_x \psi, \partial_x \cdot\rangle$, $u(\cdot)$ and $r(u(\cdot), \mu(\cdot))$ are continuous, it follows that $\mu \in \mathcal{C}([0, S], \mathbb{R})$ such that $\mu(0)$ can be uniquely determined by the formula (2.17b) in the limit $t \to 0$.

To show the projected PDE (2.17a) for $t \in (0, S]$ we just plug the equation for the speed (2.17b) into (2.16a)

$$\begin{aligned} \partial_t u &= Au + r - (M\langle \psi, Au + r\rangle)\, \psi \\ &= P(Au + r). \end{aligned}$$

To show the direction from the projected system to the PDAE we obtain from (2.17b) for $t \in (0, S]$

$$\begin{aligned} && \psi\mu &= -M\psi\langle \psi, Au + r\rangle \\ \iff && \psi\mu + M\psi\langle \psi, r\rangle &= -M\psi\langle \psi, Au\rangle \\ \iff && \psi\mu + P^{\perp} r &= -P^{\perp}(Au). \end{aligned}$$

to obtain (2.16a)

$$\begin{aligned} \partial_t u &= P(Au + r) \\ &= (I - P^{\perp})(Au) + Pr \\ &= Au + \psi\mu + P^{\perp} r + Pr \\ &= Au + \psi\mu + r. \end{aligned}$$

The algebraic constraint is always fulfilled on the projected subspace, which concludes the proof. □

For the projected PDE (2.17a) we have a solution representation via a variation-of-constants formula by using the semigroup generated by $PA = P\partial_x^2$ by

$$u(t) = e^{tP\partial_x^2}u_0 + \int_0^t e^{(t-s)P\partial_x^2} Pr(u(s), \mu(s))ds.$$

Using $r(u, \mu) = g(u) + \mu\partial_x u$ we get the implicit solution representation of (2.6) by

$$\begin{cases} u(t) = e^{tP\partial_x^2}u_0 + \int_0^t e^{(t-s)P\partial_x^2} P\left(g(u) + \mu\partial_x u\right) ds & \text{(2.18a)} \\ \mu = M\langle \partial_x\psi, \partial_x u\rangle - M\langle \psi, g(u) + \mu\partial_x u\rangle, & \text{(2.18b)} \end{cases}$$

for $t \in [0, T]$. To simplify the notation, we write u, μ instead of $u(s), \mu(s)$. We will use this solution representation to prove local convergence of the time discretization of the method of freezing using splitting methods. We obtain

$$\begin{aligned} && \mu &= M\langle \partial_x\psi, \partial_x u\rangle - M\langle \psi, g(u) + \mu\partial_x u\rangle \\ \iff && \mu(1 + M\langle \psi, \partial_x u\rangle) &= M\langle \partial_x\psi, \partial_x u\rangle - M\langle \psi, g(u)\rangle \\ \iff && \mu &= \frac{M\langle \partial_x\psi, \partial_x u\rangle - M\langle \psi, g(u)\rangle}{1 + M\langle \psi, \partial_x u\rangle} \end{aligned} \tag{2.19}$$

if $1 + M\langle \psi, \partial_x u\rangle > 0$. To see that this is indeed the case recall that the variable u is in the transformed system $u = v - \hat{u}$ and with $\psi = \partial_x\hat{u}$ we obtain

$$\begin{aligned} && 1 + \langle \partial_x\hat{u}, \partial_x\hat{u}\rangle^{-1}\langle \partial_x\hat{u}, \partial_x u(t)\rangle &> 0 \\ \iff && \langle \partial_x\hat{u}, \partial_x\hat{u}\rangle + \langle \partial_x\hat{u}, \partial_x(v(t) - \hat{u})\rangle &> 0 \\ \iff && \langle \partial_x\hat{u}, \partial_x v(t)\rangle &> 0 \end{aligned}$$

for $t \in [0, T]$. The last inequality holds true if v is sufficiently close to the traveling wave $\bar{u}$ with Assumption 1.3.1 (ii). This will later be handled with Assumption 2.3.1 (I).

2.1.5 Properties of the Projected Solution

For the convergence proof we will assume more regularity for the solution and for the right-hand side of the evolution equation of the PDAE (2.6), which was given by

$$\begin{cases} \partial_t u = Au + g(u) + \mu\partial_x u + \mu\psi, & (t \in [0, T]) \\ 0 = \langle \psi, u\rangle, & \\ u(0) = u_0. & \end{cases} \tag{2.20}$$

These properties are given in

Assumption 2.1.27. *We assume that there is a solution* $(u,\mu) : [0,T] \to \big(H^2(\mathbb{R}) \cap \mathcal{R}(P)\big) \times \mathbb{R}$ *of* (2.20) *in the sense of Definition 2.1.7 satisfying the following properties with* $h(u,\mu) = g(u) + \mu\partial_x u + \mu\psi$.

(i) $h(u(\cdot),\mu(\cdot)) : [0,T] \to L^2(\mathbb{R})$ *is continuously differentiable*

(ii) $u : [0,T] \to H^1(\mathbb{R})$ *is continuously differentiable,* $u(t) \in H^2(\mathbb{R})$ *for* $t \in [0,T]$ *and* $u(0) = u_0$

(iii) μ *is continuously differentiable in* $[0,T]$

(iv) $\partial_t u(t) = Au(t) + h(u(t),\mu(t))$ *for* $t \in [0,T]$

Next, we show that the time derivative of the exact speed μ occurring in (2.6) is uniformly bounded for $t \in [0,T]$. For this we use the representation given in (2.19). The uniform bound of the time derivative can be obtained by using the PDE (2.17a) to exchange the time derivative for a derivative in space and is precisely given in

Lemma 2.1.28. *Assume that* (u,μ) *is a solution of the PDAE* (2.6) *satisfying Assumption 2.1.27. If there is* $\varepsilon_\psi > 0$ *only depending on* ψ *such that* $(1+M\langle\psi,\partial_x u(t)\rangle) \geq \varepsilon_\psi > 0$ *for* $t \in [0,T]$*, then the time-derivative of the exact speed* μ *from* (2.18b) *is bounded. If* $\mu(t)$*,* $\|g(u(t))\|_{L^2}$ *and* $\|\partial_t g(u(t))\|_{L^2}$ *are uniformly bounded in* $t \in [0,T]$*, then* $|\mu'(t)|$ *is uniformly bounded as well and we have*

$$|\mu'(t)| \leq K_2\varepsilon_\psi^{-2}(1 + \|u\|_{L^2} + \|u\|_{L^2}^2) \quad (t \in [0,T]),$$

with a positive constant $K_2 = K_2\left(|\mu|, \|\psi\|_{H^4}, M, \|g(u)\|_{L^2}, \|\partial_t g(u)\|_{L^2}\right)$.

Proof. We start with the representation of μ given by (2.19). By the quotient rule and integration by parts we obtain

$$\begin{aligned}\partial_t\mu(t) &= \partial_t\left(\frac{M\langle\partial_x\psi,\partial_x u\rangle - M\langle\psi,g(u)\rangle}{(1+M\langle\psi,\partial_x u\rangle)}\right)\\ &= \frac{1}{(1+M\langle\psi,\partial_x u\rangle)^2}\Big[\Big(-M\langle\partial_x^2\psi,\partial_t u\rangle - M\langle\psi,\partial_t g(u)\rangle\Big)\left(1 - M\langle\partial_x\psi,u\rangle\right)\\ &\qquad + \Big(-M\langle\partial_x^2\psi,u\rangle - M\langle\psi,g(u)\rangle\Big)\left(M\langle\partial_x\psi,\partial_t u\rangle\right)\Big].\end{aligned}$$

By assumption we have $(1 + M\langle\psi,\partial_x u\rangle) \geq \varepsilon_\psi$ for an $\varepsilon_\psi > 0$ such that we obtain

$$\begin{aligned}|\partial_t\mu(t)| \leq \varepsilon_\psi^{-2}M\Big[&\Big(|\langle\partial_x^2\psi,\partial_t u\rangle| + |\langle\psi,\partial_t g(u)\rangle|\Big)\left(1 + M|\langle\partial_x\psi,u\rangle|\right)\\ &+ \Big(|\langle\partial_x^2\psi,u\rangle| + |\langle\psi,g(u)\rangle|\Big)\left(M|\langle\partial_x\psi,\partial_t u\rangle|\right)\Big].\end{aligned}$$

As mentioned, we use the PDE (2.17a) to exchange the time derivative for a derivative in space for the term $\langle \partial_x^2 \psi, \partial_t u\rangle$. Note that the PDE also holds true for $t = 0$ by Assumption 2.1.27. For $\phi \in \{\partial_x^2\psi, \partial_x\psi\}$ it follows by the definition of the projection that

$$\begin{aligned}
|\langle \phi, \partial_t u\rangle| &= |\langle \phi, P[Au + g(u) + \mu\partial_x u]\rangle| \\
&= |\langle \phi, Au + g(u) + \mu\partial_x u\rangle - \langle \phi, \psi\rangle M \langle \psi, Au + g(u) + \mu\partial_x u\rangle| \\
&\le |\langle \partial_x^2 \phi, u\rangle + \langle \phi, g(u)\rangle - \mu\langle \partial_x\phi, u\rangle - \langle \phi, \psi\rangle M(\langle \partial_x^2\psi, u\rangle + \langle \psi, g(u)\rangle - \mu\langle \partial_x\psi, u\rangle)| \\
&\le K\left(|\mu|, \|\psi\|_{H^4}, M\right)\Big(\|u\|_{L^2} + \|g(u)\|_{L^2}\Big)
\end{aligned}$$

with a constant $K = K\left(|\mu|, \|\psi\|_{H^4}, M\right) > 0$. This yields

$$\begin{aligned}
|\partial_t\mu(t)| \le{}& \varepsilon_\psi^{-2} M\Big[\Big(K(\|u\|_{L^2} + \|g(u)\|_{L^2}) + |\langle \psi, \partial_t g(u)\rangle|\Big)(1 + M|\langle \partial_x\psi, u\rangle|) \\
&+ \Big(|\langle \partial_x^2\psi, u\rangle| + |\langle \psi, g(u)\rangle|\Big) MK(\|u\|_{L^2} + \|g(u)\|_{L^2})\Big] \\
\le{}& \varepsilon_\psi^{-2} M\Big[\Big(K(\|u\|_{L^2} + \|g(u)\|_{L^2}) + \|\psi\|_{L^2}\|\partial_t g(u)\|_{L^2}\Big)(1 + M\|\partial_x\psi\|_{L^2}\|u\|_{L^2}) \\
&+ \Big(\left\|\partial_x^2\psi\right\|_{L^2}\|u\|_{L^2} + \|\psi\|_{L^2}\|g(u)\|_{L^2}\Big) MK(\|u\|_{L^2} + \|g(u)\|_{L^2})\Big] \\
\le{}& K_2\left(|\mu|, \|\psi\|_{H^4}, M, \|g(u)\|_{L^2}, \|\partial_t g(u)\|_{L^2}\right)\varepsilon_\psi^{-2}(1 + \|u\|_{L^2} + \|u\|_{L^2}^2)
\end{aligned}$$

with a constant $K_2 = K_2\left(|\mu|, \|\psi\|_{H^4}, M, \|g(u)\|_{L^2}, \|\partial_t g(u)\|_{L^2}\right) > 0$. This constant can be bounded from above if the speed $|\mu(t)|$ and nonlinear terms $\|g(u(t))\|_{L^2}$ and $\|\partial_t g(u(t))\|_{L^2}$ are uniformly bounded in $t \in [0, T]$. □

2.2 Lie Splitting for Freezing Waves

We are going to approximate solutions of

$$\begin{cases} \partial_t u = \partial_x^2 u + g(u) + \mu\partial_x u + \mu\psi, & \quad (t \in (0,T]) \qquad (2.21a) \\ \quad 0 = \langle \psi, u\rangle, & \qquad (2.21b) \\ u(0) = u_0 \in H^1(\mathbb{R}) \cap \mathcal{R}(P) \end{cases}$$

with the Lie splitting introduced in Section 1.4. We assume that the initial value for the exact solution lies in $H^4(\mathbb{R})$. Nevertheless, the concept of mild solution is necessary since the approximations by the Lie splitting will only lie in $H^1(\mathbb{R})$. Throughout this chapter we will denote the exact solution with $(\underline{u}(t), \underline{\mu}(t))$ for $t \in [0, T]$ and a fixed $u_0 \in H^4(\mathbb{R}) \cap \mathcal{R}(P)$.

2.2.1 How to Apply the Splitting Method

The goal of this chapter is to introduce a splitting scheme for the PDAE (2.21). The first question for splitting methods is often which parts of the equation should be grouped and solved together. As motivated in Section 1.4 we divide the right-hand side of the evolution equation of (2.21) in linear and nonlinear parts. By this approach we obtain a linear PDAE including the algebraic constraint and a nonlinear ODE without constraint similar to [AO17]. The algebraic constraint is enforced by applying the projector P introduced in Definition 2.1.3 in the last step of the splitting approach. In the remaining chapter we use the exact solutions of the subproblems and derive a convergence result of the splitting scheme. We are able to apply an implicit scheme to the linear subproblem and solve the nonlinear subproblem with an explicit numerical scheme in Section 3.2 to obtain a full time discrete approximation. Note that we use a different numerical approach for the viscous Burgers' equation in Chapter 6. The convergence results we obtain in Chapters 2 and 3 take only the time discretizations into account. Spatial discretization is only considered in the numerical simulations in Chapters 5 and 6.

First, we define $0 \leq t_n := n\tau \leq T < \infty$ for a time step size $\tau > 0$. We extend the transformed system (2.6) by an additional term and then apply the splitting approach. We start by discussing a single step of the splitting scheme with a smooth and consistent initial value z at time t_n and then define the full splitting scheme by recursion. We apply a splitting approach for a single step to the problem

$$\begin{cases} \partial_t u = \partial_x^2 u + g(u) + \mu\partial_x u + \mu\psi + q_n - q_n, \\ \quad 0 = \langle \psi, u \rangle, \\ u(t_n) = z. \end{cases} \qquad (t \in (t_n, t_{n+1}]) \tag{2.22a}$$

The choice of q_n will be discussed below. The additional term $q_n - q_n$ does not change the solution of this problem but the two terms are handled separately. The red part is considered in the linear subproblem whereas the blue part is handled in the nonlinear subproblem of the splitting scheme. The function q_n is typically called a *correction term*.

In some cases operator splitting suffers from an order reduction. For example in the case of constrained PDEs as in [EO15, EO16, AO17], the Strang splitting without a correction term yields only first order convergence although one expects second order convergence. But the splitting approach with the correction term overcomes the order reduction. Note that the order reduction often only occurs for the Strang splitting and the Lie splitting converges typically with first order without a correction. Thus, we do not expect an order reduction of the scheme which we introduce in this section. But it turns out that the correction term is useful for approximating traveling waves as well. In Section 4.1 we are able to prove that the corrected version preserves a steady state in a certain way. Even though one has to require that q_n is an approximation to $g(\underline{u}(t_n))$ of order one, there are multiple choices for the correction term. But it turns out that in the setting of the co-moving frame only the choice

$$q_n := g(z),$$

i.e. the nonlinearity evaluated at the initial value, seems reasonable with the given assumptions. Since we will show that – in the sense of the global error – the initial value z of (2.22) is an first-order approximation to $\underline{u}(t_n)$ in the splitting scheme, the required property $g(z) \approx g(\underline{u}(t_n))$ is fulfilled. For convenience we will leave the general framework and will only use $g(z)$ as correction term. In the first step of the splitting scheme we solve the linear inhomogeneous problem

$$\begin{cases} \partial_t v = \partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + \lambda\psi + g(z), & (t \in (t_n, t_{n+1}]) \\ 0 = \langle \psi, v \rangle, & \\ v(t_n) = z, & \end{cases} \tag{2.23}$$

where we fix the speed $\tilde{\lambda}(u_n^*)$ in front of the advection term. The choice of $\tilde{\lambda}(u_n^*)$ is discussed below. To solve this problem exactly, we use the solution representation constructed in the previous section. The time discretization of this linear subproblem will be discussed later in Section 3.2. Note that the correction $g(z)$ is constant on each time interval $[t_n, t_{n+1}]$. The crucial part for the convergence proof is that we **fix the speed** $\tilde{\lambda}(u_n^*)$ in front of the part $\tilde{\lambda}(u_n^*)\partial_x v$ obtained from the co-moving frame in each splitting step. Further, we choose the speed $\tilde{\lambda}(u_n^*)$ – at least at a formal level – independently of the initial value z. This is achieved by an additional dependence of the solution operator on u_n^*. Otherwise two different semigroups would appear in the stability estimate as we will see later. These different semigroups do not allow suitable estimates with standard semigroup theory necessary for the convergence proof. In order to obtain the two mentioned properties we define each $\tilde{\lambda}(u_n^*)$ by calculating the speed for the PDAE via an approximation u_n^* to $\underline{u}(t_n)$ of order one in the H^1-norm, i.e. there exists a constant $K > 0$

$$\|u_n^* - \underline{u}(t_n)\|_{H^1} \leq \tau K.$$

For a given function $u^* \in H^1(\mathbb{R})$ with $1 + M\langle \psi, \partial_x u^* \rangle \neq 0$ we define the speed $\tilde{\lambda}(u^*)$ by

$$\tilde{\lambda}(u^*) := \frac{M\langle \partial_x \psi, \partial_x u^* \rangle - M\langle \psi, g(u^*) \rangle}{1 + M\langle \psi, \partial_x u^* \rangle}. \tag{2.24}$$

Using the approximation u_n^* this defines the speed $\tilde{\lambda}(u_n^*)$ in (2.23). How this formula is derived from the PDAE (2.21) will be discussed later in detail and we will give an implicit relation for the speed in (2.38). The constraint of the PDAE (2.23) is fulfilled by the Lagrange multiplier $\lambda(t)$ for $t_n \leq t \leq t_{n+1}$. We choose the auxiliary function $g(z)$ at a formal level independently of u_n^*. This allows to pose lower regularity assumptions in the proof of the local error estimate. Note that this concept differs from the ideas in [AO17, EO15], where the correction term is independent of the initial value. Since in (2.23) the Lagrange multiplier, the term from the co-moving frame and the algebraic constraint occur again, we can apply Lemma 2.1.26 to obtain the projected system

$$\begin{cases} \partial_t v = P[\partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + g(z)], & (t \in (t_n, t_{n+1}]) \\ \lambda = M\langle \partial_x \psi, \partial_x v\rangle - M\langle \psi, g(z) + \tilde{\lambda}(u_n^*)\partial_x v\rangle & \\ v(t_n) = z. & \end{cases} \tag{2.25}$$

The value $\tilde{\lambda}(u_n^*)$ will be the approximation to the exact speed $\underline{\mu}(t_n)$. The term including the Lagrange multiplier vanishes in the projected evolution equation, so the unknown $\lambda(t)$ is no longer of interest. Its only purpose was to fulfill the algebraic constraint of the PDAE (2.23). Thus, we obtain the system

$$\begin{cases} \partial_t v = P[\partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + g(z)], & (t \in (t_n, t_{n+1}]) \\ \tilde{\lambda}(u_n^*) = \dfrac{M\langle \partial_x \psi, \partial_x u_n^*\rangle - M\langle \psi, g(u_n^*)\rangle}{1 + M\langle \psi, \partial_x u_n^*\rangle} & \\ v(t_n) = z. & \end{cases} \tag{2.26}$$

We solve this system exactly in the first splitting step for the proposed scheme by using the variation-of-constants formula as a solution representation for this subproblem. The time discretization is discussed in Chapter 3. We abbreviate the generator with the advection term by

$$B(u^*) \coloneqq \partial_x^2 + \tilde{\lambda}(u^*)\partial_x \tag{2.27}$$

with domain $\mathcal{D}(B(u^*)) = H^2(\mathbb{R})$ for $u^* \in H^1(\mathbb{R})$. Since we have two generators of analytic quasicontractive semigroups in the evolution equation, i.e.

$$P\partial_x^2 \quad \text{and} \quad PB(u_n^*) = P\partial_x^2 + \tilde{\lambda}(u_n^*)P\partial_x,$$

we have two solution representations for $t \in [t_n, t_{n+1}]$ given by

$$v(t) = e^{(t-t_n)P\partial_x^2} z + \int_{t_n}^t e^{(t-s)P\partial_x^2} P\left[\tilde{\lambda}(u_n^*)\partial_x v(s) + g(z)\right] ds, \tag{2.28a}$$

$$v(t) = e^{(t-t_n)PB(u_n^*)} z + \int_{t_n}^t e^{(t-s)PB(u_n^*)} Pg(z) ds. \tag{2.28b}$$

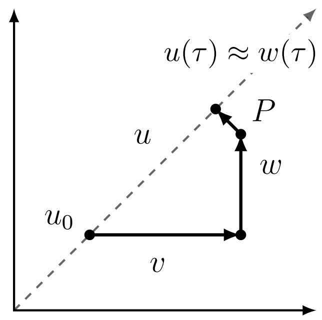

Figure 2.3: Splitting ansatz using the projection P in each step.

We will use the first one to prove second order estimates of the local error and the second one to prove the stability of the splitting scheme. Here we denote the growth constants from Lemmas 2.1.13 and 2.1.23 with ω and ω_n for the generators $P\partial_x^2$ and PB_n, respectively. Typically, τ is small and therefore the value satisfies $e^{\tau\omega} \approx 1$ since $e^{\tau\omega} \to 1$ for $\tau \to 0$. Thus, this additional factor arising in the case of quasicontractive semigroups does not matter in the local error as we will see below and is only important for the global error recursion. Back to the definition of the splitting scheme, the solution of v of the PDAE (2.26) defines the mapping

$$\Phi_v^t : (z, u^*) \mapsto \Phi_v^t(z; u^*) := e^{tPB(u^*)}z + \int_0^t e^{(t-s)PB(u^*)}Pg(z)ds \tag{2.29}$$

for $t \in [0, \tau]$. Then with (2.28b) we have $v(t) = \Phi_v^{t-t_n}(z; u_n^*)$. Note that the dependency on the approximation u_n^* turns out to be crucial for the convergence proof. This is the first step of the splitting scheme.

In the second (nonlinear) step we solve an ODE which handles the remaining parts from the evolution equation (2.22a). These are the nonlinearity g and the correction term $-g(z)$ such that we obtain the ODE

$$\partial_t w(t) = g(w(t)) - g(z), \quad w(t_n) = w_0, \qquad (t \in [t_n, t_{n+1}]) \tag{2.30}$$

where we use as initial value the solution from the first subproblem, i.e. $w_0 = v(t_{n+1})$. We denote the solution of the ODE (2.30) for $t \in [t_n, t_{n+1}]$ by

$$\Phi_w^{t-t_n}(w_0; z) := w(t). \tag{2.31}$$

For the splitting scheme we use a Taylor expansion of the exact solution with a second order remainder term to obtain the solution at time t_{n+1} by

$$w(t_{n+1}) = w(t_n) + \tau\,[g(w(t_n)) - g(z)] + \mathcal{R}_1(\tau^2). \tag{2.32}$$

The error term $\mathcal{R}_1(\tau^2)$ is discussed below in (2.44). We note here that the nonlinear problem does not involve any algebraic constraint. It turns out that the solution of this ODE in the second step still lies, up to order two, on the subspace $\mathcal{R}(P)$ where the algebraic constraint is fulfilled (Lemma 2.3.8). Even though this may lead to a convergent splitting scheme, we project the solution of the nonlinear step into the subspace $\mathcal{R}(P)$ such that we do not have to deal with inconsistent initial data for the next linear step. The evaluation of the projection is very cheap such that the total computational costs do not increase significantly. Thus, the mapping for the second step of the Lie splitting is given by

$$P\Phi_w^\tau : (v(t_{n+1}); z) \mapsto Pw(t_{n+1}) = P\Phi_w^\tau(v(t_{n+1}); z) \in \mathcal{R}(P).$$

The dependency on the initial value z for the initial problem (2.22) is a consequence of the correction term $g(z)$. To sum up the splitting is defined via

$$\begin{aligned} \mathcal{L}_\tau(z; u^*) &\coloneqq P\Phi_w^\tau(\Phi_v^\tau(z; u^*); z), \\ \mathcal{L}_\tau(z) &= \mathcal{L}_\tau(z; z), \end{aligned} \tag{2.33}$$

where the latter definition is an abbreviation to obtain the recursion of the splitting scheme. The obtained splitting scheme is illustrated in Figure 2.3. A step in the horizontal direction in Figure 2.3 amounts in solving the linear subproblem (2.26), whereas a step in the vertical direction amounts to solve the nonlinear ODE (2.30). This step is followed by the projection P.

As suggested in [AO17] to obtain the $(n+1)$-th approximation by the splitting scheme denoted with u_{n+1} we can choose $u_n^* = u_n$. Since we will prove the first order convergence of the scheme, the required property $\|u_n^* - \underline{u}(t_n)\|_{H^1} \leq \tau K$ for some constant $K > 0$ is fulfilled. To handle this argument correctly, we have to use a proof by induction technique, which is given in detail in the convergence proof of Theorem 2.3.9. With the initial value u_0 of the exact problem (2.21) we obtain the approximations by

$$u_n \coloneqq \mathcal{L}_\tau^n(u_0) \approx \underline{u}(t_n),$$

i.e. we apply n-times the splitting scheme with the operator introduced above. Note that $\underline{u}$ denotes the exact solution of the PDAE (2.21) as described in the beginning of this chapter.

The existence of solutions for the subproblems (2.23) and (2.30) are discussed later. For the linear problem we can apply standard semigroup techniques as given in Lemma 2.3.3 and the nonlinear ODE can be handled by the Picard-Lindelöf Theorem.

2.3 First Order Convergence of the Lie Splitting

In this section we derive a convergence proof for the splitting scheme introduced in Section 2.2.1 approximating the solution u of the PDAE (2.21). The PDAE was given by

$$\begin{cases} \partial_t u = Au + g(u) + \mu\partial_x u + \mu\psi, & \qquad (2.21a) \\ \quad 0 = \langle \psi, u\rangle, & (t \in (0,T]) \qquad (2.21b) \\ u(0) = u_0 \in H^1(\mathbb{R}) \cap \mathcal{R}(P). \end{cases}$$

The basic ideas for the local error and convergence proof itself are based on [AO17]. Nevertheless, the proof given in this section is quite different since in our setting we have the additional advection term $\mu\partial_x u$, which we treat in a different way than the correction term. As already mentioned we couple the correction term to the initial value and use an approximation u_n^* to calculate the speed λ_n in each step. Additionally, in the proposed scheme we get different semigroups in each splitting step due to the variance of speed λ_n which is not the case in [AO17]. These semigroups have to be handled carefully with the concept of quasicontractivity, cf. Section 2.1.2. Thus, the techniques used in [AO17] are more standard than the approach chosen in this work. Nevertheless, for numerical simulations we proceed in the usual way: the value u_n^* can be chosen as the previous value in the Lie splitting such that the correction and speed λ_n only depend on u_n. We derive a convergence proof of the splitting scheme provided certain assumptions on the nonlinearity, which hold true in the case that the nonlinearity g is a polynomial operator. Before we consider such operators in Section 2.3.3, we work in a more general framework.

For this we define three neighborhoods U, U^*, U^+ of the exact solution $\underline{u}$ of the PDAE (2.21). Let $\varepsilon^*, \varepsilon_2 > 0$ and $\delta^+ > \delta^* + \varepsilon^* > 0$, $\delta^* > \delta + \varepsilon_2 > 0$. We define

$$\begin{aligned} U \ &:= \Big\{ z \in H^1(\mathbb{R}) \;\Big|\; \exists t^* = t^*(z) \in [0,T] : \quad \|z - \underline{u}(t^*)\|_{H^1} < \delta \Big\}, \\ U^* &:= \Big\{ z \in H^1(\mathbb{R}) \;\Big|\; \exists t^* = t^*(z) \in [0,T] : \quad \|z - \underline{u}(t^*)\|_{H^1} < \delta^* \Big\}, \\ U^+ &:= \Big\{ z \in H^1(\mathbb{R}) \;\Big|\; \exists t^* = t^*(z) \in [0,T] : \quad \|z - \underline{u}(t^*)\|_{H^1} < \delta^+ \Big\}, \end{aligned} \tag{2.35}$$

i.e. we have a δ, δ^* and δ_+-neighborhood of the exact solution $\underline{u}$ with respect to the H^1-norm. In particular, there is a constant $C_{U^+} > 0$ such that

$$\|z\|_{H^1} \le C_{U^+} \qquad (z \in U^+). \tag{2.36}$$

For the neighborhoods we have the relations

$$\{\, \underline{u}(t) \mid t \in [0,T] \,\} \subset U \subset U^* \subset U^+ \subset H^1(\mathbb{R}).$$

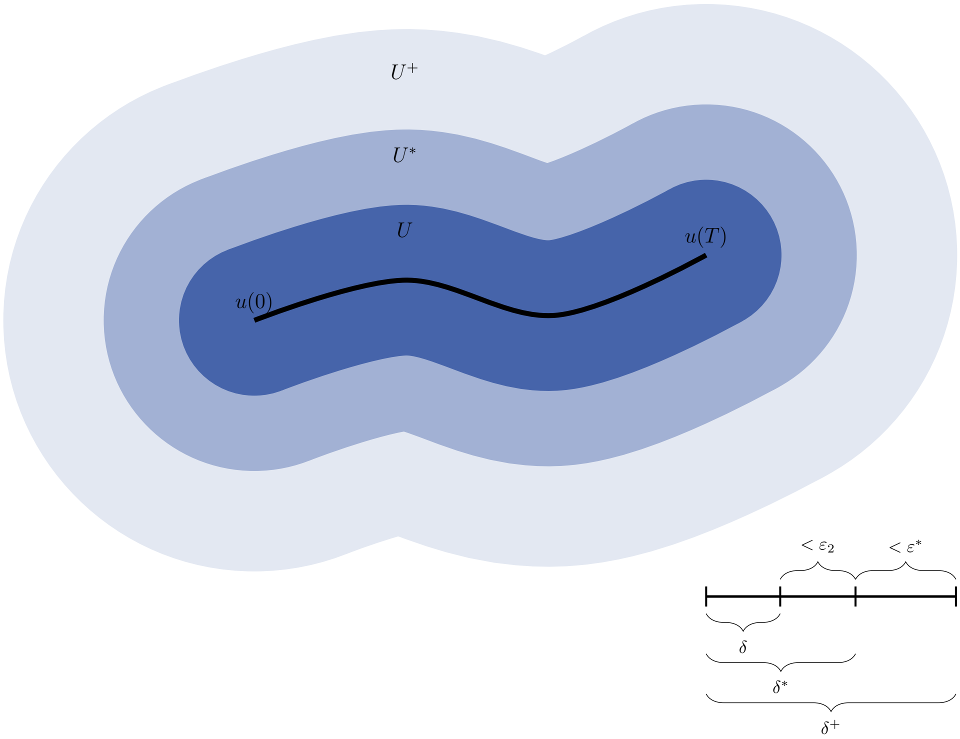

Figure 2.4: ε-neighborhoods U, U^*, U^+

These neighborhoods will be used to state the following main assumptions for the convergence proof.

Assumption 2.3.1. *In addition to Assumption 1.3.1 we assume that*

(I) the reference function $\hat{u} \in H^6_{ca}(\mathbb{R})$ satisfies Assumption 1.3.1 (ii) and there is $\varepsilon_\psi > 0$ only depending on ψ such that

$$1 + M\langle \psi, \partial_x z \rangle > \varepsilon_\psi \qquad (z \in U^+);$$

(II) the nonlinearity $g : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ is Fréchet differentiable and there is a constant $C_{Dg}(U^+) > 0$ such that

$$\|Dg(z)\|_{H^1 \leftarrow H^1} \leq C_{Dg}(U^+) \qquad (z \in U^+).$$

With the mean value theorem it follows that $g : U^+ \to H^1(\mathbb{R})$ is Lipschitz continuous with Lipschitz constant $L = L(U^+)$;

(III) the nonlinearity g is uniformly bounded in U^+, i.e. there is $C_g(U^+) > 0$ such that

$$\|g(z)\|_{H^1} \leq C_g(U^+) \qquad (z \in U^+);$$

(IV) the initial value $u_0 = v_0 - \hat{u}$ lies in $H^4(\mathbb{R})$ and is consistent, i.e. $\langle \psi, u_0 \rangle = 0$;

(V) there exists a bounded solution $(\underline{u}, \underline{\mu}) : [0,T] \to H^4(\mathbb{R}) \times \mathbb{R}$ of the PDAE (2.21) satisfying Assumption 2.1.27 such that $\underline{u} \in \mathcal{C}([0,T], H^4(\mathbb{R}))$ and $\underline{\mu} \in \mathcal{C}^1([0,T],\mathbb{R})$, in particular there are $C_u, C_\mu > 0$ such that

$$\|\underline{u}(t)\|_{H^4} \le C_u, \quad |\underline{\mu}(t)| \le C_\mu \qquad (t \in [0,T]);$$

(VI) for the nonlinearity g applied to the exact solution there is $C_{g,u} > 0$ such that

$$\|g(\underline{u}(t))\|_{H^4} \le C_{g,u} \qquad (t \in [0,T])$$

for g as a mapping $g : H^4(\mathbb{R}) \to H^4(\mathbb{R})$.

The first assumption (I) ensures that the speed representation for μ in (2.19) and $\tilde{\lambda}(u^*)$ in (2.24) for all $u^* \in U^+$ are well defined and bounded as shown in Lemma 2.3.4 (i) below. The last part in (V) follows since $t \mapsto \|\underline{u}(t)\|_{H^4}$ is a composition of continuous maps.

Remark 2.3.2. As mentioned before, we are going to motivate the definition of the speed $\tilde{\lambda}(u_n^*)$ as given in (2.24). The linear PDAE (2.23) in the first step of the splitting scheme originates from the PDAE (2.22) and is given without the fixed speed by

$$\begin{cases} \partial_t v = \partial_x^2 v + \lambda(t)\partial_x v + \lambda(t)\psi + g(z), \\ \quad 0 = \langle \psi, v \rangle, \\ v(t_n) = z. \end{cases} \qquad (t \in (t_n, t_{n+1}])$$

The first idea behind the choice of $\tilde{\lambda}(u_n^*)$ is that we choose the speed for the initial time $t = t_n$. By the equivalence to the projected system as given in Lemma 2.1.26 we have the implicit relation

$$\lambda(t_n) = M\langle \partial_x \psi, \partial_x v(t_n) \rangle - M\langle \psi, \lambda(t_n)\partial_x v(t_n) + g(z) \rangle.$$

We obtain as before

$$\begin{aligned} \lambda(t_n) &= M\langle \partial_x \psi, \partial_x v(t_n) \rangle - M\langle \psi, \lambda(t_n)\partial_x v(t_n) + g(z) \rangle \\ \iff \quad (1 + M\langle \psi, \partial_x v(t_n) \rangle)\, \lambda(t_n) &= M\langle \partial_x \psi, \partial_x v(t_n) \rangle - M\langle \psi, g(z) \rangle \\ \iff \quad \lambda(t_n) &= \frac{M\langle \partial_x \psi, \partial_x v(t_n) \rangle - M\langle \psi, g(z) \rangle}{1 + M\langle \psi, \partial_x v(t_n) \rangle}, \end{aligned}$$

where $1 + M\langle \psi, \partial_x v(t_n) \rangle > \varepsilon_\psi$ by Assumption 2.3.1 (I) if $v(t_n) \in U^+$. Note that for the initial value we have $v(t_n) = z$. If one uses $\lambda(t_n)$ for the fixed speed in the splitting approach, this would lead to the fact that the operator $B_{\lambda(t_n)}$ as defined in (2.9) would depend on the initial value z in each step. Thus, the semigroup generated by $B_{\lambda(t_n)}$ would depend on z and differs for different initial values. In the stability estimate where we start with the different initial values $u(t_n), u_n$ it is crucial that we have the same semigroups. An approach to handle the advection term in the inhomogeneity leads to a reduction of regularity in each step. As a remedy we replace the dependence on z by an dependence to an approximation u_n^* such that we end up with (2.24). Note that (2.24) is equivalent to the implicit relation

$$\tilde{\lambda}(u^*) = M\langle \partial_x \psi, \partial_x u^* \rangle - M\langle \psi, \tilde{\lambda}(u^*)\partial_x u^* + g(u^*) \rangle \tag{2.38}$$

for every $u^* \in U^+$.

We can show the existence of a unique mild solution of the linear subproblem for initial values in $H^1(\mathbb{R})$.

Lemma 2.3.3. *For $z \in H^1(\mathbb{R}) \cap \mathcal{R}(P), u_n^* \in H^1(\mathbb{R})$ there exists a unique (mild) solution $v \in \mathcal{C}([t_n, t_n + \tau], H^1(\mathbb{R}))$ of the linear problem of the splitting scheme*

$$\begin{cases} \partial_t v = \partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + \lambda\psi + g(z), \\ \quad 0 = \langle \psi, v \rangle, \\ v(t_n) = z \end{cases} \qquad (t \in (t_n, t_n + \tau])$$

for $\tau > 0$ sufficient small. If in addition z lies in $H^2(\mathbb{R})$, then v is the unique classical solution, i.e. $v \in \mathcal{C}^1([0,T], L^2(\mathbb{R}))$ and $\partial_t v = \partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + \lambda\psi + g(z)$ holds true for all $t \in [t_n, t_n + \tau]$.

Proof. We use Lemma 2.1.26 to obtain the equivalent system

$$\begin{cases} \partial_t v = P(\partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + g(z)) & (t \in (t_n, t_n + \tau]) \\ \quad \lambda = M\langle \partial_x \psi, \partial_x v \rangle - M\langle \psi, \tilde{\lambda}(u_n^*)\partial_x v + g(z) \rangle & (t \in [t_n, t_n + \tau]) \\ v(t_n) = z. \end{cases}$$

The PDE of this system can also be written as

$$\partial_t v = PB(u_n^*)v + Pg(z),$$

where $PB(u_n^*)$ is a generator of a strongly continuous semigroup on $H^1(\mathbb{R})$ by applying Lemma 2.1.25. Since the inhomogeneity $t \mapsto Pg(z)$ is independent of v and t, it is an element of $\mathcal{C}^1([t_n, t_n + \tau], H^1(\mathbb{R}))$ and locally Lipschitz continuous. The initial value z lies $H^1(\mathbb{R})$, therefore we can apply Theorem A.1.1 to obtain a unique mild solution of the PDE and further also of the linear problem in the splitting step. Since we are not interested in the maximal existence interval, we can slightly shrink the interval to obtain the desired property that the solution v lies in $\mathcal{C}([t_n, t_n + \tau], H^1(\mathbb{R}))$ for sufficient small $\tau > 0$ by the fixed point argument in the proof of the theorem as given in [Paz83, Theorem 6.1.4, p. 185]. If $z \in H^2(\mathbb{R}) = \mathcal{D}(\partial_x^2)$, the last assertion of the Lemma follows by [Sch, Theorem 2.9, p. 50]. □

Lemma 2.3.4. *Under Assumption 2.3.1 the following properties for the solutions v and w of* (2.23) *and* (2.30)*, respectively, hold true.*

(i) There is a constant $C_\lambda(U^+) > 0$ only depending on $\psi, \varepsilon_\psi, g, U^+$ such that

$$|\tilde{\lambda}(z)| \le C_\lambda(U^+) \qquad (z \in U^+).$$

(ii) There is $\omega^* > 0$ such that for $s \in \{1, 4\}$ the semigroup generated by $PB(z)$ satisfies

$$\left\| e^{tPB(z)} \right\|_{H^s \leftarrow H^s} \le e^{t\omega^*} \qquad (z \in U^+),$$

where $B(z)$ is defined above in (2.27)*.*

(iii) There is $\tau_1 > 0$ such that for $z \in U \cap \mathcal{R}(P)$ and $z^+ \in U^+$ it holds

$$\Phi_v^\tau(z; z^+) \in U^* \qquad (\tau < \tau_1).$$

(iv) There is $\tau_2 > 0$ such that for $z^* \in U^*$ and $z^+ \in U^+$ it holds

$$\Phi_w^\tau(z^*; z^+) \in U^+ \qquad (\tau < \tau_2).$$

(v) There is $C_v > 0$ and $\tau_3 > 0$ such that for every $t \in [0, T]$ and $z^+ \in U^+$ it holds

$$\left\| \Phi_v^\tau(u(t); z^+) \right\|_{H^4} \le C_v \qquad (\tau < \tau_3).$$

The solution of v will be estimated using the variation-of-constants formula. For the ODE in the nonlinear step we apply the Picard-Lindelöf Theorem, which is stated in

Theorem 2.3.5 (Picard-Lindelöf)**.** *Suppose $(E, \|\cdot\|)$ is a Banach space, $z_0 \in E$, $R > 0$, $D \subseteq E$ with $\overline{B}(z_0, R) \subseteq D$ and $f : D \to E$ Lipschitz continuous. Let*

$$\tilde{M} := \left\{ \|f(x)\| \mid x \in \overline{B}(z_0, R) \right\},$$
$$\alpha := \min \left\{ \frac{R}{\tilde{M}}, \frac{1}{2L} \right\}.$$

If $\tilde{M} < \infty$ *then the initial value problem*

$$\begin{cases} z' = f(z) \\ z(0) = z_0 \end{cases}$$

has a unique solution on $[0, \alpha]$ *with values in* $\overline{B}(z_0, R)$*.*

This theorem is an adapted version of [AE08, Theorem 7.8.14]. First, we used [AE08, Remark 7.8.14] to extend the Theorem to the case that the Banach space E is not finite dimensional by replacing this assumption by $\tilde{M} < \infty$. Further, the last assertion that the solution has values in $\overline{B}(x_0, R)$ follows by the Banach fixed point theorem in the proof of [AE08, Theorem 7.8.14].

Proof of Lemma 2.3.4. All parts of this lemma will be proven separately.

Proof of part (i). Let $z \in U^+$. By Assumption 2.3.1 (I) we have $(1 + M\langle\psi, \partial_x z\rangle) > \varepsilon_\psi$ and using (2.24) we obtain

$$\begin{aligned} |\tilde{\lambda}(z)| &\leq \frac{1}{\varepsilon_\psi} M |\langle\partial_x\psi, \partial_x z\rangle - \langle\psi, g(z)\rangle| \\ &\leq \frac{1}{\varepsilon_\psi} M \left(\|\psi\|_{H^1} \|z\|_{H^1} + \|\psi\|_{L^2} \|g(z)\|_{L^2}\right) \\ &\leq \frac{1}{\varepsilon_\psi} M \left(\|\psi\|_{H^1} C_{U^+} + \|\psi\|_{L^2} C_g(U^+)\right) \\ &=: C_\lambda(U^+). \end{aligned}$$

The constant C_{U^+} is given in (2.36) and $C_g(U^+)$ by Assumption 2.3.1 (III).

Proof of part (ii). Let $s \in \{1, 4\}$, then Lemma 2.1.25 yields

$$\left\|e^{tPB(z)}\right\|_{H^s \leftarrow H^s} \leq e^{\omega(z)t} \quad \text{for } t \geq 0$$

with

$$\begin{aligned} \omega(z) &= M \|\psi\|_{H^s} \|\psi\|_{H^2} (1 + |\tilde{\lambda}(z)|) \\ &\leq M \|\psi\|_{H^s} \|\psi\|_{H^2} (1 + C_\lambda(U^+)|) \\ &=: \omega^* \end{aligned}$$

using (i).

Proof of part (iii). Let $z \in U$ and $z^+ \in U^+$. By the definition of U there is $t^* \in [0,T]$ such that

$$\|z - \underline{u}(t^*)\|_{H^1} < \delta.$$

We have

$$\left\|\Phi_v^\tau(z;z^+) - \underline{u}(t^*)\right\|_{H^1} \leq \left\|\Phi_v^\tau(z;z^+) - e^{\tau PB(z^+)}\underline{u}(t^*)\right\|_{H^1} + \left\|e^{\tau PB(z^+)}\underline{u}(t^*) - \underline{u}(t^*)\right\|_{H^1}.$$

The existence of the solution is guaranteed by Lemma 2.3.3. In the following estimates we will often use (ii) without further notice. For the first part of the right-hand side we obtain

$$\begin{aligned}\left\|\Phi_v^\tau(z;z^+) - e^{\tau PB(z^+)}\underline{u}(t^*)\right\|_{H^1} &\leq \left\|\int_0^\tau e^{(\tau-s)PB(z^+)}Pg(z)ds\right\|_{H^1} \\ &\quad + \left\|e^{\tau PB(z^+)}\left(z - \underline{u}(t^*)\right)\right\|_{H^1} \\ &\leq \tau e^{\tau\omega^*}\|P\|_{H^1}\|g(z)\|_{H^1} + e^{\tau\omega^*}\delta \\ &\leq \tau e^{\tau\omega^*}\|P\|_{H^1} C_g(U^+) + e^{\tau\omega^*}\delta\end{aligned}$$

with $C_g(U^+)$ from Assumption 2.3.1 (III). For the second part of the right-hand side above we calculate

$$\begin{aligned}\left\|e^{\tau PB(z^+)}\underline{u}(t^*) - \underline{u}(t^*)\right\|_{H^1} &= \left\|\left(e^{\tau PB(z^+)} - I\right)\underline{u}(t^*)\right\|_{H^1} \\ &= \left\|PB(z^+)\int_0^\tau e^{sPB(z^+)}\underline{u}(t^*)ds\right\|_{H^1} \\ &\leq \|P\|_{H^1}\left\|\left(\partial_x^2 + \tilde{\lambda}(z^+)\partial_x\right)\int_0^\tau e^{sPB(z^+)}\underline{u}(t^*)ds\right\|_{H^1} \\ &\leq \|P\|_{H^1}\tau e^{\tau\omega*}\left(\|\underline{u}(t^*)\|_{H^3} + |\tilde{\lambda}(z^+)|\,\|\underline{u}(t^*)\|_{H^2}\right) \\ &\leq \tau e^{\tau\omega^*}\|P\|_{H^1} C_u\left(1 + |\tilde{\lambda}(z^+)|\right) \\ &\leq \tau e^{\tau\omega^*}\|P\|_{H^1} C_u\left(1 + C_\lambda(U^+)\right),\end{aligned}$$

where $C_\lambda(U^+)$ is the constant arising in (i) and C_u from Assumption 2.3.1 (V). To sum up we have

$$\left\|\Phi_v^\tau(z;z^+) - \underline{u}(t^*)\right\|_{H^1} \leq \tau e^{\tau\omega^*}K + e^{\tau\omega^*}\delta$$

with $K := \|P\|_{H^1}\left(C_g(U^+) + C_u(1 + C_\lambda(U^+))\right)$. To finish the proof we have to show that the right-hand side is smaller than δ^*. We chose $\tau_1 > 0$ so small that

$$\tau_1 e^{\tau_1\omega^*}K < \frac{\varepsilon_2}{2}$$

and

$$\sum_{n=1}^{\infty} \frac{(\tau_1 \omega^*)^n}{n!} = \tau_1 \omega^* + \tfrac{1}{2}(\tau_1 \omega^*)^2 + \cdots < \frac{\varepsilon_2}{2\delta},$$

where ε_2 is given by the definition of U^* as in (2.35). For $\tau < \tau_1$ this yields

$$\begin{aligned} \left\| \Phi_v^\tau(z, z^+) - \underline{u}(t^*) \right\|_{H^1} &\leq \tau e^{\tau\omega^*} K + e^{\tau\omega^*} \delta \\ &\leq \frac{\varepsilon_2}{2} + \delta(1 + \frac{\varepsilon_2}{2\delta}) \\ &= \frac{\varepsilon_2}{2} + \delta + \frac{\varepsilon_2}{2} \\ &= \delta + \varepsilon_2 < \delta^*. \end{aligned}$$

Hence $\Phi_v^\tau(z; z^+) \in U^*$ for $\tau < \tau_1$. This concludes the proof.

Proof of part (iv). The proof is based on the well-known Picard-Lindelöf Theorem as stated in Theorem 2.3.5. We chose $R = \varepsilon^*$ where $\varepsilon^* > 0$ is given by the definition of U^+ above in (2.35), where we have $\delta^* + \varepsilon^* < \delta_+$. Let $z^* \in U^*$ and $z^+ \in U^+$. Recall that the solution operator $\Phi_w^\tau(z^*; z^+)$ solves the ODE

$$\begin{cases} \partial_t w = g(w) - g(z^+), \\ w(0) = z^*. \end{cases}$$

The right-hand side, $g(w) - g(z^+)$, as a mapping in w is Lipschitz continuous on U^+ by Assumption 2.3.1 (II) such that we can apply the Picard-Lindelöf Theorem 2.3.5. Thus, it exists a unique solution w for $0 \leq s < \alpha(z^*, z^+, \varepsilon^*) = \min\left\{\frac{\varepsilon^*}{\tilde{M}}, \frac{1}{2L}\right\}$, where

$$\tilde{M} := \max\left\{ \left\| g(z) - g(z^+) \right\|_{H^1} \,\middle|\, z \in \overline{B}(z^*, \varepsilon^*) \right\}$$

and

$$\|w(0) - w(s)\|_{H^1} \leq \varepsilon^*.$$

Note that $w(0) = z^* \in U^*$ and therefore $w(s) \in U^+$ since $\delta^* + \varepsilon^* < \delta_+$. The maximal time of existence α depends on z^*, but we can bound α from below. We define

$$M^* := \sup\left\{ \left\| g(z) - g(z^+) \right\|_{H^1} \,\middle|\, z, z^+ \in U^+ \right\}.$$

Using Assumption 2.3.1 (III) we have $\tilde{M} \leq M^* \leq 2C_g(U^+)$. This yields

$$\alpha = \min\left\{\frac{\varepsilon^*}{\tilde{M}}, \frac{1}{2L}\right\} \geq \min\left\{\frac{\varepsilon^*}{M^*}, \frac{1}{2L}\right\} \geq \min\left\{\frac{\varepsilon^*}{2C_g(U^+)}, \frac{1}{2L}\right\} =: \alpha^*.$$

Thus, we have the minimal existence interval $[0, \alpha^*]$, which is independent of z^* and z^+. The assertion follows with $\tau_2 = \alpha^*$.

Proof of part (v). Let $t \in [0,T]$ and $z^+ \in U^+$. By the variation-of-constants formula we have with $\underline{u}(t) \in H^4(\mathbb{R})$

$$\Phi_v^\tau(\underline{u}(t); z^+) = e^{\tau PB(z^+)}\underline{u}(t) + \int_0^\tau e^{(\tau-s)PB(z^+)}Pg(\underline{u}(t))ds.$$

This yields with Lemma 2.3.4 (ii) for $\tau < \tau_3$

$$\begin{aligned}\left\|\Phi_v^\tau(\underline{u}(t); z^+)\right\|_{H^4} &\le e^{\tau\omega^*}\left\|\underline{u}(t)\right\|_{H^4} + \tau e^{\tau\omega^*}\left\|P\right\|_{H^4}\left\|g(\underline{u}(t))\right\|_{H^4}\\ &\le e^{\tau\omega^*}C_u + \tau e^{\tau\omega^*}\left\|P\right\|_{H^4}C_{g,u}\\ &\le e^{\tau_3\omega^*}C_u + \tau_3 e^{\tau_3\omega^*}\left\|P\right\|_{H^4}C_{g,u}\\ &=: C_v,\end{aligned}$$

where the constant C_u is given by Assumption 2.3.1 (V) and $C_{g,u}$ by Assumption 2.3.1 (VI). □

In the error bound for the local error we are using a Taylor expansion of the inhomogeneity and therefore need a bound of the time derivative of $g(u)$. We will need the following

Lemma 2.3.6. *If Assumption 2.3.1 holds true, then there is $C_{\partial_t g} > 0$*

$$\left\|\partial_t g(\underline{u}(t))\right\|_{H^1} < C_{\partial_t g} \quad \text{for } t \in [0,T],$$

where the constant is independent of the time t, i.e. the time derivative of g along the exact solution is uniformly bounded.

Proof. The proof of this statement makes use of the chain rule and the fact that the Fréchet derivative $Dg(v) : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ for $v \in U^+$ is a linear bounded operator. We obtain for $t \in [0,T]$ with the PDE (2.21)

$$\begin{aligned}\left\|\partial_t g(\underline{u}(t))\right\|_{H^1} &= \left\|Dg(\underline{u}(t))\left[\partial_t\underline{u}(t)\right]\right\|_{H^1}\\ &\le \sup_{z\in U}\left\|Dg(z)\left[\partial_t\underline{u}(t)\right]\right\|_{H^1}\\ &\le \sup_{z\in U}\left\|Dg(z)\right\|_{H^1\leftarrow H^1}\left\|\partial_t\underline{u}(t)\right\|_{H^1}\\ &\le C_{Dg}(U^+)\left\|\partial_x^2\underline{u}(t) + g(\underline{u}(t)) + \underline{\mu}(t)\partial_x\underline{u}(t) + \underline{\mu}(t)\psi\right\|_{H^1}\\ &\le C_{Dg}(U^+)\Big(\left\|\underline{u}(t)\right\|_{H^3} + \left\|g(\underline{u}(t))\right\|_{H^1} + |\underline{\mu}(t)|\left\|\underline{u}(t)\right\|_{H^2} + |\underline{\mu}(t)|\left\|\psi\right\|_{H^1}\Big)\\ &\le C_{Dg}(U^+)\Big(C_u + C_{g,u} + C_\mu C_u + C_\mu\left\|\psi\right\|_{H^1}\Big)\\ &=: C_{\partial_t g},\end{aligned}$$

with all constants arising from Assumption 2.3.1 and Lemma 2.3.4 (i). □

2.3.1 Estimates of the Local Error for a Single Lie Step

Recall that we have the time-steps $0 \leq t_n := n\tau \leq T < \infty$ for a time step size $\tau > 0$. In order to prove the convergence of the scheme (2.33) we will let τ tend to zero such that n tends to infinity. As already mentioned we denote with u_n the n-th splitting approximation via the scheme given in (2.33), i.e.

$$u_n = \mathcal{L}_\tau^n(u_0)$$

with the exact initial value $u_0 = \underline{u}(0)$. In the error accumulation in the final step of the convergence proof we will have to use estimates for the local error with initial value $\underline{u}(t_n)$ at time t_n. Thus, to analyze the local error we use $\underline{u}(t_n)$ as initial value for the Lie splitting $\mathcal{L}_\tau(\underline{u}(t_n); u_n^*)$ for some approximation u_n^* and the exact solution

$$\underline{u}(t_{n+1}) = \Phi_u^\tau(\underline{u}(t_n)).$$

Here the step size τ has to be sufficient small. We choose τ so small that all assertions of Lemma 2.3.4 are fulfilled, in particular it should be smaller than

$$\tau_0 := \min\left\{\tau_1, \tau_2, \tau_3\right\}, \tag{2.41}$$

where τ_1, τ_2, τ_3 are constants given in Lemma 2.3.4. Now we state the estimate of the local error in

Lemma 2.3.7. *We impose Assumption 2.3.1 and let $n \in \mathbb{N} \cap [0, \frac{T}{\tau})$ for $\tau < \tau_0$. For a given first order approximation $u_n^* \in U^+$ to the exact solution at time t_n in the H^1-norm, i.e.*

$$\|u_n^* - \underline{u}(t_n)\|_{H^1} \leq \tilde{C}\tau$$

for some constant $\tilde{C} > 0$ independent of n, the local error at time t_{n+1} is bounded from above by

$$\|\mathcal{L}_\tau(\underline{u}(t_n); u_n^*) - \Phi_u^\tau(\underline{u}(t_n))\|_{H^1} \leq C\tau^2,$$

where the constant C is independent of τ and n.

Note that the usual local error for numerical schemes applied to differential equations differs from the definition we consider in this lemma. Here we require an additional dependence on an approximation u_n^* to handle the advection term obtained by the method of freezing in the convergence proof.

Proof. Let $n \in \mathbb{N}$. Note that for the local error the correction term of the introduced splitting scheme $\mathcal{L}_\tau(\underline{u}(t_n); u_n^*)$ is given by $g(\underline{u}(t_n))$. For the linear subproblem we define v in this proof by (2.29) as

$$\begin{aligned} v(t) &= \Phi_v^{t-t_n}(\underline{u}(t_n), u_n^*) \\ &= e^{(t-t_n)PB(u_n^*)}\underline{u}(t_n) + \int_0^{t-t_n} e^{(t-t_n-s)PB(u_n^*)} Pg(\underline{u}(t_n))ds \\ &= e^{(t-t_n)PB(u_n^*)}\underline{u}(t_n) + \int_{t_n}^{t} e^{(t-s)PB(u_n^*)} Pg(\underline{u}(t_n))ds \end{aligned}$$

for $t \in [t_n, t_{n+1}]$ with u_n^* the approximation from the assumption. Hence v is a solution of the system (2.26) with $z = \underline{u}(t_n)$, i.e. of the system

$$\begin{cases} \partial_t v = P[\partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + g(z)], & (t \in (t_n, t_{n+1}]) \\ \tilde{\lambda}(u_n^*) = \dfrac{M\langle \partial_x \psi, \partial_x u_n^* \rangle - M\langle \psi, g(u_n^*)\rangle}{1 + M\langle \psi, \partial_x u_n^* \rangle} \\ v(t_n) = \underline{u}(t_n). \end{cases} \tag{2.42}$$

We set $\lambda_n = \tilde{\lambda}(u_n^*)$. In the proof we will make use of the property that v is continuously differentiable in $[t_n, t_{n+1}]$ by Lemma 2.3.3 since the initial value $\underline{u}(t_n)$ lies in $H^4(\mathbb{R})$ by Assumption 2.3.1 (V). We use the solution formulas (2.18a) and (2.28a) to represent the exact solution $\underline{u}$ and the solution v of the PDE (2.26), respectively, i.e.

$$\begin{aligned} \underline{u}(t_{n+1}) = \Phi_u^\tau(\underline{u}(t_n)) \qquad &= e^{\tau P \partial_x^2}\underline{u}(t_n) + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds, \\ v(t_{n+1}) = \Phi_v^\tau(\underline{u}(t_n); u_n^*) &= e^{\tau P \partial_x^2}\underline{u}(t_n) + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[\lambda_n \partial_x v(s) + g(\underline{u}(t_n))\right] ds. \end{aligned}$$

Note that the first equation for $\underline{u}$ is part of a system including the speed $\underline{\mu}$, whereas the speed λ_n is fixed in each time step of the scheme by (2.24). The speed λ_n depends on the first order approximation u_n^*. For the nonlinear ODE (2.30) we use a Taylor expansion for a solution representation with a remainder term of second order. This is given by

$$w(t_{n+1}) = w(t_n) + \tau\left[g(w(t_n)) - g(\underline{u}(t_n))\right] + \mathcal{R}_1(\tau^2), \tag{2.43}$$

with $z = \underline{u}(t_n)$ in (2.32) and $w(t_n) = w_0 = v(t_{n+1})$ where the error term is given by

$$\mathcal{R}_1(\tau^2) = \tau^2 \partial_t g(w(\xi)) \tag{2.44}$$

for some $\xi \in [t_n, t_{n+1}]$. Next we show that $\mathcal{R}_1(\tau^2)/\tau^2$ can be bounded from above independently of n and τ. The bound of the first part in (2.44) follows similar to Lemma 2.3.6

by exploiting Lemma 2.3.4. We obtain

$$\begin{aligned}\|\partial_t g(w(\xi))\|_{H^1} &= \left\|Dg(w(\xi))\Big[g(w(\xi)) - g(\underline{u}(t_n))\Big]\right\|_{H^1} \\ &\leq \|Dg(w(\xi))\|_{H^1 \leftarrow H^1} \|g(w(\xi)) - g(\underline{u}(t_n))\|_{H^1} \\ &\leq \|Dg(w(\xi))\|_{H^1 \leftarrow H^1} L \|w(\xi) - \underline{u}(t_n)\|_{H^1}\end{aligned}$$

for $\xi \in [t_n, t_{n+1}]$. Here L is the Lipschitz constant from Assumption 2.3.1 (II). To exploit the Lipschitz continuity of g we have to show that $w(\xi) \in U^+$. Since $\underline{u}(t_n) \in U, u_n^* \in U^+$ by assumption, it follows with Lemma 2.3.4 (iii) that $v(t_{n+1}) = w_0 = w(t_n) \in U^*$. Thus, with $\tau < \tau_0$ the assumption of Lemma 2.3.4 (iv) is fulfilled such that

$$w(t) = \Phi_w^{t-t_n}(v(t_{n+1}); \underline{u}(t_n)) \in U^+ \qquad \text{for } t \in [t_n, t_{n+1}].$$

This yields

$$\begin{aligned}\|\partial_t g(w(\xi))\|_{H^1} &\leq \|Dg(w(t))\|_{H^1 \leftarrow H^1} L 2 C_{U^+} \\ &\leq C_{Dg}(U^+) L 2 C_{U^+}\end{aligned}$$

with constants C_{U^+} from (2.36) and $C_{Dg}(U^+)$ from Assumption 2.3.1 (II) independent from n and τ. Thus,

$$\left\|\mathcal{R}_1(\tau^2)\right\|_{H^1} \leq \tau^2 2 L C_{Dg}(U^+) C_{U^+}. \tag{2.45}$$

For the local error we obtain

$$\begin{aligned}\|\mathcal{L}_\tau(\underline{u}(t_n); u_n^*) - \underline{u}(t_{n+1})\|_{H^1} &= \left\|P\Phi_w^\tau\Big(\Phi_v^\tau(\underline{u}(t_n); u_n^*); \underline{u}(t_n)\Big) - P\underline{u}(t_{n+1})\right\|_{H^1} \\ &\leq \|P\|_{H^1} \left\|\Phi_w^\tau\Big(\Phi_v^\tau(\underline{u}(t_n); u_n^*); \underline{u}(t_n)\Big) - \underline{u}(t_{n+1})\right\|_{H^1},\end{aligned} \tag{2.46}$$

since $\underline{u}(t) \in \mathcal{R}(P)$ and therefore $\underline{u}(t) = P\underline{u}(t)$ for $t \in [0, T]$. Hence using $w(t_n) = w_0 = v(t_{n+1})$ (cf. Figure 2.3) we have

$$\begin{aligned}&\Phi_w^\tau\Big(\Phi_v^\tau(\underline{u}(t_n); u_n^*); \underline{u}(t_n)\Big) - \underline{u}(t_{n+1}) \\ &\quad = v(t_{n+1}) + \tau\left[g(v(t_{n+1})) - g(\underline{u}(t_n))\right] - \underline{u}(t_{n+1}) + \mathcal{R}_1(\tau^2) \\ &\quad = e^{\tau P \partial_x^2}\underline{u}(t_n) - e^{\tau P \partial_x^2}\underline{u}(t_n) + \tau\left[g(v(t_{n+1})) - g(\underline{u}(t_n))\right] \\ &\qquad + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\Big[\lambda_n \partial_x v(s) + g(\underline{u}(t_n)) - g(\underline{u}(s)) - \underline{\mu}(s)\partial_x \underline{u}(s)]ds + \mathcal{R}_1(\tau^2) \\ &\quad = \tau\left[g(v(t_{n+1})) - g(\underline{u}(t_n))\right] + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\Big[g(\underline{u}(t_n)) - g(\underline{u}(s))\Big]ds \\ &\qquad + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\Big[\lambda_n \partial_x v(s) - \underline{\mu}(s)\partial_x \underline{u}(s)\Big]ds + \mathcal{R}_1(\tau^2) \\ &\quad = T_1 + T_2 + \mathcal{R}_1(\tau^2),\end{aligned}$$

where we define

$$T_1 := \tau\left[g(v(t_{n+1})) - g(\underline{u}(t_n))\right] + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\Big[g(\underline{u}(t_n)) - g(\underline{u}(s))\Big]ds,$$
$$T_2 := \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\Big[\lambda_n \partial_x v(s) - \underline{\mu}(s)\partial_x \underline{u}(s)\Big]ds.$$

In the following we will derive estimates for these terms, which will then be divided in smaller parts as well. The first part is a typical quadrature error whereas the second term is obtained from the co-moving frame.

Estimation of T_2. In this part we derive an estimate of the H^1-norm of the second term T_2. First, we define

$$\rho(s) := e^{(t_{n+1}-s)P\partial_x^2} P\Big[\lambda_n \partial_x v(s) - \underline{\mu}(s)\partial_x \underline{u}(s)\Big]$$

for $s \in [t_n, t_{n+1}]$. We use a Taylor expansion of $\rho(s)$ at t_n to find that

$$\begin{aligned} T_2 &= \int_{t_n}^{t_{n+1}} \rho(s)ds \\ &= \int_{t_n}^{t_{n+1}} \rho(t_n) + (s-t_n)\rho'(\xi)ds \\ &= \tau\rho(t_n) + \tfrac{1}{2}\rho'(\xi)\tau^2 \end{aligned} \tag{2.47}$$

for some $\xi \in [t_n, t_{n+1}]$. We have to check that $\rho'(\xi)$ is bounded. Since the initial value $v(t_n) = \underline{u}(t_n)$ lies in $H^4(\mathbb{R})$, the solution $v(t)$ for $t \in [t_n, t_{n+1}]$ also lies in $H^4(\mathbb{R})$ by the variation-of-constants formula. By Lemma 2.3.3 we know that v is continuously differentiable on $[t_n, t_{n+1}]$ and satisfies the evolution equation of the PDE (2.42) for all $t \in [t_n, t_{n+1}]$. We can differentiate $\rho(s)$ and the semigroup within since $P\Big[\lambda_n\partial_x v(s) - \underline{\mu}(s)\partial_x\underline{u}(s)\Big] \in \mathcal{D}(P\partial_x^2) = H^2(\mathbb{R})$, cf. [Paz83, Theorem 1.2.4, p. 4]. We obtain with the chain rule and $s \in [t_n, t_{n+1}]$

$$\begin{aligned} \rho'(s) = &\left(-e^{(t_{n+1}-s)P\partial_x^2} P\partial_x^2\right)\left(P\Big[\lambda_n\partial_x v(s) - \underline{\mu}(s)\partial_x\underline{u}(s)\Big]\right) \\ &+ e^{(t_{n+1}-s)P\partial_x^2} P\Big(\lambda_n\partial_t\partial_x v(s) - \underline{\mu}'(s)\partial_x\underline{u}(s) - \underline{\mu}(s)\partial_t\partial_x\underline{u}(s)\Big) \\ = &\left(-e^{(t_{n+1}-s)P\partial_x^2} P\partial_x^2\right)\left(P\Big[\lambda_n\partial_x v(s) - \underline{\mu}(s)\partial_x\underline{u}(s)\Big]\right) \\ &+ \left(e^{(t_{n+1}-s)P\partial_x^2}\right) P\Big(\lambda_n\partial_x(P[\partial_x^2 v(s) + \lambda_n\partial_x v(s) + g(\underline{u}(t_n))]) \\ &- \underline{\mu}'(s)\partial_x\underline{u}(s) - \underline{\mu}(s)\partial_x(P[\partial_x^2\underline{u}(s) + g(\underline{u}(s)) + \underline{\mu}(s)\partial_x\underline{u}(s)])\Big) \end{aligned}$$

using the PDE (2.21a) and Lemma 2.1.26. Since λ_n is constant on $[t_n, t_{n+1}]$, the time derivative for this part vanishes. We calculate

$$\begin{aligned} \|\rho'(s)\|_{H^1} \le{}& \left\|e^{(t_{n+1}-s)P\partial_x^2}\right\|_{H^1} \|P\|_{H^1} \|P\|_{H^3} \left(|\lambda_n| \|v(s)\|_{H^4} + |\underline{\mu}(s)| \|\underline{u}(s)\|_{H^4}\right) \\ &+ \left\|e^{(t_{n+1}-s)P\partial_x^2}\right\|_{H^1} \|P\|_{H^1} \\ &\cdot \Big(|\lambda_n| \|P\|_{H^2} \left[\|v(s)\|_{H^4} + |\lambda_n| \|v(s)\|_{H^3} + \|g(\underline{u}(t_n))\|_{H^2} \right] \\ &+ |\underline{\mu}'(s)| \|u(s)\|_{H^2} + |\underline{\mu}(s)| \|P\|_{H^2} \Big[\|\underline{u}(s)\|_{H^4} + \|g(\underline{u}(s))\|_{H^2} \\ &+ |\underline{\mu}(s)| \|\underline{u}(s)\|_{H^3} \Big] \Big). \end{aligned} \tag{2.48}$$

We have

$\lvert\lambda_n\rvert < C_\lambda(U^+)$		by Lemma 2.3.4 (i),
$\lvert\underline{\mu}(s)\rvert < C_\mu$	for $s \in [0,T]$	by Assumption 2.3.1 (V),
$\|\underline{u}(s)\|_{H^4} < C_u$	for $s \in [0,T]$	by Assumption 2.3.1 (V),
$\|g(\underline{u}(s))\|_{H^4} < C_{g,u}$	for $s \in [0,T]$	by Assumption 2.3.1 (VI),
$\left\|\Phi_v^{s-t_n}(\underline{u}(t_n);u_n^*)\right\|_{H^4} < C_v$	for $s \in [t_n,t_{n+1}]$	by Lemma 2.3.4 (v),
$\left\|e^{(t_{n+1}-s)P\partial_x^2}\right\|_{H^1} < e^{\omega\tau}$	for $s \in [t_n,t_{n+1}]$	by Lemma 2.1.13.

Note that $v(s) = \Phi_v^{s-t_n}(\underline{u}(t_n);u_n^*)$ for $s \in [t_n,t_{n+1}]$. In addition to these estimates, we need a bound for $|\underline{\mu}'(s)|$. For this we use Lemma 2.1.28. By Lemma 2.3.6 we have the uniform bound of $\|\partial_t g(\underline{u}(t))\|_{L^2} \le C_{\partial_t g}$ in t on $[0,T]$. We obtain with the constant K_2 from Lemma 2.1.28

$$\begin{aligned} \varepsilon_\psi^{-2} K_2 &= \varepsilon_\psi^{-2} K_2 \left(|\underline{\mu}(s)|, \|\psi\|_{H^4}, M, \|g(\underline{u}(s))\|_{L^2}, \|\partial_t g(\underline{u}(s))\|_{L^2}\right) \\ &\le K_3 = K_3\left(C_\mu, \|\psi\|_{H^4}, M, C_{g,u}, C_{\partial_t g}, \varepsilon_\psi^{-2}\right), \end{aligned}$$

with $K_3 > 0$ depending only on terms which itself are independent of n or τ. To sum up we obtain with the quasicontractive semigroup bound (cf. Lemma 2.1.13) the uniform bound

$$\begin{aligned} \|\rho'(s)\|_{H^1} \le{}& e^{\tau_0\omega} \|P\|_{H^1} \|P\|_{H^3} \left(C_\lambda(U^+)C_v + C_\mu C_u\right) \\ &+ e^{\tau_0\omega} \|P\|_{H^1} \\ &\cdot \Big(C_\lambda(U^+) \|P\|_{H^2} \left[C_v + C_\lambda(U^+)C_v + C_{g,u}\right] \\ &+ K_3 \cdot (1 + C_u + C_u^2)C_u + C_\mu \|P\|_{H^2} \left[C_u + C_{g,u} + C_\mu C_u\right] \Big) \end{aligned}$$

for $s \in [t_n,t_{n+1}]$. The value τ_0 is given in (2.41). This proves that $\rho'(\xi)$ of (2.47) is bounded independently of τ.

It remains to show $\tau\rho(t_n) = \mathcal{O}(\tau^2)$ to prove $T_2 = \mathcal{O}(\tau^2)$. Since we start the splitting step with the initial value $v(t_n) = \underline{u}(t_n)$ in the local error it follows that

$$\begin{aligned}\|\tau\rho(t_n)\|_{H^1} &= \tau \left\| e^{\tau P\partial_x^2} P[\lambda_n \partial_x v(t_n) - \underline{\mu}(t_n)\partial_x \underline{u}(t_n)] \right\|_{H^1} \\ &= \tau \left\| e^{\tau P\partial_x^2} P[\lambda_n \partial_x \underline{u}(t_n) - \underline{\mu}(t_n)\partial_x \underline{u}(t_n)] \right\|_{H^1} \\ &\leq \tau e^{\tau\omega} \|P\|_{H^1} |\lambda_n - \underline{\mu}(t_n)| \, \|\underline{u}(t_n)\|_{H^2}\end{aligned} \tag{2.49}$$

with Lemma 2.1.13. We are going to derive an estimate for the error of the speed $|\lambda_n - \underline{\mu}(t_n)|$. For the speed λ_n we use the implicit relation given in (2.38), i.e.

$$\lambda_n = M\langle \partial_x\psi, \partial_x u_n^*\rangle - M\langle \psi, \lambda_n \partial_x u_n^* + g(u_n^*)\rangle$$

and for μ we use (2.18b),

$$\underline{\mu}(t_n) = M\langle \partial_x\psi, \partial_x \underline{u}(t_n)\rangle - M\langle \psi, g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x \underline{u}(t_n)\rangle.$$

This yields

$$\begin{aligned}\lambda_n - \underline{\mu}(t_n) &= M\langle \partial_x\psi, \partial_x(u_n^* - \underline{u}(t_n))\rangle \\ &\qquad - M\langle \psi, \lambda_n\partial_x u_n^* + g(u_n^*) - \underline{\mu}(t_n)\partial_x\underline{u}(t_n) - g(\underline{u}(t_n))\rangle \\ &= M\langle \partial_x^2\psi, \underline{u}(t_n) - u_n^*\rangle + M\langle \psi, g(\underline{u}(t_n)) - g(u_n^*)\rangle \\ &\qquad + M\langle \psi, \underline{\mu}(t_n)\partial_x\underline{u}(t_n) - \lambda_n\partial_x u_n^*\rangle \\ &= M\langle \partial_x^2\psi, \underline{u}(t_n) - u_n^*\rangle + M\langle \psi, g(\underline{u}(t_n)) - g(u_n^*)\rangle \\ &\qquad - \underline{\mu}(t_n)M\langle \partial_x\psi, \underline{u}(t_n) - u_n^*\rangle + M\langle \psi, \partial_x u_n^*\rangle(\underline{\mu}(t_n) - \lambda_n),\end{aligned}$$

where we used the intermediate step

$$\underline{\mu}(t_n)\partial_x\underline{u}(t_n) - \lambda_n\partial_x u_n^* = \underline{\mu}(t_n)\partial_x\underline{u}(t_n) - \underline{\mu}(t_n)\partial_x u_n^* + \underline{\mu}(t_n)\partial_x u_n^* - \lambda_n\partial_x u_n^*.$$

Hence,

$$\begin{aligned}(\lambda_n - \underline{\mu}(t_n))(1 + M\langle \psi, \partial_x u_n^*\rangle) &= M\langle \partial_x^2\psi, \underline{u}(t_n) - u_n^*\rangle + M\langle \psi, g(\underline{u}(t_n)) - g(u_n^*)\rangle \\ &\qquad - \underline{\mu}(t_n)M\langle \partial_x\psi, \underline{u}(t_n) - u_n^*\rangle\end{aligned}$$

and

$$\begin{aligned}|\lambda_n - \underline{\mu}(t_n)| &\leq \frac{1}{1 + M\langle \psi, \partial_x u_n^*\rangle}\Big(M\|\psi\|_{H^2}\|\underline{u}(t_n) - u_n^*\|_{L^2} \\ &\qquad + ML\|\psi\|_{L^2}\|\underline{u}(t_n) - u_n^*\|_{L^2} + |\underline{\mu}(t_n)|M\|\psi\|_{H^1}\|\underline{u}(t_n) - u_n^*\|_{L^2}\Big) \\ &\leq \frac{1}{\varepsilon_\psi}\Big(M\|\psi\|_{H^2} + ML\|\psi\|_{L^2} + C_\mu M\|\psi\|_{H^1}\Big)\|\underline{u}(t_n) - u_n^*\|_{L^2}\end{aligned} \tag{2.50}$$

As one can see here, the correction $g(u_n^*)$ in the definition of the speed λ_n is necessary to obtain a first order approximation of the speed λ_n to the exact speed $\underline{\mu}(t_n)$. This is somewhat intuitive because without the correction, the speed would only depend on the linear problem, but the speed of a traveling wave typically arises by the interaction of the linear and nonlinear dynamics. Because we have that $\|u(t_n) - u_n^*\|_{H^1} \leq \tilde{C}\tau$ by assumption and with the additional τ from the Taylor expansion, see (2.47) and (2.49), we have finished the proof that $\|T_2\|_{H^1} \leq C\tau^2$ for some constant $C > 0$ independent of n. In particular, we obtain

$$\begin{aligned}
\|T_2\|_{H^1} &= \left\| \int_{t_n}^{t_{n+1}} \rho(s) ds \right\|_{H^1} \\
&= \left\| \tau\rho(t_n) + \tfrac{1}{2}\rho'(\xi)\tau^2 \right\|_{H^1} \\
&\leq \tau^2 e^{\tau_0\omega} \|P\|_{H^1} \frac{\tilde{C}}{\varepsilon_\psi} \Big(M\|\psi\|_{H^2} + ML\|\psi\|_{L^2} + C_\mu M \|\psi\|_{H^1} \Big) C_u(U^+) \\
&\quad + \tau^2 \tfrac{1}{2} e^{\tau_0\omega} \|P\|_{H^1} \|P\|_{H^3} \Big(C_\lambda(U^+) C_v + C_\mu C_u \Big) \\
&\quad + \tau^2 \tfrac{1}{2} e^{\tau_0\omega} \|P\|_{H^1} \\
&\quad \cdot \Big(C_\lambda(U^+) \|P\|_{H^2} \Big[C_v + C_\lambda(U^+) C_v + C_{g,u} \Big] \\
&\quad + K_3 \cdot (1 + C_u + C_u^2) C_u + C_\mu \|P\|_{H^2} \Big[C_u + C_{g,u} + C_\mu C_u \Big] \Big).
\end{aligned} \tag{2.51}$$

Estimate of T_1. As a next step we prove a second order estimate for

$$T_1 = \tau \left[g(v(t_{n+1})) - g(\underline{u}(t_n)) \right] + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P \Big[g(\underline{u}(t_n)) - g(\underline{u}(s)) \Big] ds.$$

Parts of the proof follow the lines of [AO17]. We are able to skip some parts of the proof since we use a fixed correction term $g(\underline{u}(t_n))$, whereas the authors in [AO17] discuss a more general approach. We define

$$\phi(s) := e^{(t_{n+1}-s)P\partial_x^2} P \Big[g(\underline{u}(t_n)) - g(\underline{u}(s)) \Big], \quad \hat{\phi}(s) := g(\underline{u}(t_n)) - g(\underline{u}(s))$$

for $s \in [t_n, t_{n+1}]$. Hence,

$$\begin{aligned}
\|T_1\|_{H^1} \leq \tau \left\| g(v(t_{n+1})) - g(\underline{u}(t_n)) \right\|_{H^1} \\
+ \left\| \int_{t_n}^{t_{n+1}} \phi(s) ds \right\|_{H^1} \\
=: \mathcal{A} + \mathcal{B},
\end{aligned}$$

where $\mathcal{A}, \mathcal{B}$ are given by each line of the right-hand side of the equation.

Estimate of part $\mathcal{B}$. For the second part $\mathcal{B}$ we calculate with a Taylor expansion

$$\begin{aligned}\int_{t_n}^{t_{n+1}} \phi(s)ds &= \int_{t_n}^{t_{n+1}} \phi(t_n) + (s-t_n)\phi'(\xi)ds \\ &= \tau\phi(t_n) + \tfrac{1}{2}\phi'(\xi)\tau^2,\end{aligned}$$

for some $\xi \in [t_n, t_{n+1}]$. Since it holds $\phi(t_n) = 0$, it remains to show the boundedness of the derivative ϕ' in order to get a second order estimate for $\mathcal{B}$. Here the derivative is given by

$$\phi'(s) = e^{(t_{n+1}-s)P\partial_x^2}\left(-P\partial_x^2 P\hat{\phi}(s) + P\hat{\phi}'(s)\right).$$

By Assumption 2.3.1 (VI) we have $\|g(\underline{u}(s))\|_{H^4} < C_{g,u}$ for $s \in [0,T]$ such that $\hat{\phi}(s) \in H^4$ is uniformly bounded in s on $[0,T]$. Thus, the first part can be bounded uniformly in s with

$$\begin{aligned}\left\|e^{(t_{n+1}-s)P\partial_x^2} P\partial_x^2 P\hat{\phi}(s)\right\|_{H^1} &\leq \left\|e^{(t_{n+1}-s)P\partial_x^2}\right\|_{H^1} \|P\|_{H^1} \|P\|_{H^3} \left\|\hat{\phi}(s)\right\|_{H^3} \\ &\leq e^{\tau_0\omega} \|P\|_{H^1} \|P\|_{H^3} 2C_{g,u},\end{aligned}$$

with Lemma 2.1.13 and Assumption 2.3.1 (VI). Further, it holds $\|\partial_t g(\underline{u}(t))\|_{H^1} < C_{\partial_t g}$ for $t \in [0,T]$ by Lemma 2.3.6 and we obtain for the second part

$$\begin{aligned}\left\|e^{(t_{n+1}-s)P\partial_x^2} P\hat{\phi}'(s)\right\|_{H^1} &\leq \left\|e^{(t_{n+1}-s)P\partial_x^2}\right\|_{H^1} \|P\|_{H^1} \left\|\hat{\phi}'(s)\right\|_{H^1} \\ &\leq e^{\tau_0\omega} \|P\|_{H^1} \|\partial_t g(\underline{u}(s))\|_{H^1} \\ &\leq e^{\tau_0\omega} \|P\|_{H^1} C_{\partial_t g}.\end{aligned}$$

This sums up to the estimate

$$\|\phi'(s)\|_{H^1} \leq e^{\tau_0\omega} \|P\|_{H^1} \left[\|P\|_{H^3} 2C_{g,u} + C_{\partial_t g}\right],$$

to finish the second order estimate for $\mathcal{B}$.

Estimate of part $\mathcal{A}$. Note that Lemma 2.3.4 (iii) yields that $v(t_{n+1})$ lies in U^* since

$\tau < \tau_1$ by assumption. For the term $\mathcal{A}$ we obtain

$$
\begin{aligned}
\tau \| g(v(t_{n+1})) - g(\underline{u}(t_n)) \|_{H^1} & \\
&\leq \tau L \left\| v(t_{n+1}) - \underline{u}(t_n) \right\|_{H^1} \\
&= \tau L \left\| v(t_{n+1}) - v(t_n) + v(t_n) - \underline{u}(t_n) \right\|_{H^1} \\
&= \tau L \left\| v(t_{n+1}) - v(t_n) \right\|_{H^1} \\
&= \tau L \left\| \int_{t_n}^{t_{n+1}} \partial_t v(s) ds \right\|_{H^1} \\
&\leq \tau L \left\| \tau \sup_{s \in [t_n, t_{n+1}]} \partial_t v(s) \right\|_{H^1} \\
&\leq \tau^2 L \sup_{s \in [t_n, t_{n+1}]} \left\| P \left[\partial_x^2 v(s) + \lambda_n \partial_x v(s) + g(\underline{u}(t_n)) \right] \right\|_{H^1} \\
&\leq \tau^2 L \left\| P \right\|_{H^1} \sup_{s \in [t_n, t_{n+1}]} \Big(\left\| v(s) \right\|_{H^3} + |\lambda_n| \left\| v(s) \right\|_{H^2} + \left\| g(\underline{u}(t_n)) \right\|_{H^1} \Big) \\
&\leq \tau^2 L \left\| P \right\|_{H^1} \Big(C_v + C_\lambda(U^+) C_v + C_{g,u} \Big)
\end{aligned}
$$

where the constant $C_{g,u}$ is given by Assumption 2.3.1 (VI) and the constant $C_\lambda(U^+)$ by Lemma 2.3.4 (i). The Lipschitz constant L is given in Assumption 2.3.1 (II). For the last step we used

$$
\left\| v(s) \right\|_{H^4} = \left\| \Phi_v^{s-t_n}(\underline{u}(t_n); u_n^*) \right\|_{H^4} < C_v \qquad \text{for } s \in [t_n, t_{n+1}]
$$

by Lemma 2.3.4 (v). Therefore $\mathcal{A}$ is of second order as well.

Together with the estimate of $\mathcal{B}$ we obtain

$$
\begin{aligned}
\left\| T_1 \right\|_{H^1} &\leq \mathcal{A} + \mathcal{B} \\
&\leq \tau^2 L \left\| P \right\|_{H^1} \Big(C_v + C_\lambda(U^+) C_v + C_{g,u} \Big) \\
&\qquad + \frac{1}{2} \tau^2 e^{\tau_0 \omega} \left\| P \right\|_{H^1} \left[\left\| P \right\|_{H^3} 2 C_{g,u} + C_{\partial_t g} \right].
\end{aligned} \tag{2.52}
$$

Combining the estimates for T_1 in (2.52), T_2 in (2.51) and $\mathcal{R}_1(\tau^2)$ in (2.45) we obtain for the local error as in (2.46)

$$
\begin{aligned}
&\|\mathcal{L}_\tau(\underline{u}(t_n);u_n^*)-\underline{u}(t_{n+1})\|_{H^1}\\
&\qquad\le \|P\|_{H^1}\left\|\Phi_w^\tau\Big(\Phi_v^\tau(\underline{u}(t_n);u_n^*);\underline{u}(t_n)\Big)-\underline{u}(t_{n+1})\right\|_{H^1}\\
&\qquad\le \|P\|_{H^1}\left\|T_1+T_2+\mathcal{R}_1(\tau^2)\right\|_{H^1}\\
&\qquad\le \|P\|_{H^1}\Big(\|T_1\|_{H^1}+\|T_2\|_{H^1}+\left\|\mathcal{R}_1(\tau^2)\right\|_{H^1}\Big)\\
&\qquad\le \|P\|_{H^1}\Big[\tau^2L\,\|P\|_{H^1}\Big(C_v+C_\lambda(U^+)C_v+C_{g,u}\Big)\\
&\qquad\quad+\frac{1}{2}\tau^2e^{\tau_0\omega}\,\|P\|_{H^1}\,[\|P\|_{H^3}\,2C_{g,u}+C_{\partial_t g}]\\
&\qquad\quad+\tau^2e^{\tau_0\omega}\,\|P\|_{H^1}\,\frac{\tilde{C}}{\varepsilon_\psi}\Big(M\,\|\psi\|_{H^2}+ML\,\|\psi\|_{L^2}+C_\mu M\,\|\psi\|_{H^1}\Big)C_u(U^+)\\
&\qquad\quad+\frac{1}{2}\tau^2e^{\tau_0\omega}\,\|P\|_{H^1}\,\|P\|_{H^3}\Big(C_\lambda(U^+)C_v+C_\mu C_u\Big)\\
&\qquad\quad+\frac{1}{2}\tau^2e^{\tau_0\omega}\,\|P\|_{H^1}\\
&\qquad\quad\cdot\Big(C_\lambda(U^+)\,\|P\|_{H^2}\Big[C_v+C_\lambda(U^+)C_v+C_{g,u}\Big]\\
&\qquad\quad+K_3\cdot(1+C_u+C_u^2)C_u+C_\mu\,\|P\|_{H^2}\Big[C_u+C_{g,u}+C_\mu C_u\Big]\Big)\\
&\qquad\quad+C_{Dg}(U^+)L2C_{U^+}\Big]\\
&\qquad=:\tau^2C.
\end{aligned}
$$

This finishes the proof of the second order estimate of the local error in the H^1-norm. □

For the constructed Lie splitting scheme the following holds.

Lemma 2.3.8. *Let Assumption 2.3.1 hold true. For every $z\in H^3(\mathbb{R})\cap U$ and $u_n^*\in U^+$ the splitting scheme* (2.33) *satisfies*

$$\left\|P\Phi_w^\tau\Big(\Phi_v^\tau(z;u_n^*);z\Big)-\Phi_w^\tau\Big(\Phi_v^\tau(z;u_n^*);z\Big)\right\|_{H^1}\le C_p\tau^2$$

where the constant $C_p>0$ is independent of τ and n but depends on $\|z\|_{H^3}$.

This means that without the projection in the last step of the splitting scheme, cf. Figure 2.3, we obtain a solution which lies up to order two in the correct subspace provided that the initial value is sufficiently regular. Although this is an interesting fact to understand the splitting of PDAEs and their algebraic constraint, we cannot use this lemma for the convergence proof. In the recursion of the splitting scheme (2.33)

$$u_{n+1}=\mathcal{L}_\tau(u_n;u_n)$$

we apply the scheme to the value $u_n \in H^1(\mathbb{R})$ as we will show in the convergence proof. Hence, the initial values in the splitting approach are not sufficiently regular for this lemma.

Proof. Here we only give the basic ideas. Since $e^{tP\partial_x^2}$ is a strongly continuous semigroup, it follows from [Paz83, Theorem 1.2.4, p. 5]

$$P\partial_x^2 \int_0^\tau e^{sP\partial_x^2} u ds = (e^{\tau P\partial_x^2} - I)u, \qquad u \in L^2(\mathbb{R}).$$

Thus, we get the estimate

$$\begin{aligned} \left\| (e^{\tau P\partial_x^2} - I)u \right\|_{H^1} &= \left\| P\partial_x^2 \int_0^\tau e^{sP\partial_x^2} u ds \right\|_{H^1} \\ &\le \|P\|_{H^1} \left\| \int_0^\tau e^{sP\partial_x^2} u ds \right\|_{H^3} \\ &\le \tau e^{\tau\omega} \|P\|_{H^1} \|u\|_{H^3} \end{aligned} \tag{2.53}$$

using Lemma 2.1.13. We have

$$\left\| P\Phi_w^\tau\Big(\Phi_v^\tau(z; u_n^*); z\Big) - \Phi_w^\tau\Big(\Phi_v^\tau(z; u_n^*); z\Big) \right\|_{H^1} = \left\| P^\perp \Phi_w^\tau\Big(\Phi_v^\tau(z; u_n^*); z\Big) \right\|_{H^1}.$$

Let

$$v(t) = \Phi_v^{t-t_n}(z; u_n^*), \qquad w(t) = \Phi_w^{t-t_n}(v(t_{n+1}); z)$$

for $t \in [t_n, t_{n+1}]$ using (2.29) and (2.31). Then it holds

$$\begin{aligned} P^\perp w(t_{n+1}) &= M\psi\langle \psi, w(t_{n+1})\rangle \\ &= M\psi\langle \psi, v(t_{n+1}) + \tau\left[g(v(t_{n+1})) - g(z)\right]\rangle + P^\perp \mathcal{R}_1(\tau^2) \\ &= M\psi\langle \psi, v(t_{n+1})\rangle + \tau M\psi\langle \psi, g(v(t_{n+1})) - g(z)\rangle + P^\perp \mathcal{R}_1(\tau^2) \\ &= \tau M\psi\langle \psi, g(v(t_{n+1})) - g(z)\rangle + P^\perp \mathcal{R}_1(\tau^2) \end{aligned}$$

since $v(t_{n+1}) \in \mathcal{R}(P)$. Here $\mathcal{R}_1(\tau^2)$ is the error term given in (2.44). We only have to estimate the first term on the right-hand side $\tau M\psi\langle \psi, g(v(t_{n+1})) - g(z)\rangle$ to get a second order estimate. We calculate

$$|\langle \psi, g(v(t_{n+1})) - g(z)\rangle| \le \|\psi\|_{L^2} L \|v(t_{n+1}) - z\|_{H^1} \tag{2.54}$$

using the Lipschitz continuity of g, cf. Assumption 2.3.1 (II).

$$\begin{aligned} \|v(t_{n+1}) - z\|_{H^1} &= \left\| e^{\tau P\partial_x^2} z - z + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P[\lambda_n \partial_x v(s) + g(z)] ds \right\|_{H^1} \\ &\le \left\| (e^{\tau P\partial_x^2} - I)z \right\|_{H^1} + \mathcal{O}(\tau) \\ &\le \tau e^{\tau\omega} \|P\|_{H^1} \|z\|_{H^3} + \mathcal{O}(\tau) \end{aligned} \tag{2.55}$$

using the estimate from (2.53) in the last step. Thus, we obtain

$$\begin{aligned}\left\|P^{\perp}w(t_{n+1})\right\|_{H^1} &\leq \tau^2 M \left\|\psi\right\|_{H^1} \left\|\psi\right\|_{L^2} L(C_7 + e^{\tau\omega} \left\|P\right\|_{H^1} \left\|z\right\|_{H^3}) + \left\|P^{\perp}\mathcal{R}_1(\tau^2)\right\|_{H^1} \\ &\leq C_p\tau^2,\end{aligned}$$

for some constant $C_7 > 0$ arising from (2.55). For the last estimate we use (2.45). Note that without the use of a correction term, here $g(z)$, the part given in (2.54) would only be of order zero. □

2.3.2 First Order Convergence in Time for the Lie Splitting

The time steps are given by $0 \leq t_n := n\tau \leq T < \infty$ for $\tau > 0$. We define by

$$\begin{aligned} u_{n+1} &= \mathcal{L}_\tau(u_n; u_n) \\ &= \mathcal{L}_\tau^{n+1}(u_0) \end{aligned} \tag{2.56}$$

the Lie approximations to the exact solution $\underline{u}(t_{n+1})$ as given in (2.33). In addition to the restriction of the time step size $\tau < \tau_0$ given in (2.41), we assume that τ is sufficiently small such that it holds

$$\tau\mathcal{K} < \delta$$

with

$$\begin{aligned} \mathcal{K} &:= Te^{T\omega^*}\left(W^* + C\right)\left[1 + Te^{T\omega^*}\left(K^* + E^*\right)e^{Te^{T\omega^*}(K^*+E^*)}\right] \\ K^* &:= e^{\tau_0\omega^*}\left\|P\right\|_{H^1} L \\ E^* &:= \left\|P\right\|_{H^1} L\left(1 + e^{\tau_0\omega^*} + \tau_0 e^{\tau_0\omega^*}\left\|P\right\|_{H^1} L\right), \\ W^* &:= 4C_{Dg}(U^+)LC_{U^+}\left\|P\right\|_{H^1}, \end{aligned} \tag{2.57}$$

where C is the constant given in the local error in Lemma 2.3.7, $L = L(U^+)$ the Lipschitz constant from Assumption 2.3.1 (II) and δ is given in (2.35). The constant $\mathcal{K}$ may seem artificial, but fixing it in advance gives a better understanding of the proof on a formal level. This second condition on the step size ensures that the numerical solution u_n stays in the neighborhood U as long as $\tau n \leq T$. In addition, this will be used to ensure that all constants arising in the convergence proof do not grow for $n \to \infty$ and is therefore an important part for the convergence proof. For completeness, we list the constant $\mathcal{K}$ resolved into its constituent parts in Remark A.1.2.

Theorem 2.3.9. *Under Assumption 2.3.1 the Lie splitting with step size* $\tau < \min\{\tau_0, \frac{\delta}{\mathcal{K}}\}$ *is convergent of first order in the* H^1*-norm, i.e.*

$$\|u_n - \underline{u}(t_n)\|_{H^1} \leq \mathcal{K}\tau, \qquad (n \in \mathbb{N}_0 \cap [0, \tfrac{T}{\tau}])$$

where the constant $\mathcal{K} > 0$ *is given in* (2.57)*. In particular, it is independent of* n *and* τ*, but depends on* T*.*

Proof. In order to prove the convergence of the Lie splitting we need stability estimates of the splitting scheme in addition to the local error, which we analyzed in Section 2.3.1. Let $e_n := u_n - \underline{u}(t_n)$ denote the global error at time $t = t_n = n\tau$. We are using a proof by induction technique as in [HLR13] to prove $\|u_n - \underline{u}(t_n)\|_{H^1} \leq \mathcal{K}\tau$ and $u_n \in \mathcal{R}(P) \cap U$, where U is the neighborhood of the exact solution as given in (2.35).

In the base case $n = 0$ the splitting scheme starts with u_0, cf. (2.56), and therefore we have $e_0 = 0$. The starting value for the splitting scheme lies in $\mathcal{R}(P) \cap U$ by Assumption 2.3.1 (IV) and the definition of U.

In the inductive step we assume that $\|u_k - \underline{u}(t_k)\|_{H^1} \leq \mathcal{K}\tau$ and $u_k \in \mathcal{R}(P) \cap U$ hold true for $0 \leq k \leq n$ and prove $\|u_{n+1} - \underline{u}(t_{n+1})\|_{H^1} \leq \mathcal{K}\tau$ and $u_{n+1} \in \mathcal{R}(P) \cap U$ for a fixed $n \in \mathbb{N}_0$. We assume $(n+1)\tau \leq T$ since we only approximate the solution up to the end time T. The property $u_{n+1} \in \mathcal{R}(P)$ follows because we project on the subspace $\mathcal{R}(P)$ in the last step of the splitting, cf. (2.33). In order to prove the estimate for the global error we start with

$$\begin{aligned} e_{n+1} &= u_{n+1} - \underline{u}(t_{n+1}) \\ &= \mathcal{L}_\tau(u_n; u_n) - \underline{u}(t_{n+1}) \\ &= \mathcal{L}_\tau(u_n; u_n) - \mathcal{L}_\tau(\underline{u}(t_n); u_n) + \mathcal{L}_\tau(\underline{u}(t_n); u_n) - \underline{u}(t_{n+1}), \\ &= \mathcal{L}_\tau(u_n; u_n) - \mathcal{L}_\tau(\underline{u}(t_n); u_n) + \delta_{n+1}, \end{aligned} \tag{2.58}$$

where $\delta_{n+1} = \mathcal{L}_\tau(\underline{u}(t_n); u_n) - \underline{u}(t_{n+1})$ is the local error already analyzed in Lemma 2.3.7 with $u_n^* = u_n$. The assumption $\|u_n - \underline{u}(t_n)\|_{H^1} \leq \mathcal{K}\tau$ of Lemma 2.3.7 is fulfilled with the induction hypothesis. Thus, to get an estimate of the global error e_{n+1} we need a stability estimate for the splitting scheme, i.e. we derive an estimate for the term $\|\mathcal{L}_\tau(u_n; u_n) - \mathcal{L}_\tau(\underline{u}(t_n); u_n)\|_{H^1}$. For this we define v as the solution to the linear problem (2.26) with initial value u_n and $\tilde{v}$ as the solution to the same problem with initial value $\underline{u}(t_n)$, i.e.

$$v(t) = \Phi_v^{t-t_n}(u_n; u_n), \qquad \tilde{v}(t) = \Phi_v^{t-t_n}(\underline{u}(t_n); u_n)$$

for $t \in [t_n, t_{n+1}]$ with the notation given in Section 2.2.1. Both solutions v and $\tilde{v}$ use $u_n^* = u_n$ in (2.26). Since $u_n \in \mathcal{R}(P)$ the initial values are consistent and therefore the solutions are well-defined. Both solutions can be represented via the variation-of-constants formula given by (2.28b) with initial value u_n or $\underline{u}(t_n)$, respectively. Here the crucial part is that both solutions use the *same speed* $\tilde{\lambda}(u_n)$ which is coupled to u_n and not directly linked to the initial value by the construction of the scheme. We define

$$B_n = B(u_n) = \partial_x^2 u_n + \tilde{\lambda}(u_n)\partial_x$$

using (2.27). Since we use the initial value for the correction term, we have $g(u_n)$ for v and $g(\underline{u}(t_n))$ for $\tilde{v}$ as inhomogeneity of the underlying PDEs. The solutions $v(t), \tilde{v}(t)$ are consistent for $t \in [t_n, t_{n+1}]$, in particular it holds $v(t_{n+1}), \tilde{v}(t_{n+1}) \in \mathcal{R}(P)$, and we obtain

$$\begin{aligned}
\mathcal{L}_\tau(u_n; u_n) - &\mathcal{L}_\tau(\underline{u}(t_n); u_n) \\
&= P\Big(v(t_{n+1}) + \tau[g(v(t_{n+1})) - g(u_n)]\Big) \\
&\qquad - P\Big(\tilde{v}(t_{n+1}) + \tau[g(\tilde{v}(t_{n+1})) - g(\underline{u}(t_n))]\Big) + \tau^2 W_{n+1} \\
&= v(t_{n+1}) - \tilde{v}(t_{n+1}) + \tau P\left[g(v(t_{n+1})) - g(\tilde{v}(t_{n+1}))\right] \\
&\qquad + \tau P\left[g(\underline{u}(t_n)) - g(u_n)\right] + \tau^2 W_{n+1} \\
&= e^{\tau P B_n} u_n - e^{\tau P B_n} \underline{u}(t_n) \\
&\qquad + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)PB_n} P\left[g(u_n) - g(\underline{u}(t_n))\right] ds \\
&\qquad + \tau P\left[g(v(t_{n+1})) - g(\tilde{v}(t_{n+1}))\right] \\
&\qquad + \tau P\left[g(\underline{u}(t_n)) - g(u_n)\right] + \tau^2 W_{n+1} \\
&= e^{\tau P B_n} e_n + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)PB_n} P\left[g(u_n) - g(\underline{u}(t_n))\right] ds \\
&\qquad + \tau P\left[g(v(t_{n+1})) - g(\tilde{v}(t_{n+1}))\right] \\
&\qquad + \tau P\left[g(\underline{u}(t_n)) - g(u_n)\right] + \tau^2 W_{n+1},
\end{aligned} \tag{2.59}$$

where W_{n+1} consists of both remainder terms of the Taylor expansion for the solution representation of the nonlinear subproblem (2.30) as given in (2.44) and will be analyzed below. We solve the error recursion below by defining

$$\begin{aligned}
K_{n+1} &\coloneqq \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)PB_n} P\left[g(u_n) - g(\underline{u}(t_n))\right] ds, \\
E_{n+1} &\coloneqq \tau P\left[g(v(t_{n+1})) - g(\tilde{v}(t_{n+1})) + g(\underline{u}(t_n)) - g(u_n)\right], \\
W_{n+1} &\coloneqq P\partial_t g\left(\Phi_w^{\xi_1 - t_n}(v(t_{n+1}); u_n)\right) - P\partial_t g\left(\Phi_w^{\xi_2 - t_n}(\tilde{v}(t_{n+1}); u_n)\right),
\end{aligned}$$

for some $\xi_1, \xi_2 \in [t_n, t_{n+1}]$. We derive some estimates for those terms in advance.

Estimate for K_{n+1}. We have

$$\begin{aligned}\|K_{n+1}\|_{H^1} &= \left\|\int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)PB_n} P\left[g(u_n) - g(\underline{u}(t_n))\right] ds\right\|_{H^1} \\ &\leq \int_{t_n}^{t_{n+1}} \left\|e^{(t_{n+1}-s)PB_n}\right\|_{H^1} \|P\|_{H^1} \|g(u_n) - g(\underline{u}(t_n))\|_{H^1} ds \\ &\leq \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)\omega^*} \|P\|_{H^1} \|g(u_n) - g(\underline{u}(t_n))\|_{H^1} ds \\ &\leq \tau e^{\tau\omega^*} \|P\|_{H^1} \|g(u_n) - g(\underline{u}(t_n))\|_{H^1} \\ &\leq \tau e^{\tau\omega^*} \|P\|_{H^1} L \|u_n - \underline{u}(t_n)\|_{H^1} \\ &\leq \tau e^{\tau_0\omega^*} \|P\|_{H^1} L \|e_n\|_{H^1} \\ &= \tau K^* \|e_n\|_{H^1}\end{aligned} \tag{2.60}$$

using Lemma 2.3.4 (ii) and the definition of K^* in (2.57).

Estimate for E_{n+1}. Using the local Lipschitz continuity in the first term and the fact that e^{tPB_n} is a quasicontractive semigroup on H^1, cf. Lemma 2.3.4 (ii), we obtain

$$\begin{aligned}\|E_{n+1}\|_{H^1} &\leq \tau \|P\|_{H^1} \left(\|g(v(t_{n+1})) - g(\tilde{v}(t_{n+1}))\|_{H^1} + \|g(\underline{u}(t_n)) - g(u_n)\|_{H^1}\right) \\ &\leq \tau \|P\|_{H^1} \left(L \|v(t_{n+1}) - \tilde{v}(t_{n+1})\|_{H^1} + L \|e_n\|_{H^1}\right) \\ &= \tau \|P\|_{H^1} L\Bigg(\left\|e^{\tau PB_n} e_n + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)PB_n} P\left[g(u_n) - g(\underline{u}(t_n))\right] ds\right\|_{H^1} \\ &\qquad + \|e_n\|_{H^1}\Bigg) \\ &\leq \tau \|P\|_{H^1} L \left(e^{\tau\omega^*} \|e_n\|_{H^1} + \|K_{n+1}\|_{H^1} + \|e_n\|_{H^1}\right) \\ &\leq \tau \|P\|_{H^1} L \left(1 + e^{\tau\omega^*} + \tau e^{\tau\omega^*} \|P\|_{H^1} L\right) \|e_n\|_{H^1} \\ &\leq \tau \|P\|_{H^1} L \left(1 + e^{\tau_0\omega^*} + \tau_0 e^{\tau_0\omega^*} \|P\|_{H^1} L\right) \|e_n\|_{H^1} \\ &= \tau E^* \|e_n\|_{H^1}\end{aligned} \tag{2.61}$$

with the definition of E^* in (2.57). Here we used the estimate for $\|K_{n+1}\|_{H^1}$ which was obtained above.

Estimate for W_{n+1}. Both parts of W_{n+1} will be estimated separately. For the first part we have

$$\partial_t w = g(w) - g(u_n), \quad w(t_n) = v(t_{n+1}).$$

By Lemma 2.3.4 (iii) it holds $v(t_{n+1}) \in U^*$ since $u_n \in U$ by the induction hypothesis. Thus, Lemma 2.3.4 (iv) yields

$$w(\xi_1) = \Phi_w^{\xi_1 - t_n}(v(t_{n+1}); u_n) \in U^+ \subseteq H^1(\mathbb{R}).$$

We obtain

$$
\begin{aligned}
\left\|\partial_t g\left(\Phi_w^{\xi_1-t_n}(v(t_{n+1});u_n)\right)\right\|_{H^1} &= \|\partial_t g(w(\xi_1))\|_{H^1} \\
&= \|Dg(w(\xi_1))\,[\partial_t w(\xi_1)]\|_{H^1} \\
&= \|Dg(w(\xi_1))\,[g(w(\xi_1)) - g(u_n)]\|_{H^1} \\
&\le \|Dg(w(\xi_1))\|_{H^1\leftarrow H^1} \|g(w(\xi_1)) - g(u_n)\|_{H^1} \\
&\le \|Dg(w(\xi_1))\|_{H^1\leftarrow H^1} L\,\|w(\xi_1) - u_n\|_{H^1} \\
&\le \|Dg(w(\xi_1))\|_{H^1\leftarrow H^1} L\Big(\|w(\xi_1)\|_{H^1} + \|u_n\|_{H^1}\Big) \\
&\le C_{Dg}(U^+)L2C_{U^+}
\end{aligned}
$$

with Assumption 2.3.1 (II) and (2.36). For the second part of W_{n+1} we have the ODE

$$
\partial_t\tilde{w} = g(\tilde{w}) - g(\underline{u}(t_n)), \quad \tilde{w}(t_n) = \tilde{v}(t_{n+1})
$$

such that we obtain in a similar way

$$
\begin{aligned}
\left\|\partial_t g\left(\Phi_w^{\xi_2-t_n}(\tilde{v}(t_{n+1});u_n)\right)\right\|_{H^1} &= \|\partial_t g(\tilde{w}(\xi_2))\|_{H^1} \\
&\le C_{Dg}(U^+)L2C_{U^+}.
\end{aligned}
$$

In the end we get

$$
\begin{aligned}
\|W_{n+1}\|_{H^1} &\le 4C_{Dg}(U^+)LC_{U^+}\|P\|_{H^1} \\
&\coloneqq W^*,
\end{aligned}
$$

where the right-hand side is independent of n and τ.

As a next step in showing the stability estimate we solve the error recursion. Because the ordering of the semigroups is important, we define the product of operators $H_k, \dots, H_n$ for $k \le n \in \mathbb{N}$ via

$$
\prod_{\ell=k}^{n} H_\ell \coloneqq H_n \cdot \ldots \cdot H_k
$$

and set for $k > n$ the product $\prod_{\ell=k}^{n} H_\ell \coloneqq I$ as the identity on the given space. To sum up we have from (2.58) and (2.59)

$$
e_{n+1} = e^{\tau PB_n}e_n + K_{n+1} + E_{n+1} + \tau^2 W_{n+1} + \delta_{n+1}.
$$

In the same way we obtain in the steps before, i.e. $0 \le k \le n$

$$
e_k = e^{\tau PB_{k-1}}e_{k-1} + K_k + E_k + \tau^2 W_k + \delta_k.
$$

Solving the recursion we obtain

$$
\begin{aligned}
e_{n+1} &= e^{\tau PB_n}\left(e^{\tau PB_{n-1}}e_{n-1} + K_n + E_n + \tau^2 W_n + \delta_n\right) \\
&\quad + K_{n+1} + E_{n+1} + \tau^2 W_{n+1} + \delta_{n+1} \\
&= e^{\tau PB_n}\Big(e^{\tau PB_{n-1}}\left(e^{\tau PB_{n-2}}e_{n-2} + K_{n-1} + E_{n-1} + \tau^2 W_{n-1} + \delta_{n-1}\right) \\
&\quad + K_n + E_n + \tau^2 W_n + \delta_n\Big) + K_{n+1} + E_{n+1} + \tau^2 W_{n+1} + \delta_{n+1} \\
&= \sum_{k=0}^{n}\left(\prod_{\ell=n+1-k}^{n} e^{\tau PB_\ell}\right)\left(K_{n+1-k} + E_{n+1-k} + \tau^2 W_{n+1-k} + \delta_{n+1-k}\right) \qquad (2.62) \\
&\quad + \prod_{\ell=0}^{n} e^{\tau PB_\ell} e_0.
\end{aligned}
$$

For an easier understanding we write down the special cases

$$\underline{k=0}: \quad \underbrace{\left(\prod_{\ell=n+1}^{n} e^{\tau PB_\ell}\right)}_{=I}(K_{n+1} + E_{n+1} + \tau^2 W_{n+1} + \delta_{n+1}),$$

$$\underline{k=1}: \quad \underbrace{\left(\prod_{\ell=n}^{n} e^{\tau PB_\ell}\right)}_{=e^{\tau PB_n}}(K_n + E_n + \tau^2 W_n + \delta_n),$$

$$\underline{k=n}: \quad \underbrace{\left(\prod_{\ell=1}^{n} e^{\tau PB_\ell}\right)}_{=e^{\tau PB_n}\cdot\ldots\cdot e^{\tau PB_1}}(\underbrace{K_1}_{\|\cdot\|_{H^1}=0} + \underbrace{E_1}_{\|\cdot\|_{H^1}=0} + \tau^2 W_1 + \delta_1).$$

We recall $B_k = B(u_k) = \partial_x^2 + \tilde{\lambda}(u_k)\partial_x$ as given in (2.27). By the induction hypothesis, we have $u_k \in U$ for $0 \le k \le n$ such that Lemma 2.3.4 (ii) yields for $m \in \{1, \ldots, n+1\}$

$$
\begin{aligned}
\left\|\prod_{\ell=m}^{n} e^{\tau PB_\ell}\right\|_{H^1\leftarrow H^1} &\le \prod_{\ell=m}^{n}\left\|e^{\tau PB_\ell}\right\|_{H^1\leftarrow H^1} &&\le \prod_{\ell=m}^{n} e^{\tau\omega^*} \\
&\le \prod_{\ell=1}^{n} e^{\tau\omega^*} &&= \left(e^{\tau\omega^*}\right)^n \\
&= e^{n\tau\omega^*} &&\le e^{T\omega^*}.
\end{aligned}
$$

Since $\|e_0\|_{H^1} = 0$ it follows

$$\left\|\prod_{\ell=0}^{n} e^{\tau PB_\ell} e_0\right\|_{H^1} = 0. \qquad (2.63)$$

Further we estimate with (2.62)

$$\begin{aligned}\|e_{n+1}\|_{H^1} &\leq \left\|\sum_{k=0}^{n}\left(\prod_{\ell=n+1-k}^{n} e^{\tau PB_\ell}\right)\Big(K_{n+1-k}+E_{n+1-k}+\tau^2 W_{n+1-k}+\delta_{n+1-k}\Big)\right\|_{H^1}\\ &\leq \sum_{k=0}^{n}\left\|\left(\prod_{\ell=n+1-k}^{n} e^{\tau PB_\ell}\right)\right\|_{H^1}\left\|\Big(K_{n+1-k}+E_{n+1-k}+\tau^2 W_{n+1-k}+\delta_{n+1-k}\Big)\right\|_{H^1}\\ &\leq \sum_{k=0}^{n} e^{T\omega^*}\left\|K_{n+1-k}+E_{n+1-k}+\tau^2 W_{n+1-k}+\delta_{n+1-k}\right\|_{H^1}.\end{aligned}$$

The estimates above for K_{n+1}, E_{n+1} and W_{n+1} also hold true for a smaller index such that we can use the estimates above for K_{n+1-k}, E_{n+1-k} and W_{n+1-k} as long as $0 \leq k \leq n$, i.e.

$$\begin{aligned}\|E_{n+1-k}\|_{H^1} &\leq \tau E^* \|e_{n-k}\|_{H^1}\\ \|K_{n+1-k}\|_{H^1} &\leq \tau K^* \|e_{n-k}\|_{H^1}\end{aligned}$$

by (2.60) and (2.61) . We have $\|E_1\|_{H^1} = 0$ since $\|e_0\|_{H^1} = 0$. The local error δ_{n+1-k} is of order two and W_{n+1-k} is bounded independently of n as mentioned above. We conclude

$$\begin{aligned}\|e_{n+1}\|_{H^1} &\leq \sum_{k=0}^{n} e^{T\omega^*}\left\|K_{n+1-k}+E_{n+1-k}+\tau^2 W_{n+1-k}+\delta_{n+1-k}\right\|_{H^1}\\ &\leq \sum_{k=0}^{n} e^{T\omega^*}\Big(\tau(K^*+E^*)\|e_{n-k}\|_{H^1}+\tau^2(W^*+C)\Big)\\ &\leq (n+1)e^{T\omega^*}\tau^2(W^*+C)+\sum_{k=0}^{n} e^{T\omega^*}\tau(K^*+E^*)\|e_k\|_{H^1}.\end{aligned}$$

We obtain using Lemma A.1.3

$$\begin{aligned}
\|e_{n+1}\|_{H^1} &\leq (n+1)e^{T\omega^*}\tau^2(W^*+C) \\
&\quad + \sum_{k=0}^{n} k e^{T\omega^*}\tau^2(W^*+C)e^{T\omega^*}\tau(K^*+E^*) \prod_{j=k+1}^{n} \left(1+e^{T\omega^*}\tau(K^*+E^*)\right) \\
&\leq Te^{T\omega^*}\tau(W^*+C) \\
&\quad + \sum_{k=0}^{n} k e^{T\omega^*}\tau^2(W^*+C)e^{T\omega^*}\tau(K^*+E^*) \prod_{j=k+1}^{n} \exp\left(e^{T\omega^*}\tau(K^*+E^*)\right) \\
&\leq Te^{T\omega^*}\tau(W^*+C) \\
&\quad + \sum_{k=0}^{n} k e^{T\omega^*}\tau^2(W^*+C)e^{T\omega^*}\tau(K^*+E^*) \exp\left((n-k)e^{T\omega^*}\tau(K^*+E^*)\right) \\
&\leq Te^{T\omega^*}\tau(W^*+C) \\
&\quad + \sum_{k=0}^{n} k e^{T\omega^*}\tau^2(W^*+C)e^{T\omega^*}\tau(K^*+E^*) \exp\left(Te^{T\omega^*}(K^*+E^*)\right) \\
&\leq Te^{T\omega^*}\tau(W^*+C) + T^2e^{T\omega^*}\tau(W^*+C)e^{T\omega^*}(K^*+E^*)\exp\left(Te^{T\omega^*}(K^*+E^*)\right) \\
&= \tau Te^{T\omega^*}(W^*+C)\left(1+Te^{T\omega^*}(K^*+E^*)e^{Te^{T\omega^*}(K^*+E^*)}\right) \\
&= \tau\mathcal{K}
\end{aligned}$$

since $(n+1)\tau \leq T$. The error terms K^*, E^*, W^* are given in (2.57) and C is the constant from the local error as given in Lemma 2.3.7. So we have the desired property

$$\|e_{n+1}\|_{H^1} = \|u_{n+1} - \underline{u}(t_{n+1})\|_{H^1} \leq \mathcal{K}\tau,$$

with $\mathcal{K}$ given in (2.57). By assumption we have $\tau < \frac{\delta}{\mathcal{K}}$ and we obtain

$$\begin{aligned}
\|u_{n+1} - \underline{u}(t_{n+1})\|_{H^1} &\leq \tau\mathcal{K} \\
&< \tfrac{\delta}{\mathcal{K}}\mathcal{K} \\
&= \delta.
\end{aligned}$$

It follows $u_{n+1} \in U$ by the definition of U as in (2.35) and therefore $u_{n+1} \in \mathcal{R}(P) \cap U$.

Note that the constant $\mathcal{K}$ depends exponentially on the end time T and the growth constant ω^* of the semigroups. Since we derived bounds for the constants arising in the convergence proof which are independent of τ and n, the constant $\mathcal{K}$ is independent of τ and n as well. Thus, the splitting scheme converges for $n \to \infty$ to the exact solution. □

Note that one can replace the initial value of the splitting scheme by an initial value u_0^* lying in a H^1-neighborhood of the exact initial value u_0, i.e.

$$u_0^* \in H^1(\mathbb{R}) \quad \text{with} \quad \|u_0^* - u_0\|_{H^1} \leq \varepsilon_3$$

for some $\varepsilon_3 > 0$. Hence we have $\|e_0\|_{H^1} \leq \varepsilon_3$ and we obtain an additional term by (2.63)

$$\left\| \prod_{\ell=0}^{n} e^{\tau PB_\ell} e_0 \right\|_{H^1} \leq e^{T\omega^*} \varepsilon_3$$

in the global error estimate by Theorem 2.3.9. Thus, the estimate in this case is given by

$$\|u_n - \underline{u}(t_n)\|_{H^1} \leq \mathcal{K}\tau + e^{T\omega^*}\varepsilon_3. \qquad (n \in \mathbb{N}_0 \cap [0, \tfrac{T}{\tau}])$$

Remark 2.3.10. *The crucial part in the convergence proof is to fix the speed λ_n in front of the $\partial_x u$-term independently of the initial value of the PDE* (2.23)*. This allows us to use the same semigroups e^{tPB_n} for v and $\tilde{v}$ in the stability estimate.*

The quasicontractivity of the generator PB_n is an important property for the convergence proof as well. Recall that in the error recursion (2.62) *we deal with terms of the form*

$$\prod_{l=k}^{n} e^{\tau PB_l}, \qquad \text{for } k = 0, \dots, n+1$$

with $B_l = \partial_x^2 + \tilde{\lambda}(u_l)\partial_x$. Assume that PB_l is not a generator of quasicontractive semigroup on $H^1(\mathbb{R})$. In this case, Lemma 2.1.9 yields an estimate

$$\left\| e^{\tau PB_l} \right\|_{H^1} \leq \tilde{M}_l e^{\tau\omega_l}$$

with $\tilde{M}_l > 1$. Note that $\tilde{M}_l$ and ω_l are typically chosen as small as possible. Similar to Lemma 2.3.4 (ii) we assume there are $\tilde{M}^* > 1$ and $\omega^* \geq 0$ such that

$$\left\| e^{\tau PB(z)} \right\|_{H^1} \leq \tilde{M}^* e^{\tau\omega^*}$$

for all $z \in U^+$, cf. Lemma 2.1.9. For every $k \in \{0, \dots, n+1\}$ we obtain the estimate

$$\begin{aligned} \left\| \prod_{l=k}^{n} e^{\tau PB_l} \right\|_{H^1} &\leq \prod_{l=k}^{n} \tilde{M}_l e^{\tau\omega_l} \\ &\leq \prod_{l=k}^{n} \tilde{M}^* e^{\tau\omega^*} \\ &= \left(\tilde{M}^*\right)^{n-k} e^{(n-k)\tau\omega^*} \\ &\leq \left(\tilde{M}^*\right)^{n-k} e^{T\omega^*}. \end{aligned}$$

Since $\tilde{M}^* > 1$ we do not obtain a convergence of the right-hand side since $\left(\tilde{M}^*\right)^{n-k} \to \infty$ for $n \to \infty$. Thus, we only obtain a suitable estimate if $\tilde{M}^* = 1$ which is only the case if the operators $PB(z)$ for $z \in U^+$ are generators of a quasicontractive semigroup.

Remark 2.3.11. *In the PDAE* (2.26) *there occurs an advection term* $\lambda_n \partial_x v$. *We consider this term as belonging to the semigroup. Another ansatz would be to treat it as part of the inhomogeneity. In this case, in the stability estimate* (2.59) *one would include the advection term in the integral part of the variation-of-constants formula and obtain an error term of the form*

$$\int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[\lambda_n \partial_x v(s) - \lambda_n \partial_x \tilde{v}(s)\right] ds.$$

Because of the spatial derivative, we were not able to get a suitable estimate for the global error.

Corollary 2.3.12. *If the assumptions of Theorem 2.3.9 hold true, the following estimate for the speed* λ_n *is satisfied*

$$|\lambda_n - \underline{\mu}(t)| \le C_6 \left\| u_n - \underline{u}(t) \right\|_{L^2} \quad (t \in [t_n, t_{n+1}])$$

for $n \in \mathbb{N}_0 \cap [0, \frac{T}{\tau}]$, *where the constant* C_6 *depends on* ψ, μ *and* u_n. *In particular, it holds*

$$|\lambda_n - \underline{\mu}(t_n)| \le C_6 \left\| u_n - \underline{u}(t_n) \right\|_{L^2}.$$

Proof. The last assertion is a direct consequence of (2.50). The first assertion follows with the same calculations by replacing t_n with t. □

2.3.3 Polynomial Nonlinearity

The convergence proof in the last section relies on specific assumptions on the nonlinearity g in the transformed system (2.4). The function g is given by (2.5). The required properties are stated in Assumption 2.3.1 (II), (III) and (VI). The main goal of this section is to prove that these assumptions are fulfilled if we choose f occurring in the original problem as a polynomial of a certain form. To obtain the transformed system we first apply the method of freezing (1.6) and go into the co-moving frame and then apply a transformation given by (2.4). We will discuss these two steps separately and analyze which form f has to take to end up with a suitable nonlinearity g.

Transformation of the PDAE

First we look at the original problem in the co-moving frame without the transformation. The PDAE was given in (2.1) by

$$\begin{cases} \partial_t u = \partial_x^2 u + f(u) + \mu \partial_x u, \quad u(0) = u_0, \\ \quad 0 = \langle \partial_x \hat{u}, u - \hat{u} \rangle \end{cases}$$

We recall that we are searching for a traveling wave

$$(\bar{u}, \bar{\mu}) \in \mathbb{H}^4_+(\mathbb{R}) \times \mathbb{R}$$

connecting the left asymptotic state $u_- \in \mathbb{R}$ to the right asymptotic state $u_+ \in \mathbb{R}$. Let $\hat{u} \in H^6_{\mathrm{ca}}(\mathbb{R})$ with the triple $(u_-, u_+, R) \in \mathbb{R}^3$ as given in Definition 1.2.2 be the reference function for the fixed phase condition. Suppose the nonlinearity f occurring in the original system (2.3) satisfies

Assumption 2.3.13. *We assume that $f : \mathbb{H}^1_+(\mathbb{R}) \to \mathbb{H}^1_+(\mathbb{R})$ is a polynomial with coefficients in $\mathbb{R}$, i.e. there is $l \in \mathbb{N}$ such that*

$$f(z(x)) = a_l z(x)^l + \cdots + a_1 z(x) + a_0 \qquad (z \in \mathbb{H}^1_+(\mathbb{R})),$$

with $a_l, \ldots, a_0 \in \mathbb{R}$. In addition we assume that

$$\begin{aligned} f(u_-) &= a_l u_-^l + \cdots + a_1 u_- + a_0 = 0, \\ f(u_+) &= a_l u_+^l + \cdots + a_1 u_+ + a_0 = 0. \end{aligned}$$

Note that $f(z) \in \mathbb{H}^1_+(\mathbb{R})$ for every $z \in \mathbb{H}^1_+(\mathbb{R})$ by Lemma 1.2.5 (iv). We recall that the transformation of the nonlinearity is given in (2.5) with $s = 4$ by the nonlinear operator

$$\begin{aligned} g : H^1(\mathbb{R}) &\to H^1(\mathbb{R}) \\ u &\mapsto g(u) = f(u + \hat{u}) + \psi' \end{aligned} \tag{2.64}$$

cf. Lemma 2.1.2. One of the important property of this transformed nonlinearity is stated in

Lemma 2.3.14. *Let $s \in \{1, \ldots, 4\}$. Under Assumption 2.3.13 the nonlinearity $g : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ in the transformed system (2.4) satisfies $g(z) \in H^s(\mathbb{R})$ for all $z \in H^s(\mathbb{R})$. In particular it holds*

$$\begin{aligned} \|g(z)\|_{H^s(\mathbb{R})} \leq \sum_{j=1}^{l} \sum_{k=0}^{j-1} \binom{j}{k} K(a_j \hat{u}^k) C(s,c)^{j-k-1} \|z\|_{H^s}^{j-k} \\ + \|f(\hat{u}) + \psi'\|_{H^s} \end{aligned} \qquad (z \in H^s(\mathbb{R}))$$

with $K(a_j \hat{u}^k)$ and $C(s,c)$ from Lemma 1.2.5. The nonlinearity g is a nonlinear operator of the form

$$g(z) = b_l z^l + \cdots + b_1 z + b_0 \qquad (z \in H^1(\mathbb{R})),$$

with $b_l, \ldots, b_0 \in \mathbb{H}^4_+$.

Proof. The proof mainly uses the properties of the space $\mathbb{H}^4_+(\mathbb{R})$ as given in Lemma 1.2.5. Let $s \in \{1, \dots, 4\}$ and $z \in H^s(\mathbb{R})$. We evaluate the j-th monomial of f with $j = 1, \dots, l$ at $z + \hat{u}$ to obtain

$$a_j(z+\hat{u})^j = a_j \sum_{k=0}^{j-1} \binom{j}{k} z^{j-k}\hat{u}^k + a_j z^0 \hat{u}^j.$$

This helps us to obtain

$$\begin{aligned} g(z) &= a_l \sum_{k=0}^{l-1} \binom{l}{k} z^{l-k}\hat{u}^k + a_l\hat{u}^l + \dots + a_2 \sum_{k=0}^{1} \binom{2}{k} z^{2-k}\hat{u}^k + a_2\hat{u}^2 \\ &\quad + a_1 z + a_1\hat{u} + a_0 + \psi' \\ &= \sum_{j=1}^{l}\sum_{k=0}^{j-1} \binom{j}{k} a_j z^{j-k}\hat{u}^k + f(\hat{u}) + \psi'. \end{aligned} \tag{2.65}$$

We check that the right-hand side of this equation lies indeed in $H^s(\mathbb{R})$. In the following we will denote with (i)-(v) the assertions of Lemma 1.2.5. By Assumption 2.3.13 and the fact that $\hat{u}$ is an element of $H^6_{\mathrm{ca}}(\mathbb{R})$ with the triple $(u_-, u_+, R) \in \mathbb{R}^3$ given by Definition 1.2.2, we know that $f(\hat{u}(x)) = 0$ for all $x \le -R$ and $x \ge R$. In addition, we know by (ii) that

$$f(\hat{u}) = a_l\hat{u}^l + \dots + a_1\hat{u} + a_0$$

is an element of $\mathbb{H}^6_+(\mathbb{R})$. Since $f(\hat{u})$ has compact support and $\mathbb{H}^6_+(\mathbb{R}) \subseteq H^6_{\mathrm{loc}}(\mathbb{R})$ it follows $f(\hat{u}) \in H^6(\mathbb{R})$. Moreover, using (v) we obtain that $\psi' = \partial_x^2\hat{u} \in H^4(\mathbb{R})$ and therefore the last part in (2.65) lies in $H^4(\mathbb{R})$. For the first part of (2.65) we know that for $j = 1, \dots, l$ and $k = 0, \dots, j-1$ we have $a_j \in \mathbb{R}$ and $a_j\hat{u}^k \in H^6_{\mathrm{ca}}(\mathbb{R})$ by (ii). From (i) we obtain $z^{j-k} \in H^s(\mathbb{R})$. Hence,

$$\binom{j}{k} a_j z^{j-k}\hat{u}^k$$

is just the multiplication of a $H^6_{\mathrm{ca}}(\mathbb{R})$-function with a $H^s(\mathbb{R})$-function with $1 \le s \le 4$. This lies in $H^s(\mathbb{R})$ by (iii). In addition, with (iii) and (i) we have

$$\begin{aligned} \left\| a_j z^{j-k}\hat{u}^k \right\|_{H^s} &\le K(a_j\hat{u}^k) \left\| z^{j-k} \right\|_{H^s} \\ &\le K(a_j\hat{u}^k) C(s,c)^{j-k-1} \left\| z \right\|_{H^s}^{j-k}. \end{aligned}$$

As a result

$$\left\| g(z) \right\|_{H^s} \le \sum_{j=1}^{l}\sum_{k=0}^{j-1} \binom{j}{k} K(a_j\hat{u}^k) C(s,c)^{j-k-1} \left\| z \right\|_{H^s}^{j-k} + \left\| f(\hat{u}) + \psi' \right\|_{H^s}.$$

Since $a_j \hat{u}^k \in \mathbb{H}^6_+(\mathbb{R})$ it follows with $f(\hat{u}), \psi' \in H^4(\mathbb{R})$ that

$$\begin{aligned} g(z) &= \sum_{j=1}^{l} \sum_{k=0}^{j-1} \binom{j}{k} a_j z^{j-k} \hat{u}^k + f(\hat{u}) + \psi' \\ &= \sum_{j=0}^{l} b_j z^j \end{aligned}$$

is a nonlinear operator which can be written as a polynomial with coefficients in $\mathbb{H}^4_+(\mathbb{R})$. In addition we have shown that $b_0 = f(\hat{u}) + \psi' \in H^4(\mathbb{R}) \subset H^s(\mathbb{R})$. □

Remark 2.3.15. *In the proof we have seen that even if the nonlinearity f is a function, the transformed nonlinearity g has to be an operator since we have*

$$g(z, \cdot) = \sum_{j=1}^{l} \sum_{k=0}^{j-1} \binom{j}{k} a_j \hat{u}(\cdot)^k z(\cdot)^{j-k} + f(\hat{u}(\cdot)) + \psi'(\cdot).$$

The coefficients $\binom{j}{k} a_j \hat{u}(\cdot)^k$ and $f(\hat{u}(\cdot)) + \psi'(\cdot)$ depend on the spatial variable and therefore g cannot be written as a function.

The nonlinearity g satisfies Assumption 2.3.1 (II) as stated in

Lemma 2.3.16. *Under Assumption 2.3.13 the nonlinear operator $g : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ is Fréchet differentiable and there is a constant $C_{Dg}(U^+) > 0$ such that*

$$\|Dg(z)\|_{H^1 \leftarrow H^1} \leq C_{Dg}(U^+) \qquad (z \in U^+).$$

In particular, $g : U^+ \to H^1(\mathbb{R})$ is Lipschitz continuous with constant $L = L(U^+)$.

Proof. Using the general binomial expansion one can easily show that the Fréchet derivative for this polynomial operator on a Banach space X is given by $Dg(z)[h] = g'(z)h$, where g' is given by

$$g'(z) := l b_l z^{l-1} + \cdots + 2b_2 z + b_1 \qquad (z \in H^1(\mathbb{R})).$$

For completeness, the calculation is given for $h \in H^1(\mathbb{R})$ by

$$\begin{aligned}
&\frac{1}{\|h\|_{H^1}} \|g(z+h) - g(z) - g'(z)h\|_{H^1} \\
&= \frac{1}{\|h\|_{H^1}} \left\| \sum_{j=0}^{l} b_j (z+h)^j - \sum_{j=0}^{l} b_j z^j - \sum_{j=1}^{l} j b_j z^{j-1} h \right\|_{H^1} \\
&= \frac{1}{\|h\|_{H^1}} \left\| \sum_{j=0}^{l} b_j \sum_{k=0}^{j} \binom{j}{k} z^{j-k} h^k - \sum_{j=0}^{l} b_j z^j - \sum_{j=1}^{l} j b_j z^{j-1} h \right\|_{H^1} \\
&= \frac{1}{\|h\|_{H^1}} \left\| \sum_{j=0}^{l} \left(b_j \sum_{k=2}^{j} \left(\binom{j}{k} z^{j-k} h^k \right) + j b_j z^{j-1} h + b_j z^j \right) - \sum_{j=0}^{l} b_j z^j - \sum_{j=0}^{l} j b_j z^{j-1} h \right\|_{H^1} \\
&= \frac{1}{\|h\|_{H^1}} \left\| \sum_{j=0}^{l} \left(b_j \sum_{k=2}^{j} \left(\binom{j}{k} z^{j-k} h^k \right) \right) \right\|_{H^1} \to 0 \text{ for } \|h\|_{H^1} \to 0
\end{aligned}$$

where we use $k \geq 2$ and Lemma 1.2.5 (iii). To show the uniform H^1-bound of Dg let $z \in U^+$ and $h \in H^1(\mathbb{R})$ with $\|h\|_{H^1} = 1$. We have

$$\begin{aligned}
\|Dg(z)[h]\|_{H^1} &= \|g'(z)h\|_{H^1} \\
&\leq \sum_{k=1}^{l} k \left\| b_k z^{k-1} h \right\|_{H^1}.
\end{aligned}$$

Even in the case $k = 1$, i.e. $\|b_1 h\|_{H^1}$, we multiply a $\mathbb{H}^4_+(\mathbb{R})$-function with a $H^1(\mathbb{R})$-function. So we can apply Lemma 1.2.5 (iii) and obtain

$$\begin{aligned}
\|Dg(z)[h]\|_{H^1} &\leq \sum_{k=1}^{l} k K(b_k) \left\| z^{k-1} h \right\|_{H^1} \\
&\leq \sum_{k=1}^{l} k K(b_k) C(1,c) \left\| z^{k-1} \right\|_{H^1} \\
&\leq \sum_{k=1}^{l} k K(b_k) C(1,c)^{k-1} \|z\|_{H^1}^{k-1} \\
&\leq \sum_{k=1}^{l} k K(b_k) C(1,c)^{k-1} C_{U^+}^{k-1} =: C_{Dg}(U^+).
\end{aligned}$$

Here we applied Lemma 1.2.5 (i) and (2.36).

Since $g : U^+ \to H^1(\mathbb{R})$ is continuous, the Lipschitz continuity with respect to the $H^1(\mathbb{R})$ norm on U^+ follows immediately by the mean value theorem for Fréchet derivatives, cf. [Wlo71, Theorem 5, p. 161]. □

It remains to prove that g as given in (2.64) satisfies Assumption 2.3.1 (III) and (VI).

Lemma 2.3.17. *Under Assumption 2.3.13 there is $C_g(U^+) > 0$ and $C_{g,u} > 0$ such that*

$$\|g(z)\|_{H^1} \leq C_g(U^+) \qquad (z \in U^+)$$

and

$$\|g(\underline{u}(t))\|_{H^4} \leq C_{g,u} \qquad (t \in [0,T]).$$

Proof. For the first estimate we use Lemma 2.3.14. For $z \in U^+$ this yields

$$\begin{aligned}
\|g(z)\|_{H^1} &\leq \sum_{j=1}^{l}\sum_{k=0}^{j-1}\binom{j}{k}K(a_j\hat{u}^k)C(s,c)^{j-k-1}\|z\|_{H^1}^{j-k} + \|f(\hat{u}) + \psi'\|_{H^1} \\
&\leq \sum_{j=1}^{l}\sum_{k=0}^{j-1}\binom{j}{k}K(a_j\hat{u}^k)C(s,c)^{j-k-1}C_{U^+}^{j-k} + \|f(\hat{u}) + \psi'\|_{H^1} \\
&=: C_g(U^+)
\end{aligned}$$

with (2.36). For the second estimate let $\tilde{U} \subset H^4(\mathbb{R})$ be a neighborhood around the exact solution $\{\underline{u}(t) : t \in [0,T]\}$. The mapping $g : \tilde{U} \to H^4(\mathbb{R})$ is continuous by Lemma 2.3.14. As a consequence it follows that

$$\begin{aligned}
G : [0,T] &\to \mathbb{R} \\
t &\mapsto \|g(\underline{u}(t))\|_{H^4}
\end{aligned}$$

is a continuous function on a compact set $[0,T]$ with real values. Thus, this function is bounded, i.e. there is $C_{g,u} > 0$ such that $|G(t)| \leq C_{g,u}$ for all $t \in [0,T]$, where $C_{g,u}$ is independent of t. This concludes the proof. □

Note that even in the case that the nonlinearity $f : \mathbb{H}^1_+(\mathbb{R}) \to \mathbb{H}^1_+(\mathbb{R})$ in the frozen system is a nonlinear operator the same properties in this section can be shown. But it turns out that due to the change of coordinates in the method of freezing the nonlinearity can change. Even in the case of a polynomial nonlinearity with space dependent coefficients, the method of freezing adds a time dependence to the coefficients of the nonlinearity as we will see below. We do not elaborate on the case of time dependent coefficients in the present thesis, though it might be possible to obtain a convergence result following the strategy we presented in the previous section in this case as well.

Change of Coordinates by the Method of Freezing

As a next step we consider the transition from the original problem to the co-moving frame and its impact on the nonlinearity.

Remark 2.3.18. *Given a nonlinear function $f : \mathbb{R} \to \mathbb{R}$ in the original problem* (1.4) *the method of freezing does not change the nonlinearity. In particular, this is the case if f has the form in Assumption 2.3.13.*

To see this we recall that the ansatz for the method of freezing (1.5) is given by

$$\begin{aligned} u(x,t) &= v(x-\gamma(t),t), \\ \partial_t \gamma(t) &= \mu(t). \end{aligned}$$

Applying it to the original problem this yields the PDE

$$(\partial_t v)(x-\gamma(t),t) = (\partial_x^2 v)(x-\gamma(t),t) + f(v(x-\gamma(t),t)) + \mu(t)(\partial_x v)(x-\gamma(t),t)$$

which is the same as

$$\partial_t v = \partial_x^2 v + f(v) + \mu \partial_x v$$

in the coordinates $(\xi, t) = (x-\gamma(t), t)$. This holds true for every function $f : \mathbb{R} \to \mathbb{R}$. In particular, this holds true for f as given in Assumption 2.3.13, i.e.

$$f(z(x)) = a_l z(x)^l + \cdots + a_1 z(x) + a_0$$

with $a_l, \ldots, a_0 \in \mathbb{R}$ and $z \in \mathbb{H}^1_+(\mathbb{R})$. Since $a_l, \ldots, a_0$ do not depend on the spatial variable x, we have

$$\begin{aligned} f(v(x-\gamma(t),t)) &= a_l v(x-\gamma(t),t)^l + \cdots + a_1 v(x-\gamma(t),t) + a_0 \\ &= a_l v(\xi,t)^l + \cdots + a_1 v(\xi,t) + a_0 \\ &= f(v(\xi,t)). \end{aligned}$$

Remark 2.3.19. *The assertion in Remark 2.3.18 does not hold true for a general non-linear operator $f : \mathbb{H}^1_+(\mathbb{R}) \to \mathbb{H}^1_+(\mathbb{R})$.*

Even in the simple case $f(z,\cdot) = a(\cdot)z(\cdot)$ with $a \in H^s(\mathbb{R})$ the ansatz of the method of freezing leads to

$$(\partial_t v)(x-\gamma(t),t) = (\partial_x^2 v)(x-\gamma(t),t) + f(v(x-\gamma(t),t),x) + \mu(t)(\partial_x v)(x-\gamma(t),t).$$

In the coordinates $(\xi,t) = (x-\gamma(t),t)$ we have

$$\begin{aligned} (\partial_t v)(\xi,t) &= (\partial_x^2 v)(\xi,t) + f(v(\xi,t),x) + \mu(t)(\partial_x v)(\xi,t) \\ &= (\partial_x^2 v)(\xi,t) + f(v(\xi,t),\xi+\gamma(t)) + \mu(t)(\partial_x v)(\xi,t) \\ &= (\partial_x^2 v)(\xi,t) + a(\xi+\gamma(t))v(\xi,t) + \mu(t)(\partial_x v)(\xi,t) \end{aligned}$$

such that $f(z, \cdot) = a(\cdot + \gamma(t))z(\cdot)$ in the new coordinates is a time dependent nonlinear operator.

2.3.4 Side Notes on the Splitting Approach

In the previous sections we introduced a scheme based on the Lie-Trotter splitting to approximate traveling wave solutions. Provided certain assumptions on the nonlinearity and regularity of the exact solution of the corresponding PDAE we were able to show that this scheme is convergent of first order on finite-time intervals. Before we consider a time discretization of the scheme in the next chapter and later validate the results numerically we conclude the present chapter by stating some thoughts on how to proceed based on the techniques introduced so far.

Second Order using Strang Splitting

The scheme we constructed in Section 2.2.1 is of first order. In their work [AO17] the authors construct a second order version of the Splitting scheme based on Strang splitting. One of the important ideas of the proof is the usage of analytic semigroups and their parabolic smoothing property. We already gave a proof that the projected operators of the PDAE generate analytic semigroups in Section 2.1.2. With that in mind, we are confident that one can show convergence of a scheme constructed analogously to the one we introduced but using Strang splitting instead of Lie splitting. Then we expect that the convergence proof follows in a straightforward way combining the techniques provided in this thesis with the estimates by the parabolic smoothing property in [AO17].

Nevertheless, one gains no further advantages pursuing this strategy in our setting. The setting in [AO17] and the purpose of the numerical scheme differ from the one given here. Altmann and Ostermann aim to solve constrained partial differential equations in a classical way in the sense of evolution equations, whereas in the present thesis we target the calculation and approximation of traveling waves by long-time forward simulations. In doing so we have to require a certain stability property of the traveling wave. If the exact solution does not converge to the traveling wave in a neighborhood of the traveling wave, one cannot expect that the numerical long-time simulation will be able to get any reasonable approximation of the traveling wave. Such a stability property determines the speed of convergence of the numerical scheme to the fixed point of the numerical scheme. We show that the traveling wave of the original problem coincides with a fixed point of the proposed scheme, cf. Section 4.1. Thus, the convergence rate in time for $\tau \to 0$ does

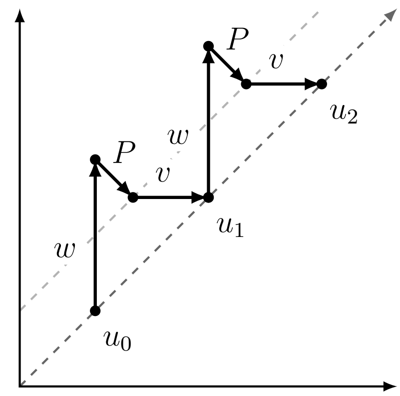

Figure 2.5: Splitting ansatz in the reversed order. The projection P is applied between the nonlinear and linear subproblem.

not play an important role for the approximation of the traveling wave. In particular, the obtained steady state is independent of τ as we see in Chapter 5. To put it in a nutshell, the time convergence does not have a large impact and therefore it is sufficient to use a scheme with first order in time to approximate traveling wave solutions. Note that, apart from the setting in [AO17], there are situations where second order schemes are useful. In Chapter 6 we consider the Burgers' equation and show via numerical simulations that in this case the steady states depend on the time step size τ. Therefore in this situation we also regard a second order scheme based on the Strang splitting.

Splitting in Reversed Order

While using operator splitting methods, one can choose in which order one handles the subproblems. So we can reverse the order of the subproblems in the splitting approach given in Section 2.2.1. In each splitting step one would solve the nonlinear ODE at first, apply the projector P and use this solution as initial value for the linear subproblem as illustrated in Figure 2.5. A similar reversed ansatz was chosen in [AO17]. We are confident that also for the reversed scheme one can show a convergence result analogously to Theorem 2.3.9. Note that in this case due to the correction term the solution operator for the nonlinear problem is the identity. Since we are confident that the proof should be very similar to the proof of Theorem 2.3.9 we do not elaborate on the details in this thesis.

CHAPTER

THREE

TIME DISCRETIZATION OF THE LINEAR SUBPROBLEM

In Chapter 2 we derived a splitting approach to approximate the exact solution of the PDAE (2.21) which was given by

$$\begin{cases} \partial_t u = \partial_x^2 u + g(u) + \mu \partial_x u + \mu \psi, \\ \quad 0 = \langle \psi, u \rangle \\ u(0) = u_0 \in H^4(\mathbb{R}) \cap \mathcal{R}(P). \end{cases} \qquad (t \in (0, T])$$

A step of the splitting scheme was defined via (2.33),

$$\mathcal{L}_\tau(z; u_n^*) \coloneqq P\Phi_w^\tau(\Phi_v^\tau(z; u_n^*); z) \tag{3.2}$$

for an approximation u_n^*. Here Φ_v^τ is the exact solution operator corresponding to the first linear subproblem

$$\begin{cases} \partial_t v = \partial_x^2 v + \tilde{\lambda}(u_n^*) \partial_x v + \lambda \psi + g(z), \\ \quad 0 = \langle \psi, v \rangle, \\ v(t_n) = z, \end{cases} \qquad (t \in (t_n, t_{n+1}]) \tag{3.3}$$

as given in (2.23). For the second nonlinear subproblem

$$\partial_t w(t) = g(w(t)) - g(z), \quad w(t_n) = w_0, \qquad (t \in [t_n, t_{n+1}]) \tag{3.4}$$

cf. (2.30), the exact solution operator is given by $\Phi_w^{t-t_n}(w_0, z)$.

Since one cannot use the exact flows of the subproblems given above for numerical simulations, we apply certain time discretizations to the subproblems in this chapter. There are different ways to pass over to a time discrete setting. In Section 3.1 we discuss an approach to use an approximation to the Lagrange multiplier λ. Instead of requiring that the algebraic constraint is fulfilled at every time $t \in [t_n, t_{n+1}]$, we fix the Lagrange multiplier in the same way we fixed the speed in front of the advection term in Chapter 2. This leads to a second order perturbation of the linear subproblem (3.3). Beside this change, we use the same approach for the splitting scheme. The main result is the convergence of the splitting scheme with discrete Lagrange multiplier in Theorem 3.1.2. This approach gives a better understanding of how the algebraic constraint can be handled for splitting methods applied to a PDAE obtained by the method of freezing.

In Section 3.2 we look at the full time discretization of the problem. Instead of using the exact solutions of the subproblems, we apply the backward Euler method to the linear subproblem (3.3) and use the forward Euler method as an approximation to the exact solution of the nonlinear subproblem (3.4). The iteration of these approximative solutions similar to (3.2) leads to a convergent splitting scheme as shown in the proof of Theorem 3.2.6.

3.1 Approximation of the Algebraic Constraint

For an implementation on a computer we have to efficiently solve the PDAE (2.23). We discuss in this section an approach to discretize the algebraic constraint. We recall the linear subproblem

$$\begin{cases} \partial_t v = \partial_x^2 v + \tilde{\lambda}(u_n^*)\partial_x v + \lambda\psi + g(z), & (t \in (t_n, t_{n+1}]) \\ \quad 0 = \langle \psi, v \rangle, & \\ v(t_n) = z, & \end{cases}$$

where the speed $\tilde{\lambda}(u_n^*)$ was defined in (2.24) by

$$\tilde{\lambda}(u_n^*) = \frac{M\langle \partial_x \psi, \partial_x u_n^* \rangle - M\langle \psi, g(u_n^*)\rangle}{1 + M\langle \psi, \partial_x u_n^* \rangle}.$$

with $u^* = u_n^*$. Instead of solving the algebraic constraint exactly and obtaining a projected version of the PDAE by applying Lemma 2.1.26, we use the already calculated speed $\tilde{\lambda}(u_n^*)$ in front of ψ instead of the Lagrange multiplier λ. This yields

$$\begin{cases} \partial_t \tilde{v} = \partial_x^2 \tilde{v} + \tilde{\lambda}(u_n^*)\partial_x \tilde{v} + \tilde{\lambda}(u_n^*)\psi + g(z), & (t \in (t_n, t_{n+1}]) \\ \tilde{v}(t_n) = z. & \end{cases} \tag{3.6}$$

For this PDE there exists a unique mild solution $\tilde{v} \in \mathcal{C}([t_n, t_{n+1}], H^1(\mathbb{R}))$ for $z \in H^1(\mathbb{R})$ by the same arguments as of Lemma 2.3.3. Note that the algebraic constraint is no longer required since the unknown variable $\lambda(t)$ was replaced by $\tilde{\lambda}(u_n^*)$. As a result we cannot apply Lemma 2.1.26 to obtain a projected version of this PDE. We represent the solution for the PDE (3.6) and the PDAE (2.23) by the variation-of-constants formula

$$\begin{aligned} \tilde{v}(t) &= e^{(t-t_n)\partial_x^2} z + \int_{t_n}^t e^{(t-s)\partial_x^2} \left[\tilde{\lambda}(u_n^*)\partial_x \tilde{v}(s) + g(z) + \tilde{\lambda}(u_n^*)\psi\right] ds, \\ v(t) &= e^{(t-t_n)\partial_x^2} z + \int_{t_n}^t e^{(t-s)\partial_x^2} \left[\tilde{\lambda}(u_n^*)\partial_x v(s) + g(z) + \lambda(s)\psi\right] ds, \end{aligned} \tag{3.7}$$

for $t \in [t_n, t_{n+1}]$ where v is the solution of the PDAE (2.23). The solution $\tilde{v}$ depends on z and an approximation $u^* = u_n^*$ such that we define the solution operator

$$\Phi_{\tilde{v}}^t(z; u^*) := e^{tB(u^*)} z + \int_0^t e^{(t-s)B(u^*)} \left[g(z) + \tilde{\lambda}(u^*)\psi\right] ds \tag{3.8}$$

with $t \in [0, \tau]$ and $B(u^*) = \partial_x^2 + \tilde{\lambda}(u^*)\partial_x$ as given in (2.27). We solve the nonlinear problem as before such that we define the splitting scheme with discrete Lagrange multiplier by

$$\begin{aligned} \tilde{\mathcal{L}}_\tau(z; u^*) &:= P\Phi_w^\tau \left(\Phi_{\tilde{v}}^\tau(z; u^*); z\right) \\ \tilde{\mathcal{L}}_\tau(z) &:= \tilde{\mathcal{L}}_\tau(z; z). \end{aligned}$$

We define now the approximations $u_n \approx \underline{u}(t_n)$ to the exact solution obtained by the splitting scheme with discrete Lagrange multiplier by

$$\begin{aligned} u_{n+1} &:= \tilde{\mathcal{L}}_\tau(u_n) \\ &= \tilde{\mathcal{L}}_\tau^{n+1}(u_0). \end{aligned}$$

We define the neighborhoods U, U^*, U^+ as in (2.35). Similar to the proof of Theorem 2.3.9 we will prove a convergence result where we use Assumption 2.3.1 and Lemma 2.3.4 in the same way as before. The only difference is that we have to show that the solution $\Phi_{\tilde{v}}^\tau$ of (3.6) lies in the correct neighborhood. Similar to Lemma 2.3.4 (iii) we have the following result.

Lemma 3.1.1. *There is $\tau_1^* > 0$ such that for $z \in U \cap \mathcal{R}(P)$ and $z^+ \in U^+$ it holds*

$$\Phi_{\tilde{v}}^\tau(z; z^+) \in U^* \qquad (\tau < \tau_1^*).$$

Proof. The basic ideas for the proof are the same as for the proof of Lemma 2.3.4 (iii). Nevertheless, since we are working with the non-projected operator $B(z^+)$, there are certain changes.

Let $z \in U$ and $z^+ \in U^+$. By the definition of U there is $t^* \in [0, T]$ such that

$$\|z - \underline{u}(t^*)\|_{H^1} < \delta.$$

We have

$$\left\|\Phi_{\tilde{v}}^{\tau}(z;z^{+}) - \underline{u}(t^{*})\right\|_{H^1} \leq \left\|\Phi_{\tilde{v}}^{\tau}(z;z^{+}) - e^{\tau B(z^{+})}\underline{u}(t^{*})\right\|_{H^1} + \left\|e^{\tau B(z^{+})}\underline{u}(t^{*}) - \underline{u}(t^{*})\right\|_{H^1}$$

with the definition of the solution operator given in (3.8). In the following estimates we will use that $B(z^{+})$ is a generator of a contraction semigroup on $H^s(\mathbb{R})$ for $s \geq 0$ by Lemma 2.1.25. For the first part of the right-hand side we obtain

$$\begin{aligned}\left\|\Phi_{\tilde{v}}^{\tau}(z;z^{+}) - e^{\tau B(z^{+})}\underline{u}(t^{*})\right\|_{H^1} &\leq \left\|\int_0^{\tau} e^{(\tau-s)B(z^{+})}\left[g(z) + \tilde{\lambda}(z^{+})\psi\right] ds\right\|_{H^1} \\ &\quad + \left\|e^{\tau B(z^{+})}\left(z - \underline{u}(t^{*})\right)\right\|_{H^1} \\ &\leq \tau\left(\|g(z)\|_{H^1} + \tilde{\lambda}(z^{+})\|\psi\|_{H^1}\right) + \delta \\ &\leq \tau\left(C_g(U^{+}) + C_\lambda(U^{+})\|\psi\|_{H^1}\right) + \delta\end{aligned}$$

with $C_g(U^{+})$ from Assumption 2.3.1 (III) and $C_\lambda(U^{+})$ from Lemma 2.3.4 (i). For the second part of the right-hand side above we calculate

$$\begin{aligned}\left\|e^{\tau B(z^{+})}\underline{u}(t^{*}) - \underline{u}(t^{*})\right\|_{H^1} &= \left\|\left(e^{\tau B(z^{+})} - I\right)\underline{u}(t^{*})\right\|_{H^1} \\ &\leq \left\|B(z^{+})\int_0^{\tau} e^{sB(z^{+})}\underline{u}(t^{*})ds\right\|_{H^1} \\ &\leq \left\|\left(\partial_x^2 + \tilde{\lambda}(z^{+})\partial_x\right)\int_0^{\tau} e^{sB(z^{+})}\underline{u}(t^{*})ds\right\|_{H^1} \\ &\leq \tau\left(\|\underline{u}(t^{*})\|_{H^3} + |\tilde{\lambda}(z^{+})|\,\|\underline{u}(t^{*})\|_{H^2}\right) \\ &\leq \tau C_u\left(1 + |\tilde{\lambda}(z^{+})|\right) \\ &\leq \tau C_u\left(1 + C_\lambda(U^{+})\right),\end{aligned}$$

where $C_\lambda(U^{+})$ is the constant arising in Lemma 2.3.4 (i) and C_u from Assumption 2.3.1 (V). To sum up we have

$$\left\|\Phi_{\tilde{v}}^{\tau}(z;z^{+}) - \underline{u}(t^{*})\right\|_{H^1} \leq \tau K + \delta$$

with $K := C_g(U^{+}) + C_\lambda(U^{+})\|\psi\|_{H^1} + C_u\left(1 + C_\lambda(U^{+})\right)$. To finish the proof we have to show that the right-hand side is smaller than δ^*. We chose $\tau_1^* > 0$ small enough such that

$$\tau_1^* K \leq \varepsilon_2$$

where ε_2 is given by the definition of U^* as in (2.35). For $\tau < \tau_1^*$ this yields

$$\begin{aligned}\left\|\Phi_{\tilde{v}}^{\tau}(z;z^{+}) - \underline{u}(t^{*})\right\|_{H^1} &\leq \tau K + \delta \\ &< \varepsilon_2 + \delta < \delta^*.\end{aligned}$$

Hence $\Phi_{\tilde{v}}^{\tau}(z;z^{+}) \in U^*$ for $\tau < \tau_1$. This concludes the proof.

□

We have to slightly adapt τ_0 using τ_1^* from Lemma 3.1.1 to obtain

$$\tau_0 := \min\left\{\tau_1^*, \tau_2, \tau_3\right\}.$$

The following Theorem 3.1.2 yields a similar estimate for the global error as Theorem 2.3.9. Since we consider $\tilde{\mathcal{L}}_\tau$ instead of $\mathcal{L}_\tau$, the error constant changes. In contrast to (2.57) the new global error constant contains an additional term $\mathcal{A}^*$. We have

$$\mathcal{K} := Te^{T\omega^*}\left(W^* + C + \mathcal{A}^*\right)\left[1 + Te^{T\omega^*}\left(K^* + E^*\right)e^{Te^{T\omega^*}(K^*+E^*)}\right] \tag{3.9}$$

with

$$\begin{aligned}
\mathcal{A}^* &:= \Big(\|P\|_{H^1} K_5(1+\tau_0 L) + 4LC_{Dg}(U^+)C_{U^+}\Big)\\
K_5 &:= \|\psi\|_{H^1} M(1+|\lambda_n|)\\
&\quad\cdot\Big(\|\psi\|_{H^4} C_{U^+} + C_\lambda(U^+)C_{U^+} + C_g(U^+) + C_{\lambda,v}\|\psi\|_{L^2}\Big),\\
C_{\lambda,v} &:= M\|\psi\|_{H^1} C_{U^+} + M\|\psi\|_{L^2}\Big(C_g(U^+) + C_\lambda(U^+)C_{U^+}\Big)
\end{aligned}$$

where K^*, E^* and W^* are defined in (2.57) and C is given in Lemma 2.3.7. With this preliminaries we can show the following convergence theorem.

Theorem 3.1.2. *Under Assumption 2.3.1 the Lie splitting $\tilde{\mathcal{L}}_\tau$ with a given step size $\tau < \min\{\tau_0, \frac{\delta}{\mathcal{K}}\}$ is convergent of first order in the H^1-norm, i.e.*

$$\|u_n - \underline{u}(t_n)\|_{H^1} \le \mathcal{K}\tau, \qquad (n \in \mathbb{N}_0 \cap [0, \tfrac{T}{\tau}])$$

where the constant $\mathcal{K} > 0$ is given in (3.9). *In particular, it is independent of n and τ, but depends on T.*

Proof. We only have to slightly modify the proof by induction of Theorem 2.3.9. We prove that

1. $u_n \in U \cap \mathcal{R}(P)$,
2. $\|u_n - \underline{u}(t_n)\|_{H^1} \le \tau\mathcal{K}$

is satisfied for all $n \in \mathbb{N}_0$ with $n\tau \le T$. For the inductive step we assume as before that $u_k \in U \cap \mathcal{R}(P)$ and $\|u_k - u(t_k)\|_{H^1} \le \tau\mathcal{K}$ hold true for all $0 \le k \le n$ and show that $u_{n+1} \in U \cap \mathcal{R}(P)$ and $\|u_{n+1} - \underline{u}(t_{n+1})\|_{H^1} \le \tau\mathcal{K}$ are satisfied. We assume $(n+1)\tau \le T$ since we only approximate the solution up to the end time T.

We estimate the global error $e_{n+1} \coloneqq u_{n+1} - \underline{u}(t_{n+1})$ by

$$\begin{aligned}
\|e_{n+1}\|_{H^1} &= \left\| \tilde{\mathcal{L}}_\tau(u_n; u_n) - \underline{u}(t_{n+1}) \right\|_{H^1} \\
&\leq \left\| \tilde{\mathcal{L}}_\tau(u_n; u_n) - \mathcal{L}_\tau(u_n; u_n) \right\|_{H^1} \\
&\quad + \|\mathcal{L}_\tau(u_n; u_n) - \mathcal{L}_\tau(\underline{u}(t_n); u_n)\|_{H^1} \\
&\quad + \|\mathcal{L}_\tau(\underline{u}(t_n); u_n) - \Phi_u^\tau(\underline{u}(t_n); t_n)\|_{H^1} \\
&= \mathcal{A} + \mathcal{B} + \mathcal{C}.
\end{aligned}$$

with

$$\begin{aligned}
\mathcal{A} &\coloneqq \left\| \tilde{\mathcal{L}}_\tau(u_n; u_n) - \mathcal{L}_\tau(u_n; u_n) \right\|_{H^1}, \\
\mathcal{B} &\coloneqq \|\mathcal{L}_\tau(u_n; u_n) - \mathcal{L}_\tau(\underline{u}(t_n); u_n)\|_{H^1}, \\
\mathcal{C} &\coloneqq \|\mathcal{L}_\tau(\underline{u}(t_n); u_n) - \Phi_u^\tau(\underline{u}(t_n); t_n)\|_{H^1}.
\end{aligned}$$

The global error consists of three error terms. The last one $\mathcal{C}$ is a local error. For this, Lemma 2.3.7 already yields an second order estimate. The proof follows in a straightforward way with the new definition of u_n as well. This is due to the fact that the lemma only relies on an approximation u_n^* of order one, which we handle by induction as well. The second term $\mathcal{B}$ can be handled similar to the stability estimate in Theorem 2.3.9. Since the definition of u_n changed, we have to be careful in the convergence proof, but the occurring terms can be handled in a very similar way as before. While $\mathcal{B}$ and $\mathcal{C}$ are terms appearing in a very similar way in the proof of Theorem 2.3.9 the first term $\mathcal{A}$ requires a deeper analysis. Hence, we restrict ourselves to the discussion of this term. It is of second order and thus can be handled as the other terms in the error recursion. We define

$$\tilde{v}(t) = \Phi_{\tilde{v}}^{t-t_n}(u_n; u_n), \qquad v(t) = \Phi_v^{t-t_n}(u_n; u_n), \qquad \lambda_n = \tilde{\lambda}(u_n)$$

with $t \in [t_n, t_{n+1}]$. For the nonlinear step we use the solution representation by a Taylor expansion as well given in (2.43), to obtain

$$\begin{aligned}
\mathcal{A} &= \Big\| P\tilde{v}(t_{n+1}) + \tau P\left[g(\tilde{v}(t_{n+1})) - g(u_n)\right] \\
&\qquad - Pv(t_{n+1}) - \tau P\left[g(v(t_{n+1})) - g(u_n)\right] + \mathcal{R}_2(\tau^2) \Big\|_{H^1} \\
&\leq \|P\left(\tilde{v}(t_{n+1}) - v(t_{n+1})\right)\|_{H^1} \\
&\qquad + \tau \|P\|_{H^1} \|g(\tilde{v}(t_{n+1})) - g(u_n) - g(v(t_{n+1}) + g(u_n))\|_{H^1} + \left\|\mathcal{R}_2(\tau^2)\right\|_{H^1} \\
&\leq \|P\left(\tilde{v}(t_{n+1}) - v(t_{n+1})\right)\|_{H^1} \\
&\qquad + \tau \|P\|_{H^1} L \|\tilde{v}(t_{n+1}) - v(t_{n+1})\|_{H^1} + \left\|\mathcal{R}_2(\tau^2)\right\|_{H^1} \\
&= \|P\|_{H^1} (1 + \tau L) \|\tilde{v}(t_{n+1}) - v(t_{n+1})\|_{H^1} + \left\|\mathcal{R}_2(\tau^2)\right\|_{H^1}
\end{aligned}$$

using the Lipschitz continuity given in Assumption 2.3.1 (II) with Lemma 3.1.1. The remainder term $\mathcal{R}_2(\tau^2)$ consists of the remainders from both Taylor expansions as in (2.44) and is given by

$$\mathcal{R}_2(\tau^2) = \tau^2 \partial_t g(\tilde{w}(\xi_1)) - \tau^2 \partial_t g(w(\xi_2)),$$

with $w(t) = \Phi_w^{t-t_n}(v(t_{n+1}); u_n)$ and $\tilde{w}(t) = \Phi_w^{t-t_n}(\tilde{v}(t_{n+1}); u_n)$ for $\xi_1, \xi_2 \in [t_n, t_{n+1}]$. We have $v(t_{n+1}), \tilde{v}(t_{n+1}) \in U^*$ with Lemma 2.3.4 (iii) and Lemma 3.1.1, respectively. Thus with Lemma 2.3.4 (iv) it holds $w(t), \tilde{w}(t) \in U^+$ since $\tau < \tau_0$. In the same way as for the estimate in (2.45) we obtain

$$\left\| \mathcal{R}_2(\tau^2) \right\|_{H^1} \leq \tau^2 4 L C_{Dg}(U^+) C_{U^+}.$$

We set $\lambda_n = \tilde{\lambda}(u_n)$ and we have with (3.7)

$$\tilde{v}(t_{n+1}) - v(t_{n+1}) = \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)\partial_x^2} \left(\lambda_n - \lambda(s)\right) \psi ds$$

since both solutions have the same initial value u_n and same speed λ_n in front of the advection term. It remains to derive a first order estimate of $\sup_{s \in [t_n, t_{n+1}]} |\lambda_n - \lambda(s)|$ and the remainder term $\mathcal{R}_2(\tau^2)$, which is similar to (2.44). We have with (2.25) and (2.38)

$$\begin{aligned} \lambda_n - \lambda(s) &= M\langle \partial_x \psi, \partial_x u_n \rangle - M\langle \psi, \lambda_n \partial_x u_n + g(u_n) \rangle \\ &\quad - M\langle \partial_x \psi, \partial_x v(s) \rangle + M\langle \psi, \lambda_n \partial_x v(s) + g(u_n) \rangle \\ &= M\langle \partial_x^2 \psi, v(s) - u_n \rangle - \lambda_n M\langle \partial_x \psi, v(s) - u_n \rangle \end{aligned}$$

for $s \in [t_n, t_{n+1}]$. We obtain for $\phi \in \{\partial_x \psi, \partial_x^2 \psi\}$

$$\begin{aligned} \langle \phi, v(s) - u_n \rangle &= \langle \phi, \left(e^{(s-t_n)\partial_x^2} - I \right) u_n \rangle \\ &\quad + \langle \phi, \int_{t_n}^{s} e^{(s-\xi)\partial_x^2} \left[\lambda_n \partial_x v(\xi) + g(u_n) + \lambda(\xi)\psi \right] d\xi \rangle. \end{aligned} \tag{3.10}$$

For the first term on the right-hand side we obtain

$$\begin{aligned} |\langle \phi, \left(e^{(s-t_n)\partial_x^2} - I \right) u_n \rangle| &= |\langle \phi, \partial_x^2 \int_0^{s-t_n} e^{\xi \partial_x^2} u_n d\xi \rangle| \\ &= |\langle \partial_x^2 \phi, \int_0^{s-t_n} e^{\xi \partial_x^2} u_n d\xi \rangle| \\ &\leq \|\psi\|_{H^4} \tau \sup_{\xi \in [t_n, t_{n+1}]} \left\| e^{\xi \partial_x^2} \right\|_{L^2} \|u_n\|_{L^2} \\ &\leq \tau \|\psi\|_{H^4} \|u_n\|_{L^2} \\ &\leq \tau \|\psi\|_{H^4} C_{U^+} \end{aligned}$$

for $s \in [t_n, t_{n+1}]$ using Lemma 2.1.12 and (2.36). We have by (2.25) with $z = u_n$

$$
\begin{aligned}
|\lambda(s)| &= |M\langle \partial_x \psi, \partial_x v(s)\rangle - M\langle \psi, g(u_n) + \lambda_n \partial_x v(s)\rangle| \\
&\leq M \|\psi\|_{H^1} \|v(s)\|_{H^1} + M \|\psi\|_{L^2} (\|g(u_n)\|_{L^2} + |\lambda_n| \|v(s)\|_{H^1}) \\
&\leq M \|\psi\|_{H^1} C_{U^+} + M \|\psi\|_{L^2} \left(C_g(U^+) + C_\lambda(U^+) C_{U^+}\right) \\
&=: C_{\lambda,v}
\end{aligned}
$$

using Lemma 2.3.4 (i), Lemma 2.3.4 (iii), (2.36) and Assumption 2.3.1 (III). For the term which occurs in the second term of the right-hand side of (3.10) we calculate

$$
\begin{aligned}
&\sup_{s \in [t_n, t_{n+1}]} \left\| \int_{t_n}^{s} e^{(s-\xi)\partial_x^2} \left[\lambda_n \partial_x v(\xi) + g(u_n) + \lambda(\xi)\psi\right] d\xi \right\|_{L^2} \\
&\qquad \leq \sup_{s \in [t_n, t_{n+1}]} (s - t_n) \sup_{\xi \in [t_n, t_{n+1}]} \left\| e^{(s-\xi)\partial_x^2} \right\|_{L^2} \|\lambda_n \partial_x v(\xi) + g(u_n) + \lambda(\xi)\psi\|_{L^2} \\
&\qquad \leq \tau \left(C_\lambda(U^+) C_{U^+} + C_g(U^+) + C_{\lambda,v} \|\psi\|_{L^2} \right)
\end{aligned}
$$

using Lemma 2.3.4 (i), Lemma 2.3.4 (iii) and Assumption 2.3.1 (III).

Finally, using the above estimates and $\|\phi\|_{L^2} \leq \|\psi\|_{H^2}$ we obtain

$$
\begin{aligned}
\|\tilde{v}(t_{n+1}) - v(t_{n+1})\|_{H^1} &\leq \left\| \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)\partial_x^2} (\lambda_n - \lambda(s)) \psi ds \right\|_{H^1} \\
&\leq \tau \sup_{s \in [t_n, t_{n+1}]} \left\| e^{(t_{n+1}-s)\partial_x^2} \right\|_{H^1} |\lambda_n - \lambda(s)| \|\psi\|_{H^1} \\
&\leq \tau \|\psi\|_{H^1} M(1 + |\lambda_n|) \Big(\tau \|\psi\|_{H^4} C_{U^+} \\
&\qquad + \tau \|\psi\|_{H^2} \left(C_\lambda(U^+) C_{U^+} + C_g(U^+) + C_{\lambda,v} \|\psi\|_{L^2} \right) \Big) \\
&\leq \tau^2 \|\psi\|_{H^1} M(1 + |\lambda_n|) \Big(\|\psi\|_{H^4} C_{U^+} \\
&\qquad + \|\psi\|_{H^2} \left(C_\lambda(U^+) C_{U^+} + C_g(U^+) + C_{\lambda,v} \|\psi\|_{L^2} \right) \Big) \\
&=: \tau^2 K_5.
\end{aligned}
$$

Finally we obtain

$$
\begin{aligned}
\mathcal{A} &\leq \tau^2 \|P\|_{H^1} (1 + \tau L) K_5 + \tau^2 4 L C_{Dg}(U^+) C_{U^+} \\
&\leq \tau^2 \left(\|P\|_{H^1} K_5 (1 + \tau_0 L) + 4 L C_{Dg}(U^+) C_{U^+} \right) \\
&= \tau^2 \mathcal{A}^*.
\end{aligned}
$$

The convergence follows analogously to the proof of Theorem 2.3.9 with the additional term $\tau^2 \mathcal{A}^*$ handled in the same way as the local error. □

We are confident that one can use exponential integrators [HO10] to solve the linear subproblem (3.6),

$$\begin{cases} \partial_t \tilde{v} = \partial_x^2 \tilde{v} + \tilde{\lambda}(u_n^*)\partial_x \tilde{v} + \tilde{\lambda}(u_n^*)\psi + g(z), & (t \in (t_n, t_{n+1}]) \\ \tilde{v}(t_n) = z. \end{cases}$$

We do not elaborate on this approach in details, but we give an idea on how to apply exponential integrators to the problem. The idea behind exponential integrators is to solve the variation-of-constants formula, where we have the two choices with $B_n = B(u_n^*) = \partial_x^2 + \tilde{\lambda}(u_n^*)\partial_x$

$$\tilde{v}(t_{n+1}) = e^{\tau B_n} z + \int_0^\tau e^{(\tau - s)B_n} \left[\tilde{\lambda}(u_n^*)\psi + g(z) \right] ds,$$
$$\tilde{v}(t_{n+1}) = e^{\tau \partial_x^2} z + \int_0^\tau e^{(\tau - s)\partial_x^2} \left[\tilde{\lambda}(u_n^*)\partial_x \tilde{v} \tilde{\lambda}(u_n^*)\psi + g(z) \right] ds.$$

For the first equation the operator B_n changes in each time step such that one has to calculate the exponential in each time step for this approach. In the second version the solution $\tilde{v}$ occurs in the integral part. Therefore the integral cannot be calculated in an exact way and one has to use a numerical integration formula to obtain approximations to the integral. Note that an ansatz using the projected generators PA or PB_n would also be possible, but the resulting matrices with finite differences would be dense due to the projection such that the numerical calculation of the exponential of these matrices would be expensive.

Nevertheless, using exponential integrators provide interesting approach for numerical solutions but we do not elaborate on this subject. As an alternative, we are using a backward Euler method for the time integration of the linear subproblem as discussed in the next section.

3.2 An Implicit Approach for the PDAE

In the previous section we used an explicit approach to solve the algebraic constraint in the PDAE of the linear subproblem. The linear and nonlinear subproblems were still solved without applying a time discretization. The scheme which we introduce in this section approximates a solution to the PDAE

$$\begin{cases} \partial_t u = \partial_x^2 u + g(u) + \mu \partial_x u + \mu \psi, & \\ \quad 0 = \langle \psi, u \rangle, & (t \in [0, T]) \\ u(0) = u_0 \in H^5(\mathbb{R}) \cap \mathcal{R}(P) & \end{cases} \tag{3.11}$$

by using time discretizations for the subproblems of the splitting approach introduced in Section 2.2.1. Note that we require in this section higher regularity as in Section 2.2.1, i.e. the exact solution has to lie in $H^5(\mathbb{R})$. In the convergence proof in the time-continuous case (Theorem 2.3.9) we used the variation-of-constants formula for the linear subproblem. In this section we choose an implicit approach to solve the linear PDAE by applying the backward Euler method to the evolution equation of the linear subproblem. The algebraic constraint is ensured with an implicit approach as well. For the nonlinear subproblem we apply the forward Euler method. The main result of this section is the convergence proof of the resulting scheme in Section 3.2.2.

3.2.1 Preliminaries

For the backward Euler method we use the resolvent of an operator. We give the following definitions from [EN00, Section IV.1]. The spectrum of a closed operator $(Z, \mathcal{D}(Z))$ on a Banach space X is given by

$$\sigma(Z) := \{\lambda \in \mathbb{C} \mid \lambda I - Z \text{ is not bijective }\}.$$

Moreover we have the resolvent set

$$\rho(Z) := \mathbb{C} \setminus \sigma(Z)$$

and for every $\lambda \in \rho(Z)$ we define the resolvent

$$R(\lambda, Z) := (\lambda I - Z)^{-1}.$$

In addition, we will make use of the following theorem.

Theorem 3.2.1 ([EN00, Theorem II.1.10, p. 55])**.** *Let $(T(t))_{t\geq 0}$ be a strongly continuous semigroup on the Banach space $(X, \|\cdot\|)$ and take constants $\omega \geq 0, \tilde{M} \geq 1$ such that*

$$\|T(t)\| \leq \tilde{M} e^{\omega t} \tag{3.12}$$

for $t \geq 0$. For the generator $(Z, \mathcal{D}(Z))$ of $(T(t))_{t\geq 0}$ the following properties hold.

(i) If $\lambda \in \mathbb{C}$ such that $R(\lambda)x := \int_0^\infty e^{-\lambda s} T(s) x ds$ exists for all $x \in X$, then $\lambda \in \rho(Z)$ and $R(\lambda, Z) = R(\lambda)$.

(ii) If $\operatorname{Re}\lambda > \omega$, then $\lambda \in \rho(Z)$. The resolvent is given by the integral expression in (i).

(iii) $\|R(\lambda, Z)\| \leq \frac{\tilde{M}}{\operatorname{Re}\lambda - \omega}$ for all λ with $\operatorname{Re}\lambda > \omega$.

Note that the existence of the constants ω and $\tilde{M}$ is given in Lemma 2.1.9. The second assertion will be used to show that the resolvent operator occurring by the the backward Euler method is invertible. The last assertion of this theorem will be used to bound the occurring resolvent operator in the local error and stability estimates as discussed in the next section. In advance we show the following lemma.

Lemma 3.2.2. *Let the operator* $(Z, \mathcal{D}(Z))$ *be a generator of a strongly continuous semigroup* $(T(t))_{t\geq 0}$ *on a Banach space* $(X, \|\cdot\|)$ *with constants* $\omega \geq 0, \tilde{M} \geq 1$ *such that* (3.12) *is satisfied. Then for every* $\tau \in \mathbb{R}_+$ *with* $\tau < \frac{1}{\omega}$ *the operator* $(I - \tau Z)$ *is invertible and it holds*

$$\left\|(I - \tau Z)^{-1}\right\| \leq \frac{\tilde{M}}{1 - \tau\omega}.$$

Proof. The proof relies on some basic calculations and Theorem 3.2.1. We have

$$I - \tau Z = \tau(\tfrac{1}{\tau} I - Z). \tag{3.13}$$

Theorem 3.2.1 (ii) yields that $(\frac{1}{\tau} I - Z)$ is bijective and invertible if $\frac{1}{\tau} > \omega$. In this case we obtain with (3.13)

$$\begin{aligned} (I - \tau Z)^{-1} &= \tfrac{1}{\tau} \left(\tfrac{1}{\tau} I - Z\right)^{-1} \\ &= \tfrac{1}{\tau} R(\tfrac{1}{\tau}, Z) \end{aligned}$$

and

$$\begin{aligned} \left\|(I - \tau Z)^{-1}\right\| &= \tfrac{1}{\tau} \left\|R(\tfrac{1}{\tau}, Z)\right\| \\ &\leq \tfrac{1}{\tau} \frac{\tilde{M}}{\left(\frac{1}{\tau} - \omega\right)} \\ &= \frac{\tilde{M}}{1 - \tau\omega}. \end{aligned}$$

using Theorem 3.2.1 (iii). This yields the estimate of the lemma. □

3.2.2 Convergence of the Splitting Scheme

The linear PDAE which we considered as the first subproblem in the splitting approach was given in (2.23). The system is given by

$$\begin{cases} \partial_t v = \partial_x^2 v + \tilde{\lambda}(u_n^*) \partial_x v + \lambda\psi + g(z), \\ \quad 0 = \langle \psi, v \rangle, \\ v(t_n) = z \end{cases} \qquad (t \in (t_n, t_{n+1}])$$

for a smooth and consistent initial value $z \in H^1(\mathbb{R}) \cap \mathcal{R}(P)$. For the time discretization, the approximation of the evolution equation via the backward Euler method can be done in a straightforward way. We chose the algebraic constraint such that the outcome of the linear subproblem lies in $\mathcal{R}(P)$. We denote the approximation with v_{n+1}. This yields the system

$$\begin{cases} v_{n+1} = z + \tau \left[\partial_x^2 v_{n+1} + \tilde{\lambda}(u_n^*)\partial_x v_{n+1} + \lambda^* \psi + g(z)\right], \\ \quad 0 = \langle \psi, v_{n+1} \rangle \end{cases} \tag{3.15}$$

for a given pair (z, u_n^*). The time-independent variable λ^* is uniquely determined by $0 = \langle \psi, v_{n+1} \rangle$. Similar to the time-continuous case where we showed the equivalence of systems in Lemma 2.1.26, we can derive the following system from the above equation for an initial value $z \in \mathcal{R}(P)$

$$\begin{cases} v_{n+1} = z + \tau \left[P\partial_x^2 v_{n+1} + \tilde{\lambda}(u_n^*)P\partial_x v_{n+1} + Pg(z)\right], \\ \quad \lambda^* = -M\langle \psi, \partial_x^2 v_{n+1} + \tilde{\lambda}(u_n^*)\partial_x v_{n+1} + g(z)\rangle. \end{cases} \tag{3.16}$$

with $P = I - M\psi\langle \psi, \cdot \rangle$ as before. Since both PDAEs depend on z and u_n^*, we define the solution operator for the linear subproblem by

$$\varphi_v^\tau(z; u_n^*) \coloneqq v_{n+1}. \tag{3.17}$$

By solving for the unknown variable v_{n+1} in the evolution equation of (3.15) and (3.16) we obtain the representations

$$\begin{aligned} v_{n+1} &= (I - \tau B(u_n^*))^{-1} \left(z + \tau \left[\lambda^* \psi + g(z)\right]\right), \\ v_{n+1} &= (I - \tau PB(u_n^*))^{-1} \left(z + \tau Pg(z)\right), \end{aligned} \tag{3.18}$$

where $B(u_n^*) = \partial_x^2 + \tilde{\lambda}(u_n^*)\partial_x$. Using the fact that $B(u_n^*)$ and $PB(u_n^*)$ are generators of strongly continuous semigroups (Lemma 2.1.25), Lemma 3.2.2 yields that the operators

$$(I - \tau B(u_n^*)) \text{ and } (I - \tau PB(u_n^*))$$

are indeed invertible. Note that in numerical simulations using a LU decomposition is more precise and much less expensive than computing the inverse of a matrix.

Using a fully implicit scheme for the linear subproblem seems to be the method of choice. This is motivated by the heat equation, i.e. the case where we only consider the term ∂_x^2. In this situation explicit Runge–Kutta schemes like the forward Euler method only yield good approximations for very small time step sizes.

We define the full time discrete Lie splitting by

$$\begin{aligned}\varphi_\tau(z;u^*) &\coloneqq \varphi_v^\tau(z;u^*) + \tau P\left[g(\varphi_v^\tau(z;u^*)) - g(z)\right] \\ \varphi_\tau(z) &\coloneqq \varphi_\tau(z;z).\end{aligned} \tag{3.19}$$

This is analogous to (2.33) since $\varphi_v^\tau(z;u^*) \in \mathcal{R}(P)$. The neighborhoods U, U^* and U^+ are chosen as before in (2.35). For $\varepsilon^*, \varepsilon_2 > 0$ and $\delta^+ > \delta^* + \varepsilon^* > 0$, $\delta^* > \delta + \varepsilon_2 > 0$ we have

$$\begin{aligned}U \;&\coloneqq \left\{ z \in H^1(\mathbb{R}) \;\middle|\; \exists t^* = t^*(z) \in [0,T] : \quad \|z - \underline{u}(t^*)\|_{H^1(\mathbb{R})} < \delta \right\}, \\ U^* &\coloneqq \left\{ z \in H^1(\mathbb{R}) \;\middle|\; \exists t^* = t^*(z) \in [0,T] : \quad \|z - \underline{u}(t^*)\|_{H^1(\mathbb{R})} < \delta^* \right\}, \\ U^+ &\coloneqq \left\{ z \in H^1(\mathbb{R}) \;\middle|\; \exists t^* = t^*(z) \in [0,T] : \quad \|z - \underline{u}(t^*)\|_{H^1(\mathbb{R})} < \delta^+ \right\}.\end{aligned} \tag{3.20}$$

We have to slightly modify Assumption 2.3.1 for the time discrete setting. In particular, we are going to assume a slightly adapted version of (III)-(VI) to obtain a bounded exact solution in the $H^5(\mathbb{R})$-norm. For completeness we state all assumptions in the following.

Assumption 3.2.3. *In addition to Assumption 1.3.1 we assume that*

(I)* *the reference function $\hat{u} \in H^7_{ca}(\mathbb{R})$ satisfies Assumption 1.3.1 (ii) and there is $\varepsilon_\psi > 0$ only depending on ψ such that*

$$1 + M\langle \psi, \partial_x z\rangle > \varepsilon_\psi \qquad (z \in U^+);$$

(II)* *the nonlinearity $g : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ is Fréchet differentiable and there is a constant $C_{Dg}(U^+) > 0$ such that*

$$\|Dg(z)\|_{H^1 \leftarrow H^1} \le C_{Dg}(U^+) \qquad (z \in U^+).$$

With the mean value theorem it follows that $g : U^+ \to H^1(\mathbb{R})$ is Lipschitz continuous with Lipschitz constant $L = L(U^+)$;

(III)* *the nonlinearity g is uniformly bounded in U^+, i.e. there is $C_g(U^+) > 0$ such that*

$$\|g(z)\|_{H^1} \le C_g(U^+) \qquad (z \in U^+);$$

(IV)* *the initial value $u_0 = v_0 - \hat{u}$ lies in $H^5(\mathbb{R})$ and is consistent, i.e. $\langle \psi, u_0\rangle = 0$;*

(V)* *there exists a bounded solution $(\underline{u}, \underline{\mu}) : [0,T] \to H^5(\mathbb{R}) \times \mathbb{R}$ of the PDAE (3.11) satisfying Assumption 2.1.27 such that $\underline{u} \in \mathcal{C}([0,T], H^5(\mathbb{R}))$ and $\underline{\mu} \in \mathcal{C}^1([0,T], \mathbb{R})$, in particular there are $C_u, C_\mu > 0$ such that*

$$\|\underline{u}(t)\|_{H^5} \le C_u, \quad |\underline{\mu}(t)| \le C_\mu \qquad (t \in [0,T]);$$

(VI) for the nonlinearity g applied to the exact solution there is $C_{g,u} > 0$ such that*

$$\|g(\underline{u}(t))\|_{H^5} \leq C_{g,u} \qquad (t \in [0,T])$$

for g as a mapping $g : H^5(\mathbb{R}) \to H^5(\mathbb{R})$.

Analogously to the discussion in Section 2.3.3 we can show that these assumptions are satisfied for polynomial nonlinearities. Note that in the case of the last assumption (VI*) we have to assume $\hat{u} \in H^7_{\mathrm{ca}}(\mathbb{R})$. We use the same bound of the speed $\tilde{\lambda}(z)$ and adapt the bound of the semigroup $e^{tPB(z)}$ for $z \in U^+$. Thus we slightly modify Lemma 2.3.4 to obtain

Lemma 3.2.4. *Under Assumption 2.3.1 the following properties for the solution v_{n+1} of* (3.15) *and* (3.16) *hold true.*

(i) There is a constant $C_\lambda(U^+) > 0$ only depending on $\psi, \varepsilon_\psi, g, U^+$ such that

$$|\tilde{\lambda}(z)| \leq C_\lambda(U^+) \qquad (z \in U^+).$$

(ii) There is $\omega^* > 0$ such that for $s \in \{1, \ldots, 5\}$ the semigroup generated by $PB(z)$ satisfies

$$\left\|e^{tPB(z)}\right\|_{H^s \leftarrow H^s} \leq e^{t\omega^*} \qquad (z \in U^+),$$

where $B(z) = \partial_x^2 + \tilde{\lambda}(z)\partial_x$.

(iii) There is $\tau_1 > 0$ such that for $z \in U \cap \mathcal{R}(P)$ and $z^+ \in U^+$ it holds

$$\varphi_v^\tau(z; z^+) \in U^* \qquad (\tau < \tau_1).$$

The first part was already proven in the proof of Lemma 2.3.4. Analogously to Lemma 2.3.4 (ii) we chose

$$\omega^* := M \|\psi\|_{H^5} \|\psi\|_{H^2} (1 + C_\lambda(U^+))$$

such that the semigroup generated by $PB(z)$ satisfies

$$\left\|e^{tPB(z)}\right\|_{H^s \leftarrow H^s} \leq e^{t\omega^*} \qquad (z \in U^+)$$

for $s \in \{1, \ldots, 5\}$ and $t \geq 0$. Note that

$$\begin{aligned} \left\|e^{tP\partial_x^2}\right\|_{H^s \leftarrow H^s} &\leq e^{tM\|\psi\|_{H^s}\|\psi\|_{H^2}} \\ &\leq e^{t\omega^*} \end{aligned} \tag{3.21}$$

for $s \in \{1, \dots, 5\}$ and $t \geq 0$ by Corollary 2.1.17. We define

$$\tau^* := \frac{1}{2\omega^*}.$$

By Lemma 2.1.25 we know that $B(z)$ generates a contraction semigroup and $PB(z)$ is a generator of a quasicontractive semigroup for every $z \in U^+$. Thus, Lemma 3.2.2 yields for $s \in \{1, \dots, 5\}$ and $\tau < \tau^*$

$$\begin{aligned} \left\| (I - \tau PB(z))^{-1} \right\|_{H^s} &\leq \frac{1}{1 - \tau\omega^*} \leq 2, \\ \left\| (I - \tau B(z))^{-1} \right\|_{H^s} &\leq 1. \end{aligned} \tag{3.22}$$

Note that for the first estimate the quasicontractive property of the semigroup is essential. With this definitions we can prove Lemma 3.2.4 (iii).

Proof of Lemma 3.2.4 (iii). Let $z \in U, z^+ \in U^+$. By the definition of U there is $t^* \in [0, T]$ such that $\|z - \underline{u}(t^*)\|_{H^1} < \delta$. We define

$$v_{n+1} := \varphi_v^\tau(z; z^+).$$

Using (3.18) we have

$$\begin{aligned} v_{n+1} - \underline{u}(t^*) &= (I - \tau PB(z^+))^{-1} [z + \tau Pg(z)] - \underline{u}(t^*) \\ &= (I - \tau PB(z^+))^{-1} [z + \tau Pg(z)] - (I - \tau PB(z^+))^{-1} \underline{u}(t^*) \\ &\quad + (I - \tau PB(z^+))^{-1} \underline{u}(t^*) - \underline{u}(t^*) \\ &= \mathcal{A}_1 + \mathcal{A}_2 \end{aligned}$$

with

$$\begin{aligned} \mathcal{A}_1 &:= (I - \tau PB(z^+))^{-1} [z + \tau Pg(z)] - (I - \tau PB(z^+))^{-1} \underline{u}(t^*), \\ \mathcal{A}_2 &:= (I - \tau PB(z^+))^{-1} \underline{u}(t^*) - \underline{u}(t^*). \end{aligned}$$

For the first part $\mathcal{A}_1$ we obtain

$$\begin{aligned} \|\mathcal{A}_1\|_{H^1} &\leq \left\| (I - \tau PB(z^+))^{-1} [z - \underline{u}(t^*)] \right\|_{H^1} + \tau \left\| (I - \tau PB(z^+))^{-1} Pg(z) \right\|_{H^1} \\ &\leq \frac{1}{1 - \tau\omega^*} \delta + \tau \frac{1}{1 - \tau\omega^*} \|P\|_{H^1} C_g(U^+) \end{aligned}$$

using (3.22) and Assumption 3.2.3 (III*). We chose

$$\tau < \min \left\{ \tau^*, \frac{\varepsilon_2}{6 \|P\|_{H^1} C_g(U^+)}, \frac{\varepsilon_2}{\omega^* (\varepsilon_2 + 3\delta)} \right\}$$

Since $\tau^* = \frac{1}{2\omega^*}$ this yields similar to (3.22)

$$\begin{aligned}
\|\mathcal{A}_1\|_{H^1} &\leq \frac{1}{1-\tau\omega^*}\delta + \tau 2\|P\|_{H^1} C_g(U^+) \\
&\leq \frac{1}{1-\frac{\varepsilon_2}{\omega^*(\varepsilon_2+3\delta)}\omega^*}\delta + \frac{\varepsilon_2}{6\|P\|_{H^1} C_g(U^+)} 2\|P\|_{H^1} C_g(U^+) \\
&\leq \frac{1}{1-\frac{\varepsilon_2}{\varepsilon_2+3\delta}}\delta + \frac{\varepsilon_2}{3} \\
&= \frac{\varepsilon_2+3\delta}{3\delta}\delta + \frac{\varepsilon_2}{3} \\
&= \delta + \frac{\varepsilon_2}{3} + \frac{\varepsilon_2}{3} \\
&= \delta + \frac{2}{3}\varepsilon_2.
\end{aligned}$$

For the second part we obtain by defining the bijective linear operator $D \coloneqq (I - \tau PB(z^+))$, cf. Lemma 3.2.2,

$$\begin{aligned}
\mathcal{A}_2 &= (I - \tau PB(z^+))^{-1}\underline{u}(t^*) - \underline{u}(t^*) \\
&= D^{-1}\left[\underline{u}(t^*) - D\underline{u}(t^*)\right] \\
&= D^{-1}\tau PB(z^+)\underline{u}(t^*)
\end{aligned}$$

and obtain with $\tau < \tau^*$ and (3.22)

$$\begin{aligned}
\|\mathcal{A}_2\|_{H^1} &= \left\|(I - \tau PB(z^+))^{-1}\left[\tau PB(z^+)\underline{u}(t^*)\right]\right\|_{H^1} \\
&\leq 2\left\|\tau PB(z^+)\underline{u}(t^*)\right\|_{H^1} \\
&\leq 2\left\|\tau P(\partial_x^2 + \tilde{\lambda}(z^+)\partial_x)\underline{u}(t^*)\right\|_{H^1} \\
&\leq 2\tau\|P\|_{H^1}(1 + |\tilde{\lambda}(z^+)|)\|\underline{u}(t^*)\|_{H^3} \\
&\leq 2\tau\|P\|_{H^1} C_u(1 + C_\lambda(U^+))
\end{aligned}$$

using Assumption 2.3.1 (V) and Lemma 3.2.4 (i). If we chose in addition

$$\tau < \frac{\varepsilon_2}{6\|P\|_{H^1} C_u(1 + C_\lambda(U^+))}$$

this yields

$$\|\mathcal{A}_2\|_{H^1} < \frac{\varepsilon_2}{3}$$

To sum up choosing

$$\tau < \min\left\{\tau^*, \frac{\varepsilon_2}{6\|P\|_{H^1} C_g(U^+)}, \frac{1}{\omega^*}\left(1 - \frac{1}{1+\frac{\varepsilon_2}{3\delta}}\right), \frac{\varepsilon_2}{6\|P\|_{H^1} C_u(1 + C_\lambda)}\right\} =: \tau_1$$

we obtain

$$\begin{aligned}\|v_{n+1} - \underline{u}(t^*)\|_{H^1} &= \|\mathcal{A}_1 + \mathcal{A}_2\|_{H^1} \\ &\leq \delta + \frac{2}{3}\varepsilon_2 + \frac{\varepsilon_2}{3} \\ &< \delta^*.\end{aligned}$$

Hence $\varphi_v^\tau(z; z^+) = v_{n+1} \in U^*$ by definition of U^* in (3.20).

□

As before, we are going to prove the convergence of the scheme in the $H^1(\mathbb{R})$-norm. By some technical reasons we have to reduce the step size τ in the convergence proof further. We will have to estimate

$$(1 - \tau\omega^*)^{-n}$$

where $n\tau \leq T$. We have

$$\left(1 - \frac{T\omega^*}{n}\right)^{-n} \to e^{T\omega^*} \qquad \text{for } n \to \infty.$$

Hence there is $n_0 \in \mathbb{N}$ such that

$$\left(1 - \frac{T\omega^*}{n}\right)^{-n} < e^{T\omega^*+1} \qquad (n \geq n_0).$$

It follows that

$$(1 - \tau\omega^*)^{-n} < e^{T\omega^*+1} \tag{3.23}$$

provided $n \geq n_0$ which can also be written as $\tau \leq \frac{T}{n_0}$. We are fixing τ_1 as in Lemma 3.2.4 (iii) and we set

$$\tau_0 := \min\left\{\tau^*, \tau_1, \tfrac{T}{n_0}\right\}. \tag{3.24}$$

As in the time-continuous case, cf. Lemma 2.3.7, we can show the following result for the local error.

Lemma 3.2.5. *We impose Assumption 3.2.3 and let $n \in \mathbb{N} \cap [0, \frac{T}{\tau})$ for $\tau < \tau_0$. For a given first order approximation $u_n^* \in U^+$ to the exact solution at time t_n in the H^1-norm, i.e.*

$$\|u_n^* - \underline{u}(t_n)\|_{H^1} \leq \tilde{C}\tau$$

for some constant $\tilde{C} > 0$ independent of n, the local error in the time discrete splitting scheme at time t_{n+1} is bounded from above by

$$\|\varphi_\tau(\underline{u}(t_n); u_n^*) - \Phi_u^\tau(\underline{u}(t_n))\|_{H^1} \le C\tau^2,$$

where the constant C is independent of τ and n.

Proof. We set

$$v_{n+1} = \varphi_v^\tau(\underline{u}(t_n); u_n^*), \qquad \lambda_n = \tilde{\lambda}(u_n^*), \qquad B_n = B(u_n^*)$$

using (3.16) with $z = \underline{u}(t_n)$ such that v_{n+1} solves

$$\begin{cases} v_{n+1} = \underline{u}(t_n) + \tau P\left[\partial_x^2 v_{n+1} + \lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))\right], \\ \lambda^* = -M\langle \psi, \partial_x^2 v_{n+1} + \lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))\rangle. \end{cases} \tag{3.25}$$

For the exact solution we use (2.18a) with initial value $\underline{u}(t_n)$ at time t_n to obtain

$$\underline{u}(t_{n+1}) = \Phi_u^\tau(\underline{u}(t_n)) = e^{\tau P\partial_x^2}\underline{u}(t_n) + \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds.$$

We obtain for the local error

$$\begin{aligned}
&\varphi_\tau(\underline{u}(t_n); u_n^*) - \Phi_u^\tau(\underline{u}(t_n)) \\
&\qquad = v_{n+1} + \tau P[g(v_{n+1}) - g(\underline{u}(t_n))] - \underline{u}(t_{n+1}) \\
&\qquad = \underline{u}(t_n) + \tau P\left[\partial_x^2 v_{n+1} + \lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))\right] \\
&\qquad\quad + \tau P[g(v_{n+1}) - g(\underline{u}(t_n))] \\
&\qquad\quad - e^{\tau P\partial_x^2}\underline{u}(t_n) - \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds \\
&\qquad = \underline{u}(t_n) + \tau P\partial_x^2 v_{n+1} - e^{\tau P\partial_x^2}\underline{u}(t_n) \\
&\qquad\quad + \tau P[\lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))] \\
&\qquad\quad - \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds \\
&\qquad\quad + \tau P[g(v_{n+1}) - g(\underline{u}(t_n))] \\
&\qquad = \mathcal{A} + \mathcal{B} + \mathcal{C}
\end{aligned}$$

with

$$\begin{aligned}
\mathcal{A} &\coloneqq \underline{u}(t_n) + \tau P\partial_x^2 v_{n+1} - e^{\tau P\partial_x^2}\underline{u}(t_n), \\
\mathcal{B} &\coloneqq \tau P[\lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))] - \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds, \\
\mathcal{C} &\coloneqq \tau P[g(v_{n+1}) - g(\underline{u}(t_n))].
\end{aligned}$$

First we show that $\|v_{n+1}\|_{H^5}$ is bounded. We have using (3.18) with $z = \underline{u}(t_n)$ and exploiting (3.22)

$$\begin{aligned}\|v_{n+1}\|_{H^5} &= \left\|(I-\tau P B_n)^{-1}\left(\underline{u}(t_n)+\tau P g(\underline{u}(t_n))\right)\right\|_{H^5}\\&\leq \frac{1}{1-\tau\omega^*}\left\|\underline{u}(t_n)+\tau P g(\underline{u}(t_n))\right\|_{H^5}\\&\leq \frac{1}{1-\tau_0\omega^*}\left(C_u+\tau\|P\|_{H^5}C_{g,u}\right)\\&= 2\left(C_u+\tau\|P\|_{H^5}C_{g,u}\right),\end{aligned} \tag{3.26}$$

where $\|\underline{u}(t_n)\|_{H^5} \leq C_u$ by Assumption 3.2.3 (V*) and $\|g(\underline{u}(t_n))\|_{H^5} \leq C_{g,u}$ by Assumption 3.2.3 (VI*). In the second to last step we used the assumption $\tau < \tau_0 = \frac{1}{2\omega^*}$.

Estimation of $\mathcal{A}$. By (3.25) we obtain

$$\begin{aligned}\mathcal{A} &= \underline{u}(t_n)+\tau P\partial_x^2 v_{n+1} - e^{\tau P\partial_x^2}\underline{u}(t_n)\\&= \underline{u}(t_n)+\tau P\partial_x^2\Big(\underline{u}(t_n)+\tau P\left[\partial_x^2 v_{n+1}+\lambda_n\partial_x v_{n+1}+g(\underline{u}(t_n))\right]\Big) - e^{\tau P\partial_x^2}\underline{u}(t_n)\\&= (I+\tau P\partial_x^2 - e^{\tau P\partial_x^2})\underline{u}(t_n)+\tau^2 P\partial_x^2 P\left[\partial_x^2 v_{n+1}+\lambda_n\partial_x v_{n+1}+g(\underline{u}(t_n))\right].\end{aligned}$$

Thus,

$$\begin{aligned}\|\mathcal{A}\|_{H^1} \leq &\left\|(I+\tau P\partial_x^2 - e^{\tau P\partial_x^2})\underline{u}(t_n)\right\|_{H^1}\\&+\tau^2\left\|P\partial_x^2 P\left[\partial_x^2 v_{n+1}+\lambda_n\partial_x v_{n+1}+g(\underline{u}(t_n))\right]\right\|_{H^1}\end{aligned}$$

For the first term on the right-hand side observe that

$$\begin{aligned}-\int_0^\tau\int_0^s \left(P\partial_x^2\right)^2 e^{rP\partial_x^2}\underline{u}(t_n)\,dr\,ds &= -\int_0^\tau P\partial_x^2\left[e^{rP\partial_x^2}\right]_{r=0}^s \underline{u}(t_n)\,ds\\&= -\int_0^\tau \left(P\partial_x^2 e^{sP\partial_x^2} - P\partial_x^2\right)\underline{u}(t_n)\,ds\\&= -\left[e^{sP\partial_x^2} - sP\partial_x^2\right]_{s=0}^\tau \underline{u}(t_n)\\&= \left(I+\tau P\partial_x^2 - e^{\tau P\partial_x^2}\right)\underline{u}(t_n).\end{aligned}$$

We use $\left\|e^{\tau P\partial_x^2}\right\|_{H^1} \leq e^{\tau\omega^*}$ by (3.21) to bound the semigroup. We obtain a bound if $\underline{u}(t_n) \in H^5$ by

$$\begin{aligned}\left\|\left(I+\tau P\partial_x^2 - e^{\tau P\partial_x^2}\right)\underline{u}(t_n)\right\|_{H^1} &\leq \frac{\tau^2}{2}\sup_{\xi\in[0,\tau]}\left\|e^{\xi P\partial_x^2}\right\|_{H^1}\left\|P\partial_x^2 P\partial_x^2\underline{u}(t_n)\right\|_{H^1}\\&\leq \tau^2\tfrac{1}{2}e^{\tau\omega^*}\|P\|_{H^1}\|P\|_{H^3}\|\underline{u}(t_n)\|_{H^5}\\&\leq \tau^2\tfrac{1}{2}e^{\tau\omega^*}\|P\|_{H^1}\|P\|_{H^3}C_u\end{aligned}$$

using Assumption 3.2.3 (V*) and Lemma 3.2.4 (ii). To sum up we obtain

$$\begin{aligned}
\|\mathcal{A}\|_{H^1} &\le \tau^2 \tfrac{1}{2} e^{\tau\omega^*} \|P\|_{H^1} \|P\|_{H^3} C_u \\
&\quad + \tau^2 \|P\|_{H^1} \|P\|_{H^3} \left(\|v_{n+1}\|_{H^5} + |\lambda_n| \|v_{n+1}\|_{H^4} + \|g(\underline{u}(t_n))\|_{H^3}\right) \\
&\le \tau^2 \tfrac{1}{2} e^{\tau_0\omega^*} \|P\|_{H^1} \|P\|_{H^3} C_u \\
&\quad + \tau^2 \|P\|_{H^1} \|P\|_{H^3} \Big((1 + C_\lambda(U^+))2\left(C_u + \tau_0 \|P\|_{H^5} C_{g,u}\right) + C_{g,u}\Big) \\
&=: \tau^2 C_{\mathcal{A}}
\end{aligned}$$

using (3.26), Assumption 3.2.3 (VI*) and Lemma 3.2.4 (i). This finishes the second order estimate of $\mathcal{A}$.

Estimation of $\mathcal{B}$. We divide $\mathcal{B}$ into two parts by

$$\begin{aligned}
\mathcal{B} &:= \tau P[\lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))] - \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds \\
&= \tau P[\lambda_n \partial_x v_{n+1} - \underline{\mu}(t_n)\partial_x v_{n+1}] \\
&\quad + \tau P[\underline{\mu}(t_n)\partial_x v_{n+1} + g(\underline{u}(t_n))] - \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds \\
&= \mathcal{B}_1 + \mathcal{B}_2
\end{aligned}$$

with

$$\begin{aligned}
\mathcal{B}_1 &:= \tau P[(\lambda_n - \underline{\mu}(t_n))\partial_x v_{n+1}], \\
\mathcal{B}_2 &:= \tau P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x v_{n+1}] - \int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right] ds.
\end{aligned}$$

To obtain a second order estimate of $\mathcal{B}_1$ we use the already derived estimate

$$|\lambda_n - \underline{\mu}(t_n)| \le \frac{1}{\varepsilon_\psi}\Big(M \|\psi\|_{H^2} + ML \|\psi\|_{L^2} + C_\mu M \|\psi\|_{H^1}\Big) \|\underline{u}(t_n) - u_n^*\|_{L^2}$$

as in (2.50). Note that λ_n is chosen in the same way as in the setting of this estimate. Using here the assumption $\|u_n^* - \underline{u}(t_n)\|_{H^1} \le \tilde{C}\tau$ we obtain

$$\|\mathcal{B}_1\|_{H^1} \le \tau^2 \|P\|_{H^1} \frac{1}{\varepsilon_\psi}\Big(M \|\psi\|_{H^2} + ML \|\psi\|_{L^2} + C_\mu M \|\psi\|_{H^1}\Big)\tilde{C} 2\left(C_u + \tau \|P\|_{H^5} C_{g,u}\right)$$

using (3.26).

For the second part $\mathcal{B}_2$ we define

$$\rho(s) := e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x \underline{u}(s)\right].$$

and apply a Taylor expansion similar as in (2.47) to obtain

$$\begin{aligned}\int_{t_n}^{t_{n+1}} e^{(t_{n+1}-s)P\partial_x^2} P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x\underline{u}(s)\right] ds &= \int_{t_n}^{t_{n+1}} \rho(s)ds \\ &= \int_{t_n}^{t_{n+1}} \rho(t_n) + (s-t_n)\rho'(\xi)ds \\ &= \tau\rho(t_n) + \tfrac{1}{2}\rho'(\xi)\tau^2.\end{aligned}$$

This yields

$$\mathcal{B}_2 = \tau P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x v_{n+1}] - \tau e^{\tau P\partial_x^2} P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x\underline{u}(t_n)] - \tfrac{1}{2}\rho'(\xi)\tau^2.$$

Using (3.16) we obtain

$$\begin{aligned}&\tau P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x v_{n+1}] - \tau e^{\tau P\partial_x^2} P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x\underline{u}(t_n)] \\ &\quad= \tau(I - e^{\tau P\partial_x^2})P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x\underline{u}(t_n)] \\ &\qquad+ \tau^2 P\underline{\mu}(t_n)\partial_x P\left[\partial_x^2 v_{n+1} + \lambda_n\partial_x v_{n+1} + g(\underline{u}(t_n))\right].\end{aligned}$$

With (2.53) and (3.21) it follows

$$\begin{aligned}\|\mathcal{B}_2\|_{H^1} &\le \tau\left\|(I - e^{\tau P\partial_x^2})P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x\underline{u}(t_n)]\right\|_{H^1} \\ &\quad+ \tau^2\left\|P\underline{\mu}(t_n)\partial_x P\left[\partial_x^2 v_{n+1} + \lambda_n\partial_x v_{n+1} + g(\underline{u}(t_n))\right]\right\|_{H^1} + \tau^2\tfrac{1}{2}\|\rho'(\xi)\|_{H^1} \\ &\le \tau^2 e^{\tau\omega^*}\|P\|_{H^1}\left\|P[g(\underline{u}(t_n)) + \underline{\mu}(t_n)\partial_x\underline{u}(t_n)]\right\|_{H^3} \\ &\quad+ \tau^2\left\|P\underline{\mu}(t_n)\partial_x P\left[\partial_x^2 v_{n+1} + \lambda_n\partial_x v_{n+1} + g(\underline{u}(t_n))\right]\right\|_{H^1} + \tau^2\tfrac{1}{2}\|\rho'(\xi)\|_{H^1} \\ &\le \tau^2 e^{\tau_0\omega^*}\|P\|_{H^1}\|P\|_{H^3}[\|g(\underline{u}(t_n))\|_{H^3} + C_\mu\|\underline{u}(t_n)\|_{H^4}] \\ &\quad+ \tau^2\|P\|_{H^1} C_\mu\|P\|_{H^2}\left[\|v_{n+1}\|_{H^4} + C_\lambda(U^+)\|v_{n+1}\|_{H^3} + \|g(\underline{u}(t_n))\|_{H^2}\right] \\ &\quad+ \tau^2\tfrac{1}{2}\|\rho'(\xi)\|_{H^1}\end{aligned}$$

It remains to obtain a bound of $\rho'(\xi)$ in the H^1-norm. We have for $s \in [t_n, t_{n+1}]$

$$\begin{aligned}\rho'(s) &= -e^{(t_{n+1}-s)P\partial_x^2} P\partial_x^2 P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x\underline{u}(s)\right] \\ &\quad+ e^{(t_{n+1}-s)P\partial_x^2} P\left[\partial_t g(\underline{u}(s)) + \underline{\mu}'(s)\partial_x\underline{u}(s) + \underline{\mu}(s)\partial_x\partial_t\underline{u}(s)\right] \\ &= -e^{(t_{n+1}-s)P\partial_x^2} P\partial_x^2 P\left[g(\underline{u}(s)) + \underline{\mu}(s)\partial_x\underline{u}(s)\right] \\ &\quad+ e^{(t_{n+1}-s)P\partial_x^2} P\Big[\partial_t g(\underline{u}(s)) + \underline{\mu}'(s)\partial_x\underline{u}(s) \\ &\quad+ \underline{\mu}(s)\partial_x P\left(\partial_x^2\underline{u}(s) + g(\underline{u}(s)) + \underline{\mu}(s)\partial_x\underline{u}(s)\right)\Big],\end{aligned}$$

where we used (3.11) with Lemma 2.1.26. All this terms already occurred in (2.48). Using the estimates derived there this yields an upper bound for $\|\rho'(\xi)\|_{H^1}$, which is independent of n and τ. To sum up we have a bound $\|\mathcal{B}\|_{H^1} \leq \tau^2 C_{\mathcal{B}}$ with a constant $C_{\mathcal{B}} > 0$ independent of n and τ.

Estimation of $\mathcal{C}$. We have

$$\begin{aligned}\|\mathcal{C}\|_{H^1} &= \tau \left\|P[g(v_{n+1}) - g(\underline{u}(t_n))]\right\|_{H^1} \\ &\leq \tau \|P\|_{H^1} L \left\|v_{n+1} - \underline{u}(t_n)\right\|_{H^1}\end{aligned}$$

using the local Lipschitz continuity as given in Assumption 3.2.3 (II*). Note that $v_{n+1} \in U^*$ by Lemma 3.2.4 (iii). For the estimate of $\|v_{n+1} - \underline{u}(t_n)\|_{H^1}$ we use (3.16) and (3.26) to obtain

$$\begin{aligned}\|\mathcal{C}\|_{H^1} &\leq \tau^2 \|P\|_{H^1} L \left\|P\left(\partial_x^2 v_{n+1} + \lambda_n \partial_x v_{n+1} + g(\underline{u}(t_n))\right)\right\|_{H^1} \\ &\leq \tau^2 \|P\|_{H^1}^2 L\Big((1 + C_\lambda(U^+))2\left(C_u + \tau \|P\|_{H^5} C_{g,u}\right) + C_{g,u}\Big) \\ &=: \tau^2 C_{\mathcal{C}}.\end{aligned}$$

This finishes the second order estimate of the local error. We have

$$\begin{aligned}\|\varphi_\tau(\underline{u}(t_n); u_n^*) - \Phi_u^\tau(\underline{u}(t_n))\|_{H^1} &\leq \|\mathcal{A}\|_{H^1} + \|\mathcal{B}\|_{H^1} + \|\mathcal{C}\|_{H^1} \\ &\leq \tau^2 \left(C_{\mathcal{A}} + C_{\mathcal{B}} + C_{\mathcal{C}}\right) \\ &=: \tau^2 C,\end{aligned}$$

where the constant C is independent of n and τ. □

Let u_{n+1} denote the approximations to the exact solution with the scheme described in (3.19), i.e.

$$\begin{aligned}u_{n+1} &= \varphi_\tau(u_n; u_n) \\ &= \varphi_\tau(u_n) \\ &= \varphi_\tau^{n+1}(u_0).\end{aligned} \tag{3.27}$$

We define the constant

$$\mathcal{K} := T e^{T\omega^* + 1} e^{T\|P\|_{H^1} L} e^{2T\|P\|_{H^1} L} C. \tag{3.28}$$

Similar to the splitting approach described in Section 2.2.1 we can show that the approximations u_n obtained by the splitting scheme (3.27) converge to the exact solution. Let τ_0 be as in (3.24), i.e. $\tau_0 = \min\left\{\tau^*, \tau_1, \frac{T}{n_0}\right\}$.

Theorem 3.2.6. *Under Assumption 3.2.3 the time discrete Lie splitting with step size* $\tau < \min\{\tau_0, \frac{\delta}{\mathcal{K}}\}$ *is convergent of first order in the* H^1*-norm, i.e.*

$$\|u_n - \underline{u}(t_n)\|_{H^1} \leq \mathcal{K}\tau, \qquad (n \in \mathbb{N}_0 \cap [0, \tfrac{T}{\tau}])$$

where the constant $\mathcal{K} > 0$ *is given in* (3.28)*. In particular,* $\mathcal{K}$ *is independent of* n *and* τ*, but depends on* T*.*

Proof. As before we define the global error at time t_n by

$$e_n \coloneqq u_n - \underline{u}(t_n).$$

Similar to the time-continuous case the proof is done via induction. We prove that

1. $u_n \in U \cap \mathcal{R}(P)$,
2. $\|u_n - \underline{u}(t_n)\|_{H^1} \leq \tau\mathcal{K}$.

is satisfied for all $n \in \mathbb{N}_0$ with $n\tau \leq T$. The base case $n = 0$ follows as in the proof of Theorem 2.3.9. For the inductive step we assume that $u_k \in U \cap \mathcal{R}(P)$ and $\|u_k - u(t_k)\|_{H^1} \leq \tau\mathcal{K}$ hold true for all $0 \leq k \leq n$ and show that $u_{n+1} \in U \cap \mathcal{R}(P)$ and $\|u_{n+1} - \underline{u}(t_{n+1})\|_{H^1} \leq \tau\mathcal{K}$ are satisfied. We assume $(n+1)\tau \leq T$ since we only approximate the solution up to the end time T. For the global error we have with (3.27)

$$\begin{aligned} e_{n+1} &= \varphi_\tau(u_n; u_n) - \underline{u}(t_{n+1}) \\ &= \varphi_\tau(u_n; u_n) - \varphi_\tau(\underline{u}(t_n); u_n) + \varphi_\tau(\underline{u}(t_n); u_n) - \underline{u}(t_{n+1}), \end{aligned}$$

i.e. the global error consists of a stability term and the local error. As we have seen in Lemma 3.2.5, the local error can be bounded by $C\tau^2$. We set

$$v_{n+1} = \varphi_v^\tau(u_n; u_n), \qquad \tilde{v}_{n+1} = \varphi_v^\tau(\underline{u}(t_n); u_n)$$

where φ_v^τ is defined in (3.17) and use $B_n = \partial_x^2 + \lambda_n \partial_x$ with $\lambda_n = \tilde{\lambda}(u_n)$. This yields

$$\begin{aligned} &\varphi_\tau(u_n; u_n) - \varphi_\tau(\underline{u}(t_n); u_n) \\ &\qquad = v_{n+1} + \tau P[g(v_{n+1}) - g(u_n)] - \tilde{v}_{n+1} - \tau P[g(\tilde{v}_{n+1}) - g(\underline{u}(t_n))] \\ &\qquad = v_{n+1} - \tilde{v}_{n+1} + \tau P[g(v_{n+1}) - g(\tilde{v}_{n+1})] - \tau P[g(u_n) - g(\underline{u}(t_n))]. \end{aligned}$$

For the terms occurring in the right-hand side we get

$$\begin{aligned} \|\tau P[g(u_n) - g(\underline{u}(t_n))]\|_{H^1} &\leq \tau \|P\|_{H^1} L \|u_n - \underline{u}(t_n)\|_{H^1} \\ &\leq \tau \|P\|_{H^1} L \|e_n\|_{H^1} \end{aligned}$$

and

$$
\begin{aligned}
&\|v_{n+1}-\tilde{v}_{n+1}\|_{H^1} \\
&\quad \le \left\|(I-\tau PB_n)^{-1}\left[u_n+\tau Pg(u_n)-\underline{u}(t_n)-\tau Pg(\underline{u}(t_n))\right]\right\|_{H^1} \\
&\quad \le \frac{1}{1-\tau\omega^*}\left(\|e_n\|_{H^1}+\tau\|P\|_{H^1}L\|e_n\|_{H^1}\right) \\
&\quad = \frac{1}{1-\tau\omega^*}\|e_n\|_{H^1}\left(1+\tau\|P\|_{H^1}L\right)
\end{aligned}
$$

with (3.22). We obtain

$$
\begin{aligned}
&\|\varphi_\tau(u_n;u_n)-\varphi_\tau(\underline{u}(t_n);u_n)\|_{H^1} \\
&\qquad \le \frac{1}{1-\tau\omega^*}\|e_n\|_{H^1}\left(1+\tau\|P\|_{H^1}L\right) \\
&\qquad\quad +\tau\|P\|_{H^1}L\frac{1}{1-\tau\omega^*}\|e_n\|_{H^1}\left(1+\tau\|P\|_{H^1}L\right) \\
&\qquad\quad +\tau\|P\|_{H^1}L\|e_n\|_{H^1} \\
&\qquad \le \frac{1}{1-\tau\omega^*}\|e_n\|_{H^1}\left(1+\tau\|P\|_{H^1}L\right) \\
&\qquad\quad +\tau\|P\|_{H^1}L\frac{1}{1-\tau\omega^*}\|e_n\|_{H^1}\left(1+\tau\|P\|_{H^1}L\right) \\
&\qquad\quad +\tau\|P\|_{H^1}L\|e_n\|_{H^1}\frac{1}{1-\tau\omega^*}\left(1+\tau\|P\|_{H^1}L\right) \\
&\qquad = \|e_n\|_{H^1}\frac{1}{1-\tau\omega^*}\left(1+\tau\|P\|_{H^1}L\right)\left(1+2\tau\|P\|_{H^1}L\right) \\
&\qquad = \|e_n\|_{H^1}C_{\text{stab}}
\end{aligned}
$$

since $(1+\tau\|P\|_{H^1}L)\ge 1$ and $\frac{1}{1-\tau\omega^*}\ge 1$. We have

$$
\begin{aligned}
C_{\text{stab}} &= \frac{1}{1-\tau\omega^*}\left(1+\tau\|P\|_{H^1}L\right)\left(1+2\tau\|P\|_{H^1}L\right) \\
&\ge 1
\end{aligned}
$$

and obtain with $n\tau\le T$

$$
\begin{aligned}
(C_{\text{stab}})^n &= \left(\frac{1}{1-\tau\omega^*}\right)^n\left(1+\tau\|P\|_{H^1}L\right)^n\left(1+2\tau\|P\|_{H^1}L\right)^n \\
&\le e^{T\omega^*+1}e^{T\|P\|_{H^1}L}e^{2T\|P\|_{H^1}L}
\end{aligned}
$$

using (3.23). Note that the term $\frac{1}{1-\tau\omega^*}$ is obtained by Lemma 3.2.2 using the quasicontractivity of the semigroup $PB(z)$ as in (3.22). Here, the quasicontractivity proves to be essential for the proof, since otherwise the constant C_{stab} would contain a term of the form $\frac{\tilde{M}}{1-\tau\omega^*}$ for some $\tilde{M} > 1$. Hence,

$$\left(\frac{\tilde{M}}{1-\tau\omega^*}\right)^n \to \infty \quad \text{for } n \to \infty$$

and we do not obtain a suitable estimate.

Finally we obtain

$$\begin{aligned}
\|e_{n+1}\|_{H^1} &\leq \|e_n\|_{H^1} C_{\text{stab}} + C\tau^2 \\
&\leq \|e_0\|_{H^1} (C_{\text{stab}})^{n+1} + (n+1)(C_{\text{stab}})^n C\tau^2 \\
&= T(C_{\text{stab}})^n C\tau \\
&\leq T e^{T\omega^*+1} e^{T\|P\|_{H^1}L} e^{2T\|P\|_{H^1}L} C\tau \\
&= \mathcal{K}\tau
\end{aligned}$$

with $\|e_0\|_{H^1} = 0$, $(n+1)\tau \leq T$ and $C_{\text{stab}} \geq 1$. The constant $\mathcal{K}$ was given in (3.28). Since $\mathcal{K}\tau < \delta$ by assumption we obtain

$$\begin{aligned}
\|u_{n+1} - \underline{u}(t_{n+1})\|_{H^1} &\leq \mathcal{K}\tau \\
&\leq \delta.
\end{aligned}$$

This implies $u_{n+1} \in U$ by the definition of U, cf. (2.35). The remaining property $u_{n+1} \in \mathcal{R}(P)$ follows by

$$\begin{aligned}
u_{n+1} &= v_{n+1} + \tau P[g(v_{n+1}) - g(u_n)] \\
&= P v_{n+1} + \tau P[g(v_{n+1}) - g(u_n)] \in \mathcal{R}(P)
\end{aligned}$$

since $v_{n+1} \in \mathcal{R}(P)$. This concludes the proof of the global error estimate. $\square$

CHAPTER

FOUR

ASYMPTOTIC STATES

So far we focused on finding traveling wave solutions of the original problem (1.4) with the linear differential operator ∂_x^2,

$$\partial_t u = \partial_x^2 u + f(u) \qquad (t \in [0, T]). \tag{4.1}$$

To achieve this we applied the method of freezing to the original problem and transformed the system to an equivalent PDAE using Lemma 2.1.26. Considering this transformation process, the question arises as to what the counterpart of a traveling wave solution is in the new setting. As we will show in this chapter the counterpart is a steady state. Note that the link between a traveling wave of the original system and a steady state in the frozen system was already discussed in [Thü05, RM12] in a slightly different setting.

For a steady state $\bar{u}$ the initial value and the solution $u(x,t)$ of a Cauchy problem coincides by using $u(x,t) = \bar{u}(x)$ since the solution does not change in time. Therefore, we will omit the initial values for the Cauchy problems in this sections for convenience.

Definition 4.0.1. *Let X be a Banach space and $F : Y \subseteq X \to X$ a smooth mapping. Given a differential equation of the type*

$$\partial_t u = F(u)$$

we call $\bar{u} \in X$ a steady state of the system if $\partial_t \bar{u} = F(\bar{u}) = 0$ is satisfied.

For a discrete dynamical system $(X, \mathbb{N}_0, \phi)$ with generator ϕ we call $\bar{u} \in X$ a steady state of ϕ if

$$\phi(\bar{u}) = \bar{u},$$

i.e. $\bar{u}$ is a fixed point of the generator ϕ.

Note that a lot of numerical schemes induce discrete dynamical systems. For example the splitting schemes $\mathcal{L}_\tau$ and φ_τ we defined in Sections 2.2.1 and 3.2 yield the discrete dynamical systems $(H^1(\mathbb{R}), \mathbb{N}_0, \mathcal{L}_\tau)$ and $(H^1(\mathbb{R}), \mathbb{N}_0, \varphi_\tau)$.

As we show below, traveling wave solutions of the PDE (4.1) correspond to steady states for the PDAE

$$\begin{cases} \partial_s w = \partial_\xi^2 w + g(w) + \mu\partial_x w + \mu\psi, \\ \quad 0 = \langle \psi, w \rangle \end{cases} \qquad (s \in [0,T]) \tag{4.2}$$

in the coordinates $(\xi, s) = (x - \gamma(t), t)$. To see this we have to consider the change of coordinates by the method of freezing in Section 1.3 and the transformation of the system given in Lemma 2.1.2.

Lemma 4.0.2. *Let $(\bar{u}, \bar{\mu})$ be a traveling wave solution of the PDE* (4.1) *and assume that $\bar{u} - \hat{u} \in \mathcal{R}(P)$. Then $(\bar{u} - \hat{u}, \mu)$ is a steady state of* (4.2).

In addition, a steady state of (4.2) *yields a traveling wave solution of the PDE* (4.1).

We are confident that the assumption $\bar{u} - \hat{u} \in \mathcal{R}(P)$ can be omitted. We do not elaborate on the details but it seems possible that one can always find a $x_0 \in \mathbb{R}$ such that

$$\langle \psi, \bar{u}(\cdot - x_0) - \hat{u} \rangle = 0.$$

The main reason for this is that the reference function $\hat{u}$ is chosen with

$$\lim_{x \to \pm\infty} (\bar{u}(x) - \hat{u}(x)) = 0$$

as in (1.8). Note that for every $x_0 \in \mathbb{R}$ the shifted profile $\bar{u}(\cdot - x_0)$ yields a traveling wave as well.

Proof. Assume that $(\bar{u}, \bar{\mu})$ is a traveling wave solution of (4.1) with $\bar{u} - \hat{u} \in \mathcal{R}(P)$, i.e. $\bar{u}(x - \mu t)$ solves (4.1). We have for all $x \in \mathbb{R}, t \geq 0$

$$\begin{aligned} 0 &= -\partial_t(\bar{u}(x - \mu t)) + \partial_x^2(\bar{u}(x - \mu t)) + f(\bar{u}(x - \mu t)) \\ &= \mu \bar{u}'(x - \mu t) + \bar{u}''(x - \mu t) + f(\bar{u}(x - \mu t)) \end{aligned}$$

hence

$$\mu \bar{u}'(\xi) + \bar{u}''(\xi) + f(\bar{u}(\xi)) = 0 \tag{4.3}$$

holds for all $\xi \in \mathbb{R}$. As in Section 1.3 we choose the ansatz

$$\begin{aligned} &u(x,t) = v(x - \gamma(t), t), \\ &\partial_t \gamma(t) = \mu \end{aligned}$$

for the method of freezing and we choose $\gamma(0) = 0$, hence $\gamma(t) = \mu t$. We set $\bar{w} := \bar{u} - \hat{u}$ and show that $\bar{w}$ is a steady state of (4.1) in the new coordinates $(\xi, s) = (x - \mu t, t)$. With $g(w) = f(w + \hat{u}) + \partial_\xi^2 \hat{u}$ we have

$$\begin{aligned}
\partial_\xi^2 \bar{w}(\xi) &+ g(\bar{w})(\xi) + \mu \partial_\xi \bar{w}(\xi) + \mu \psi(\xi) \\
&= \partial_\xi^2 \bar{u}(\xi) - \partial_\xi^2 \hat{u}(\xi) + f(\bar{u}(\xi)) + \partial_\xi^2 \hat{u}(\xi) + \mu \left(\partial_\xi \bar{u}(\xi) - \partial_\xi \hat{u}(\xi)\right) + \mu \partial_\xi \hat{u}(\xi) \\
&= \partial_\xi^2 \bar{u}(\xi) + f(\bar{u}(\xi)) + \mu \partial_\xi \bar{u}(\xi) \\
&= 0
\end{aligned}$$

by (4.3). Moreover, since $\partial_s \bar{w} = 0$ and we have $\langle \psi, \bar{u} - \hat{u} \rangle = 0$ by assumption the algebraic constraint of (4.2) is fulfilled for every $s \in [0, T]$.

In order to show the second assertion recall that the transformation of the PDAE was obtained by the mapping $u \mapsto u - \hat{u}$ as shown in the proof of Lemma 2.1.2. The transformation of the coordinates was given by $\xi = x - \gamma(t)$ as in (1.6), where $\partial_t \gamma(t) = \bar{\lambda}$. If we assume that $(\bar{v}, \bar{\lambda})$ is a steady state in the coordinates (ξ, t) of (4.2) then we obtain a traveling wave solution for (4.1) by

$$u(x,t) = \left(\bar{v} + \hat{u}\right)(x - \bar{\lambda} t) \qquad (x \in \mathbb{R}, t \geq 0)$$

with profile $\bar{u} + \hat{u}$ and speed $\bar{\lambda}$. This can be verified by an easy calculation. □

4.1 Preservation of Steady States of the Lie Splitting

In this section we show that the Lie splitting scheme constructed in Chapter 2 preserves steady states of the PDAE (4.2). Note that steady states for this system yield traveling wave solutions of the PDE (4.1), cf. Lemma 4.0.2.

Lemma 4.1.1. *Suppose* $(\bar{u}, \bar{\mu}) \in (H^2(\mathbb{R}) \cap \mathcal{R}(P)) \times \mathbb{R}$ *is a steady state of the PDAE* (4.2)*. Then the Lie splitting* $\mathcal{L}_\tau$ *given in* (2.33) *and the full time discrete Lie splitting* φ_τ *given in* (3.19) *preserve the steady state* $(\bar{u}, \bar{\mu})$*, i.e.*

$$\begin{aligned}
\mathcal{L}_\tau(\bar{u}; \bar{u}) &= \bar{u}, \\
\varphi_\tau(\bar{u}; \bar{u}) &= \bar{u},
\end{aligned}$$

where $\bar{\mu}$ *can be directly calculated from* $\bar{u}$ *similar to* (2.19).

Proof. Let $(\bar{u}, \bar{\mu}) \in (H^2(\mathbb{R}) \cap \mathcal{R}(P)) \times \mathbb{R}$ be a steady state of the PDAE (4.2). We handle the Lie splitting $\mathcal{L}_\tau$ and the full time discrete Lie splitting φ_τ separately. First we look at the Lie splitting $\mathcal{L}_\tau$, which was given by (2.33)

$$\mathcal{L}_\tau(z;u^*) = P\Phi_w^\tau(\Phi_v^\tau(z;u^*);z)$$

for some initial value z and approximations u^*. In the last step we apply the projection P. It is clear that the projection preserves every consistent steady state, i.e. for a steady state $(\bar{u},\bar{\mu})$ with $\bar{u} \in \mathcal{R}(P)$ we have $P\bar{u} = \bar{u}$. We are going to show that even the flows of the subproblems preserve a steady state $\bar{u}$ by showing

$$\Phi_v^\tau(\bar{u};\bar{u}) = \bar{u}, \qquad \Phi_w^\tau(\bar{u};\bar{u}) = \bar{u}.$$

For the nonlinear subproblem we see that the solution $\Phi_w^t(w_0;z)$ of the ODE given in (2.30)

$$\partial_t w = g(w(t)) - g(z), \quad w(0) = w_0, \qquad\qquad (t \in [0,\tau])$$

has at least the steady state z. This steady state is only a solution of the initial value problem if the initial value property $w_0 = z$ is satisfied. Additional steady states may occur if $g(w) - g(z) = 0$ is satisfied. With $w_0 = z = \bar{u}$ we have $\Phi_w^\tau(\bar{u};\bar{u}) = \bar{u}$.

It remains to show that the linear subproblem preserves a steady state. The linear subproblem for $\mathcal{L}_\tau$ was given in (2.23). We use $z = u_n^* = \bar{u}$ and obtain

$$\begin{cases} \partial_t v = \partial_x^2 v + \tilde{\lambda}(\bar{u})\partial_x v + \lambda\psi + g(\bar{u}), & (t \in (t_n, t_{n+1}]) \\ 0 = \langle \psi, v\rangle, & \\ v(t_n) = \bar{u}. & \end{cases} \tag{4.4}$$

By (2.24) we have

$$\tilde{\lambda}(\bar{u}) = \frac{M\langle \partial_x\psi, \partial_x\bar{u}\rangle - M\langle \psi, g(\bar{u})\rangle}{1 + M\langle \psi, \partial_x\bar{u}\rangle}.$$

Using $\bar{u}$ as initial value for the PDAE (4.2) and applying Lemma 2.1.26 we obtain

$$\bar{\mu} = \frac{M\langle \partial_x\psi, \partial_x\bar{u}\rangle - M\langle \psi, g(\bar{u})\rangle}{1 + M\langle \psi, \partial_x\bar{u}\rangle},$$

hence $\tilde{\lambda}(\bar{u}) = \bar{\mu}$. Since $(\bar{u},\bar{\mu})$ is a steady state of (4.2) we have $\partial_t\bar{u} = 0$ and

$$\begin{cases} 0 = \partial_x^2\bar{u} + \bar{\mu}\partial_x\bar{u} + \bar{\mu}\psi + g(\bar{u}), \\ 0 = \langle \psi, \bar{u}\rangle. \end{cases}$$

It immediately follows that $(\bar{u},\bar{\mu})$ is a solution of (4.4), i.e. $\mathcal{L}_\tau(\bar{u},\bar{u}) = \bar{u}$.

The full time discrete Lie splitting φ_τ was given in (3.19),

$$\begin{aligned}\varphi_\tau(z;u^*) &= \varphi_v^\tau(z;u^*) + \tau P\left[g(\varphi_v^\tau(z;u^*)) - g(z)\right]\\ &= P\Big(\varphi_v^\tau(z;u^*) + \tau\left[g(\varphi_v^\tau(z;u^*)) - g(z)\right]\Big)\end{aligned}$$

since $\varphi_v^\tau(z;u^*) \in \mathcal{R}(P)$. The projection preserves every consistent steady state. We define

$$\varphi_w^\tau(w_0;z) \coloneqq w_0 + \tau[g(w_0) - g(z)].$$

as the approximation to solution of the nonlinear subproblem via forward Euler method. We are going to show that the flows of the subproblems preserve a steady state $\bar{u}$ by showing

$$\varphi_v^\tau(\bar{u};\bar{u}) = \bar{u}, \qquad \varphi_w^\tau(\bar{u};\bar{u}) = \bar{u}.$$

For the nonlinear subproblem we obtain

$$\varphi_w^\tau(w_0;z) = z + \tau\left[g(w_0) - g(z)\right].$$

Thus, the forward Euler method preserves a steady state if the initial value w_0 and value for the correction z coincides. Therefore we have $\varphi_w^\tau(\bar{u};\bar{u}) = \bar{u}$. Note that all Runge-Kutta methods retain all steady states of the underlying differential equation as shown for example in [SH96, Theorem 5.3.3, p. 374].

For the linear subproblem we have for $\varphi_v^\tau(\bar{u};\bar{u}) = v_{n+1}$ the equation

$$\begin{aligned}v_{n+1} &= \bar{u} + \tau P\left[\partial_x^2 v_{n+1} + \tilde{\lambda}(\bar{u})\partial_x v_{n+1} + g(\bar{u})\right]\\ &= \bar{u} + \tau P\left[\partial_x^2 v_{n+1} + \bar{\mu}\partial_x v_{n+1} + g(\bar{u})\right]\end{aligned} \tag{4.5}$$

using $\tilde{\lambda}(\bar{u}) = \bar{\mu}$ as above. We have by Lemma 2.1.26 applied to (4.2)

$$\begin{cases}\partial_t u = P[\partial_x^2 u + g(u) + \mu\partial_x u], \\ \quad \mu = M\langle\partial_x\psi, \partial_x u\rangle - M\langle\psi, g(u) + \mu\partial_x u\rangle.\end{cases} \qquad (t \in [0,T])$$

Since $\bar{u}$ is a steady state of (4.2) we have $\partial_t\bar{u} = 0$ and $P[\partial_x^2\bar{u} + g(\bar{u}) + \bar{\mu}\partial_x\bar{u}] = 0$. Hence, we have

$$\bar{u} = \bar{u} + \tau P\left[\partial_x^2\bar{u} + \mu\partial_x\bar{u} + g(\bar{u})\right]$$

and $\bar{u}$ solves (4.5). Thus, $\bar{u}$ is a steady state of φ_τ, i.e. $\varphi_\tau(\bar{u},\bar{u}) = \bar{u}$. This concludes the proof. □

Although we were not able to show that a steady state of the splitting scheme yields a steady state of the PDAE (4.2), in all numerical experiments done for this thesis we only observed steady states of the splitting scheme which were induced by steady states of the PDAE (4.2). Nevertheless there may be spurious solutions of the fixed point equation. Hence, in numerical experiments one should vary the time step size τ to verify one has indeed a fixed point. This is motivated by that fact that spurious solutions for Runge–Kutta methods in the finite dimensional case exist but leave every bounded domain for $\tau \to 0$. In Chapter 5 we are able to verify for the Nagumo equation using numerical experiments that the steady states of the splitting scheme coincide with the steady states of the PDAE.

CHAPTER

FIVE

NUMERICAL EXPERIMENTS FOR THE FROZEN NAGUMO EQUATION

In Section 2.2.1 we introduced a splitting scheme which we can apply to a frozen PDAE by the method of freezing. Based on this, we derived a full time discrete splitting approach in Chapter 3. In this chapter we discuss numerical simulations to validate the convergence results proven in the previous chapters. Furthermore, we see that the method is able to approximate traveling wave solutions by calculating steady states of the splitting scheme as described in Chapter 4.

We test a full discrete numerical scheme with finite differences based on the splitting approach in Section 3.2 for the *Nagumo equation*

$$\partial_t u = \partial_x^2 u + u(1-u)(u-\alpha) \tag{5.1}$$

with $\alpha \in (0, \frac{1}{2})$. Since $f(u) = u(1-u)(u-\alpha)$ is a polynomial function in u, this nonlinearity satisfies Assumption 2.3.13 with $u_- = 0$ and $u_+ = 1$. Therefore, the assumptions on the nonlinearity in the Theorems 2.3.9 and 3.2.6 are fulfilled. With a suitable choice of the reference function $\hat{u}$ we know that the Lie splitting given in Section 2.2.1 and the time discrete Lie splitting given in Section 3.2 converge to the exact solution for a finite-time interval. For the numerical simulation we use a spatial discretization as well. We use the splitting scheme to approximate traveling wave solutions of the Nagumo equation by a direct long-time forward simulation.

Before we are able to describe the splitting scheme for the Nagumo equation, we have to apply the method of freezing as given in Section 1.3 and have to consider the transformation as given by Lemma 2.1.2. We are going to approximate solutions of the PDAE in the co-moving frame given by

$$\begin{cases} \partial_t u = \partial_x^2 u + f(u) + \mu \partial_x u, \quad u(0) = u_0 \\ \quad 0 = \langle \psi, u - \hat{u} \rangle, \end{cases} \qquad (x \in \mathbb{R}) \tag{5.2}$$

where $\psi = \partial_x \hat{u}$ is the first derivative of the reference function $\hat{u}$. This system is considered in the new coordinates $(\xi, t) = (x - \gamma(t), t)$. In this section we do not approximate the position of the co-moving frame but this can be done in a straightforward way by numerical integration over μ, since $\partial_t \gamma = \mu$. We refer to Chapter 6 for a detailed explanation in the context of the Burgers' equation and we omit the approximation in this chapter. Thus, we only calculate the solutions in the new coordinates in this section. After applying the transformation $u \mapsto u - \hat{u}$ as in Lemma 2.1.2 we obtain the PDAE

$$\begin{cases} \partial_t u = \partial_x^2 u + g(u) + \mu \partial_x u + \mu \psi, \quad u(0) = u_0 \\ \quad 0 = \langle \psi, u \rangle, \end{cases} \qquad (x \in \mathbb{R}) \tag{5.3}$$

where $g(u) = f(u + \hat{u}) + \partial_x^2 \hat{u}$. We use the full time discrete splitting scheme

$$\begin{aligned} u_{n+1} &:= \varphi_\tau(u_n; u_n) \\ &= \varphi_\tau^n(u_0) \end{aligned}$$

for some initial value u_0 and a time step size $\tau > 0$. We have

$$\varphi_\tau(u_n; u_n) := \varphi_v^\tau(u_n; u_n) + \tau P \left[g(\varphi_v^\tau(u_n; u_n)) - g(u_n) \right]$$

as given in (3.19) with $z = u^* = u_n$. For the linear subproblem we solve the system (3.15) given by

$$\begin{cases} v_{n+1} = u_n + \tau \left[\partial_x^2 v_{n+1} + \tilde{\lambda}(u_n) \partial_x v_{n+1} + \lambda^* \psi + g(u_n) \right], \\ \quad 0 = \langle \psi, v_{n+1} \rangle, \end{cases} \tag{5.4}$$

with $\varphi_\tau(u_n; u_n) = v_{n+1}$. For the spatial discretization we use finite differences of second order with Dirichlet boundary conditions. We denote with ∂_0^2 the discrete Laplacian, i.e. the difference quotient of second order as an approximation to the second derivative, and with ∂_0 we denote the difference quotient of second order as approximation to the first derivative, both with Dirichlet boundary conditions. To be more specific, we use a grid with uniform step size $h > 0$ on a compact interval $[x_-, x_+] \subseteq \mathbb{R}$ and we assume that we can write the grid for $\tilde{M} \in \mathbb{N}$ as

$$\mathbb{K} = \left\{ x_j := hj + x_- \;\middle|\; 0 \le j \le \frac{x_+ - x_-}{h} = \tilde{M} + 1 \right\}.$$

For a given function $w = u_n$ at a fixed time t_n we denote with $w^1, \dots, w^{\tilde{M}}$ the discrete version in space evaluated at the grid points $x_1, \dots, x_M^{\tilde{M}}$. We can write the difference quotients as

$$\begin{aligned}
\partial_0 w &= \frac{1}{2h}\left[w^2 - B_\ell, w^3 - w^1, \dots, w^{\tilde{M}} - w^{\tilde{M}-2}, B_r - w^{\tilde{M}-1}\right], \\
\partial_0^2 w &= \frac{1}{h^2}\Big[w^2 - 2w^1 + B_\ell, w^3 - 2w^2 + w^1, \dots, w^{\tilde{M}} - 2w^{\tilde{M}-1} + w^{\tilde{M}-2}, \\
&\qquad B_r - 2w^{\tilde{M}} + w^{\tilde{M}-1}\Big],
\end{aligned} \tag{5.5}$$

where B_ℓ and B_r are the left and right Dirichlet boundary values, respectively.

We now discuss the splitting scheme with spatial discretization using the vectors $u_n, v_{n+1}, \hat{u} \in \mathbb{R}^{\tilde{M}}$. As a discrete version of the L^2-inner product $\langle q, r\rangle$ we use $hq^\top r$ for $q, r \in \mathbb{R}^{\tilde{M}}$. We define the approximation of the speed $\tilde{\lambda}(u_n)$ by

$$\lambda_n = -\frac{hM(\partial_0\hat{u})^\top\left(\partial_0^2 u_n + g(u_n)\right)}{1 + hM(\partial_0\hat{u})^\top\partial_0 u_n}$$

with $M = h(\partial_0\hat{u})^\top\partial_0\hat{u}$. After rearranging the system (5.4) and applying a spatial discretization we obtain the system for v_{n+1} and λ^* by

$$\left(\begin{array}{c|c} I - \tau\partial_0^2 - \lambda_n\tau\partial_0 & -\tau\partial_0\hat{u} \\ \hline h(\partial_0\hat{u})^\top & 0 \end{array}\right)\left(\begin{array}{c} v_{n+1} \\ \hline \lambda^* \end{array}\right) = \left(\begin{array}{c} u_n + \tau g(u_n) \\ \hline 0 \end{array}\right).$$

Note that we do not have any boundary values in the right-hand side of the system since we will assume that the boundary values are zero. We solve this system with a LU decomposition. For the discrete version of the projector we use

$$\tilde{P}u = z - hM(\partial_0\hat{u})^\top z, \qquad M = h(\partial_0\hat{u})^\top\partial_0\hat{u}$$

for $z \in \mathbb{R}^{\tilde{M}}$. Finally, we obtain the splitting scheme

$$u_{n+1} = v_{n+1} + \tau\tilde{P}\left[g(v_{n+1}) - g(u_n)\right],$$

where we choose the starting value u_0 below.

For the Nagumo equation one already knows traveling wave solutions, cf. [CG92]. Therefore, it is a good candidate to test the splitting scheme. In the original system (5.1) there are traveling wave solutions given by

$$\bar{u}(x,t) = \bar{v}(x - \mu t) \quad \text{with} \quad \bar{v}(x) = \frac{1}{1 + \exp(-\frac{x}{\sqrt{2}})}, \qquad \bar{\mu} = -\sqrt{2}(\tfrac{1}{2} - \alpha),$$

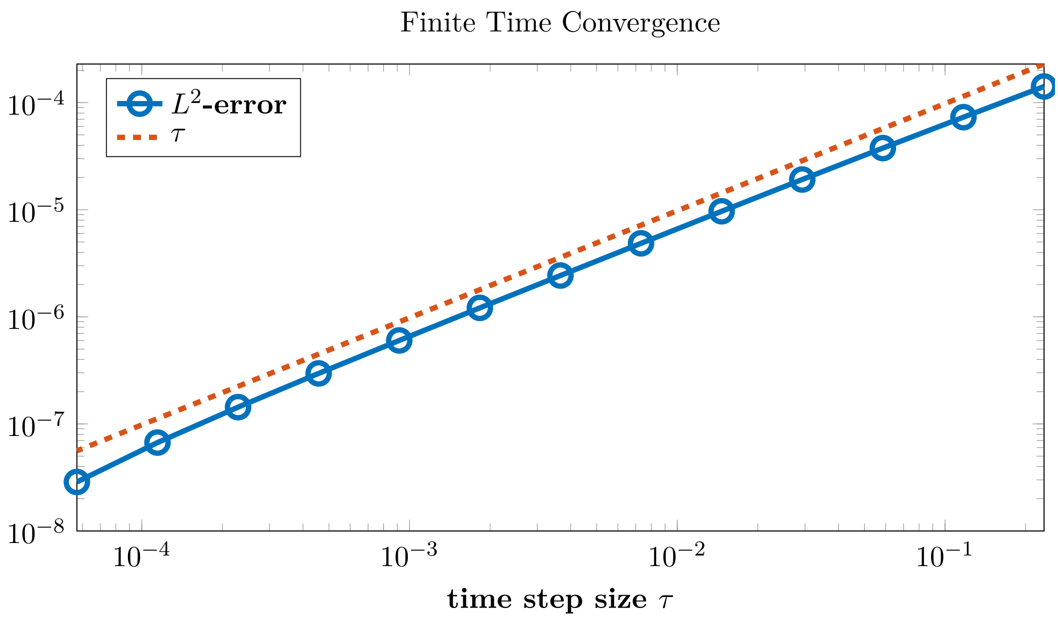

Figure 5.1: Finite time convergence of the splitting approach by using the maximal error over all times. Here we used $h = \frac{70}{1200}$ and the time step size τ is given on the axis of abscissas.

where the speed of the traveling wave directly depends on the parameter $\alpha \in (0, \frac{1}{2})$. We have the asymptotic states $\lim_{x\to\pm\infty} \bar{v}(x) = u_\pm$ with $u_- = 0$ and $u_+ = 1$. Hence, we can choose the reference function as $\hat{u}(x) = \frac{1}{2}\tanh(x) + \frac{1}{2}$ and obtain $\lim_{x\to\pm\infty} \hat{u}(x) = u_\pm$.

Based on the described scheme we ran several numerical simulations. We discuss the main observations obtained by those experiments in regard to the finite time convergence and approximation of traveling waves. In all simulations we used the following parameters

$$\begin{aligned} \alpha &= \tfrac{1}{4}, & [x_-, x_+] &= [-35, 35], & u_0(x_j) &= 0, \\ f(u) &= u(1-u)(u-\alpha), & T &= 180, & \hat{u}(x_j) &= \tfrac{1}{2}\tanh(x_j) + \tfrac{1}{2}, \\ g(u) &= f(u+\hat{u}) + \partial_0^2 \hat{u}, & B_\ell &= B_r = 0, \end{aligned}$$

where B_ℓ, B_r are the Dirichlet boundary values of the differential operators as given in (5.5). The time step size τ and the value h for the spatial grid varied in the different experiments. Note that since the solutions of the splitting scheme are in the transformed system, we have to use the mapping $u \mapsto u + \hat{u}$ to obtain the numerical solutions in the system of the co-moving frame (5.2).

In Figure 5.1 we used a spatial grid with 1200 points but varied the time step size τ. The axis of abscissas shows the time step size τ and on the ordinate the error over all times is shown. Since we do not know the exact solution of the time evolution, we use a

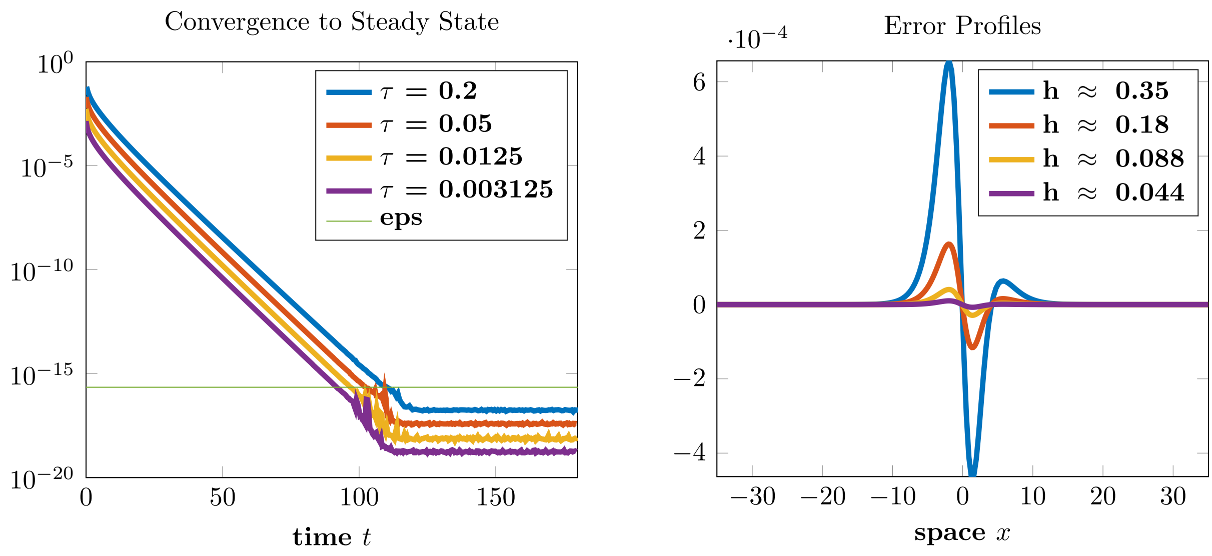

Figure 5.2: On the left-hand side we plot $\|u_{n+1} - u_n\|_{L^2}$ and see that the scheme yields a steady state in finite time. On the right-hand side we observe different numerical steady states for different h.

reference solution u_{ref} calculated via the splitting scheme with a very small time step size $\tau = \frac{30}{32*2^{16}} \approx 0.0000143$. Given a time step size τ the error is calculated by

$$\max_{n \in \mathbb{N} \cap [0, \frac{T}{\tau}]} \|u_{\text{ref}}(t_n) - \varphi_\tau^n(u_0)\|_{L^2},$$

where $\varphi_\tau^n(u_0)$ is an approximation obtained with the splitting method described above. Note that we use a discrete version of the L^2-norm. In Figure 5.1 we see that the splitting scheme converges with order one to the reference solution on the finite-time interval $[0, T]$. This coincides with Theorem 2.3.9.

Next we want to discuss to what extend the splitting scheme is able to approximate traveling wave solutions of (5.1). In Chapter 4 we were only able to show that steady states of (5.3) yield steady states of the splitting scheme as in Lemma 4.1.1 and not vice versa. However, in all numerical experiments we only observed steady states of the splitting scheme which were in fact induced by a steady state of the PDAE (4.2). Note that a steady state of (5.3) yields a traveling wave solution of (5.1) by Lemma 4.0.2. In the following we will see that this splitting scheme is able to approximate traveling wave solutions of the Nagumo equation.

On the left-hand side of Figure 5.2 we plot $u_{n+1} - u_n$ in the L^2-norm and see that the scheme yields a steady state in finite time. The time when the difference falls below

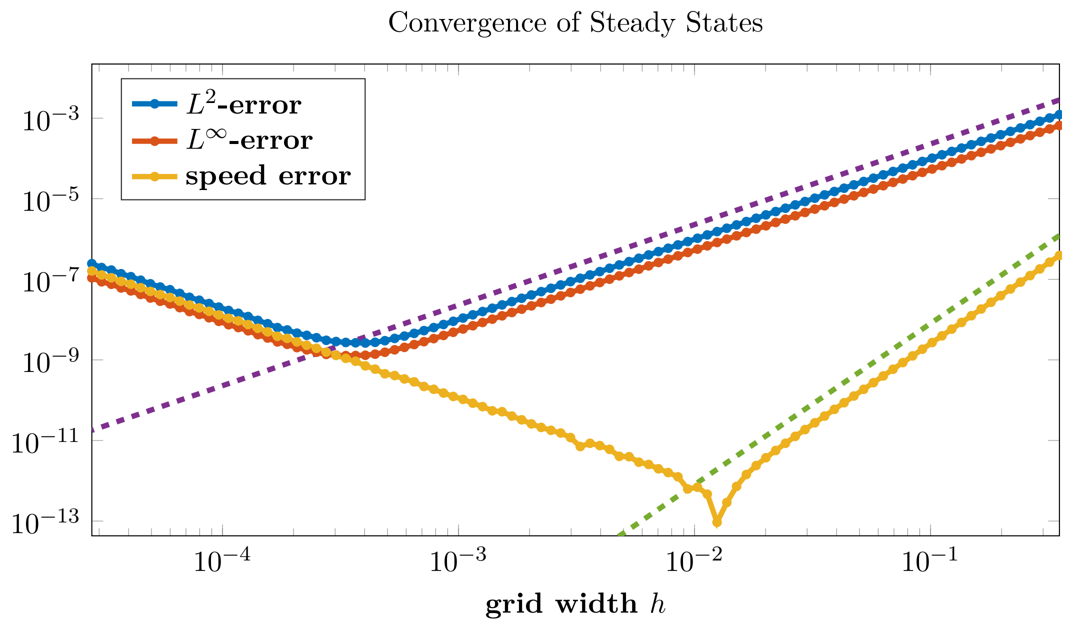

Figure 5.3: Steady state of the splitting scheme converges to the steady state of the exact solution. Dashed lines are second and forth order references.

machine precision, which we denote with *eps*, varies for different τ. The calculations for this plot were done with 400 grid points in space. On the right-hand side of Figure 5.2 we use the time step size $\tau = 0.2$ and vary the grid width h. We compare the computed steady states at the end time $T = 180$ to the exact steady state $\bar{v}$ of (5.2). For this we have to transform the steady states of the numerical simulation by using the mapping $u \mapsto u + \hat{u}$. We obtain the error by $\bar{v} - u_n - \hat{u}$ at the final time step $n = \frac{180}{0.2}$. We see that the error of the profile shrinks with smaller value of h. Note that the errors dominate in a small interval around zero. This is also the domain where the profile $\bar{v}$ varies the most.

For Figure 5.3 we used the time step size $\tau = 0.5$ and vary the grid width h. Instead of plotting the error profiles as in the right-hand side of Figure 5.2, the errors $\|\bar{v} - u_n - \hat{u}\|_{L^2}$ and $\|\bar{v} - u_n - \hat{u}\|_{L^\infty}$ are displayed for different h at the final time step $n = \frac{180}{0.5}$. We observe that the steady states computed by the numerical scheme converge to the exact steady state with second order until $h \approx 0.0005$. This second order convergence up to 10^{-9} with a fixed time step size $\tau = 0.5$ is explained by the preservation of steady states by the schemes described above. Therefore, we only see an error in space and do not see a dominating constant error from the time discretization. This agrees with the expectation since we used second order finite differences. For the speed we see fourth order convergence. For this we calculated $\lambda_n - \bar{\mu}$, where n corresponds to the end time $T = 180$. This is called a superconvergence phenomenon and was observed in numerical experiments concerning the Nagumo equation in the co-moving frame in [Thü05, Chapter 5.2, p. 125] as well. Note that it was not necessary to reduce the time step size since we do not see a Courant–Friedrichs–Lewy (CFL) condition in the numerical experiments. Therefore, we were able to obtain numerical results with very small grid width h. It turns out that the condition number of the matrix describing the difference quotient ∂_0^2 tends to infinity for $h \to 0$ and therefore we obtain large rounding errors. These rounding errors explain why the errors become larger again when h gets very small. Since the condition number of the matrix ∂_0^2 can be computed, one can estimate the expected error of ∂_0^2 in advance.

CHAPTER

SIX

BURGERS' NONLINEARITY

The preceding work, in particular Chapter 2, dealt with Cauchy problems for semilinear PDEs of the form

$$\partial_t u = \partial_x^2 u + f(u),$$

where $f : H^1(\mathbb{R}) \to H^1(\mathbb{R})$ is a locally Lipschitz continuous function. In this section we construct a numerical scheme based on splitting methods to approximate traveling wave solutions of PDEs which do not fit into the setting from before. As a toy example we consider the Cauchy problem for the viscous Burgers' equation

$$\begin{cases} \partial_t u + \partial_x(\frac{1}{2}u^2) = \partial_x^2 u \qquad (t \in [0,\infty)) \\ u(0) = u_0 \end{cases} \tag{6.1}$$

such that the nonlinearity is given by

$$\begin{aligned} f : H^1(\mathbb{R}) &\to L^2(\mathbb{R}) \\ u &\mapsto u\partial_x u. \end{aligned}$$

General nonlinear problems are way more challenging than the semilinear case since we cannot use the Lipschitz continuity from $H^1(\mathbb{R})$ to $H^1(\mathbb{R})$. In particular, the convergence analysis for these equations is out of scope for this thesis. Nevertheless, in this section we want to explain how to apply a splitting approach to the PDAE obtained from the Burgers' equation by the method of freezing and discuss numerical results. The main intent behind this approach is to treat the hyperbolic subproblem

$$\partial_t u + \partial_x(\tfrac{1}{2}u^2) = 0$$

in the setting of hyperbolic conservation laws. The solution may obtain shocks or rarefaction waves due to the nonlinear characteristics in finite time. Shock waves occur if the characteristic curves of the solution meet in one point and therefore the derivative of the solution tends to infinity in finite time. Rarefaction waves occur if the characteristic curves in one point run into different directions such that mass or information emerge in that point.

A challenging task is to resolve such phenomena in a suitable way in numerical simulations. A standard scheme to solve hyperbolic PDEs is the Lax-Friedrichs scheme, see for example [LeV92], which is based on finite differences. It is well-known that this scheme adds arbitrary viscosity to the numerical solution. Therefore it is not very suitable to handle shock and rarefaction waves or phenomena which induce those, since the Lax-Friedrichs scheme smoothes the solution. An extension to the classical Lax-Friedrichs scheme, which is better suited to resolve the already described phenomena, are the schemes introduced by Kurganov and Tadmore in [KT00]. In contrast to the classical methods, the additional viscosity has less impact and these extensions allow a semi-discrete formulation of the problem.

The Burgers' equation is often used as a test equation for coupled hyperbolic-parabolic equations by adding a parameter in front of the viscosity $\partial_x^2 u$, i.e.

$$\partial_t u + \partial_x \left(\frac{1}{2} u^2 \right) = \nu \partial_x^2 u$$

for $\nu \in [0,1]$. For $\nu = 1$ we have the viscous Burgers' equation and for $\nu = 0$ the inviscid Burgers' equation. By varying the parameter ν in numerical experiments, one can change the impact of the parabolic viscous part to test equations where either the hyperbolic part is dominating or the parabolic part. For simplicity we will restrict to the case of the viscous Burgers' equation, i.e. to the case $\nu = 1$. The scheme for $\nu \neq 1$ can be derived in an analogous way.

The remaining part of this chapter was already published in [FRM18]. It is an substantial part of this thesis since, even if one regards a different setting while approximating traveling waves for the Burgers' equation, the same techniques were used. Thus, this chapter gives a good insight how to combine splitting methods and the method of freezing for nonlinear problems as well.

The article is joint work with Jens Rottmann-Matthes. In particular, the numerical simulations were done by the author of this thesis.
We recall that traveling waves are solutions $(\bar{u}, \bar{\mu})$ of the form

$$u(x,t) = \bar{u}(x - \bar{\mu}t), \quad x \in \mathbb{R}, \quad t \in \mathbb{R},$$

where $\bar{u} : \mathbb{R} \to \mathbb{R}$ is the non-constant profile and $\bar{\mu} \in \mathbb{R}$ the velocity of the wave, cf. Definition 1.1.1. For Burgers' equation there is a family of traveling wave solutions, see for example [KL89, Theorem 4.4.4, p. 147],

$$\begin{aligned} u(x,t) &= \varphi(x - \bar{\mu}t) + \tfrac{1}{2}(b+c) = \bar{u}(x - \bar{\mu}t), \\ \varphi(x) &= a\frac{1-e^{ax}}{1+e^{ax}}, \qquad a = \tfrac{1}{2}(b-c), \qquad \bar{\mu} = \tfrac{1}{2}(b+c), \end{aligned}$$

parametrized by the asymptotic states $\lim_{x\to-\infty} \bar{u}(x) = b > c = \lim_{x\to\infty} \bar{u}(x)$.

Since we use a long-time forward simulation to approximate traveling waves, we apply the method of freezing introduced in Section 1.3 as before. In Burgers' case the method of freezing transforms (6.1) into the PDAE

$$\begin{cases} \partial_t v = \partial_x^2 v - \partial_x(\tfrac{1}{2}v^2) + \mu\partial_x v, \\ \quad 0 = \Psi(v,\mu), \\ \partial_t \gamma = \mu, \end{cases} \qquad \begin{aligned} v(0) &= v_0, \\ \gamma(0) &= 0. \end{aligned} \tag{6.2}$$

In this chapter we also approximate the position $\gamma(t)$ of the co-moving frame and therefore we include the simple ODE $\partial_t \gamma = \mu$ in the above system. We restrict to the two standard choices for the phase condition, the *orthogonal phase condition* given by

$$\Psi(v,\mu) := \langle \partial_t v, \partial_x v \rangle = \langle \partial_x^2 v - \partial_x(\tfrac{1}{2}v^2) + \mu\partial_x v, \partial_x v \rangle \tag{6.3}$$

and the *fixed phase condition* given by

$$\Psi(v,\mu) := \langle v - \hat{v}, \partial_x \hat{v} \rangle \tag{6.4}$$

with $\hat{v}$ an appropriately chosen reference function.

For the numerical approximation of (6.2) we use splitting methods as described in Section 1.4. In [HLR13], the authors show that the Strang splitting is second order convergent for the viscous Burgers' PDE provided the solution is sufficiently regular. To apply splitting methods to the freezing PDAE (6.2), we split the equation into two parts to separate the hyperbolic and parabolic problem. Then we solve each part with a method which is particularly adapted to the respective subproblem. Namely we solve the hyperbolic problem with an explicit scheme from Kurganov and Tadmor [KT00]. The parabolic subproblem is solved by an implicit second order finite-difference approximation, due to the restrictive CFL condition.

The main focus in this chapter is on approximating the limits of the time evolution and, different from Theorem 2.3.9 and [HLR13], not on the finite-time convergence properties of the scheme. In particular, we aim to understand the preservation of steady states and their stability for the schemes introduced in this chapter. In the case of ordinary differential equations there is a well-established theory for numerical steady states. For example in [SH96] there are results which state that one-step methods preserve fixed points and their stability in a shrinking neighborhood which depends on the step size using Lipschitz assumptions. An analogous result holds for the Strang splitting:

Theorem 6.0.1 ([Flo13]). *Let $A, B \in C^3(\mathbb{R}^m, \mathbb{R}^m)$ and assume that $\hat{u}$ is a hyperbolic fixed point of* (1.10). *Let φ_A and φ_B be one-step methods approximating Φ_A and Φ_B, respectively. If φ_A, φ_b are second order Runge-Kutta methods then there are $\tau_0, K > 0$, such that the Strang splitting, $U^{n+1} = \varphi^\tau(U^n) = \varphi_B^{\tau/2} \circ \varphi_A^\tau \circ \varphi_B^{\tau/2}(U^n)$, has a fixed point $\hat{U}$ which is unique in the ball $B(\hat{u}; K\tau^2)$ for all $0 < \tau \leq \tau_0$. Furthermore, $\hat{U}$ is a stable (resp. unstable) fixed point of φ^τ if $\hat{u}$ is a stable (resp. unstable) steady state of* (1.10).

There are several results which show that one can obtain good approximations to traveling waves using the method of freezing, for example results on the preservation of asymptotic stability of traveling waves for certain problem classes in the continuous and semi-discrete case, cf. [RM12, BOR14, Thü05]. But the time-asymptotic behavior of a discretization with a splitting approach has not been discussed in the literature prior to this work.

A different approach to apply adapted schemes for different parts of the freezing PDAE appears in [RM19], where the freezing method is used to capture similarity solutions of the multidimensional Burgers' equation. There an IMEX-Runge-Kutta approach is used and second order convergence for the time dependent problem is shown on finite-time intervals.

6.1 The Splitting Scheme

We now explicitly state the numerical scheme. We split (6.2) into two subproblems as follows: Let $\Phi_A^t : (z_0, \gamma_0, \mu_0) \mapsto \big(z(t), \gamma(t), \mu(t)\big)$ be the solution operator to the parabolic problem

$$\begin{cases} \partial_t z = \partial_x^2 z, & z(\cdot, 0) = z_0, \\ \partial_t \gamma = 0, & \gamma(0) = \gamma_0, \\ \partial_t \mu = 0, & \mu(0) = \mu_0, \end{cases} \tag{6.5}$$

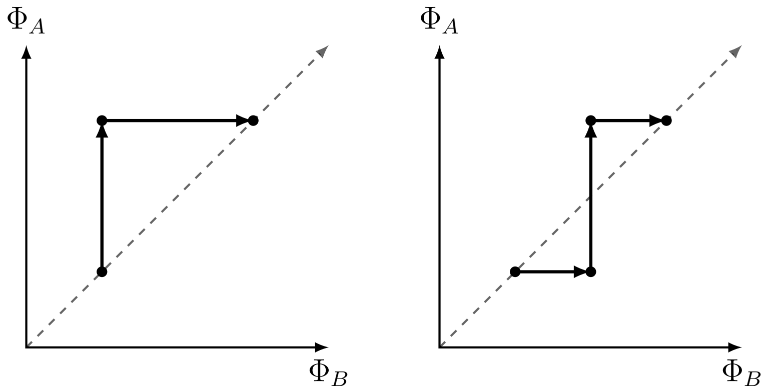

Figure 6.1: Diagram of the Lie-Trotter splitting on the left and the Strang splitting on the right.

let $\Phi_B^t : (w_0, \gamma_0, \mu_0) \mapsto \big(w(t), \gamma(t), \mu(t)\big)$ be the solution operator to

$$\begin{cases} \partial_t w = -\partial_x(\tfrac{1}{2}w^2) + \mu\partial_x w, \\ \quad 0 = \Psi(w, \mu), \\ \partial_t \gamma = \mu, \end{cases} \qquad \begin{aligned} w(\cdot, 0) &= w_0, \\ \gamma(0) &= \gamma_0. \end{aligned} \tag{6.6}$$

Here Ψ is one of the phase conditions (6.3) or (6.4). Note that the initial value μ_0 is ignored for this operator (6.6), because it is uniquely determined by the constraint. Since the splitting approach now iterates both solution operators consecutively, the question when and how to solve the algebraic constraint arises. For the orthogonal phase condition we choose an explicit and for the fixed phase condition we use a half-explicit approach. Thus we calculate the speed μ prior to solving the nonlinear PDE, the $\mu\partial_x w$ part is then discretized by using finite differences. Lie and Strang splitting are illustrated by diagrams in Figure 6.1. A step in the vertical direction in Figure 6.1 amounts in numerically solving the Cauchy problem for the heat equation (6.5), whereas a step in the horizontal direction amounts to solve the hyperbolic PDAE (6.6). Only states on the dashed diagonal line might be considered as approximations to solutions to the original problem. In addition, the order of the subproblems (6.5), (6.6) in the splitting approach is chosen such that the phase condition is satisfied at the end of a full time step. More details about how to calculate the speed with the algebraic constraint can be found in the description of the schemes, cf. equations (6.7), (6.8), (6.11) and (6.12). A schematic overview of the schemes is given in Figure 6.2.

convergence	**order 1**		**order 2**	
full problem	$\partial_t u + \partial_x\left(\frac{1}{2}u^2\right) = \partial_x^2 u$			
freezing method	orthogonal or fixed p.c.		fixed p.c.	
subproblem	$\partial_t w = -\partial_x(\frac{1}{2}w^2)$	$\partial_t z = \partial_x^2 z$	$\partial_t w = -\partial_x(\frac{1}{2}w^2)$	$\partial_t z = \partial_x^2 z$
semi-discrete formulation	Rusanov Scheme	discrete Laplacian	Kurganov-Tadmor	discrete Laplacian
time discretization	forward Euler	backward Euler	Heun's method	Crank-Nicolson
splitting method	Lie		Strang	

Figure 6.2: Overview of the applied numerical schemes for the presented schemes which offer a numerical steady state.

6.1.1 First Order Scheme

We first present a first order scheme. For this we use a method of lines (MOL) approach for (6.6): We choose a finite interval $[L_-, L_+]$ and a spatial grid with uniform step size h. We assume that we can write the grid as

$$\mathbb{K} = \left\{ x_j := hj + \frac{L_+ + L_-}{2} \;\middle|\; -\frac{L_+ - L_-}{2h} \le j \le \frac{L_+ - L_-}{2h} =: M + 1 \right\}.$$

For a given function $w(t)$ at a fixed time t we denote with $w_{-M}(t), \dots, w_M(t)$ the discrete version in space evaluated at the grid points $x_{-M}, \dots, x_M$. We spatially discretize with the semi-discrete version of the Rusanov scheme using Dirichlet boundary conditions. It is worth mentioning here that well-known methods like the Lax–Friedrichs (LxF) scheme [Lax54] or Nessyahu–Tadmor (NT) scheme [NT90] do not offer a semi-discrete version. The *Rusanov scheme (RS)* in its semi-discrete form for a nonlinear conservation law of the form $\partial_t u + \partial_x f(u) = 0$ is given by

$$\begin{aligned}
\frac{d}{dt} u_j(t) &= -\frac{f\big(u_{j+1}(t)\big) - f\big(u_{j-1}(t)\big)}{2h} \\
&\quad + \frac{\kappa}{2h}[u_{j+1}(t) - 2u_j(t) + u_{j-1}(t)] \\
&= -\partial_0 f\big(u(t)\big)_j + \kappa \tfrac{h}{2} \partial_0^2 u(t)_j \\
&=: \mathrm{RS}^h(u(t)),
\end{aligned}$$

where ∂_0 is the central difference quotient, $\partial_0 u_j = \frac{1}{2h}(u_{j+1} - u_{j-1})$, ∂_0^2 the discrete Laplacian, both with Dirichlet boundary conditions and $\kappa = \max_j u(jh, 0)$ is the maximum over the initial value evaluated at all grid points. The term including the value κ is a smoothing term of order $\mathcal{O}(h)$ which adds viscosity to the numerical solution and allows for a semi-discrete version of the scheme.

This scheme is in a simplified form: Since the local maximal speeds, used in the Rusanov and Kurganov-Tadmor scheme, ensure that all information of the Riemann fans stay in each cell of the discretized problem, they can be replaced by an upper bound. In the case of the Burgers' nonlinearity this upper bound is given by the maximal absolute value of the solution, which, in turn, is given by the maximal absolute value κ of the initial function u_0 due to the maximum principle.

The time discretization is done with a uniform step size τ, for the first order version we use the forward Euler method. The numerical approximation of Φ_B^τ will be denoted by $\phi_{B,\mathrm{RS}\,h}^\tau$ and $\varphi_{B,\mathrm{RS}\,h}^\tau$ for the two different phase conditions (6.3) and (6.4), respectively. The operator $\phi_{B,\mathrm{RS}\,h}^\tau$ is given as the function which maps w_0, γ_0, μ_0 to the solution w^1, γ^1, μ^1 of the system

$$\begin{cases} w^1 = w^0 + \tau\,\mathrm{RS}^h(w^0) + \tau\mu^*\partial_0 w^0, & \\ \mu^* = -\dfrac{(\partial_0 w^0)^\top \left(\partial_0^2 w^0 - w^0\partial_0 w^0\right)}{(\partial_0 w^0)^\top \partial_0 w^0}, & w^0 = w_0, \\ \gamma^1 = \gamma_0 + \tau\mu^1, & \gamma^0 = \gamma_0, \\ \mu^1 = -\dfrac{(\partial_0 w^1)^\top \left(\partial_0^2 w^1 - w^1\partial_0 w^1\right)}{(\partial_0 w^1)^\top \partial_0 w^1}, & \end{cases} \tag{6.7}$$

where we use a discrete version of the orthogonal phase condition (6.3). Note that the speeds μ^* and μ^1 are obtained by a simple calculation of (6.3) at time 0 and τ for this subproblem using finite differences. The value γ^1 is the approximation of the position of the co-moving frame, cf. Section 1.3. For the fixed phase condition (6.4) the operator $\varphi_{B,\mathrm{RS}\,h}^\tau$ is given as the mapping, which maps w_0, γ_0, μ_0 to the solution w^1, γ^1, μ^1 of the system

$$\begin{cases} w^1 = w^0 + \tau\,\mathrm{RS}^h(w^0) + \tau\mu^1\partial_0 w^0, & \\ \mu^1 = -\dfrac{\partial_0\hat{v}^\top\left(w^0 + \tau\,\mathrm{RS}^h(w^0) - \hat{v}\right)}{\tau\partial_0\hat{v}^\top\partial_0 w}, & w^0 = w_0, \quad \gamma^0 = \gamma_0. \\ \gamma^1 = \gamma_0 + \tau\mu^1, & \end{cases} \tag{6.8}$$

Also for the subproblem (6.5) we use a MOL approach, namely we spatially discretize (6.5) by finite differences, i.e. the discrete Laplacian with Dirichlet boundary conditions,

∂_0^2, is used to approximate the second spatial derivative,

$$\frac{d}{dt} z_j = \partial_0^2 z_j, \quad z_j(0) = z_j^0.$$

For the time discretization we use backward Euler, because implicit methods have better stability properties for this type of equation. Using the linearity of ∂_0^2, this leads to $\phi^\tau_{A,\mathrm{BE}\,h} : (z_0, \gamma_0, \mu_0) \mapsto (z^1, \gamma^1, \mu^1)$ where

$$\begin{cases} z^1 = (I - \tau\partial_0^2)^{-1} z^0, & z^0 = z_0, \\ \gamma^1 = \gamma^0, & \gamma^0 = \gamma_0, \\ \mu^1 = \mu^0, & \mu^0 = \mu_0, \end{cases}$$

such that $\phi^\tau_{A,\mathrm{BE}\,h} \approx \Phi^\tau_A$.

By using the Lie splitting (1.13), the full scheme for the freezing PDAE (6.2) is given by

$$\begin{pmatrix} v^{n+1} \\ \gamma^{n+1} \\ \mu^{n+1} \end{pmatrix} := \phi^\tau_{B,\mathrm{RS}\,h} \circ \phi^\tau_{A,\mathrm{BE}\,h} \begin{pmatrix} v^n \\ \gamma^n \\ \mu^n \end{pmatrix} \tag{6.9}$$

for the orthogonal phase condition and by

$$\begin{pmatrix} v^{n+1} \\ \gamma^{n+1} \\ \mu^{n+1} \end{pmatrix} := \varphi^\tau_{B,\mathrm{RS}\,h} \circ \phi^\tau_{A,\mathrm{BE}\,h} \begin{pmatrix} v^n \\ \gamma^n \\ \mu^n \end{pmatrix} \tag{6.10}$$

for the fixed phase condition.

6.1.2 Second Order Scheme

As already mentioned in Section 2.3.4, in the context of the Burgers' equation one gains an advantage using a second order version of the Splitting scheme. The reason for this is that the steady states obtained by the splitting approach in this chapter depend on the time step size τ in contrast to the setting in Chapter 2.

To construct a scheme with quadratic convergence in time and space we have to replace the numerical solution operators by suitable second order schemes and use Strang splitting instead of Lie splitting. For the nonlinear hyperbolic part we use the second order semi-discrete scheme from [KT00]. For a nonlinear conservation law of the form $\partial_t u + \partial_x f(u) = 0$

it is given by

$$\begin{aligned}\frac{d}{dt}u_j(t) &= -\frac{1}{2h}\Big(f\Big(u^+_{j+1/2}(t)\Big) + f\Big(u^-_{j+1/2}(t)\Big) - f\Big(u^+_{j-1/2}(t)\Big) - f\Big(u^-_{j-1/2}(t)\Big)\Big)\\ &\quad + \frac{\kappa}{2h}\Big(u^+_{j+1/2}(t) - u^-_{j+1/2}(t) - u^+_{j-1/2}(t) + u^-_{j-1/2}(t)\Big)\\ &=: \mathrm{KT}^h(u(t)),\end{aligned}$$

where

$$u^{\pm}_{j+\frac{1}{2}}(t) := u_{j+\frac{1}{2}\pm\frac{1}{2}}(t) \mp \frac{h}{2}(u_x)_{j+\frac{1}{2}\pm\frac{1}{2}}(t)$$

for $j = -M, \dots, M$ with $u(t) \in \mathbb{R}^{2M+1}$ and $u_j(t) \in \mathbb{R}$ its j-th element. The slopes are approximated using the minmod limiter

$$(u_x)^n_j = \operatorname{minmod}\left(\frac{u^n_j - u^n_{j-1}}{h}, \frac{u^n_{j+1} - u^n_j}{h}\right),$$

where $\operatorname{minmod}(a,b) := \frac{1}{2}[\operatorname{sgn}(a) + \operatorname{sgn}(b)] \cdot \min(|a|,|b|)$. The term including the value κ is again a smoothing term of order $\mathcal{O}(h)$ adding viscosity to the approximation. For the time integration we use Heun's method. In the case of (6.3), $\phi^\tau_{B,\mathrm{KT}\,h}$ is the mapping $\phi^\tau_{B,\mathrm{KT}\,h} : (w_0, \gamma_0, \mu_0) \mapsto (w^1, \gamma^1, \mu^1)$ given by the solution of

$$\begin{cases} w^* = w^0 + \tau\,\mathrm{KT}^h(w^0) + \tau\mu^*\partial_0 w^0, \\ w^1 = \frac{1}{2}w^0 + \frac{1}{2}\Big(w^* + \tau\,\mathrm{KT}^h(w^*) + \tau\mu^*\partial_0 w^*\Big), \\ \mu^* = -\dfrac{(\partial_0 w^0)^\top\left(\partial_0^2 w^0 - w^0\partial_0 w^0\right)}{(\partial_0 w^0)^\top\partial_0 w^0}, & w^0 = w_0, \\ \gamma^1 = \gamma_0 + \tau\mu^1 & \gamma^0 = \gamma_0. \\ \mu^1 = -\dfrac{(\partial_0 w^1)^\top\left(\partial_0^2 w^1 - w^1\partial_0 w^1\right)}{(\partial_0 w^1)^\top\partial_0 w^1}, \end{cases} \tag{6.11}$$

For the fixed phase condition (6.4) we define $\varphi^\tau_{B,\mathrm{KT}\,h}$ as the mapping $(w_0, \gamma_0, \mu_0) \mapsto (w^1, \gamma^1, \mu^1)$

$$\begin{cases} w^* = w^0 + \tau\,\mathrm{KT}^h(w^0) + \tau\mu^1\partial_0 w^0, \\ w^1 = \frac{1}{2}w^0 + \frac{1}{2}\Big(w^* + \tau\,\mathrm{KT}^h(w^*) + \tau\mu^1\partial_0 w^*\Big), & w^0 = w_0, \\ \mu^1 = -\dfrac{\partial_0\hat{v}^\top\Big(w^0 + \tau\,\mathrm{KT}^h(w^0) - \hat{v}\Big)}{\partial_0\hat{v}^\top\partial_0 w}, & \gamma^0 = \gamma_0. \\ \gamma^1 = \gamma_0 + \tau\mu^1, \end{cases} \tag{6.12}$$

For the heat equation, we use the Crank-Nicolson method to discretize in time and, as in the first order version, the discrete Laplacian with Dirichlet boundary conditions, ∂_0^2, is used in space. The solution operator $\phi^{\tau}_{A,\mathrm{CN}\,h}$ is given by the mapping $(z_0, \gamma_0, \mu_0) \mapsto (z^1, \gamma^1, \mu^1)$ of

$$\begin{cases} z^1 = (I - \frac{\tau}{2}\partial_0^2)^{-1}(I + \frac{\tau}{2}\partial_0^2)z^0, & z^0 = z_0, \\ \gamma^1 = \gamma^0, & \gamma^0 = \gamma_0, \\ \mu^1 = \mu^0, & \mu^0 = \mu_0. \end{cases}$$

These methods where chosen, because they offer quadratic convergence for the individual problems and thus we can hope for quadratic convergence of the full problem with Strang splitting. Strang splitting (1.14) leads to our second order scheme given by

$$\begin{pmatrix} v^{n+1} \\ \gamma^{n+1} \\ \mu^{n+1} \end{pmatrix} = \phi^{\tau/2}_{B,\mathrm{KT}\,h} \circ \phi^{\tau}_{A,\mathrm{CN}\,h} \circ \phi^{\tau/2}_{B,\mathrm{KT}\,h} \begin{pmatrix} v^{n} \\ \gamma^{n} \\ \mu^{n} \end{pmatrix} \tag{6.13}$$

for the orthogonal phase condition and by

$$\begin{pmatrix} v^{n+1} \\ \gamma^{n+1} \\ \mu^{n+1} \end{pmatrix} = \varphi^{\tau/2}_{B,\mathrm{KT}\,h} \circ \phi^{\tau}_{A,\mathrm{CN}\,h} \circ \varphi^{\tau/2}_{B,\mathrm{KT}\,h} \begin{pmatrix} v^{n} \\ \gamma^{n} \\ \mu^{n} \end{pmatrix} \tag{6.14}$$

for the fixed phase condition.

6.2 Numerical Results

The purpose of our schemes is to calculate viscous profiles by a simple forward simulation and thus we are interested in the quality of those profiles obtained at the end of a long-time simulation. Note that we do not consider the convergence order on finite intervals. For all following simulations we use

$$\begin{aligned} \hat{v}(x_j) &= -\tanh(x_j) + \tfrac{1}{2}, \qquad & b &= 1.5, \qquad & c &= -0,5, \\ v^0(x_j) &= -\tanh(x_j) + \tfrac{1}{2}, \qquad & \gamma^0 &= \mu^0 = 0, \qquad & [L_-, L_+] &= [-15, 15], \end{aligned}$$

and Dirichlet boundary conditions. Since we are looking for numerical steady states in the co-moving frame, we have to check if our numerical schemes yield steady states. A steady state has the property $\frac{d}{dt}u(t) = 0$, which translates in the numerical case to $u^{n+1} = u^n$. In Figure 6.3 we plot the time against the discrete L^2-distance $\|u^{n+1} - u^n\|_{L^2}$ and see that our schemes yield steady states at around $t \approx 100$ for (6.9), (6.10) and (6.14) since $\|u^{n+1} - u^n\|_{L^2}$ is close to machine precision. For the Strang splitting scheme with

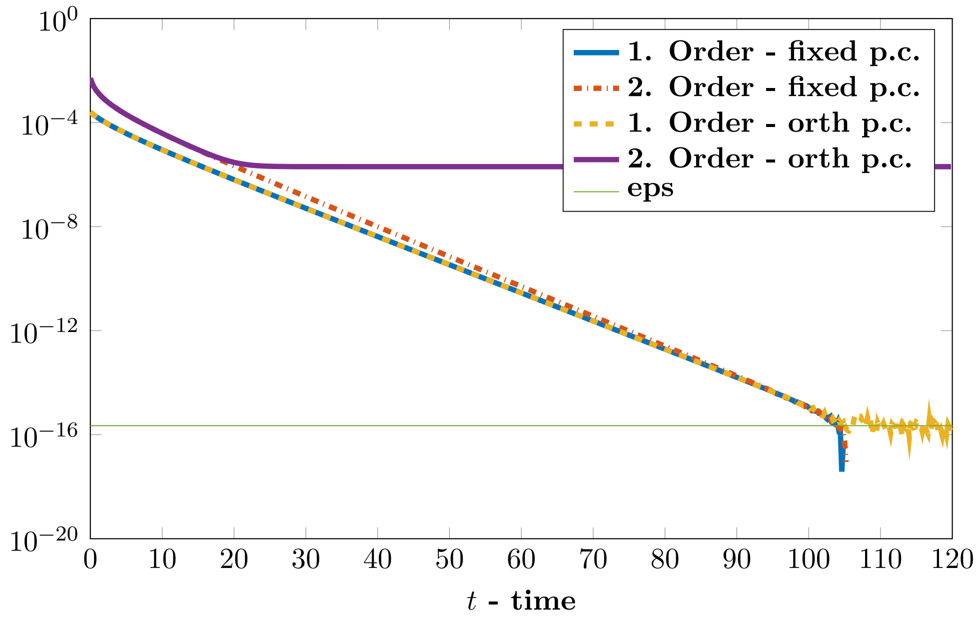

Figure 6.3: Convergence to a numerical steady state except for the second order scheme with orthogonal phase condition.

orthogonal phase condition (6.13) we see that $\|u^{n+1} - u^n\|_{L^2}$ does not converge to zero and the scheme does not offer a steady state. This can be explained by the statement that the orthogonality phase condition is not very robust as mentioned in [BOR14]. Solutions for this scheme leave the co-moving frame because the approximation of the speed is incorrect in this case. For these computations we use 300 grid point, i.e. $h = 0.1$, and $\tau = \frac{h}{10}$.

Next, we consider the error profiles of the calculated steady states with different step sizes. This result is shown in Figure 6.4. Obviously, we get different numerical steady states for different $\tau = \frac{h}{10}$, which approximates the exact steady state better for smaller steps sizes. In addition, we observe that the dominant error occurs around the center and there is hardly any error at the boundary.

The most interesting observation in our case is the convergence of our numerical steady states to the exact one, cf. Figure 6.5. Here we plot the discrete L^2-error of the resulting states in comparison to the exact state for different time step sizes and grid widths with $\tau = \frac{h}{2}$. One can observe that the numerical steady states converge linearly to the exact solution for the first order scheme while the second order scheme yields quadratic convergence.

Finally, we note that usually the exact solution of the traveling wave is unknown. Therefore one has to guess some suitable reference function. In Figure 6.6 we see that a rough guess is sufficient for the initial value as well as for the reference function $\hat{v}$. The

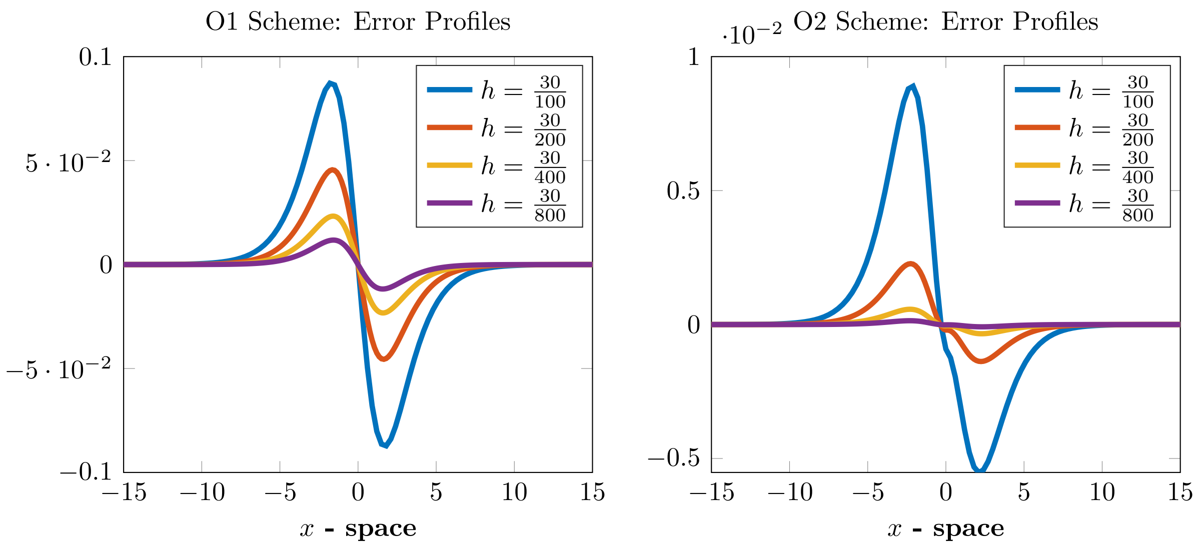

Figure 6.4: Different numerical steady states for different $\tau = \frac{h}{10}$. Note that the errors dominate where the profile varies the most and not at the boundary.

forward simulation approximates the traveling wave as before.

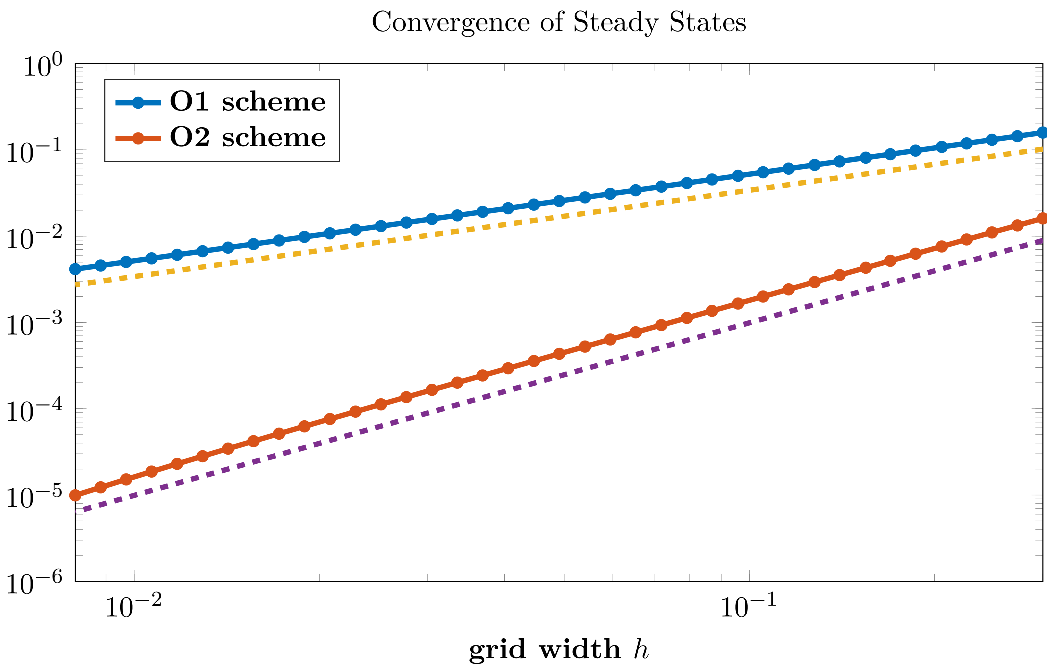

Figure 6.5: Convergence rates of the numerical steady states to the exact steady state using $\tau = \frac{h}{2}$. The scheme (6.10) was omitted because it produces the same results as (6.9), whereas the scheme (6.13) was ignored because it does not offer steady states. Dashed lines are first and second order references.

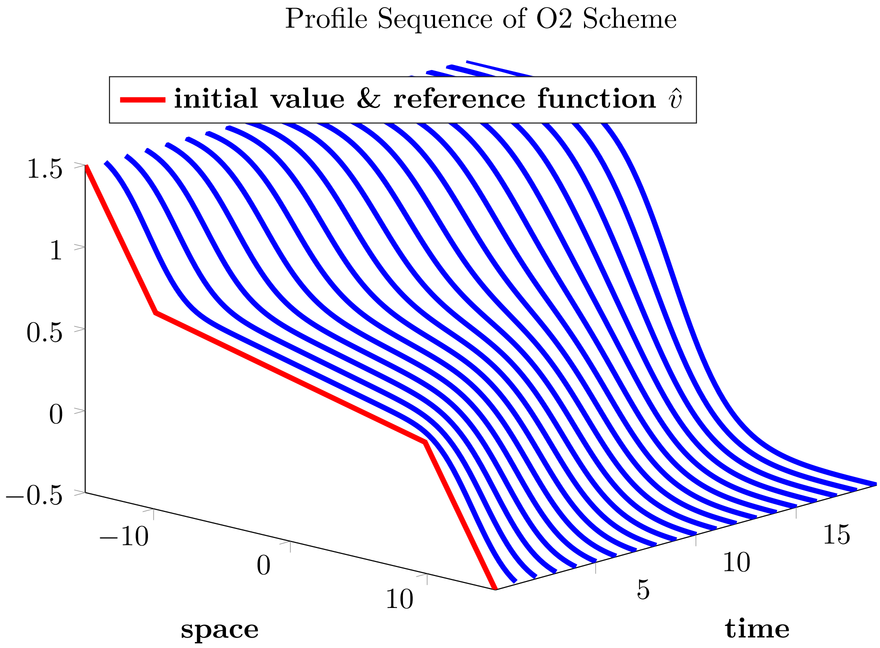

Figure 6.6: Solution using initial value and reference function which only covers the rough behavior of the solution. For this we used $h = 0.3$ and $\tau = \frac{h}{40}$.

APPENDIX

A

APPENDIX

A.1 Some Statements Used in the Convergence Proof

Theorem A.1.1 ([Paz83, Theorem 6.1.4, p. 185])**.** *Let $f : [0,\infty) \times X \to X$ be continuous in t for $t \geq 0$ and locally Lipschitz continuous in u, uniformly in t on bounded intervals. If $-A$ is the infinitesimal generator of a C_0 semigroup $T(t)$ on X then for every $u_0 \in X$ there is a $t_{max} \leq \infty$ such that the initial value problem*

$$\begin{cases} \partial_t u + Au(t) = f(t, u(t)), & t > 0 \\ \quad u(0) = u_0 \end{cases}$$

has a unique mild solution u on $[0, t_{max})$. Moreover, if $t_{max} < \infty$ then

$$\lim_{t \to t_{max}} \|u(t)\| = \infty.$$

Remark A.1.2. *The constant $\mathcal{K}$ of the global error as given in* (2.57) *and used in Theorem 2.3.9 is given by*

$$
\begin{aligned}
\mathcal{K} \coloneqq Te^{T\omega^*}\Big[&1 + Te^{T\omega^*}\Big(e^{\tau_0\omega^*}\left\|P\right\|_{H^1}L + \left\|P\right\|_{H^1}L\Big(1 + e^{\tau_0\omega^*} + \tau_0 e^{\tau_0\omega^*}\left\|P\right\|_{H^1}L\Big)\Big) \\
&\cdot e^{Te^{T\omega^*}\left(e^{\tau_0\omega^*}\left\|P\right\|_{H^1}L + \left\|P\right\|_{H^1}L\left(1+e^{\tau_0\omega^*}+\tau_0 e^{\tau_0\omega^*}\left\|P\right\|_{H^1}L\right)\right)}\Big] \\
&\cdot \Big(4C_{Dg}(U^+)LC_{U^+}\left\|P\right\|_{H^1} \\
&+ \left\|P\right\|_{H^1}\Big[L\left\|P\right\|_{H^1}\left(C_v + C_\lambda(U^+)C_v + C_{g,u}\right) \\
&+ \frac{1}{2}e^{\tau_0\omega}\left\|P\right\|_{H^1}[\left\|P\right\|_{H^3}2C_{g,u} + C_{\partial_t g}] \\
&+ e^{\tau_0\omega}\left\|P\right\|_{H^1}\frac{\tilde{C}}{\varepsilon_\psi}\Big(M\left\|\psi\right\|_{H^2} + ML\left\|\psi\right\|_{L^2} + C_\mu M\left\|\psi\right\|_{H^1}\Big)C_u(U^+) \\
&+ \frac{1}{2}e^{\tau_0\omega}\left\|P\right\|_{H^1}\left\|P\right\|_{H^3}\left(C_\lambda(U^+)C_v + C_\mu C_u\right) \\
&+ \frac{1}{2}e^{\tau_0\omega}\left\|P\right\|_{H^1} \\
&\cdot \Big(C_\lambda(U^+)\left\|P\right\|_{H^2}\Big[C_v + C_\lambda(U^+)C_v + C_{g,u}\Big] \\
&+ K_3\cdot(1 + C_u + C_u^2)C_u + C_\mu\left\|P\right\|_{H^2}\Big[C_u + C_{g,u} + C_\mu C_u\Big]\Big) \\
&+ C_{Dg}(U^+)L2C_{U^+}\Big]\Big)
\end{aligned}
$$

Discrete Gronwall's inequality

There are many different versions of Gronwall's inequality or sometimes called Gronwall's Lemma. The following version was found online, see [Hol], and we were not able to find a reference in the literature. For completeness we give the proof for this version of Gronwall's inequality based on the ideas in [Hol].

Define

$$
G_j^{(m)} \coloneqq 1 + \sum_{j<k<m} g_k \prod_{j<i<k}(1 + g_i) \tag{A.1}
$$

for $j \in \mathbb{N}, m > j$. It holds

$$
G_j^{(m)} = \prod_{j<i<m}(1 + g_i). \tag{A.2}
$$

Proof. We prove the statement by induction on m for fixed $j \in \mathbb{N}$. In the base case $m = j + 1$ we have $1 = 1$. We assume that (A.2) holds true for m and show that it holds true for $m+1$ as well. We have

$$\begin{aligned}
G_j^{(m+1)} &= 1 + \sum_{j<k<m+1} g_k \prod_{j<i<k} (1+g_i) \\
&= 1 + \sum_{j<k<m} g_k \prod_{j<i<k} (1+g_i) + g_m \prod_{j<i<m} (1+g_i) \\
&\overset{\text{i.h.}}{=} \left(\prod_{j<i<m} (1+g_i) \right) (1+g_m) \\
&= \prod_{j<i<m+1} (1+g_i).
\end{aligned}$$

This concludes the claim. □

Lemma A.1.3. *Assume $(y_n)_{n\in\mathbb{N}_0}, (f_n)_{n\in\mathbb{N}_0}$ and $(g_n)_{n\in\mathbb{N}_0}$ are nonnegative sequences and*

$$y_n \le f_n + \sum_{0\le k<n} g_k y_k \quad \textit{for } n \ge 0. \tag{A.3}$$

Then it holds

$$y_n \le f_n + \sum_{0\le k<n} f_k g_k \prod_{k<j<n} (1+g_j). \tag{A.4}$$

Proof. For $n=0$ we have $y_0 \le f_0$ for (A.3) and thus (A.4) holds. Let $m>0$ and we assume that (A.4) holds for $0 \le n < m$. We have to show

$$y_m \le f_m + \sum_{0\le k<m} f_k g_k \prod_{k<j<m} (1+g_j).$$

We have by using the induction hypothesis

$$\begin{aligned}
y_m &\le f_m + \sum_{0\le k<m} g_k y_k \\
&\le f_m + \sum_{0\le k<m} g_k \left(f_k + \sum_{0\le j<k} f_j g_j \prod_{j<i<k} (1+g_i) \right)
\end{aligned} \tag{A.5}$$

We show that

$$\sum_{0\le k<m} g_k \left(f_k + \sum_{0\le j<k} f_j g_j \prod_{j<i<k} (1+g_i) \right) = \sum_{0\le j<m} f_j g_j \left(1 + \sum_{j<k<m} g_k \prod_{j<i<k} (1+g_i) \right)$$

holds true. We have

$$\begin{aligned}
&\sum_{0\le k<m} g_k \left(f_k + \sum_{0\le j<k} f_j g_j \prod_{j<i<k} (1+g_i) \right) \\
&\quad = \sum_{0\le k<m} g_k f_k + \sum_{0\le k<m} \sum_{0\le j<k} g_k f_j g_j \prod_{j<i<k} (1+g_i) \\
&\quad = \sum_{0\le k<m} g_k f_k + \sum_{0\le j<m-1} \sum_{j<k<m} g_k f_j g_j \prod_{j<i<k} (1+g_i) \\
&\quad = \sum_{0\le j<m} g_j f_j + \sum_{0\le j<m-1} \sum_{j<k<m} g_k f_j g_j \prod_{j<i<k} (1+g_i) \\
&\quad = g_{m-1} f_{m-1} + \sum_{0\le j<m-1} g_j f_j \left(1 + \sum_{j<k<m} g_k \prod_{j<i<k} (1+g_i) \right) \\
&\quad = \sum_{0\le j<m} g_j f_j G_j^{(m)}.
\end{aligned}$$

where we use (A.1) and $G_{m-1}^{(m)} = 1$. We continue (A.5) to obtain

$$\begin{aligned}
y_m &\le f_m + \sum_{0\le k<m} g_k \left(f_k + \sum_{0\le j<k} f_j g_j \prod_{j<i<k} (1+g_i) \right) \\
&= f_m + \sum_{0\le j<m} f_j g_j G_j^{(m)} \\
&= f_m + \sum_{0\le j<m} f_j g_j \prod_{j<i<m+1} (1+g_i)
\end{aligned}$$

using (A.2), which concludes the proof. □

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