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DIPLOMA THESIS

Numerical Integration of Nonlinear Evolution Equations

Analysis and Implementation
of Various Numerical Procedures

written at the
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supervised by
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Place and date

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Abstract

This diploma thesis deals with the analysis and the numerical implementation of integration schemes for evolution equations, as well as asymptotically correct defect-based local error estimators. Recent work in [5] introduced the symmetrized defect for the linear, autonomous Schrödinger-type evolution equation, which proved to be of a higher asymptotical order than the well known classical defect, in the case of symmetric time-stepping. In [3] this result was proven to hold true also for nonlinear and nonautonomous evolution equations. In this thesis we recapitulate these results in a concise, but complete manner, whereby we set citations in a more general then detailed way. After that, we apply them to established, as well as newly constructed splitting schemes. To provide numerical verification of the theory, we consider several linear/nonlinear, autonomous/nonautonomous model problems.

I declare that I have authored this thesis independently, that I have not used other than the declared sources or resources, and that I have explicitly marked all material which has been quoted either literally or by content from the used sources.

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Acknowledgments

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Contents

Chapter 1

Introduction

In many fields of natural sciences one encounters a class of differential equations, where the system is modelled over time, called *evolution equations*. Their most general form discussed in this thesis is the *nonlinear, nonautonomous* initial value problem,

$$\frac{\mathrm{d}}{\mathrm{dt}}u(t) = F(t, u(t)), \quad u(t_0) = u_0. \tag{1.1}$$

Prominent representatives of an evolution equation are *Schrödinger-type evolution equations*, which provide the explicit problems presented in this thesis. Since the complexity of the underlying problem often does not allow an analytically determinable solution $u(t)$ of (1.1), we desire numerical methods that approximate that solution. These methods are called *integration schemes*. Although there exists a distinct number of different approaches, in this thesis we explicitly focus on so called *splitting schemes* and *defect-based schemes*.
A splitting/defect-based scheme is a so called *one-step integrator* that approximates the exact solution (at a certain time) one time step after another. Consistent one-step integrators are asymptotically correct, i.e., the error converges to 0 if the time step goes to 0. The thereby occuring convergence order is called the *order of the integration scheme*.
Since one should always try to keep the computational costs of a numerical method as low as possible, we desire schemes of a high order, which allow to iterate over bigger time steps with the same accuracy as lower order schemes. However, as often in computer science, in general this comes with the trade-off of more complex formulas for higher order schemes. It is one of our main tasks here to find 'cheap' integration schemes that still are of high order.
Another approach to lower the computational costs are *adaptive algorithms* that adjust the step size of the integration scheme as indicated by so called *defect-based local error estimators*. Altough we do not discuss adaptivity in this thesis, we intensely talk about the *classical defect*, as well as the newly developed *symmetrized defect* associated with an integration scheme. In the case of *symmetric integration schemes* the symmetrized defect proves to be of a higher asymptotical order than the classical defect. This was initially discussed in [5] for the linear, autonomous Schrödinger-type evolution equation, while in [3] this interesting result was proven to remain true also for nonlinear, nonautonomous evolution equations. The key elements for the construction of the symmetrized defect are the *funda-*

mental identity associated with an evolution equation and the *Gröbner-Alekseev Lemma*. Furthermore, with the help of these defect-based local error estimators one is able to construct defect-based integration schemes associated with a basic integrator of order p. We call these schemes also the *corrected schemes* associated with an integrator. The classical defect-based corrected scheme has order $p+1$, while (in the symmetric case) the symmetrized defect-based scheme proves to be of order $p+2$. In this thesis we apply these methods to various splitting schemes with the objective of finding efficient one-step integrators.
We remark that in this thesis we develop integrators suitable for linear and nonlinear, autonomous and nonautonomous evolution equations, thus covering a wide range of applications in natural sciences. In many cases efficient algorithms are presented, which allow a general numerical implementation of the integration schemes applied to different problems.

Outline
In Chapter 2 we introduce the nonlinear evolution equation and its associated flow, along with the important fundamental identity. We define general one-step integration schemes of order p and give a notion of the classical and symmetrized defect associated with it. We present and prove important properties of the defects and their corrected schemes. Moreover, since in Chapter 4 we consider a specific *composition method*, we introduce this class of integrators in general form.
Within the next Chapter 3 we generalize the theoretical results from Chapter 2 for nonlinear evolution equations in nonautonomous form. We do this by introducing relative time into the problem (1.1). Thereby we show that here an adapted version of the fundamental identity still holds true, which yields representations of the defects in the case of nonlinear, nonautonomous evolution equations. An important part of this thesis is presented in the end of that chapter, when we develop efficient strategies for the evaluation of (non)linear, nonautonomous defect-based integration schemes. We also provide these in algorithmic form, which allow a numerical realization on the computer.
The results from Chapters 2 and 3 are then applied to specific integration schemes in Chapter 4. We consider linear, nonautonomous integrators in Sections 4.1–4.4, while in Sections 4.5 and 4.6 nonlinear, nonautonomous schemes are presented.
Ultimately in Chapter 5 we introduce four different problems to empirically verify the expected orders of all the integration schemes in this thesis. These problems are:

- A linear, nonautonomous Schrödinger equation with exact solution,
- the same kind of problem, but with a numerically computed reference solution, approximated on a very fine mesh with a higher order scheme,
- a cubic, nonlinear, nonautonomous Schrödinger equation with known solution,
- and the *Rosen-Zener model* with a numerical approximation, sufficiently close to the unknown exact solution.

The numerical verifications of the theoretical results are presented in the form of convergence tables. Additional informations left out of the previous chapters are found in the Appendix.

Chapter 2

Problem specification and definitions

2.1 Nonlinear evolution equation

We follow [3, pp.2sqq.] and consider the nonlinear evolution equation

$$\frac{\mathrm{d}}{\mathrm{dt}}u(t) = F(u(t)), \quad u(0) = u_0, \tag{2.1}$$

and denote the exact flow associated with (2.1) by $\mathcal{E}(t, u)$, so that

$$u(t) = \mathcal{E}(t, u_0). \tag{2.2}$$

Throughout this thesis we denote partial derivatives by ∂_1 and ∂_2, so that in case of the flow $\mathcal{E}$ we write

$$\begin{aligned} \partial_1\mathcal{E}(t, u_0) &:= \tfrac{\partial}{\partial t}\mathcal{E}(t, u_0), \\ \partial_2\mathcal{E}(t, u_0) &:= \tfrac{\partial}{\partial u_0}\mathcal{E}(t, u_0). \end{aligned} \tag{2.3}$$

Then, by definition $\mathcal{E}(t, u_0)$ satisfies

$$\partial_1\mathcal{E}(t, u_0) = F(\mathcal{E}(t, u_0)), \quad \mathcal{E}(0, u_0) = u_0. \tag{2.4}$$

The basis for the subsequent constructions is the following fundamental identity, which, as stated in [3, p.2], is a consequence of the first-order variational equation for $\mathcal{E}(t, u)$, see [10, Theorem I.14.3].

Theorem 2.1.1 (Fundamental identity)**.** *As a consequence of the initial value problem* (2.1) *there holds the fundamental identity*

$$\big[\partial_1\mathcal{E}(t, u_0) = \big]F(\mathcal{E}(t, u_0)) = \partial_2\mathcal{E}(t, u_0) \cdot F(u_0). \tag{2.5}$$

Proof. An elegant proof for the identity (2.5) is given in [3, p.3] and originates from [8, (3.7)]. We present in this thesis a different proof with similar argumentation: From the definition of the flow (2.2) we derive

$$u_0 = \mathcal{E}(-t, u(t)), \tag{2.6}$$

and

$$u(t) = \mathcal{E}(t, \mathcal{E}(-t, u(t))). \tag{2.7}$$

From the identities (2.6) and (2.7) and the chain rule we obtain:

$$\begin{aligned}
& \tfrac{\partial}{\partial t}u(t) &&= \tfrac{\partial}{\partial t}\big(\mathcal{E}(t, \mathcal{E}(-t, u(t)))\big) \\
\Leftrightarrow \quad & \tfrac{\partial}{\partial t}u(t) &&= \partial_1\mathcal{E}(t, \underbrace{\mathcal{E}(-t, u(t))}_{=u_0}) + \partial_2\mathcal{E}(t, \mathcal{E}(-t, u(t))) \cdot \tfrac{\partial}{\partial t}\big(\mathcal{E}(-t, u(t))\big) \\
\Leftrightarrow \quad & \tfrac{\partial}{\partial t}u(t) &&= \partial_1\mathcal{E}(t, u_0) + \partial_2\mathcal{E}(t, u_0) \cdot \partial_1\mathcal{E}(-t, u(t))(-1) \\
& && \quad + \partial_2\mathcal{E}(t, \mathcal{E}(-t, u(t))) \cdot \partial_2\mathcal{E}(-t, u(t)) \cdot \tfrac{\partial}{\partial t}u(t) \\
\Leftrightarrow \quad & \tfrac{\partial}{\partial t}u(t) &&= \partial_1\mathcal{E}(t, u_0) - \partial_2\mathcal{E}(t, u_0) \cdot F(\mathcal{E}(-t, u(t))) \\
& && \quad + \tfrac{\partial}{\partial u_0}\big(\mathcal{E}(-t, \mathcal{E}(t, u_0))\big) \cdot \tfrac{\partial}{\partial t}u(t) \\
\Leftrightarrow \quad & \tfrac{\partial}{\partial t}u(t) &&= \partial_1\mathcal{E}(t, u_0) - \partial_2\mathcal{E}(t, u_0) \cdot F(u_0) + \mathrm{Id} \cdot \tfrac{\partial}{\partial t}u(t) \\
\Leftrightarrow \quad & \partial_1\mathcal{E}(t, u_0) &&= \partial_2\mathcal{E}(t, u_0) \cdot F(u_0),
\end{aligned}$$

since

$$\begin{aligned}
\mathrm{Id} &= \tfrac{\partial}{\partial u_0}\big(u_0\big) = \tfrac{\partial}{\partial u_0}\big(\mathcal{E}(-t, \mathcal{E}(t, u_0)\big) = \partial_2\mathcal{E}(-t, \mathcal{E}(t, u_0)) \cdot \tfrac{\partial}{\partial u_0}\big(\mathcal{E}(t, u_0)\big) \\
&= \partial_2\mathcal{E}(-t, \mathcal{E}(t, u_0)) \cdot \partial_2\mathcal{E}(t, u_0) = \partial_2\mathcal{E}(-t, u(t)) \cdot \partial_2\mathcal{E}(t, \mathcal{E}(-t, u(t)).
\end{aligned}$$

This concludes the proof. ■

2.2 One-step integrators

Throughout this thesis we consider various approximation schemes to the problem (2.1). In [3, p.3] or [4, pp.183–184] they are defined as follows.

Definition 2.2.2. *A one-step approximation scheme $\mathcal{S}(t, u)$ to the initial value problem* (2.1) *with exact flow* (2.4)*, with stepsize t and starting point $(0, u_0)$ is characterized by the property*

$$\mathcal{S}(t, u_0) \approx \mathcal{E}(t, u_0), \quad \mathcal{S}(0, u_0) = u_0.$$

We say that the scheme has order p, if the local error, defined by

$$\mathcal{L}(t, u) := \mathcal{S}(t, u) - \mathcal{E}(t, u), \tag{2.8}$$

satisfies $\mathcal{L}(t, u_0) = \mathcal{O}(t^{p+1})$, for $t \to 0$.

2.3 Classical and symmetrized defect for one-step integrators

In view of defining defect-based a-posteriori estimators of the local error (2.8) we introduce the classical defect and the symmetrized defect.

2.3.1 Classical defect

The defining property (2.4) of the flow justifies to define the so-called classical defect associated with an integrator $\mathcal{S}$.

Definition 2.3.3. *Consider a one-step approximation scheme $\mathcal{S}$ of order p as introduced in Definition 2.2.2. The classical defect associated with $\mathcal{S}(t,u)$ is then defined as*

$$\mathcal{D}_c(t,u) := \partial_1 \mathcal{S}(t,u) - F(\mathcal{S}(t,u)). \tag{2.9}$$

Due to its construction, we at least expect $\mathcal{D}_c(t,u_0) = \mathcal{O}(t^p)$.

Remark 2.3.4. One observes $\mathcal{D}_c(t,u_0) = \mathcal{O}(t^p)$ due to:

$$\begin{aligned}\mathcal{D}_c(t,u_0) &= \partial_1 \mathcal{S}(t,u_0) - F(\mathcal{S}(t,u_0)) - \big(\underbrace{\partial_1 \mathcal{E}(t,u_0) - F(\mathcal{E}(t,u_0))}_{=0,\text{ due to (2.4)}}\big) \\ &= \partial_1\big(\underbrace{\mathcal{S}(t,u_0) - \mathcal{E}(t,u_0)}_{=\mathcal{O}(t^{p+1}),\text{ due to } Def.\ 2.2.2}\big) - \big(\underbrace{F(\mathcal{S}(t,u_0)) - F(\mathcal{E}(t,u_0))}_{=\mathcal{O}(t^{p+1}),\text{ due to } F \text{ Lip.-cont.}}\big).\end{aligned}$$

//

The following theorem allows us to represent the local error in terms of the classical defect via the so-called Gröbner-Alekseev Lemma, which is for instance also stated in [3, Theorem 1] and [10, Theorem I.14.5].

Theorem 2.3.5. *In terms of the classical defect* (2.9)*, the local error defined in* (2.8) *satisfies the integral representation*

$$\mathcal{L}(t,u_0) = \int_0^t \partial_2 \mathcal{E}(t-s, \mathcal{S}(s,u_0)) \cdot \mathcal{D}_c(s,u_0)\, ds. \tag{2.10}$$

Proof. A concise proof originating from [8] is given in [3, p.4], making use of the fundamental identity (2.5), see Theorem 2.1.1. ■

This representation provides a way to derive the proposition

$$\mathcal{L}(t,u_0) = \tfrac{t}{p+1}\mathcal{D}_c(t,u_0) + \mathcal{O}(t^{p+2}).$$

We discuss this in detail in Section 2.4.

2.3.2 Symmetrized defect

We first define the adjoint scheme to a given scheme, as well as self-adjoint schemes, see [11, p.42].

Definition 2.3.6. *Consider a one-step approximation scheme $\mathcal{S}$ as introduced in Definition 2.2.2. The adjoint scheme $\mathcal{S}^*$ of $\mathcal{S}$ is defined as*

$$\mathcal{S}^*(t, u_0) := \mathcal{S}^{-1}(-t, u_0),$$

i.e., it is the inverse map of the original scheme with reversed time step $-t$.
$\mathcal{S}$ is called symmetric (self-adjoint, time-reversible), if

$$\mathcal{S}^*(t, u_0) = \mathcal{S}(t, u_0),$$

which implies

$$\mathcal{S}(-t, \mathcal{S}(t, u_0)) = u_0. \tag{2.11}$$

Remark 2.3.7. We remark that the exact flow $\mathcal{E}(t, u_0)$ is self-adjoint, i.e., $\mathcal{E}(-t, \mathcal{E}(t, u_0)) = u_0$, which was a key element in the proof of Theorem 2.1.1. //

Self-adjoint schemes have some interesting properties, in particular they have even order p. We state this property in the next theorem.

Theorem 2.3.8. *Consider the exact flow $\mathcal{E}$ from* (2.2) *and a corresponding scheme S of order p, as defined in Definition 2.2.2. Due to* (2.8) *we can write*

$$\mathcal{S}(t, u_0) = \mathcal{E}(t, u_0) + C(u_0)t^{p+1} + \mathcal{O}(t^{p+2}),$$

where C is a function not depending on t. The adjoint scheme $\mathcal{S}^*$ of $\mathcal{S}$ has the same order p and can be written as

$$\mathcal{S}^*(t, u_0) = \mathcal{E}(t, u_0) + (-1)^p C(u_0)t^{p+1} + \mathcal{O}(t^{p+2}).$$

Moreover, if $\mathcal{S}$ is self-adjoint it inevitably has even order p.

Proof. A proof of these properties is given in [11, Theorem II.3.2]. ■

In this thesis we apply the symmetrized defect only to self-adjoint schemes $\mathcal{S}$, since later results depend on this property. However, it is justified to define the symmetrized defect for arbitrary schemes. The fundamental identity (2.5) motivates its definition, introduced in [3, p.6]

Definition 2.3.9. *Consider a one-step approximation scheme $\mathcal{S}$ as introduced in Definition 2.2.2. The symmetrized defect associated with $\mathcal{S}(t,u)$ is defined as*

$$\mathcal{D}_s(t,u) := \partial_1\mathcal{S}(t,u) - \tfrac{1}{2}\big(F(\mathcal{S}(t,u)) + \partial_2\mathcal{S}(t,u)\cdot F(u)\big). \tag{2.12}$$

Due to its construction, we at least expect $\mathcal{D}_s(t,u) = \mathcal{O}(t^p)$.

Remark 2.3.10. In addition to $\mathcal{D}_s(t,u) = \mathcal{O}(t^p)$ we even have

$$\mathcal{D}_s(t,u) = \mathcal{D}_c(t,u) + \mathcal{O}(t^{p+1}),$$

which can easily be deduced due to the fundamental identity (2.5):

$$\begin{aligned}
\mathcal{D}_s(t,u) &= \partial_1\mathcal{S}(t,u) - \tfrac{1}{2}\big(F(\mathcal{S}(t,u)) + \partial_2\mathcal{S}(t,u)\cdot F(u)\big)\\
&= \big(\partial_1\mathcal{S}(t,u) - F(\mathcal{S}(t,u))\big) + \tfrac{1}{2}\big(F(\mathcal{S}(t,u)) - \partial_2\mathcal{S}(t,u)\cdot F(u)\big)\\
&= \mathcal{D}_c(t,u) + \tfrac{1}{2}\big(\underbrace{F(\mathcal{E}(t,u)) - \partial_2\mathcal{E}(t,u)\cdot F(u)}_{=0,\ \text{due to (2.5)}}\big)\\
&\quad + \tfrac{1}{2}\big(\underbrace{F(\mathcal{S}(t,u)) - F(\mathcal{E}(t,u))}_{=\mathcal{O}(t^{p+1}),\ \text{due to } F \text{ Lip.-cont.}}\big) + \tfrac{1}{2}\big(\underbrace{\partial_2\mathcal{E}(t,u) - \partial_2\mathcal{S}(t,u)}_{=\mathcal{O}(t^{p+1}),\ \text{due to } Def.\ 2.2.2}\big)\cdot F(u)\\
&= \mathcal{D}_c(t,u) + \mathcal{O}(t^{p+1}).
\end{aligned}$$

//

Just as with the classical defect (see Theorem 2.3.5) the local error can also be expressed in terms of the symmetrized defect, which is the statement of the following theorem.

Theorem 2.3.11. *In terms of the symmetrized defect* (2.12) *the local error defined in* (2.8) *admits the integral representation*

$$\mathcal{L}(t,u_0) = \int_0^t \partial_2\mathcal{E}(\tfrac{t-s}{2}, \mathcal{S}(s,\mathcal{E}(\tfrac{t-s}{2},u_0)))\cdot\mathcal{D}_s(s,\mathcal{E}(\tfrac{t-s}{2},u_0))\,ds. \tag{2.13}$$

Proof. A detailed proof following the idea of [10, Theorem I.14.5] is given in [3, Theorem 2]. The proof expands the ideas of the proof to Theorem 2.3.5 and also makes use of the fundamental identity (2.5). ■

2.4 Classical and symmetrized, defect-based local error estimator

The idea for the defect-based local error estimator is due to [5] and [4]. We recall the local error integral representations in (2.10) and (2.13) and denote the integrands by $\Theta(s)$. We also

set $\mathcal{D}(t,u_0)=\mathcal{D}_c(t,u_0)$ and $\mathcal{D}_s(t,u_0)$, respectively. Due to the construction of the defects, we at least expect $\mathcal{D}(s,u_0)=\mathcal{O}(s^p)$, so $\Theta(s)=\mathcal{O}(s^p)$. Consequently

$$\begin{aligned}\mathcal{L}(t,u_0)=\int_0^t \Theta(s)\,ds \approx \int_0^t \tfrac{s^p}{p!}\Theta^{(p)}(0)\,ds = \tfrac{t^{p+1}}{(p+1)!}\Theta^{(p)}(0)\\ \approx \tfrac{t}{p+1}\Theta(t)=\tfrac{t}{p+1}\mathcal{D}(t,u_0),\end{aligned} \tag{2.14}$$

where $\approx$ means asymptotic approximation at level $\mathcal{O}(t^{p+2})$. Hence,

$$\mathcal{L}(t,u_0)=\tfrac{t}{p+1}\mathcal{D}(t,u_0)+\mathcal{O}(t^{p+2}), \tag{2.15}$$

for $\mathcal{D}(t,u_0)=\mathcal{D}_c(t,u_0)$ and $\mathcal{D}(t,u_0)=\mathcal{D}_s(t,u_0)$, respectively. In the following we show that in the self-adjoint case and with the symmetrized defect there even holds

$$\mathcal{L}(t,u_0)=\tfrac{t}{p+1}\mathcal{D}_s(t,u_0)+\mathcal{O}(t^{p+3}). \tag{2.16}$$

First we define the corrected schemes.

Definition 2.4.12. *Consider a one-step approximation scheme $\mathcal{S}$ of order p as introduced in Definition 2.2.2. The corrected scheme for the classical defect* (2.9) *is defined as*

$$\widehat{\mathcal{S}}_c(t,u):=\mathcal{S}(t,u)-\tfrac{t}{p+1}\mathcal{D}_c(t,u). \tag{2.17}$$

The corrected scheme for the symmetrized defect (2.12) *is defined as*

$$\widehat{\mathcal{S}}_s(t,u):=\mathcal{S}(t,u)-\tfrac{t}{p+1}\mathcal{D}_s(t,u). \tag{2.18}$$

We formulate (2.15) and (2.16) as theorems. These are the central theorems of [3].

Theorem 2.4.13. *Consider a one-step approximation scheme $\mathcal{S}$ of order p, applied to an evolution equation* (2.1). *The local error of the corrected scheme* (2.17), $\widehat{\mathcal{L}}_c(t,u):=\widehat{\mathcal{S}}_c(t,u)-\mathcal{E}(t,u)$ *satisfies*

$$\widehat{\mathcal{L}}_c(t,u_0)=\mathcal{O}(t^{p+2}), \tag{2.19}$$

i.e., $\widehat{S}_c$ has order $p+1$.

Proof. The proposition in (2.19) is simply a reformulation of (2.15), since

$$\begin{aligned}\widehat{\mathcal{L}}_c(t,u_0)=\widehat{\mathcal{S}}_c(t,u_0)-\mathcal{E}(t,u_0)\overset{(2.17)}{=}\mathcal{S}(t,u_0)-\tfrac{t}{p+1}\mathcal{D}_c(t,u_0)-\mathcal{E}(t,u_0)\\ \overset{(2.8)}{=}\mathcal{L}(t,u_0)-\tfrac{t}{p+1}\mathcal{D}_c(t,u_0)\overset{(2.15)}{=}\mathcal{O}(t^{p+2}).\end{aligned}$$

The proof for (2.15) is given in (2.14). ■

Theorem 2.4.14. *Consider a self-adjoint one-step scheme $\mathcal{S}$ of (even) order $p \geq 2$, satisfying* (2.11)*, applied to an evolution equation* (2.1)*. Then the corrected scheme* (2.18) *is almost self-adjoint, i.e.,*

$$\widehat{\mathcal{S}}_s(-t, \widehat{\mathcal{S}}_s(t, u_0)) = u_0 + \mathcal{O}(t^{2p+2}). \tag{2.20}$$

Moreover, the local error $\widehat{\mathcal{L}}_s(t,u) := \widehat{\mathcal{S}}_s(t,u) - \mathcal{E}(t,u)$ of the corrected scheme satisfies

$$\widehat{\mathcal{L}}_s(t, u_0) = \mathcal{O}(t^{p+3}), \tag{2.21}$$

i.e., $\widehat{S}_s$ has even order $p+2$.

Proof. The proof for this theorem is given in [3, pp.7–9]. In consideration of its significance for this thesis we present it here.
We apply Taylor expansion to

$$\begin{aligned}\widehat{\mathcal{S}}_s(-t, \widehat{\mathcal{S}}_s(t, u_0)) &= \mathcal{S}(-t, \widehat{\mathcal{S}}_s(t, u_0)) + \tfrac{t}{p+1}\mathcal{D}_s(-t, \widehat{\mathcal{S}}_s(t, u_0)) \\ &= \mathcal{S}(-t, \mathcal{S}(t, u_0) - \tfrac{t}{p+1}\mathcal{D}_s(t, u_0)) + \tfrac{t}{p+1}\mathcal{D}_s(-t, \mathcal{S}(t, u_0) - \tfrac{t}{p+1}\mathcal{D}_s(t, u_0))\end{aligned}$$

in $\mathcal{S}(t, u_0) - \frac{t}{p+1}\mathcal{D}_s(t, u_0)$, around $\mathcal{S}(t, u_0)$. Because $\mathcal{S}$ is by assumption self-adjoint and due to the fact that $t\mathcal{D}_s(t, u_0) = \mathcal{O}(t^{p+1})$, we have:

$$\begin{aligned}\widehat{\mathcal{S}}_s(-t, \widehat{\mathcal{S}}_s(t, u_0)) &= \mathcal{S}(-t, \mathcal{S}(t, u_0)) + \partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot \big(- \tfrac{t}{p+1}\mathcal{D}_s(t, u_0)\big) + \mathcal{O}(t^{2p+2}) \\ &\quad + \tfrac{t}{p+1}\mathcal{D}_s(-t, \mathcal{S}(t, u_0)) + \mathcal{O}(t^{2p+2}) \\ &= u_0 - \tfrac{t}{p+1}\big(\underbrace{\partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot \mathcal{D}_s(t, u_0) - \mathcal{D}_s(-t, \mathcal{S}(t, u_0))}_{\textbf{\textit{critical term}}} \big) + \mathcal{O}(t^{2p+2}).\end{aligned} \tag{2.22}$$

To prove (2.20), we have to show that the ***critical term*** equals 0. Hence, we collect the contributions to the ***critical term***. First, since

$$0 = \tfrac{\partial}{\partial t}\big(\underbrace{\mathcal{S}(-t, \mathcal{S}(t, u_0))}_{= u_0} \big) = -\partial_1\mathcal{S}(-t, \mathcal{S}(t, u_0)) + \partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot \partial_1\mathcal{S}(t, u_0), \tag{2.23}$$

we have

$$\begin{aligned}&\mathcal{D}_s(-t, \mathcal{S}(t, u_0)) = \\ &= \partial_1\mathcal{S}(-t, \mathcal{S}(t, u_0)) - \tfrac{1}{2}\big(F(\underbrace{\mathcal{S}(-t, \mathcal{S}(t, u_0))}_{= u_0}) + \partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot F(\mathcal{S}(t, u_0))\big) \\ &\overset{(2.23)}{=} \partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot \partial_1\mathcal{S}(t, u_0) - \tfrac{1}{2}F(u_0) - \tfrac{1}{2}\partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot F(\mathcal{S}(t, u_0)) \\ &= \partial_2\mathcal{S}(-t, \mathcal{S}(t, u_0)) \cdot \big(\partial_1\mathcal{S}(t, u_0) - \tfrac{1}{2}F(\mathcal{S}(t, u_0))\big) - \tfrac{1}{2}F(u_0).\end{aligned} \tag{2.24}$$

By making use of identity (2.24) and the definition of the symmetrized defect (2.12) it holds:

$$\begin{aligned}
\textbf{\textit{critical term}} &= \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\mathcal{D}_s(t,u_0)-\mathcal{D}_s(-t,\mathcal{S}(t,u_0))\\
&= \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\big(\partial_1\mathcal{S}(t,u_0)-\tfrac{1}{2}F(\mathcal{S}(t,u_0))-\tfrac{1}{2}\partial_2\mathcal{S}(t,u_0)\cdot F(u_0)\big)\\
&\quad -\partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\big(\partial_1\mathcal{S}(t,u_0)-\tfrac{1}{2}F(\mathcal{S}(t,u_0))\big)+\tfrac{1}{2}F(u_0)\\
&= -\tfrac{1}{2}\big(\partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\partial_2\mathcal{S}(t,u_0)-\mathrm{Id}\big)\cdot F(u_0)\\
&= -\tfrac{1}{2}\big(\underbrace{\tfrac{\partial}{\partial u_0}\big(\mathcal{S}(-t,\mathcal{S}(t,u_0))\big)}_{=\mathrm{Id}}-\mathrm{Id}\big)\cdot F(u_0)=0.
\end{aligned}\tag{2.25}$$

Thus, (2.22) indeed simplifies to (2.20). To prove (2.21) we proceed in the same way as for the linear case [5, Theorem 1], following the argument from [11, Theorem II.3.2]. From (2.15) we know that for some function C independent of t:

$$\widehat{\mathcal{S}}_s(t,u_0)=\mathcal{E}(t,u_0)+Ct^{p+2}+\mathcal{O}(t^{p+3}).\tag{2.26}$$

We use (2.26), the property (2.20) and Taylor expansion in $\mathcal{E}(t,u_0)+Ct^{p+2}+\mathcal{O}(t^{p+3})$ around $\mathcal{E}(t,u_0)$ to proceed in the following way:

$$\begin{aligned}
u_0+\mathcal{O}(t^{2p+2}) &\overset{(2.20)}{=} \widehat{\mathcal{S}}_s(-t,\widehat{\mathcal{S}}_s(t,u_0))\\
&\overset{(2.26)}{=} \widehat{\mathcal{S}}_s(-t,\mathcal{E}(t,u_0)+Ct^{p+2}+\mathcal{O}(t^{p+3}))\\
&\overset{(2.26)}{=} \mathcal{E}(-t,\mathcal{E}(t,u_0)+Ct^{p+2}+\mathcal{O}(t^{p+3}))+Ct^{p+2}+\mathcal{O}(t^{p+3})\\
&= \underbrace{\mathcal{E}(-t,\mathcal{E}(t,u_0))}_{=u_0}+\partial_2\mathcal{E}(-t,\mathcal{E}(t,u_0))\cdot(Ct^{p+2}+\mathcal{O}(t^{p+3}))+Ct^{p+2}+\mathcal{O}(t^{p+3})\\
&= u_0+(\underbrace{\partial_2\mathcal{E}(-t,\mathcal{E}(t,u_0))+\mathrm{Id}}_{\neq 0})Ct^{p+2}+\mathcal{O}(t^{p+3}).
\end{aligned}\tag{2.27}$$

This implies $C=0$, and (2.26) equals (2.21). To justify $\partial_2\mathcal{E}(-t,\mathcal{E}(t,u_0))\neq-\mathrm{Id}$ in (2.27) we assume the opposite and argue:

$$\begin{aligned}
\mathrm{Id} &= \tfrac{\partial}{\partial u_0}\big(\mathcal{E}(-t,\mathcal{E}(t,u_0))\big)=\underbrace{\partial_2\mathcal{E}(-t,\mathcal{E}(t,u_0))}_{=-\mathrm{Id}}\partial_2\mathcal{E}(t,u_0)\\
&\Rightarrow\ \partial_2\mathcal{E}(t,u_0)=-\mathrm{Id}\ \Leftrightarrow\ \mathcal{E}(t,u_0)=-u_0,\ \text{for all } t\geq 0,
\end{aligned}$$

which contradicts $\mathcal{E}(0,u_0)=u_0$. This concludes the proof of Theorem 2.4.14. ■

Remark 2.4.15. Analogously to [3, Remark 1] the proof to Theorem 2.4.14 remains valid, if $\mathcal{S}$ is no longer self-adjoint, but satisfies the weaker condition

$$\mathcal{S}(-t,\mathcal{S}(t,u_0))=u_0+\mathcal{O}(t^q),\ \text{for } q>p+2.\tag{2.28}$$

To understand this, we revisit the key parts of the proof:
Equation (2.23) in this case reads

$$\underline{\mathcal{O}(t^{q-1})} = \tfrac{\partial}{\partial t}\big(\underbrace{\mathcal{S}(-t,\mathcal{S}(t,u_0))}_{=u_0+\underline{\mathcal{O}(t^q)}}\big) = -\partial_1\mathcal{S}(-t,\mathcal{S}(t,u_0)) + \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\partial_1\mathcal{S}(t,u_0),$$

which alters equation (2.24) in the following way:

$$\begin{aligned}
&\mathcal{D}_s(-t,\mathcal{S}(t,u_0)) = \\
&= \partial_1\mathcal{S}(-t,\mathcal{S}(t,u_0)) - \tfrac{1}{2}\big(F(\underbrace{\mathcal{S}(-t,\mathcal{S}(t,u_0))}_{=u_0+\underline{\mathcal{O}(t^q)}}) + \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot F(\mathcal{S}(t,u_0))\big) \\
&= \underline{\mathcal{O}(t^{q-1})} + \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\partial_1\mathcal{S}(t,u_0) \\
&\quad - \tfrac{1}{2}\underbrace{F(u_0+\underline{\mathcal{O}(t^q)})}_{\overset{\text{Taylor}}{=}F(u_0)+\underline{\mathcal{O}(t^q)}} - \tfrac{1}{2}\partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot F(\mathcal{S}(t,u_0)) \\
&= \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\big(\partial_1\mathcal{S}(t,u_0) - \tfrac{1}{2}F(\mathcal{S}(t,u_0))\big) - \tfrac{1}{2}F(u_0) + \underline{\mathcal{O}(t^{q-1})}.
\end{aligned}$$

It is now easy to see that analogous calculations as in (2.25) do not eliminate the ***critial term***, but an error term $\mathcal{O}(t^{q-1})$ remains:

$$\begin{aligned}
\textbf{\textit{critical term}} &= \partial_2\mathcal{S}(-t,\mathcal{S}(t,u_0))\cdot\mathcal{D}_s(t,u_0) - \mathcal{D}_s(-t,\mathcal{S}(t,u_0)) \\
&= -\tfrac{1}{2}\big(\underbrace{\tfrac{\partial}{\partial u_0}(\mathcal{S}(-t,\mathcal{S}(t,u_0)))}_{=\mathrm{Id}} - \mathrm{Id}\big)\cdot F(u_0) + \underline{\mathcal{O}(t^{q-1})} = \underline{\mathcal{O}(t^{q-1})}.
\end{aligned}$$

Thus, we have a weaker proposition in comparison to (2.20):

$$\widehat{\mathcal{S}}_s(-t,\widehat{\mathcal{S}}_s(t,u_0)) = u_0 + \mathcal{O}(t^q). \tag{2.29}$$

However, the weaker condition (2.29) is sufficient to argue that $C = 0$ in (2.27), since $q > p+2$.

This shows that Theorem 2.4.14 can be applied to the corrected scheme $\widehat{\mathcal{S}}_s$ of a self-adjoint scheme $\mathcal{S}$ of (even) order $p \geq 4$: Since it holds that

$$\widehat{\mathcal{S}}_s(-t,\widehat{\mathcal{S}}_s(t,u_0)) = u_0 + \mathcal{O}(t^{2p+2}),$$

see (2.20), and $\widehat{\mathcal{S}}_s$ has order $p_s := p+2$, the weaker condition (2.28) is fulfilled, if

$$q = 2p+2 > (p+2)+2 = p_s+2, \tag{2.30}$$

which is true for (even) order $p \geq 4$. This argument can be repeated inductively, which leads to integrators of arbitrary order. However, this method of increasing the order by defect correction is usually not very relevant in practice due to prohibitive computational effort in comparison to a straightforward higher-order method.

This approach does not work, if we start with a basic scheme of order $p = 2$ and its symmetrized corrected scheme of order 4, since here (2.30) is not fulfilled. Nonetheless, since we fit into the usual setting of (2.15), we still expect order 5 for its subsequent symmetrized corrected scheme. In the case of some integrators it proves to be reasonable in terms of computational effort to proceed like this. We explore this possibility in Section 4.1. //

In Chapter 5 we consider the application of corrected schemes based on a number of specific integrators, introduced in Chapter 4, and find numerical verifications of Theorems 2.4.13 and 2.4.14, as well as the considerations in Remark 2.4.15.

2.5 Composition methods

In this section we give a theoretical discussion of a particular family of integration schemes. We follow [11, pp.42–44] and introduce compositions of basic, given one-step integrators of order p. They are compositions of the basic method with different step sizes and aim to increase the order while preserving some desirable properties of the basic method. This idea has mainly been developed in papers of Suzuki ([19], 1990), Yoshida ([20], 1990), and McLachlan ([17], 1995), see also [11].

Definition 2.5.16. *Consider a one-step approximation scheme $\mathcal{S}$ of order p as introduced in Definition 2.2.2. We call its composition with s step-sizes $\gamma_1 t, \gamma_2 t, \ldots, \gamma_s t$, i.e.,*

$$\mathcal{C}(t, u_0) := \mathcal{S}(\gamma_s t, \ldots \mathcal{S}(\gamma_2 t, \mathcal{S}(\gamma_1 t, u_0))), \tag{2.31}$$

the corresponding composition method.

The following theorem sets the path for an order-increasing composition method.

Theorem 2.5.17. *Consider a one-step approximation scheme $\mathcal{S}$ of order p and a composition method $\mathcal{C}$ (2.31) with s step-sizes $\gamma_1 t, \gamma_2 t, \ldots, \gamma_s t$. If*

$$\begin{aligned} \gamma_1 + \gamma_2 + \cdots + \gamma_s &= 1, \\ \gamma_1^{p+1} + \gamma_2^{p+1} + \cdots + \gamma_s^{p+1} &= 0, \end{aligned} \tag{2.32}$$

then $\mathcal{C}$ is at least of order $p + 1$.

Proof. A proof of this property is given in [11, Theorem II.4.1] and is related to the proof of Theorem 2.3.8. ■

2.5.1 The triple jump

As stated in [11, p.44], the system of equations (2.32) has no real solutions for odd p. Consequently we aim for order-increase only in the case of integrators of even order p. In

this case the smallest s that provides a real solution is $s = 3$. If we impose symmetry $\gamma_1 = \gamma_3$, we obtain

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{\frac{1}{p+1}}}, \quad \gamma_2 = 1 - 2\gamma_1 = -\frac{2^{\frac{1}{p+1}}}{2 - 2^{\frac{1}{p+1}}}, \tag{2.33}$$

and due to Theorem 2.5.17 the resulting composition method is at least of order $p + 1$. We call this method the *triple jump*. So, if we start with a basic one-step integration scheme of order $p = 2$, the composition method defined through (2.33) at least has order $p = 3$. Moreover, because we rooted for $\gamma_1 = \gamma_3$ and thus retrieved a self-adjoint integrator, we make use of Theorem 2.3.8 and know that we can actually expect even order $p = 4$.

Remark 2.5.18. A single application of the triple jump on a basic integration scheme of even order 2 increases the order to 4. One can repeat this step and retrieve a scheme of even order 6. Repetition leads to schemes of any desired even order. However, since $\gamma_2 < 0$, this involves integration backward in time. It even holds that $\gamma_1 + \gamma_2 < 0$, so a full time step of the *triple jump* combined with iterative applications involves a heavy fractal-like zigzag, see [11, p.44]. //

Chapter 3

Nonautonomous evolution equations

In prior work ([9],[5]) specific integration schemes and their defects were already applied to linear, autonomous evolution equations of the form

$$\frac{\mathrm{d}}{\mathrm{dt}}u(t) = Hu(t), \quad u(0) = u_0, \tag{3.1}$$

where $H = A + B$, or $H = A + B + C$. In this chapter these results are generalized to the linear and nonlinear, nonautonomous case. For these cases we find representations of the classical (2.9) and symmetrized defect (2.12).

3.1 The nonautonomous case

We consider a general nonautonomous evolution equation

$$\frac{\mathrm{d}}{\mathrm{dt}}u(t) = F(t, u(t)), \quad u(t_0) = u_0. \tag{3.2}$$

Here, we prefer to use local time τ relative to the initial time t_0, so that $t = t_0+\tau$. Thus, (3.2) is reformulated as

$$\frac{\partial}{\partial\tau}u(t_0 + \tau) = F(t_0 + \tau, u(t_0 + \tau)), \quad u(t_0) = u_0. \tag{3.3}$$

The exact flow associated with (3.2) ((3.3), respectively) is denoted by $\mathcal{E}(\tau, t_0, u_0)$, which satisfies

$$\frac{\partial}{\partial\tau}\mathcal{E}(\tau, t_0, u_0) = F(t_0 + \tau, \mathcal{E}(\tau, t_0, u_0)), \quad \mathcal{E}(0, t_0, u_0) = u_0.$$

Analogously to (2.3) we define the partial derivatives:

$$\begin{aligned}
\partial_1\mathcal{E}(\tau, t_0, u_0) &:= \tfrac{\partial}{\partial\tau}\mathcal{E}(\tau, t_0, u_0),\\
\partial_2\mathcal{E}(\tau, t_0, u_0) &:= \tfrac{\partial}{\partial t_0}\mathcal{E}(\tau, t_0, u_0),\\
\partial_3\mathcal{E}(\tau, t_0, u_0) &:= \tfrac{\partial}{\partial u_0}\mathcal{E}(\tau, t_0, u_0).
\end{aligned}$$

Next we follow [3, pp.13sqq.] and reformulate (3.3) in autonomous form, showing that the theoretical background of Theorems 2.4.13 and 2.4.14 directly carries over to the nonautonomous case.

3.2 Reformulation as an autonomous problem

We reformulate the problem (3.2) into an autonomous, yet nonlinear system for $U(t) := (v(t), u(t))^T$, where $v : t \mapsto t$. With

$$\begin{pmatrix} \frac{\mathrm{d}}{\mathrm{dt}} v(t) \\ \frac{\mathrm{d}}{\mathrm{dt}} u(t) \end{pmatrix} = \begin{pmatrix} 1 \\ F(v(t), u(t)) \end{pmatrix} =: \boldsymbol{F}(U(t)), \quad \begin{pmatrix} v(t_0) \\ u(t_0) \end{pmatrix} = \begin{pmatrix} t_0 \\ u_0 \end{pmatrix} =: U_0,$$

the system (3.2) reads

$$\tfrac{\mathrm{d}}{\mathrm{dt}} U(t) = \boldsymbol{F}(U(t)), \quad U(t_0) = U_0,$$

i.e., it is in autonomous form. As already mentioned above, we use the more specific notation,

$$U = \begin{pmatrix} t_0 + \tau \\ u \end{pmatrix},$$

whence system (3.3) reads

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau} U(\tau) = \boldsymbol{F}(U(\tau)), \quad U(0) = U_0,$$

with the flow

$$\boldsymbol{\mathcal{E}}(\tau, U) = \boldsymbol{\mathcal{E}}(\tau, t_0, u) = \begin{pmatrix} t_0 + \tau \\ \mathcal{E}(\tau, t_0, u) \end{pmatrix}.$$

The fundamental identity (2.5) reads

$$\big[\partial_1 \boldsymbol{\mathcal{E}}(\tau, U) = \big] \boldsymbol{F}(\boldsymbol{\mathcal{E}}(\tau, U)) = \partial_2 \boldsymbol{\mathcal{E}}(\tau, U) \cdot \boldsymbol{F}(U). \tag{3.4}$$

We desire to have representations of $\partial_1 \boldsymbol{\mathcal{E}}(\tau, U_0)$, $\partial_2 \boldsymbol{\mathcal{E}}(\tau, U_0)$ and $\boldsymbol{F}(U_0)$:

$$\begin{aligned} \partial_1 \boldsymbol{\mathcal{E}}(\tau, U_0) &= \boldsymbol{F}(\boldsymbol{\mathcal{E}}(\tau, U_0)) = \begin{pmatrix} 1 \\ F(t_0 + \tau, \mathcal{E}(\tau, t_0, u_0)) \end{pmatrix}, \quad \boldsymbol{\mathcal{E}}(0, U_0) = U_0, \\ \partial_2 \boldsymbol{\mathcal{E}}(\tau, U_0) &= \begin{pmatrix} 1 & 0 \\ \partial_2 \mathcal{E}(\tau, t_0, u_0) & \partial_3 \mathcal{E}(\tau, t_0, u_0) \end{pmatrix}, \\ \boldsymbol{F}(U_0) &= \begin{pmatrix} 1 \\ F(t_0, u_0) \end{pmatrix}. \end{aligned}$$

Evaluating the second component of (3.4) now yields the fundamental identity for the nonautonomous problem (3.2):

$$\big[\partial_1 \mathcal{E}(\tau, t_0, u_0) = \big] F(t_0 + \tau, \mathcal{E}(\tau, t_0, u_0)) = \partial_2 \mathcal{E}(\tau, t_0, u_0) + \partial_3 \mathcal{E}(\tau, t_0, u_0) \cdot F(t_0, u_0).$$

We formulate this result as a distinct theorem.

Theorem 3.2.1. *As a consequence of the initial value problem* (3.2) *there holds the fundamental identity for the nonautonomous case,*

$$\big[\partial_1\mathcal{E}(\tau,t_0,u_0)=\big]F(t_0+\tau,\mathcal{E}(\tau,t_0,u_0))=\partial_2\mathcal{E}(\tau,t_0,u_0)+\partial_3\mathcal{E}(\tau,t_0,u_0)\cdot F(t_0,u_0). \tag{3.5}$$

Proof. A verification of (3.5) based on the fundamental identity for the autonomous case (2.5) was given in the lines before the theorem. Moreover, in [3, Lemma 5] one finds an explicit proof of this proposition. ■

Over the course of the next sections we shall discuss the evaluation of the classical and the symmetrized defect for the linear and nonlinear (nonautonomous) cases.

3.3 Defect evaluation in the linear, nonautonomous case

We expand the ideas from [3, pp.14–15] and consider a linear, nonautonomous evolution equation of the form

$$\tfrac{\mathrm{d}}{\mathrm{d}t}u(t)=F(t,u(t))=Au(t)+B(t)u(t),\quad u(t_0)=u_0, \tag{3.6}$$

and its reformulation analogously to (3.3),

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}u(t_0+\tau)=F(t_0+\tau,u(t_0+\tau))=Au(t_0+\tau)+B(t_0+\tau)u(t_0+\tau),\quad u(t_0)=u_0. \tag{3.7}$$

Observe that the operator B depends on the time t, making the problem (3.6) a nonautonomous one. Since in this case the flow $\mathcal{E}$ is linear in u_0, it is written as

$$\mathcal{E}(\tau,t_0,u_0)=:\mathcal{E}(\tau,t_0)u_0,$$

satisfying

$$\partial_1\mathcal{E}(\tau,t_0)=(A+B(t_0+\tau))\mathcal{E}(\tau,t_0),\quad \mathcal{E}(0,t_0)=\mathrm{Id}.$$

Here, a one-step approximation scheme $\mathcal{S}(\tau,t_0,u_0)\approx\mathcal{E}(\tau,t_0,u_0)$ is also typically linear in u_0:

$$\mathcal{S}(\tau,t_0,u_0)=:\mathcal{S}(\tau,t_0)u_0\approx\mathcal{E}(\tau,t_0)u_0. \tag{3.8}$$

In particular, in view of Theorem 2.4.14 we again focus on self-adjoint integrators, which are characterized by the identity

$$\mathcal{S}(-\tau, t_0+\tau)\mathcal{S}(\tau, t_0) = \mathrm{Id}, \tag{3.9}$$

see also (2.11). Here, since

$$\partial_3\mathcal{E}(\tau, t_0, u_0) = \tfrac{\partial}{\partial u_0}\big(\mathcal{E}(\tau, t_0)u_0\big) = \mathcal{E}(\tau, t_0),$$

and

$$\begin{aligned} F(t_0+\tau, \mathcal{E}(\tau, t_0, u_0)) &= (A + B(t_0+\tau))\mathcal{E}(\tau, t_0)u_0, \\ F(t_0, u_0) &= (A + B(t_0))u_0, \end{aligned}$$

the fundamental identity (3.5) takes the form

$$\big[\partial_1\mathcal{E}(\tau, t_0)u_0 = \big](A + B(t_0+\tau))\mathcal{E}(\tau, t_0)u_0 = \partial_2\mathcal{E}(\tau, t_0)u_0 + \mathcal{E}(\tau, t_0)(A + B(t_0))u_0. \tag{3.10}$$

The (linear) subflows of problem (3.7) and their partial derivatives are:

$$\begin{array}{lll} \mathcal{E}_A(\tau, t_0)u_0 = e^{\tau A}u_0 & \partial_1\mathcal{E}_A(\tau, t_0)u_0 = e^{\tau A}Au_0 & \partial_2\mathcal{E}_A(\tau, t_0) = 0 \\ \mathcal{E}_B(\tau, t_0)u_0 & \partial_1\mathcal{E}_B(\tau, t_0)u_0 & \partial_2\mathcal{E}_B(\tau, t_0)u_0 \end{array} \tag{3.11}$$

Remark 3.3.2. The existences of the partial derivatives to the subflow $\mathcal{E}_B(\tau, t_0)u_0$ depend on its concrete form. Since in the specific linear, nonautonomous evolution equations considered for this thesis $B(t)$ is a time-dependent diagonal matrix, there is $\mathcal{E}_B(\tau, t_0)u_0 = e^{\tau B(t_0+\tau)}u_0$, which is well defined. In these cases the representations of the partial derivatives do exist. We present those in Section 3.5. //

Since we apply a specific kind of integrator to the linear, nonautonomous problem (3.7), we extend Definition 2.2.2:

Definition 3.3.3. *A typical splitting scheme of order $p \geq 2$ and $J \geq 1$ stages, applied to the initial value problem* (3.7)*, with stepsize τ and starting point t_0 has the form*

$$\mathcal{S}(\tau, t_0) = \mathcal{E}_B(b_J\tau, t_J)\mathcal{E}_A(a_J\tau, t_{J-1})\cdots\mathcal{E}_B(b_1\tau, t_1)\mathcal{E}_A(a_1\tau, t_0), \tag{3.12}$$

with the subflows of (3.11)*, appropriate coefficients $a_j, b_j,\ j = 1, \ldots, J$, and*

$$t_j := t_{j-1} + a_j\tau, \quad j = 1, \ldots, J.$$

I.e., the operator $\mathcal{E}_A$ propagates the time for the t_0-dependent operator $\mathcal{E}_B$.

Because the fundamental identity here takes the form (3.10), we derive the following representations of the defects (see Definitions 2.3.3 and 2.3.9) for the integrator $\mathcal{S}$ in Definition 3.3.3:

- Classical defect:

$$\mathcal{D}_c(\tau, t_0, u_0) = \mathcal{D}_c(\tau, t_0)u_0, \tag{3.13a}$$

with

$$\mathcal{D}_c(\tau, t_0) = \partial_1\mathcal{S}(\tau, t_0) - \big((A + B(t_0 + \tau))\mathcal{S}(\tau, t_0)\big). \tag{3.13b}$$

- Symmetrized defect:

$$\mathcal{D}_s(\tau, t_0, u_0) = \mathcal{D}_s(\tau, t_0)u_0, \tag{3.14a}$$

with

$$\begin{aligned}\mathcal{D}_s(\tau, t_0) &= \partial_1\mathcal{S}(\tau, t_0) - \tfrac{1}{2}\big((A + B(t_0 + \tau))\mathcal{S}(\tau, t_0) + \partial_2\mathcal{S}(\tau, t_0) + \mathcal{S}(\tau, t_0)(A + B(t_0))\big)\\ &= \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau, t_0) - \tfrac{1}{2}\big((A + B(t_0 + \tau))\mathcal{S}(\tau, t_0) + \mathcal{S}(\tau, t_0)(A + B(t_0))\big).\end{aligned} \tag{3.14b}$$

Remark 3.3.4. It is immediately clear that since $\mathcal{E}$ and $\mathcal{S}$ are linear in u_0, so are $\mathcal{D}_c$ and $\mathcal{D}_s$. This justifies the syntax $\mathcal{D}(\tau, t_0)$. //

Applied to concrete splitting schemes of the form (3.12) the evaluation of the defects requires to evaluate the partial derivatives $\partial_1\mathcal{S}(\tau, t_0)$ and $\partial_2\mathcal{S}(\tau, t_0)$. For notational reasons we define

$$\begin{aligned}u_j^A &:= \mathcal{E}_A(a_j\tau, t_{j-1}) \cdots \mathcal{E}_B(b_1\tau, t_1)\mathcal{E}_A(a_1\tau, t_0)u_0,\\ u_j^B &:= \mathcal{E}_B(b_j\tau, t_j)u_j^A,\end{aligned} \tag{3.15}$$

for $j = 1, \ldots, J$. The chain and the product rules give us general representations of the partial derivatives:

$$\begin{aligned}\partial_1\mathcal{S}(\tau, t_0) &= b_J\partial_1\mathcal{E}_B(b_J\tau, t_J)u_J^A + \mathcal{E}_B(b_J\tau, t_J)\big(a_J\partial_1\mathcal{E}_A(a_J\tau, t_{J-1})u_{J-1}^B + \mathcal{E}_A(a_J\tau, t_{J-1})\\ &\qquad \big(\cdots b_1\partial_1\mathcal{E}_B(b_1\tau, t_1)u_1^A + \mathcal{E}_B(b_1\tau, t_1)a_1\partial_1\mathcal{E}_A(a_1\tau, t_0)u_0 \ldots\big)\big),\\ \partial_2\mathcal{S}(\tau, t_0) &= \partial_2\mathcal{E}_B(b_J\tau, t_J)u_J^A + \mathcal{E}_B(b_J\tau, t_J)\mathcal{E}_A(a_J\tau, t_{J-1})\big(\cdots \partial_2\mathcal{E}_B(b_1\tau, t_1)u_1^A \ldots\big).\end{aligned} \tag{3.16}$$

Under the assumption for the subflow $\mathcal{E}_B(\tau, t_0)u_0$ made in Remark 3.3.2, we give in the subsequent Section 3.6 algorithms for the evaluation of general splitting schemes of the form (3.12) and their defects (3.13) and (3.14), that incorporate (3.16).
However, since for specific splitting schemes the algorithmic evaluation in the form (3.16) may be inefficient, we also look for explicit, efficiently computable representations. This is the main task of Chapter 4.

3.4 Defect evaluation in the nonlinear, nonautonomous case

We now consider a nonlinear, nonautonomous evolution equation of the form

$$\tfrac{\mathrm{d}}{\mathrm{dt}}u(t) = F(t, u(t)) = Au(t) + B(t)u(t) + C(u(t)), \quad u(t_0) = u_0, \tag{3.17}$$

and its reformulation analogously to (3.3),

$$\begin{aligned} \tfrac{\mathrm{d}}{\mathrm{d}\tau}u(t_0+\tau) &= F(t_0+\tau,u(t_0+\tau)) = Au(t_0+\tau)+B(t_0+\tau)u(t_0+\tau)+C(u(t_0+\tau)),\\ u(t_0) &= u_0. \end{aligned} \tag{3.18}$$

The nonlinear flow $\mathcal{E}(\tau,t_0,u_0)$ fulfills the fundamental identity (3.10), which here takes the form

$$\begin{aligned} \big[\partial_1\mathcal{E}(t,u_0) = \big](A+B(t_0+\tau))\mathcal{E}(\tau,t_0,u_0)+C(\mathcal{E}(\tau,t_0,u_0))\\ = \partial_2\mathcal{E}(\tau,t_0,u_0)+\partial_3\mathcal{E}(\tau,t_0,u_0)\cdot\big((A+B(t_0))u_0+C(u_0)\big). \end{aligned} \tag{3.19}$$

The subflows of problem (3.18) and their partial derivatives are:

$$\begin{array}{lll} \mathcal{E}_A(\tau,t_0)u_0 = e^{\tau A}u_0, & \mathcal{E}_B(\tau,t_0)u_0, & \mathcal{E}_C(\tau,t_0,u_0),\\ \partial_1\mathcal{E}_A(\tau,t_0)u_0 = e^{\tau A}Au_0, & \partial_1\mathcal{E}_B(\tau,t_0)u_0, & \partial_1\mathcal{E}_C(\tau,t_0,u_0),\\ \partial_2\mathcal{E}_A(\tau,t_0)u_0 = 0, & \partial_2\mathcal{E}_B(\tau,t_0)u_0, & \partial_2\mathcal{E}_C(\tau,t_0,u_0) = 0,\\ \partial_3\mathcal{E}_A(\tau,t_0,u_0)\cdot\phi = \mathcal{E}_A(\tau,t_0)\phi, & \partial_3\mathcal{E}_B(\tau,t_0,u_0)\cdot\phi = \mathcal{E}_B(\tau,t_0)\phi, & \partial_3\mathcal{E}_C(\tau,t_0,u_0)\cdot\phi. \end{array} \tag{3.20}$$

Remark 3.4.5. Since the existences of the partial derivatives to the subflows $\mathcal{E}_B(\tau,t_0)u_0$ and $\mathcal{E}_C(\tau,t_0,u_0)$ depend on their concrete forms, we state them here in general form. In the specific linear, nonautonomous evolution equations considered for this thesis the nonlinearity is a cubic term in $u(t)$, and $B(t)$ is a time-dependent diagonal matrix, whence $\mathcal{E}_B(\tau,t_0)u_0 = e^{\tau B(t_0+\tau)}u_0$. //

Analogously to Definition 3.3.3 we define:

Definition 3.4.6. *A typical splitting scheme of order $p\geq 2$ and $J\geq 1$ stages to the initial value problem* (3.18)*, with stepsize τ and starting point t_0 has the form*

$$\mathcal{S}(\tau,t_0,u_0) = \mathcal{E}_C\big(c_J\tau,t_J,\mathcal{E}_B(b_J\tau,t_J)\mathcal{E}_A(a_J\tau,t_{J-1})\cdots\mathcal{E}_C\big(c_1\tau,t_1,\mathcal{E}_B(b_1\tau,t_1)\mathcal{E}_A(a_1\tau,t_0)u_0\big)\ldots\big), \tag{3.21}$$

with the subflows of (3.20)*, appropriate coefficients $a_j,b_j,c_j,\ j=1,\ldots,J$, and*

$$t_j := t_{j-1}+a_j\tau,\quad j=1,\ldots,J.$$

I.e., the operator $\mathcal{E}_A$ propagates the time for the t_0-dependent operator $\mathcal{E}_B$.

With the fundamental identity (3.19) we get theses representations of the defects for the integrator $\mathcal{S}$ in Definition 3.4.6:

- Classical defect:

$$\mathcal{D}_c(\tau,t_0,u_0) = \partial_1\mathcal{S}(\tau,t_0,u_0)-\big((A+B(t_0+\tau))\mathcal{S}(\tau,t_0,u_0)+C(\mathcal{S}(\tau,t_0,u_0))\big). \tag{3.22}$$

- Symmetrized defect:

$$\begin{aligned}\mathcal{D}_s(\tau,t_0,u_0) = \partial_1\mathcal{S}(\tau,t_0,u_0) - \tfrac{1}{2}\big((A+B(t_0+\tau))\mathcal{S}(\tau,t_0,u_0) + C(\mathcal{S}(\tau,t_0,u_0))\\ + \partial_2\mathcal{S}(\tau,t_0,u_0) + \partial_3\mathcal{S}(\tau,t_0,u_0)\cdot((A+B(t_0))u_0 + C(u_0))\big).\end{aligned} \tag{3.23}$$

Analogously to (3.15) we define

$$\begin{aligned}u_j^A &:= \mathcal{E}_A(a_j\tau,t_{j-1})\mathcal{E}_C\big(c_{j-1}\tau,t_{j-1},\mathcal{E}_B(b_{j-1}\tau,t_{j-1})\cdots\mathcal{E}_A(a_1\tau,t_0)u_0\ldots\big),\\ u_j^B &:= \mathcal{E}_B(b_j\tau,t_j)u_j^A,\\ u_j^C &:= \mathcal{E}_C(c_j\tau,t_j,u_j^B),\end{aligned}$$

for $j = 1,\ldots,J$. The chain and the product rules give us general representations of the partial derivatives:

$$\begin{aligned}\partial_1\mathcal{S}(\tau,t_0,u_0) &= c_J\partial_1\mathcal{E}_C(c_J\tau,t_J,u_J^B) + \partial_3\mathcal{E}_C(c_J\tau,t_J,u_J^B)\cdot\big(b_J\partial_1\mathcal{E}_B(b_J\tau,t_J)u_J^A\\ &\quad + \mathcal{E}_B(b_J\tau,t_J)\big(a_J\partial_1\mathcal{E}_A(a_J\tau,t_{J-1})u_{J-1}^C + \mathcal{E}_A(a_J\tau,t_{J-1})\\ &\quad \big(\cdots c_1\partial_1\mathcal{E}_C(c_1\tau,t_1,u_1^B) + \partial_3\mathcal{E}_C(c_1\tau,t_1,u_1^B)\cdot\big(b_1\partial_1\mathcal{E}_B(b_1\tau,t_1)u_1^A\\ &\quad + \mathcal{E}_B(b_1\tau,t_1)a_1\partial_1\mathcal{E}_A(a_1\tau,t_0)u_0\big)\ldots\big)\big)\big),\\ \partial_2\mathcal{S}(\tau,t_0,u_0) &= \partial_3\mathcal{E}_C(c_J\tau,t_J,u_J^B)\cdot\big(\partial_2\mathcal{E}_B(b_J\tau,t_J)u_J^A + \mathcal{E}_B(b_J\tau,t_J)\mathcal{E}_A(a_J\tau,t_{J-1})\\ &\quad \big(\cdots\partial_3\mathcal{E}_C(c_1\tau,t_1,u_1^B)\cdot\big(\partial_2\mathcal{E}_B(b_1\tau,t_1)u_1^A + \mathcal{E}_B(b_1\tau,t_1)u_1^A\big)\ldots\big)\big),\\ \partial_3\mathcal{S}(\tau,t_0,u_0)\cdot\phi &= \partial_3\mathcal{E}_C(c_J\tau,t_J,u_J^B)\cdot\big(\mathcal{E}_B(b_J\tau,t_J)\mathcal{E}_A(a_J\tau,t_{J-1})\cdots\partial_3\mathcal{E}_C(c_1\tau,t_1,u_1^B)\cdot\phi\ldots\big).\end{aligned} \tag{3.24}$$

Under the assumptions for $\mathcal{E}_B(\tau,t_0)u_0$ in Remark 3.4.5 and for general integrators of the form (3.21) algorithms for the evaluation of (3.22) and (3.23), that incorporate (3.24), are presented in Section 3.6.

3.5 Derivatives of matrix exponentials occuring in our splitting schemes

In anticipation of Section 3.6 and the upcoming Chapter 4 we desire numerically computable representations of $\partial_1\mathcal{E}_B(\tau,t_0)$ and $\partial_2\mathcal{E}_B(\tau,t_0)$ (see (3.16), (3.24) for their occurrence in the partial derivatives of $\mathcal{S}(\tau,t_0,u_0)$), under the assumption that $\mathcal{E}_B(\tau,t_0)u_0 = e^{\tau B(t_0+\tau)}u_0$, with a time-dependent diagonal matrix $B(t)$. To do this, we need to know the partial derivatives of the matrix exponential, occuring in our splitting schemes,

$$\begin{pmatrix} t_0 \\ \tau \end{pmatrix} \mapsto e^{\Omega(\tau,t_0)}, \qquad \Omega(\tau,t_0) := \alpha\tau B(t_0+\beta\tau). \tag{3.25}$$

Here α, β are arbitrary, real constants. We have:

$$\begin{aligned}\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0) &= \alpha\big(B(t_0+\beta\tau)+\beta\tau B'(t_0+\beta\tau)\big),\\ \tfrac{\partial}{\partial t_0}\Omega(\tau,t_0) &= \alpha\tau B'(t_0+\beta\tau).\end{aligned}$$

The formulas (6.5) in Appendix 6.2.2, along with the integral substitution $s\tau = \sigma$ result in the following representations of the partial derivatives of the matrix exponential (3.25), which we denote by $\mathcal{R}(\tau, t_0)$:

$$\begin{aligned}\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)\big) = \tfrac{\partial}{\partial\tau}e^{\Omega(\tau,t_0)} &= \int_0^1 e^{s\Omega(\tau,t_0)}\big(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)\big)e^{(1-s)\Omega(\tau,t_0)}\,ds\\ &= \alpha\frac{1}{\tau}\Big(\int_0^\tau e^{\sigma\alpha B(t_0+\beta\tau)}\big(B(t_0+\beta\tau)+\beta\tau B'(t_0+\beta\tau)\big)e^{-\sigma\alpha B(t_0+\beta\tau)}\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)}\\ &= \alpha\Big(B(t_0+\beta\tau)+\beta\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)},\end{aligned}\tag{3.26}$$

and

$$\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega(\tau,t_0)\big) = \tfrac{\partial}{\partial t_0}e^{\Omega(\tau,t_0)} = \alpha\Big(\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)},\tag{3.27}$$

where

$$F(\sigma;\tau) := e^{\sigma\alpha B(t_0+\beta\tau)}B'(t_0+\beta\tau)e^{-\sigma\alpha B(t_0+\beta\tau)}.\tag{3.28}$$

The last simplification in (3.26) is possible, because $B(t_0+\beta\tau)$ commutes with the matrix exponentials. One may think about $\mathcal{R}(\tau,t_0)\big(\,\cdot\,\big)$ as a matrix-operator dependent on τ and t_0.

Remark 3.5.7. For second-order integrators we evaluate the integral term $\int_0^\tau F(\sigma;\tau)\,d\sigma$ numerically by applying the second-order trapezoidal quadrature formula stated in (6.7):

$$\begin{aligned}\Big(\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\tau B(t_0+\frac{\tau}{2})} &\approx \tfrac{1}{2}\tau\big(F(0;\tau)+F(\tau;\tau)\big)e^{\tau B(t_0+\frac{\tau}{2})}\\ &= \tfrac{1}{2}\tau\big(B'(t_0+\tfrac{\tau}{2})e^{\tau B(t_0+\frac{\tau}{2})}+e^{\tau B(t_0+\frac{\tau}{2})}B'(t_0+\tfrac{\tau}{2})\big),\end{aligned}\tag{3.29}$$

see Section 6.3.1 of the Appendix. Consequently, in numerical applications of second-order integrators we use the following asymptotically correct formulas based on (3.29) to evaluate

the partial derivatives of the matrix exponentials (3.26) and (3.27):

$$\begin{aligned}
&\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)\big) = \alpha\Big(B(t_0+\beta\tau)+\beta\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)}\\
&\overset{(3.29)}{\approx}\ \alpha B(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + \tfrac{1}{2}\tau\alpha\beta\big(B'(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + e^{\alpha\tau B(t_0+\beta\tau)}B'(t_0+\beta\tau)\big),\\
&\\
&\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega(\tau,t_0)\big) = \alpha\Big(\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)}\\
&\overset{(3.29)}{\approx}\ \tfrac{1}{2}\tau\alpha\big(B'(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + e^{\alpha\tau B(t_0+\beta\tau)}B'(t_0+\beta\tau)\big).
\end{aligned}\tag{3.30}$$

//

Remark 3.5.8. For fourth-order integrators we evaluate the occurring integral terms numerically by applying the fourth-order modified trapezoidal quadrature formulas of Hermite-type stated in (6.8):

$$\begin{aligned}
&\Big(\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)}\\
&\approx \tfrac{1}{2}\tau\big(F(0;\tau)+F(\tau;\tau)\big)e^{\alpha\tau B(t_0+\beta\tau)} + \tfrac{1}{12}\tau^2\big(\tfrac{\partial}{\partial\sigma}F(\sigma;\tau)\big|_{\sigma=0} - \tfrac{\partial}{\partial\sigma}F(\sigma;\tau)\big|_{\sigma=\tau}\big)e^{\alpha\tau B(t_0+\beta\tau)}\\
&= \tfrac{1}{2}\tau\big(B'(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + e^{\alpha\tau B(t_0+\beta\tau)}B'(t_0+\beta\tau)\big)\\
&\quad + \tfrac{1}{12}\tau^2\alpha\big(\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]e^{\alpha\tau B(t_0+\beta\tau)} - e^{\alpha\tau B(t_0+\beta\tau)}\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]\big),
\end{aligned}\tag{3.31}$$

see Section 6.3.2 of the Appendix. The partial derivatives of the integrand (3.28),

$$\tfrac{\partial}{\partial\sigma}F(\sigma;\tau) = \alpha\big(B(t_0+\beta\tau)F(\sigma;\tau) - F(\sigma;\tau)B(t_0+\beta\tau)\big),$$

in combination with evaluation at $\sigma=0$ and $\sigma=\tau$ are responsible for the occurrence of the commutator $\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]$. In numerical applications of second-order integrators we use the following asymptotically correct formulas based on (3.31) to evaluate the partial

derivatives of the matrix exponentials (3.26) and (3.27):

$$\begin{aligned}
&\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)\big) = \alpha\Big(B(t_0+\beta\tau)+\beta\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)}\\
&\overset{(3.31)}{\approx}\ \alpha B(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + \tfrac{1}{2}\tau\alpha\beta\big(B'(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + e^{\alpha\tau B(t_0+\beta\tau)}B'(t_0+\beta\tau)\big)\\
&\quad + \tfrac{1}{12}\tau^2\alpha^2\beta\big(\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]e^{\alpha\tau B(t_0+\beta\tau)} - e^{\alpha\tau B(t_0+\beta\tau)}\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]\big),
\end{aligned}$$

$$\begin{aligned}
&\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega(\tau,t_0)\big) = \alpha\Big(\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau B(t_0+\beta\tau)}\\
&\overset{(3.31)}{\approx}\ \tfrac{1}{2}\tau\alpha\big(B'(t_0+\beta\tau)e^{\alpha\tau B(t_0+\beta\tau)} + e^{\alpha\tau B(t_0+\beta\tau)}B'(t_0+\beta\tau)\big)\\
&\quad + \tfrac{1}{12}\tau^2\alpha^2\big(\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]e^{\alpha\tau B(t_0+\beta\tau)} - e^{\alpha\tau B(t_0+\beta\tau)}\big[B(t_0+\beta\tau),B'(t_0+\beta\tau)\big]\big).
\end{aligned} \tag{3.32}$$

//

3.6 Algorithmic realization of the defect evaluations

Here we present the corresponding algorithms for the defect-evaluations in Sections 3.3 and 3.4. Algorithms 1 and 2 take the inital values t_0, u_0, as well as the time step τ and have the approximation $\mathcal{S}(\tau,t_0,u_0)$, as well as the defects (3.13) and (3.14) as outputs. Algorithms 3 and 4 do the same for the defects (3.22) and (3.23). For instance in [18, pp.14sqq.] and [3, p.12] similar algorithms for related problems are stated.

In our algorithms the evaluations of

$$\partial_1\mathcal{E}_B(\tau,t_0)u_0 = \tfrac{\partial}{\partial\tau}e^{\tau B(t_0+\tau)}u_0 \quad\text{and}\quad \partial_2\mathcal{E}_B(\tau,t_0)u_0 = \tfrac{\partial}{\partial t_0}e^{\tau B(t_0+\tau)}u_0$$

are denoted by

$$\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\big(\tau B(t_0+\tau)\big)\big) \quad\text{and}\quad \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\big(\tau B(t_0+\tau)\big)\big),$$

respectively (cf. the previous Section 3.5), which eases a numerical implementation involving the formulas (3.30) and (3.32).

Algorithm 1 Algorithmic realization of $\mathcal{S}(\tau, t_0)u_0$ (3.12) and $\mathcal{D}_c(\tau, t_0)u_0$ (3.13)

Require: $t_0,\ u_0,\ \tau$

$t := t_0$
$\beta := 0$
$u := u_0$
$d := 0$
for $j = 1 \dots J$ **do**
  $d = d + a_j A u$
  $d = e^{a_j \tau A} d$
  $u = e^{a_j \tau A} u$
  $\beta = \beta + a_j$
  $t = t + a_j \tau$
  $d = e^{b_j \tau B(t)} d + \mathcal{R}(\tau, t)\big(b_j B(t) + b_j \beta \tau B'(t)\big) u$
  $u = e^{b_j \tau B(t)} u$
end for
$d = d - \big(Au + B(t)u\big)$
return $u,\ d$

Algorithm 2 Algorithmic realization of $\mathcal{S}(\tau, t_0)u_0$ (3.12) and $\mathcal{D}_s(\tau, t_0)u_0$ (3.14)

Require: $t_0,\ u_0,\ \tau$

$t := t_0$
$\beta := 0$
$u := u_0$
$d := -\frac{1}{2} B(t) u$
$\delta := 0$
for $j = 1 \dots J$ **do**
  $d = d + \begin{cases} (a_j - \frac{1}{2}) A u, & j = 1 \\ a_j A u, & j > 1 \end{cases}$
  $d = e^{a_j \tau A} d$
  $\delta = e^{a_j \tau A} \delta$
  $u = e^{a_j \tau A} u$
  $\beta = \beta + a_j$
  $t = t + a_j \tau$
  $d = e^{b_j \tau B(t)} d + \mathcal{R}(\tau, t)\big(b_j B(t) + b_j \beta \tau B'(t)\big) u$
  $\delta = e^{b_j \tau B(t)} \delta + \mathcal{R}(\tau, t)\big(b_j \tau B'(t)\big) u$
  $u = e^{b_j \tau B(t)} u$
end for
$d = d - \frac{1}{2}\big(Au + B(t)u + \delta\big)$
return $u,\ d$

Algorithm 3 Algorithmic realization of $\mathcal{S}(\tau, t_0, u_0)$ (3.21) and $\mathcal{D}_c(\tau, t_0, u_0)$ (3.22)

Require: $t_0,\ u_0,\ \tau$

$t := t_0$
$\beta := 0$
$u := u_0$
$d := 0$
for $j = 1 \dots J$ **do**
  $d = d + a_j A u$
  $d = e^{a_j \tau A} d$
  $u = e^{a_j \tau A} u$
  $\beta = \beta + a_j$
  $t = t + a_j \tau$
  $d = e^{b_j \tau B(t)} d + \mathcal{R}(\tau, t)\big(b_j B(t) + b_j \beta \tau B'(t)\big) u$
  $u = e^{b_j \tau B(t)} u$
  $d = \partial_3 \mathcal{E}_C(c_j \tau, t, u) \cdot d + c_j \partial_1 \mathcal{E}_C(c_j \tau, t, u)$
  $u = \mathcal{E}_C(c_j \tau, t, u)$
end for
$d = d - \big(Au + B(t)u + C(u)\big)$
return $u,\ d$

Algorithm 4 Algorithmic realization of $\mathcal{S}(\tau, t_0, u_0)$ (3.21) and $\mathcal{D}_s(\tau, t_0, u_0)$ (3.23)

Require: $t_0,\ u_0,\ \tau$

$t := t_0$

$\beta := 0$

$u := u_0$

$d := -\frac{1}{2}\big(B(t)u + C(u)\big)$

$\delta := 0$

for $j = 1 \dots J$ **do**

$$d = d + \begin{cases} (a_j - \frac{1}{2})Au, & j = 1 \\ a_j Au, & j > 1 \end{cases}$$

$d = e^{a_j \tau A} d$

$\delta = e^{a_j \tau A} \delta$

$u = e^{a_j \tau A} u$

$\beta = \beta + a_j$

$t = t + a_j \tau$

$d = e^{b_j \tau B(t)} d + \mathcal{R}(\tau, t)\big(b_j B(t) + b_j \beta \tau B'(t)\big)u$

$\delta = e^{b_j \tau B(t)} \delta + \mathcal{R}(\tau, t)\big(b_j \tau B'(t)\big)u$

$u = e^{b_j \tau B(t)} u$

$d = \partial_3 \mathcal{E}_C(c_j \tau, t, u) \cdot d + c_j \partial_1 \mathcal{E}_C(c_j \tau, t, u)$

$\delta = \partial_3 \mathcal{E}_C(c_j \tau, t, u) \cdot d$

$u = \mathcal{E}_C(c_j \tau, t, u)$

end for

$d = d - \frac{1}{2}\big(Au + B(t)u + C(u) + \delta\big)$

return $u,\ d$

Chapter 4

Integration schemes

In this chapter we introduce specific self-adjoint integration schemes $\mathcal{S}(\tau, t_0, u_0) \approx \mathcal{E}(\tau, t_0, u_0)$, i.e., they satisfy

$$\mathcal{S}(-\tau, t_0 + \tau, \mathcal{S}(\tau, t_0, u_0)) = u_0,$$

and compute efficient representations of the integrators' defects.

In the case of linear problems the integrator usually is a splitting scheme of the form (3.12), see the upcoming Sections 4.1–4.3. In Section 4.4 we also consider a symplectic integration scheme which is not of the form (3.12). In any case, the integrator is typically linear in u_0, whence there holds (3.8). We remark that in these cases the self-adjoint property reads as in (3.9),

$$\mathcal{S}(-\tau, t_0 + \tau)\mathcal{S}(\tau, t_0)u_0 = u_0.$$

However, one presented integrator, introduced in Section 4.1, is only almost self-adjoint, i.e.,

$$\mathcal{S}(-\tau, t_0 + \tau)\mathcal{S}(\tau, t_0)u_0 = u_0 + \mathcal{O}(t^q),$$

for some sufficiently large q.

Towards the end of this chapter in Section 4.5 we ultimately discuss nonlinear splitting schemes of the form (3.21) for a nonlinear problem.

4.1 Exponential midpoint scheme

Consider (3.7), with $A = 0$, i.e.,

$$\tfrac{\mathrm{d}}{\mathrm{d}\tau}u(t_0 + \tau) = B(t_0 + \tau)u(t_0 + \tau), \quad u(t_0) = u_0. \tag{4.1}$$

The second-order (self-adjoint) exponential midpoint rule, applied to (4.1), is given by

$$\mathcal{S}(\tau, t_0) = e^{\tau B(t_0 + \frac{\tau}{2})}. \tag{4.2}$$

This scheme is taken from [3, pp.15–16]. Since $p = 2$, it holds that

$$\big(\mathcal{S}(\tau, t_0) - \mathcal{E}(\tau, t_0)\big)u_0 = \mathcal{L}(\tau, t_0)u_0 = \mathcal{O}(\tau^3).$$

The integrator (4.2) is a splitting scheme (3.12) with $J = 1$ and $a_1 = \frac{1}{2}, b_1 = 1$. So, one could easily apply Algorithms 1 and 2 for the defect evaluations. However, we discuss the defects in more detail here.

In [3, p.16] the classical and the symmetrized defect to (4.2) are already calculated:

- Classical defect (3.13):

$$\mathcal{D}_c(\tau, t_0) = \mathcal{R}(\tau, t_0)\big(B(t_0 + \tfrac{\tau}{2}) + \tfrac{1}{2}\tau B'(t_0 + \tfrac{\tau}{2})\big) - B(t_0 + \tau)\mathcal{S}(\tau, t_0). \tag{4.3}$$

- Symmetrized defect (3.14):

$$\mathcal{D}_s(\tau, t_0) = \mathcal{S}(\tau, t_0)\big(B(t_0 + \tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big) - \tfrac{1}{2}B(t_0 + \tau)\mathcal{S}(\tau, t_0). \tag{4.4}$$

Remark 4.1.1. For (4.3) we recall Section 3.5 and the representaion of the derivatives of the matrix exponential in (3.26):

$$\mathcal{R}(\tau, t_0)\big(\tfrac{\partial}{\partial\tau}(\tau B(t_0 + \tfrac{\tau}{2})\big) = \mathcal{R}(\tau, t_0)\big(B(t_0 + \tfrac{\tau}{2}) + \tfrac{1}{2}\tau B'(t_0 + \tfrac{\tau}{2})\big),$$

which we evaluate numerically by applying the quadrature formula from Remark 3.5.7.
The symmetrized defect (4.4) on the other hand is crucially simplified, since here the derivatives of the matrix exponential conveniently cancel out. This leaves a computational cost of only two evaluations of the matrix exponential. //

Next, we take a closer look at the corrected schemes

$$\widehat{\mathcal{S}}_c(\tau, t_0) = \mathcal{S}(\tau, t_0) - \tfrac{\tau}{3}\mathcal{D}_c(\tau, t_0), \tag{4.5}$$

and

$$\widehat{\mathcal{S}}_s(\tau, t_0) = \mathcal{S}(\tau, t_0) - \tfrac{\tau}{3}\mathcal{D}_s(\tau, t_0), \tag{4.6}$$

to (4.2) (see (2.17) and (2.18) in Definition 2.4.12). From Theorem 2.4.13 we see that

$$\widehat{\mathcal{L}}_c(\tau, t_0)u_0 = \mathcal{O}(\tau^4),$$

i.e., $\widehat{\mathcal{S}}_c$ has order 3, and from Theorem 2.4.14, that

$$\widehat{\mathcal{L}}_s(\tau, t_0)u_0 = \mathcal{O}(\tau^5),$$

i.e., $\widehat{\mathcal{S}}_s$ has order 4.
We continue by choosing $\widehat{\mathcal{S}}_s$ as the basic scheme:

$$\mathcal{S}^{(4)}(\tau, t_0) := \widehat{S}_s(\tau, t_0), \tag{4.7}$$

of order $p = 4$. Due to Theorem 2.4.14 we observed that

$$\mathcal{S}^{(4)}(-\tau, t_0 + \tau)\mathcal{S}^{(4)}(\tau, t_0) = \mathrm{Id} + \mathcal{O}(\tau^6),$$

thus, $\mathcal{S}^{(4)}$ is no longer self-adjoint. However, as reasoned in Remark 2.4.15 we still expect the symmetrized corrected scheme to (4.7), i.e.,

$$\widehat{\mathcal{S}}_s^{(4)}(\tau, t_0) = \mathcal{S}^{(4)}(\tau, t_0) - \tfrac{\tau}{5}\mathcal{D}_s^{(4)}(\tau, t_0), \tag{4.8}$$

to be of order 5, thus $\widehat{\mathcal{L}}_s^{(4)}(\tau, t_0)u_0 = \mathcal{O}(\tau^6)$. Here $\mathcal{D}_s^{(4)}$ denotes the symmetrized defect to (4.7) and $\widehat{\mathcal{L}}_s^{(4)}$ the local error $\widehat{\mathcal{L}}_s^{(4)}(\tau, t_0) = \widehat{\mathcal{S}}_s^{(4)}(\tau, t_0) - \mathcal{E}(\tau, t_0)$.

Since the symmetrized defect $\mathcal{D}_s(\tau, t_0)$ in (4.4)

(i) requires only two evaluations of the matrix exponential and

(ii) is evaluated exactly, due to the absence of derivatives of the matrix exponential,

the scheme $\mathcal{S}^{(4)}(\tau, t_0)$ is a proper candidate for taking a closer look at its symmetrized corrected scheme (4.8), although it 'only' has order 5. On that account, we collect the contributions of

$$\mathcal{D}_s^{(4)}(\tau, t_0) = \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}^{(4)}(\tau, t_0) - \tfrac{1}{2}\big(B(t_0 + \tau)\mathcal{S}^{(4)}(\tau, t_0) + \mathcal{S}^{(4)}(\tau, t_0)B(t_0)\big).$$

They are:

- $\partial_1\mathcal{S}^{(4)}(\tau, t_0)$:

$$\begin{aligned}\partial_1\mathcal{S}^{(4)}(\tau, t_0) &= \partial_1\mathcal{S}(\tau, t_0) - \tfrac{\partial}{\partial\tau}\big(\tfrac{\tau}{3}\mathcal{D}_s(\tau, t_0)\big)\\ &= \partial_1\mathcal{S}(\tau, t_0) - \tfrac{1}{3}\mathcal{D}_s(\tau, t_0) - \tfrac{\tau}{3}\partial_1\mathcal{D}_s(\tau, t_0),\end{aligned}$$

  where

$$\begin{aligned}\partial_1\mathcal{D}_s(\tau, t_0) = \partial_1\mathcal{S}(\tau, t_0)\big(B(t_0 + \tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big) + \mathcal{S}(\tau, t_0)\big(\tfrac{1}{2}B'(t_0 + \tfrac{\tau}{2})\big)\\ - \tfrac{1}{2}B'(t_0 + \tau)\mathcal{S}(\tau, t_0) - \tfrac{1}{2}B(t_0 + \tau)\partial_1\mathcal{S}(\tau, t_0).\end{aligned} \tag{4.9}$$

- $\partial_2\mathcal{S}^{(4)}(\tau, t_0)$:

$$\begin{aligned}\partial_2\mathcal{S}^{(4)}(\tau, t_0) &= \partial_2\mathcal{S}(\tau, t_0) - \tfrac{\partial}{\partial t_0}\big(\tfrac{\tau}{3}\mathcal{D}_s(\tau, t_0)\big)\\ &= \partial_2\mathcal{S}(\tau, t_0) - \tfrac{\tau}{3}\partial_2\mathcal{D}_s(\tau, t_0),\end{aligned}$$

  where

$$\begin{aligned}\partial_2\mathcal{D}_s(\tau, t_0) = \partial_2\mathcal{S}(\tau, t_0)\big(B(t_0 + \tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big) + \mathcal{S}(\tau, t_0)\big(B'(t_0 + \tfrac{\tau}{2}) - \tfrac{1}{2}B'(t_0)\big)\\ - \tfrac{1}{2}B'(t_0 + \tau)\mathcal{S}(\tau, t_0) - \tfrac{1}{2}B(t_0 + \tau)\partial_2\mathcal{S}(\tau, t_0).\end{aligned} \tag{4.10}$$

This sums up to

$$\begin{aligned}\mathcal{D}_s^{(4)}(\tau,t_0) &= \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}^{(4)}(\tau,t_0) - \tfrac{1}{2}\big(B(t_0+\tau)\mathcal{S}^{(4)}(\tau,t_0) + \mathcal{S}^{(4)}(\tau,t_0)B(t_0)\big)\\ &= \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau,t_0) - \tfrac{1}{3}\mathcal{D}_s(\tau,t_0) - \tfrac{\tau}{3}\partial_1\mathcal{D}_s(\tau,t_0) + \tfrac{1}{2}\tfrac{\tau}{3}\partial_2\mathcal{D}_s(\tau,t_0)\\ &\quad - \tfrac{1}{2}\big(B(t_0+\tau)\mathcal{S}^{(4)}(\tau,t_0) + \mathcal{S}^{(4)}(\tau,t_0)B(t_0)\big).\end{aligned} \tag{4.11}$$

Since

$$\begin{aligned}\big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau,t_0) &= \mathcal{R}(\tau,t_0)\big(B(t_0+\tfrac{\tau}{2}) + \tfrac{1}{2}\tau B'(t_0+\tfrac{\tau}{2})\big) - \tfrac{1}{2}\mathcal{R}(\tau,t_0)\big(\tau B'(t_0+\tfrac{\tau}{2})\big)\\ &= \mathcal{R}(\tau,t_0)\big(B(t_0+\tfrac{\tau}{2})\big) = B(t_0+\tfrac{\tau}{2})\mathcal{S}(\tau,t_0) = \mathcal{S}(\tau,t_0)B(t_0+\tfrac{\tau}{2}),\end{aligned} \tag{4.12}$$

and with the identities (4.9) and (4.10), we simplify (4.11) further:

$$\begin{aligned}\mathcal{D}_s^{(4)}(\tau,t_0) &= \mathcal{S}(\tau,t_0)B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{3}\big[\mathcal{S}(\tau,t_0)\big(B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big) - \tfrac{1}{2}B(t_0+\tau)\mathcal{S}(\tau,t_0)\big]\\ &\quad - \tfrac{\tau}{3}\big[\underline{\partial_1\mathcal{S}(\tau,t_0)\big(B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big)} + \mathcal{S}(\tau,t_0)\big(\tfrac{1}{2}B'(t_0+\tfrac{\tau}{2})\big)\\ &\qquad \underline{\underline{- \tfrac{1}{2}B'(t_0+\tau)\mathcal{S}(\tau,t_0)}} - \underline{\underline{\tfrac{1}{2}B(t_0+\tau)\partial_1\mathcal{S}(\tau,t_0)}}\big]\\ &\quad + \tfrac{\tau}{6}\big[\underline{\partial_2\mathcal{S}(\tau,t_0)\big(B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big)} + \mathcal{S}(\tau,t_0)\big(B'(t_0+\tfrac{\tau}{2}) - \tfrac{1}{2}B'(t_0)\big)\\ &\qquad \underline{\underline{- \tfrac{1}{2}B'(t_0+\tau)\mathcal{S}(\tau,t_0)}} - \underline{\underline{\tfrac{1}{2}B(t_0+\tau)\partial_2\mathcal{S}(\tau,t_0)}}\big]\\ &\quad - \tfrac{1}{2}\big(B(t_0+\tau)\mathcal{S}^{(4)}(\tau,t_0) + \mathcal{S}^{(4)}(\tau,t_0)B(t_0)\big)\\ &= \mathcal{S}(\tau,t_0)B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{3}\big[\mathcal{S}(\tau,t_0)\big(B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big) - \tfrac{1}{2}B(t_0+\tau)\mathcal{S}(\tau,t_0)\big]\\ &\quad - \tfrac{\tau}{3}\big[\underbrace{\big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau,t_0)}_{=\mathcal{S}(\tau,t_0)B(t_0+\frac{\tau}{2}),\ (4.12)}\big(B(t_0+\tfrac{\tau}{2}) - \tfrac{1}{2}B(t_0)\big) - \tfrac{1}{2}B(t_0+\tau)\underbrace{\big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau,t_0)}_{=B(t_0+\frac{\tau}{2})\mathcal{S}(\tau,t_0),\ (4.12)}\\ &\qquad - \tfrac{1}{4}B'(t_0+\tau)\mathcal{S}(\tau,t_0) + \tfrac{1}{4}\mathcal{S}(\tau,t_0)B'(t_0)\big]\\ &\quad - \tfrac{1}{2}\big(B(t_0+\tau)\mathcal{S}^{(4)}(\tau,t_0) + \mathcal{S}^{(4)}(\tau,t_0)B(t_0)\big).\end{aligned}$$

Summarizing the corresponding terms results in

$$\begin{aligned}\mathcal{D}_s^{(4)}(\tau,t_0) &= \mathcal{S}(\tau,t_0)\tfrac{1}{3}\big[B(t_0+\tfrac{\tau}{2})\big(2\,\mathrm{Id} - \tau B(t_0+\tfrac{\tau}{2}) + \tfrac{\tau}{2}B(t_0)\big) + \tfrac{1}{2}B(t_0) - \tfrac{\tau}{4}B'(t_0)\big]\\ &\quad + \tfrac{1}{6}\big[B(t_0+\tau)\big(\mathrm{Id} + \tau B(t_0+\tfrac{\tau}{2})\big) + \tfrac{\tau}{2}B'(t_0+\tau)\big]\mathcal{S}(\tau,t_0)\\ &\quad - \tfrac{1}{2}\big(B(t_0+\tau)\mathcal{S}^{(4)}(\tau,t_0) + \mathcal{S}^{(4)}(\tau,t_0)B(t_0)\big).\end{aligned} \tag{4.13}$$

With the computable representations of the defects (4.3), (4.4) and (4.13) it is now possible to perform numerical experiments that verify the expected orders of the schemes $\widehat{\mathcal{S}}_c$, $\widehat{\mathcal{S}}_s$ and $\widehat{\mathcal{S}}_s^{(4)}$. We do this in Section 5.2.1.

4.2 Strang splitting combined with exponential midpoint scheme

A second-order (self-adjoint) splitting scheme, applied to the linear, nonautonomous evolution equation (3.7) is given by

$$\mathcal{S}(\tau, t_0) = e^{\frac{\tau}{2}A} e^{\tau B(t_0+\frac{\tau}{2})} e^{\frac{\tau}{2}A}. \tag{4.14}$$

This is a combination of second-order Strang splitting with the exponential midpoint scheme (cf. Section 4.1) for the time dependent part $B(t)$. This scheme was introduced in [16, p.10]. The integrator (4.14) has the form (3.12), with $J = 2$ and

$$\begin{aligned} a_1 &= \tfrac{1}{2}, \quad b_1 = 1, \\ a_2 &= \tfrac{1}{2}, \quad b_2 = 0. \end{aligned}$$

One could apply Algorithms 1 and 2 to evaluate the defects. However, since a closer look at the symmetrized defect shows some crucial simplifications, we discuss the defects in more detail here.

In this case the partial derivatives (3.16) become

$$\begin{aligned} \partial_1 \mathcal{S}(\tau, t_0) &= \tfrac{1}{2} A \mathcal{S}(\tau, t_0) + e^{\frac{\tau}{2}A} \mathcal{R}(\tau, t_0) \big(\tfrac{\partial}{\partial \tau} \Omega(\tau, t_0)\big) e^{\frac{\tau}{2}A} + \tfrac{1}{2} \mathcal{S}(\tau, t_0) A, \\ \partial_2 \mathcal{S}(\tau, t_0) &= e^{\frac{\tau}{2}A} \mathcal{R}(\tau, t_0) \big(\tfrac{\partial}{\partial t_0} \Omega(\tau, t_0)\big) e^{\frac{\tau}{2}A}. \end{aligned} \tag{4.15}$$

Here, $\Omega(\tau, t_0) = \tau B(t_0 + \frac{\tau}{2})$, so the formulas (3.25)–(3.28) can be applied with $\alpha = 1$ and $\beta = \frac{1}{2}$. Consequently the symmetrized defect (3.14) simplifies to

$$\begin{aligned} \mathcal{D}_s(\tau, t_0) &= \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau, t_0) - \tfrac{1}{2}\big((A + B(t_0+\tau))\mathcal{S}(\tau, t_0) + \mathcal{S}(\tau, t_0)(A + B(t_0))\big) \\ &= \tfrac{1}{2} A \mathcal{S}(\tau, t_0) + e^{\frac{\tau}{2}A} \mathcal{R}(\tau, t_0) \big(\tfrac{\partial}{\partial \tau} \Omega(\tau, t_0)\big) e^{\frac{\tau}{2}A} + \tfrac{1}{2} \mathcal{S}(\tau, t_0) A \\ &\quad - \tfrac{1}{2} e^{\frac{\tau}{2}A} \mathcal{R}(\tau, t_0) \big(\tfrac{\partial}{\partial t_0} \Omega(\tau, t_0)\big) e^{\frac{\tau}{2}A} \\ &\quad - \tfrac{1}{2}\big(A + B(t_0+\tau)\big)\mathcal{S}(\tau, t_0) - \tfrac{1}{2}\mathcal{S}(\tau, t_0)\big(A + B(t_0)\big) \\ &= e^{\frac{\tau}{2}A}\Big(B(t_0 + \tfrac{\tau}{2}) + \tfrac{1}{2}\int_0^\tau F(\sigma; \tau)\, d\sigma\Big) \cdot e^{\tau B(t_0+\frac{\tau}{2})} e^{\frac{\tau}{2}A} \\ &\quad - \tfrac{1}{2} e^{\frac{\tau}{2}A}\Big(\int_0^\tau F(\sigma; \tau)\, d\sigma\Big) \cdot e^{\tau B(t_0+\frac{\tau}{2})} e^{\frac{\tau}{2}A} \\ &\quad - \tfrac{1}{2} B(t_0+\tau)\mathcal{S}(\tau, t_0) - \tfrac{1}{2}\mathcal{S}(\tau, t_0) B(t_0) \\ &= -\tfrac{1}{2} B(t_0+\tau)\mathcal{S}(\tau, t_0) + e^{\frac{\tau}{2}A} B(t_0 + \tfrac{\tau}{2}) e^{\tau B(t_0+\frac{\tau}{2})} e^{\frac{\tau}{2}A} - \tfrac{1}{2}\mathcal{S}(\tau, t_0) B(t_0). \end{aligned} \tag{4.16}$$

Remark 4.2.2. This is a crucial simplification of the symmetrized defect, since we do not have to numerically evaluate the integral term $\int_0^\tau F(\sigma; \tau)\, d\sigma$. On the other hand, the

classical defect involves a single evaluation of this term, which we evaluate numerically by applying the quadrature formula from Remark 3.5.7. //

With (3.30) the classical defect (3.13) here has the (slightly simplified) explicit representation:

$$\begin{aligned}
\mathcal{D}_c(\tau,t_0) &= \partial_1\mathcal{S}(\tau,t_0) - \big(A\mathcal{S}(\tau,t_0) + B(t_0+\tau)\mathcal{S}(\tau,t_0)\big)\\
&= \underline{\tfrac{1}{2}A\mathcal{S}(\tau,t_0)} + e^{\frac{\tau}{2}A}\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)\big)e^{\frac{\tau}{2}A} + \tfrac{1}{2}\mathcal{S}(\tau,t_0)A\\
&\quad - \big(\underline{A\mathcal{S}(\tau,t_0)} + B(t_0+\tau)\mathcal{S}(\tau,t_0)\big)\\
&= e^{\frac{\tau}{2}A}B(t_0+\tfrac{\tau}{2})e^{\tau B(t_0+\frac{\tau}{2})}e^{\frac{\tau}{2}A} + \tfrac{1}{2}e^{\frac{\tau}{2}A}\Big(\int_0^\tau F(\sigma;\tau)\,d\sigma\Big)\cdot e^{\tau B(t_0+\frac{\tau}{2})}e^{\frac{\tau}{2}A}\\
&\quad + \tfrac{1}{2}\mathcal{S}(\tau,t_0)A - \tfrac{1}{2}A\mathcal{S}(\tau,t_0) - B(t_0+\tau)\mathcal{S}(\tau,t_0)\\
&\overset{(3.30)}{\approx} - \tfrac{1}{2}\big(A+2\,B(t_0+\tau)\big)\mathcal{S}(\tau,t_0) + e^{\frac{\tau}{2}A}\big(B(t_0+\tfrac{\tau}{2}) + \tfrac{1}{4}\tau B'(t_0+\tfrac{\tau}{2})\big)e^{\tau B(t_0+\frac{\tau}{2})}e^{\frac{\tau}{2}A}\\
&\quad + e^{\frac{\tau}{2}A}e^{\tau B(t_0+\frac{\tau}{2})}\tfrac{1}{4}\tau B'(t_0+\tfrac{\tau}{2})e^{\frac{\tau}{2}A} + \tfrac{1}{2}\mathcal{S}(\tau,t_0)A.
\end{aligned} \tag{4.17}$$

Since we do not apply the Algorithms 1 and 2, the evaluation of the defects (4.16) and (4.17) was implemented in the most efficient way to combine as many evaluation steps as possible. Numerical tests are discussed in Section 5.2.2.

4.3 Triple Jump applied to Strang-midpoint-scheme

We recall the composition method introduced in Section 4.2 and apply it to the basic second-order scheme (4.14),

$$\mathcal{S}(\tau,t_0) = e^{\frac{\tau}{2}A}e^{\tau B(t_0+\frac{\tau}{2})}e^{\frac{\tau}{2}A},$$

which leads to the triple jump

$$\begin{aligned}
\mathcal{C}(\tau,t_0) &= \mathcal{S}(\gamma_1\tau,t_0+(\gamma_1+\gamma_2)\tau)\mathcal{S}(\gamma_2\tau,t_0+\gamma_1\tau)\mathcal{S}(\gamma_1\tau,t_0)\\
&= e^{\frac{\gamma_1}{2}\tau A}e^{\gamma_1\tau B(t_0+(1-\frac{\gamma_1}{2})\tau)}e^{\frac{\gamma_1+\gamma_2}{2}\tau A}e^{\gamma_2\tau B(t_0+\frac{1}{2}\tau)}e^{\frac{\gamma_1+\gamma_2}{2}\tau A}e^{\gamma_1\tau B(t_0+\frac{\gamma_1}{2}\tau)}e^{\frac{\gamma_1}{2}\tau A},
\end{aligned} \tag{4.18}$$

with time steps

$$\gamma_1 = \gamma_3 = \frac{1}{2-2^{\frac{1}{3}}}, \quad \gamma_2 = 1-2\gamma_1 = -\frac{2^{\frac{1}{3}}}{2-2^{\frac{1}{3}}}.$$

A closer look at (4.18), or the reasoning in Section 2.5.1 shows that $\mathcal{C}(\tau,t_0)$ is self-adjoint, which allows it to fit into the setting of Theorem 2.4.14. Due to Theorem 2.5.17 and Remark 2.5.18, we expect the integrator (4.18) to be of order $p=4$. It also is a splitting scheme of the form (3.12) with $J=4$ and coefficients $a_j, b_j,\ j=1,\dots,4$, displayed in Table 4.1.

j	a_j	b_j
1	$\frac{\gamma_1}{2}$	γ_1
2	$\frac{\gamma_1+\gamma_2}{2}$	γ_2
3	$\frac{\gamma_1+\gamma_2}{2}$	γ_1
4	$\frac{\gamma_1}{2}$	0

Table 4.1: Coefficients for the splitting scheme (4.18) of stage $J = 4$.

We can evaluate the classical defect

$$\mathcal{D}_c(\tau, t_0) = \partial_1 \mathcal{C}(\tau, t_0) - \big((A + B(t_0 + \tau))\mathcal{C}(\tau, t_0)\big),$$

and the symmetrized defect

$$\mathcal{D}_s(\tau, t_0) = \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{C}(\tau, t_0) - \tfrac{1}{2}\big((A + B(t_0 + \tau))\mathcal{C}(\tau, t_0) + \mathcal{C}(\tau, t_0)(A + B(t_0))\big),$$

with the Algorithms 1 and 2.

Remark 4.3.3. We define

$$\begin{aligned} \Omega_1(\tau, t_0) &:= \gamma_1 \tau B(t_0 + \tfrac{\gamma_1}{2}\tau), \\ \Omega_2(\tau, t_0) &:= \gamma_2 \tau B(t_0 + \tfrac{\tau}{2}), \\ \Omega_3(\tau, t_0) &:= \gamma_1 \tau B(t_0 + (1 - \tfrac{\gamma_1}{2})\tau), \end{aligned} \tag{4.19}$$

and for the occurring partial derivatives of the matrix exponentials $\mathcal{R}(\tau, t_0)\big(\frac{\partial}{\partial \tau}\Omega_i(\tau, t_0)\big)$ and $\mathcal{R}(\tau, t_0)\big(\frac{\partial}{\partial t_0}\Omega_i(\tau, t_0)\big)$ we remind again of Section 3.5. Since the operators $\Omega_i(\tau, t_0),\ i = 1, 2, 3$, are defined as in (4.19), the formulas (3.25)–(3.28) can be applied with $\alpha = \gamma_1, \gamma_2, \gamma_1$ and $\beta = \frac{\gamma_1}{2}, \frac{1}{2}, (1 - \frac{\gamma_1}{2})$. The numerical evaluation is effected using the fourth-order quadrature formulas in (3.32) from Remark 3.5.8. //

Numerical tests for the triple jump and its corrected schemes are realized in Section 5.2.3.

4.4 Symplectic integrators with time dependent potential

Again, consider the linear, nonautonomous problem (3.7). We present the self-adjoint and linear, so called gradient symplectic fourth-order scheme, introduced in [7, p.5]. To define it, we introduce the operator

$$\widetilde{A} := A + D, \quad \text{with } D := \overleftarrow{\frac{\partial}{\partial t}}, \tag{4.20}$$

where D denotes the *forward time derivative operator*. With it we introduce the gradient symplectic scheme ($p = 4$):

$$\mathcal{S}(\tau, t_0) = e^{\frac{1}{6}\tau B(t_0+\tau)} e^{\frac{1}{2}\tau A} e^{\frac{2}{3}\tau \widetilde{B}(t_0+\frac{\tau}{2})} e^{\frac{1}{2}\tau A} e^{\frac{1}{6}\tau B(t_0)}, \tag{4.21}$$

with the commutator-containing operator

$$\begin{aligned} \widetilde{B}(t) &:= B(t) + \tfrac{1}{48}t^2[B(t), [\widetilde{A}, B(t)]] \\ &= B(t) + \tfrac{1}{48}t^2[B(t), [A, B(t)]]. \end{aligned} \tag{4.22}$$

The simplification in the last equation arises from the fact that

$$[B(t), [\widetilde{A}, B(t)]] = [B(t), [A, B(t)]] + [B(t), [D, B(t)]]$$

and $[B(t), [D, B(t)]] = 0$, since

$$\begin{aligned} [B(t), [D, B(t)]]\psi(x,t) &= \big(2B(t)DB(t) - DB(t)B(t) - B(t)B(t)D\big)\psi(x,t) \\ &= 2B(t)\overleftarrow{\tfrac{\partial}{\partial t}}\big(B(t)\psi(x,t)\big) - \overleftarrow{\tfrac{\partial}{\partial t}}\big(B(t)^2\psi(x,t)\big) - B(t)^2\overleftarrow{\tfrac{\partial}{\partial t}}\psi(x,t) \\ &= 2B(t)B'(t)\psi(x,t) + 2B(t)^2\overleftarrow{\tfrac{\partial}{\partial t}}\psi(x,t) - 2B(t)B'(t)\psi(x,t) \\ &\quad - B(t)^2\overleftarrow{\tfrac{\partial}{\partial t}}\psi(x,t) - B(t)^2\overleftarrow{\tfrac{\partial}{\partial t}}\psi(x,t) = 0, \end{aligned}$$

for a t-differentiable function $\psi(x,t)$. The integrator (4.21) proves to be self-adjoint, since

$$\begin{aligned} \mathcal{S}(-\tau, t_0+\tau) &= e^{-\frac{1}{6}\tau B((t_0+\tau)-\tau)} e^{-\frac{1}{2}\tau A} e^{-\frac{2}{3}\tau \widetilde{B}((t_0+\tau)-\frac{\tau}{2})} e^{-\frac{1}{2}\tau A} e^{-\frac{1}{6}\tau B(t_0+\tau)} \\ &= e^{-\frac{1}{6}\tau B(t_0)} e^{-\frac{1}{2}\tau A} e^{-\frac{2}{3}\tau \widetilde{B}(t_0+\frac{\tau}{2})} e^{-\frac{1}{2}\tau A} e^{-\frac{1}{6}\tau B(t_0+\tau)} = S^{-1}(\tau, t_0), \end{aligned}$$

which allows (4.21) to fit into the setting of Theorem 2.4.14.

We apply the integrator (4.21) to special linear, nonautonomous evolution equations of type (3.6) depending on space and time, i.e.,

$$\tfrac{\partial}{\partial t}\psi(x,t) = \mathrm{i}\Delta\psi(x,t) + (-\mathrm{i})V(x,t)\psi(x,t), \quad x \in \mathbb{R}^n,\ t \geq 0, \tag{4.23}$$

where Δ denotes the Laplace operator and $V(x,t)$ represents a (complex-valued) potential.

Remark 4.4.4. After spatial discretization $\mathrm{i}\Delta\psi(x,t)$ plays the role of $Au(t)$, while $-\mathrm{i}V(x,t)\psi(x,t)$ becomes $B(t)u(t)$. In Sections 5.1.1 and 5.1.2 this procedure is described in more detail. //

The setting (4.23) allows a crucial simplification of the operator (4.22). We formulate this in the following theorem.

Theorem 4.4.5. *For problems of the kind* (4.23) *the operator* $[B(t), [A, B(t)]]$ *in* (4.22)*, with* $A = \mathrm{i}\Delta$ *and* $B(t) = -\mathrm{i}V(x,t)$*, simplifies to*

$$[-\mathrm{i}V(x,t), [\mathrm{i}\Delta, -\mathrm{i}V(x,t)]] = -2\sum_{i=1}^{n}\big(\tfrac{\partial}{\partial x_i}V(x,t)\big)^2. \tag{4.24}$$

Proof. We understand (4.24) by applying the generalized product rule for the Laplace operator (see (6.2)) multiple times. For simplification we may ignore the complex unit i due to linearity:

$$\begin{aligned}
&[V(x,t),[\Delta,V(x,t)]]\psi(x,t) = \big(2V(x,t)\Delta V(x,t) - V(x,t)^2\Delta - \Delta V(x,t)^2\big)\psi(x,t)\\
&= 2V(x,t)\Delta(V(x,t)\psi(x,t)) - V(x,t)^2\Delta\psi(x,t) - \Delta(V(x,t)^2\psi(x,t))\\
&= 2V(x,t)^2\Delta\psi(x,t) + 4V(x,t)\nabla V(x,t)\cdot\nabla\psi(x,t) + 2V(x,t)\psi(x,t)\Delta V(x,t)\\
&\quad - V(x,t)^2\Delta\psi(x,t) - V(x,t)^2\Delta\psi(x,t) - 2\nabla(V(x,t)^2)\cdot\nabla\psi(x,t) + \psi(x,t)\Delta(V(x,t)^2)\\
&= 4V(x,t)\nabla V(x,t)\cdot\nabla\psi(x,t) + 2V(x,t)\psi(x,t)\Delta V(x,t) - 4V(x,t)\nabla V(x,t)\cdot\nabla\psi(x,t)\\
&\quad - \psi(x,t)V(x,t)\Delta V(x,t) + \underline{2\psi(x,t)\nabla V(x,t)\cdot\nabla V(x,t)} - \psi(x,t)V(x,t)\Delta V(x,t)\\
&= 2\nabla V(x,t)\cdot\nabla V(x,t)\psi(x,t)\\
&= 2\sum_{i=1}^{n}\big(\tfrac{\partial}{\partial x_i}V(x,t)\big)^2\psi(x,t).
\end{aligned}$$

■

In all further considerations of this section we assume the setting (4.23), whence (4.24) applies. For notational reasons we define

$$\widehat{B}(t) := [-\mathrm{i}V(x,t),[\mathrm{i}\Delta,-\mathrm{i}V(x,t)]] = -2\sum_{i=1}^{n}\big(\tfrac{\partial}{\partial x_i}V(x,t)\big)^2,$$

and rewrite the integrator (4.21),

$$\mathcal{S}(\tau,t_0) = \underbrace{e^{\frac{1}{6}\tau B(t_0+\tau)}e^{\frac{1}{2}\tau A}}_{=:\,\mathcal{S}_3(\tau,t_0)}\underbrace{e^{\frac{2}{3}\tau\widetilde{B}(t_0+\frac{\tau}{2})}}_{=:\,\mathcal{S}_2(\tau,t_0)}\underbrace{e^{\frac{1}{2}\tau A}e^{\frac{1}{6}\tau B(t_0)}}_{=:\,\mathcal{S}_1(\tau,t_0)} = \mathcal{S}_3(\tau,t_0)\mathcal{S}_2(\tau,t_0)\mathcal{S}_1(\tau,t_0), \tag{4.25}$$

and define the operators

$$\begin{aligned}
\Omega_1(\tau,t_0) &:= \tfrac{1}{6}\tau B(t_0),\\
\widehat{\Omega}_2(\tau,t_0) &:= \tfrac{1}{72}\tau^3\widehat{B}(t_0+\tfrac{\tau}{2}),\\
\Omega_2(\tau,t_0) &:= \tfrac{2}{3}\tau B(t_0+\tfrac{\tau}{2}),\\
\Omega_3(\tau,t_0) &:= \tfrac{1}{6}\tau B(t_0+\tau).
\end{aligned} \tag{4.26}$$

So, with (4.22), (4.24), (4.26) and the fact that $B(t)$ and $\widehat{B}(t)$ commute, since they are <u>diagonal matrices</u> in the setting (4.23):

$$\mathcal{S}_2(\tau,t_0) = e^{\frac{2}{3}\tau\widetilde{B}(t_0+\frac{\tau}{2})} = e^{\frac{2}{3}\tau B(t_0+\frac{\tau}{2})}e^{\frac{1}{72}\tau^3\widehat{B}(t_0+\frac{\tau}{2})} = e^{\Omega_2(\tau,t_0)}e^{\widehat{\Omega}_2(\tau,t_0)}.$$

Applying the product and chain rule, the partial derivatives of (4.25) take the form

$$\begin{aligned}\partial_1\mathcal{S}(\tau,t_0) = \quad & \partial_1\mathcal{S}_3(\tau,t_0)\mathcal{S}_2(\tau,t_0)\mathcal{S}_1(\tau,t_0)\\ &+ \mathcal{S}_3(\tau,t_0)\partial_1\mathcal{S}_2(\tau,t_0)\mathcal{S}_1(\tau,t_0)\\ &+ \mathcal{S}_3(\tau,t_0)\mathcal{S}_2(\tau,t_0)\partial_1\mathcal{S}_1(\tau,t_0),\end{aligned} \tag{4.27}$$

where

$$\begin{aligned}\partial_1\mathcal{S}_1(\tau,t_0) &= \tfrac{1}{2}A\,\mathcal{S}_1(\tau,t_0) + e^{\frac{1}{2}\tau A}\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega_1(\tau,t_0)\big),\\ \partial_1\mathcal{S}_2(\tau,t_0) &= \tfrac{\partial}{\partial\tau}\big(e^{\Omega_2(\tau,t_0)}e^{\widehat{\Omega}_2(\tau,t_0)}\big)\\ &= \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega_2(\tau,t_0)\big)e^{\widehat{\Omega}_2(\tau,t_0)} + e^{\Omega_2(\tau,t_0)}\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\widehat{\Omega}_2(\tau,t_0)\big),\\ \partial_1\mathcal{S}_3(\tau,t_0) &= \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega_3(\tau,t_0)\big)e^{\frac{1}{2}\tau A} + \mathcal{S}_3(\tau,t_0)\,\tfrac{1}{2}A,\end{aligned} \tag{4.28}$$

and

$$\begin{aligned}\partial_2\mathcal{S}(\tau,t_0) = \quad & \partial_2\mathcal{S}_3(\tau,t_0)\mathcal{S}_2(\tau,t_0)\mathcal{S}_1(\tau,t_0)\\ &+ \mathcal{S}_3(\tau,t_0)\partial_2\mathcal{S}_2(\tau,t_0)\mathcal{S}_1(\tau,t_0)\\ &+ \mathcal{S}_3(\tau,t_0)\mathcal{S}_2(\tau,t_0)\partial_2\mathcal{S}_1(\tau,t_0),\end{aligned} \tag{4.29}$$

where

$$\begin{aligned}\partial_2\mathcal{S}_1(\tau,t_0) &= e^{\frac{1}{2}\tau A}\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega_1(\tau,t_0)\big),\\ \partial_2\mathcal{S}_2(\tau,t_0) &= \tfrac{\partial}{\partial t_0}\big(e^{\Omega_2(\tau,t_0)}e^{\widehat{\Omega}_2(\tau,t_0)}\big)\\ &= \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega_2(\tau,t_0)\big)e^{\widehat{\Omega}_2(\tau,t_0)} + e^{\Omega_2(\tau,t_0)}\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\widehat{\Omega}_2(\tau,t_0)\big),\\ \partial_2\mathcal{S}_3(\tau,t_0) &= \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega_3(\tau,t_0)\big)e^{\frac{1}{2}\tau A}.\end{aligned} \tag{4.30}$$

Remark 4.4.6. Just as with the triple jump from Section 4.3, the terms

$$\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\Omega_i(\tau,t_0)\big), \quad \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\Omega_i(\tau,t_0)\big), \quad i=1,2,3,$$

are numerically evaluated with the formulas (3.32) in Remark 3.5.8. Here, $\alpha = \frac{1}{6}, \frac{2}{3}, \frac{1}{6}$ and $\beta = 0, \frac{1}{2}, 1$ in those formulas. //

What is left, is a computable formula for the partial derivatives

$$\mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\widehat{\Omega}_2(\tau,t_0)\big), \quad \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\widehat{\Omega}_2(\tau,t_0)\big),$$

originating from the partial derivatives of the matrix exponential with exponent $\widehat{\Omega}_2(\tau,t_0) = \frac{1}{72}\tau^3\widehat{B}(t_0+\frac{\tau}{2})$. Since it differs in structure from the other operators in (4.26), we can not simply refer to the formulas (3.25)–(3.28) in Section 3.5. However, these formulas require only minor adaptation: With $\alpha := \frac{1}{72}, \beta := \frac{1}{2}$ and the integrand

$$\widehat{F}(\sigma;\tau) := e^{\sigma\alpha\tau^2\widehat{B}(t_0+\beta\tau)}\widehat{B}'(t_0+\beta\tau)e^{-\sigma\alpha\tau^2\widehat{B}(t_0+\beta\tau)},$$

we get

$$\tfrac{\partial}{\partial\tau}e^{\widehat{\Omega}_2(\tau,t_0)} = \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial\tau}\widehat{\Omega}_2(\tau,t_0)\big) = \alpha\tau^2\Big(3\widehat{B}(t_0+\beta\tau) + \beta\int_0^\tau \widehat{F}(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)}, \tag{4.31}$$

and

$$\tfrac{\partial}{\partial t_0}e^{\widehat{\Omega}_2(\tau,t_0)} = \mathcal{R}(\tau,t_0)\big(\tfrac{\partial}{\partial t_0}\widehat{\Omega}_2(\tau,t_0)\big) = \alpha\tau^2\Big(\int_0^\tau \widehat{F}(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)}. \tag{4.32}$$

Analogously to (3.32) we apply the fourth-order quadrature formula in (6.8) to numerically evalute the terms (4.31) and (4.32):

$$\begin{aligned}
&\Big(\int_0^\tau \widehat{F}(\sigma;\tau)\,d\sigma\Big)\cdot e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)}\\
&\approx \big(\tfrac{1}{2}\tau\big(\widehat{F}(0;\tau)+\widehat{F}(\tau;\tau)\big) + \tfrac{1}{12}\tau^2\big(\tfrac{\partial}{\partial\sigma}\widehat{F}(\sigma;\tau)\big|_{\sigma=0} - \tfrac{\partial}{\partial\sigma}\widehat{F}(\sigma;\tau)\big|_{\sigma=\tau}\big)\big)e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)}\\
&= \tfrac{1}{2}\tau\big(\widehat{B}'(t_0+\beta\tau)e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)} + e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)}\widehat{B}'(t_0+\beta\tau)\big)\\
&+\tfrac{1}{12}\tau^4\alpha\big(\big[\widehat{B}(t_0+\beta\tau),\widehat{B}'(t_0+\beta\tau)\big]e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)} - e^{\alpha\tau^3\widehat{B}(t_0+\beta\tau)}\big[\widehat{B}(t_0+\beta\tau),\widehat{B}'(t_0+\beta\tau)\big]\big).
\end{aligned} \tag{4.33}$$

Collecting all the identities and formulas in (4.25)–(4.33), we are able to evaluate the defects for the symplectic integration scheme (4.21):

- Classical defect (3.13):

$$\mathcal{D}_c(\tau,t_0) = \partial_1\mathcal{S}(\tau,t_0) - \big((A+B(t_0+\tau))\mathcal{S}(\tau,t_0)\big). \tag{4.34}$$

- Symmetrized defect (3.14):

$$\mathcal{D}_s(\tau,t_0) = \big(\partial_1 - \tfrac{1}{2}\partial_2\big)\mathcal{S}(\tau,t_0) - \tfrac{1}{2}\big((A+B(t_0+\tau))\mathcal{S}(\tau,t_0) + \mathcal{S}(\tau,t_0)(A+B(t_0))\big). \tag{4.35}$$

In numerical tests of the symplectic integration scheme and its corrected schemes, which are realized in Section 5.2.4, we evaluate the lengthy representations of the defects (4.34) and (4.35) in the most efficient way.

4.5 Nonlinear Strang splitting combined with exponential midpoint scheme

We now focus on the nonlinear problem (3.18). The second-order nonlinear Strang splitting to (3.18) is given by (3.21), with $J = 3$ stages and coefficients $a_j, b_j, c_j,\ j = 1,2,3$, displayed in Table 4.2:

$$\mathcal{S}(\tau,t_0,u_0) = e^{\frac{1}{2}\tau A}e^{\frac{1}{2}\tau B(t_0+\frac{\tau}{2})}\mathcal{E}_C\big(\tau,t_0+\tfrac{\tau}{2},e^{\frac{1}{2}\tau B(t_0+\frac{\tau}{2})}e^{\frac{1}{2}\tau A}u_0\big). \tag{4.36}$$

j	a_j	b_j	c_j
1	$\frac{1}{2}$	$\frac{1}{2}$	1
2	0	$\frac{1}{2}$	0
3	$\frac{1}{2}$	0	0

Table 4.2: Coefficients for the splitting scheme (4.36) of stage $J = 3$.

The scheme is taken from Winfried Auzinger's website [14]. We evaluate the nonlinear integrator (4.36) and its defects (3.22) and (3.22) with Algorithm 3 and Algorithm 4, respectively. For the occuring integral terms we rely on the second-order quadrature formulas in Remark 3.5.7. Numerical tests that verify the expected orders of the corrected schemes, are presented in Section 5.2.5.

4.6 Nonlinear fourth-order splitting scheme

A fourth-order nonlinear splitting scheme for the nonlinear problem (3.18) is given by (3.21), with $J = 11$ stages and coefficients $a_j, b_j, c_j,\ j = 1, \ldots, 11$, displayed in Table 4.3. The scheme is also taken from Winfried Auzinger's website [14, Auzinger/Ketcheson 2014] and is named AK 11-4.

j	a_j	b_j	c_j
1	0.257069044488538534	0.296061717549380091	0.592448417648034871
2	0.432582164538475621	0.704720077493718759	0.819259857623654322
3	−0.031637836548173035	−0.046163676369010239	−0.911708275271689193
4	−0.158013372478841120	−0.909236237348177222	0
5	a_4	0	c_3
6	0	b_3	0
7	a_3	0	c_2
8	0	b_2	0
9	a_2	0	c_1
10	0	b_1	0
11	a_1	0	0

Table 4.3: Coefficients for the splitting scheme AK 11-4 of stage $J = 11$.

We evaluate the integrator AK 11-4 and its defects (3.22) and (3.22) with Algorithms 3 and Algorithms 4, respectively. For the occuring integral terms we rely on the fourth-order quadrature formulas in Remark 3.5.8. Numerical tests that verify the expected orders of the corrected schemes, are presented in Section 5.2.6.

Chapter 5

Numerical results

In this chapter we present the numerical results of the integration schemes discussed in Chapter 4 applied to several specific problems, introduced in the subsequent Section 5.1.

5.1 Tested examples

We introduce suitable examples of linear, nonautonomous, as well as nonlinear, nonautonomous evolution equations.

5.1.1 Linear, nonautonomous Schrödinger equation with known solution

We state the linear, nonautonomous Schrödinger equation with time-dependent potential $t \mapsto V(x,t)$,

$$\frac{\partial}{\partial t}\psi(x,t) = \tfrac{1}{2}\mathrm{i}\frac{\partial^2}{\partial x^2}\psi(x,t) - \mathrm{i}V(x,t)\psi(x,t), \quad x \in [-16,16], \quad t \geq 0, \tag{5.1}$$

where the potential has the form

$$V(x,t) = -\tfrac{1}{2}|\psi_{\mathrm{ex}}(x,t)|^2.$$

The exact solution is known:

$$\psi_{\mathrm{ex}}(x,t) = \frac{2e^{\frac{3}{2}\mathrm{i}t - \mathrm{i}x}}{\cosh(2t+2x)},$$
$$u_0 := \psi_{ex}(x,0) = \frac{2e^{-\mathrm{i}x}}{\cosh(2x)}.$$

We choose final time $T = 1$ and impose periodic boundary conditions on the interval $[-16, 16]$. Spectral collocation at 1024 equidistant mesh points transforms (5.1) into a linear, nonautonomous ODE-system of the form (3.6). Here the spatially discretized potential $t \mapsto -\mathrm{i}V(x,t)$ plays the role of $B(t)$, in the form

$$B(t) = \mathrm{diag}(\text{-}\mathrm{i}V(x,t)), \tag{5.2}$$

while the kinetic term $\frac{1}{2}\mathrm{i}\frac{\partial^2}{\partial x^2}\psi(x,t)$ plays the role of $Au(t)$. The latter is discretized in space using pseudospectral Fourier-type collocation. For more details, we refer to Appendix 6.4. In Figure 5.1 the reference solution of problem (5.1) with potential (5.2) is displayed.
In the subsequent Section 5.2 we present numerical results for suitable integrators (introduced in Chapter 4) applied to problem (5.1) with potential (5.2).

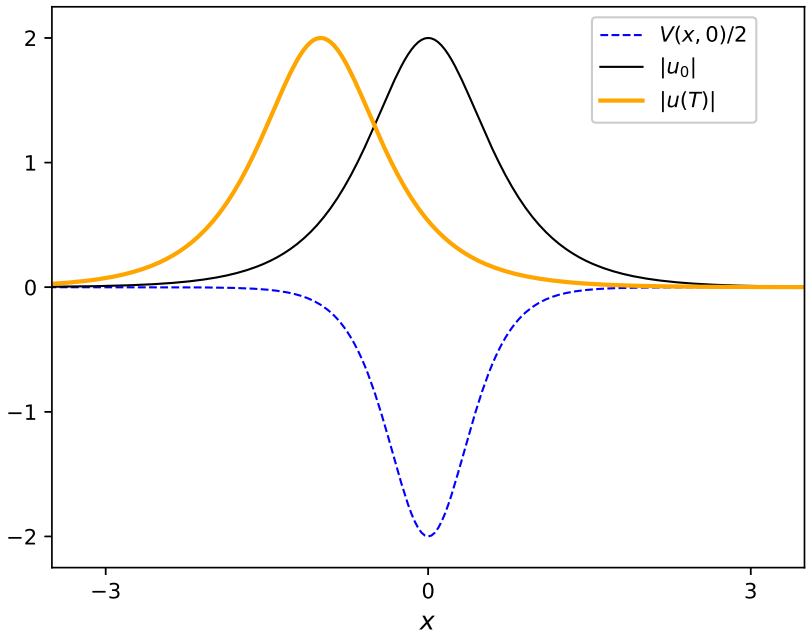

Figure 5.1: Plots of the potential $V(x,0)$, as well as the absolute values of the initial value u_0 and the complex-valued solution $u(T)$ at the final time $T = 1$, over $x = [-16, 16]$. The solution evolves from u_0 consistently to the left under the influence of V.

5.1.2 Linear, nonautonomous Schrödinger equation with unknown solution

This example is taken from [13, pp.21–22]. We state the linear, nonautonomous Schrödinger equation with time-dependent potential $t \mapsto V(x,t)$,

$$\frac{\partial}{\partial t}\psi(x,t) = \mathrm{i}\frac{\partial^2}{\partial x^2}\psi(x,t) - \mathrm{i}V(x,t)\psi(x,t), \quad x \in [-10,10], \quad t \geq 0. \tag{5.3}$$

The initial condition is a Gaussian wave packet

$$u_0(x) = (\delta\pi)^{-1/4} \exp\big(-\tfrac{1}{2\delta}(x-x_0)^2\big), \quad x_0 = -2.5, \quad \delta = 0.2,$$

which sits in the left well of a double well potential

$$V_D(x) = x^4 - 20x^2.$$

We choose $[-10,10]$ as the spatial domain and $[0,5]$ as the temporal domain of our problem. When we allow the wave function to evolve under V_D, it remains largely confined to the left well at the final time, $T = 5$ (see Figure 5.2). Superimposing a time dependent excitation to the potential, we are able to exert control on the wave function. The effective time-varying potential in this case is

$$V_S(x,t) = V_D(x,t) + 10S_{10,T}(t)x,$$

with $S_{\omega,T}(t) = \sin((\pi t/T)^2)\sin(\omega T)$. Again, spectral collocation at 512 equidistant mesh points leads to the linear, nonautonomous ODE-system (3.6). Choosing the potential $V_D(x)$ implies

$$B = B(t) = \mathrm{diag}(\text{-}\mathrm{i}V_D(x)), \tag{5.4}$$

which makes (5.3) an autonomous problem. Choosing the potential $V_S(x,t)$, we obtain

$$B(t) = \mathrm{diag}(\text{-}\mathrm{i}V_S(x,t)). \tag{5.5}$$

We proceed analogously to the previous Section 5.1.1 to determine the evaluation of $Au(t)$. In Figure 5.2 the (numerically approximated) solutions to the problem (5.3) are displayed. In the subsequent Section 5.2 we present numerical results for suitable integrators (introduced in Chapter 4) applied to the example (5.3) with potentials (5.4) and (5.5).

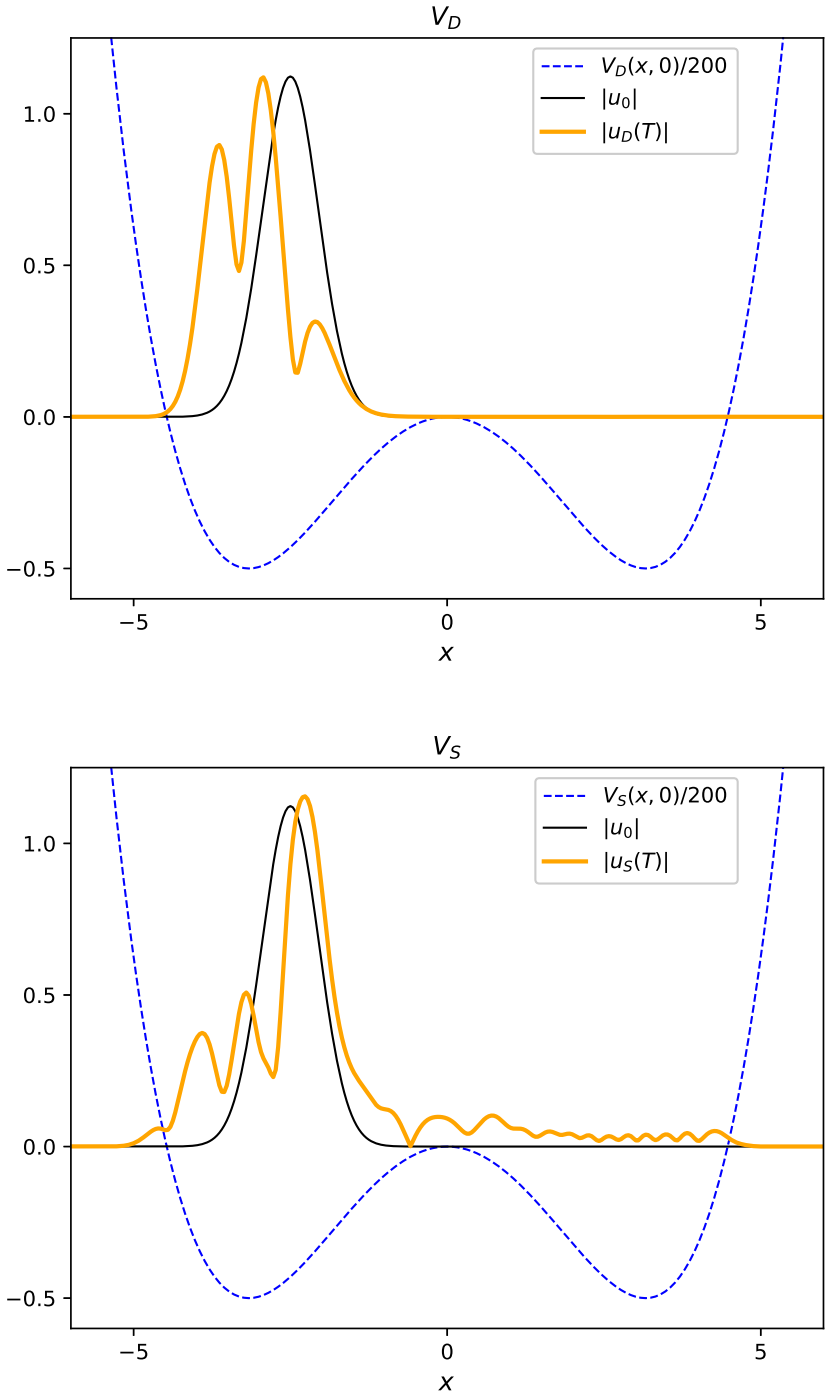

Figure 5.2: Plots of the real-valued potential $V_D(x,0) = V_S(x,0)$, as well as the absolute values of the initial value u_0 and the complex-valued solutions $u_D(T)$ and $u_S(T)$ at final time $T = 5$, over $x = [-10, 10]$. The solutions evolve from u_0 under the influence of V_D and V_S, respectively.

5.1.3 Rosen-Zener model

This example is taken from [6] and was also used in [3, p.22]. The linear, nonautonomous Schrödinger equation is given by

$$\mathrm{i}\dot{\psi}(t) = H(t)\psi(t), \tag{5.6}$$

with

$$\begin{aligned}
&H(t) = f_1(t)\sigma_1 \otimes I_{k\times k} + f_2(t)\sigma_2 \otimes R \in \mathbb{C}^{2k\times 2k}, \quad k = 100,\\
&\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix},\\
&R = \mathrm{tridiag}(1, 0, 1) \in \mathbb{R}^{k\times k}, \quad f_1(t) = V_0 \cos(\omega t)(\cosh(t/T_0))^{-1},\\
&f_2(t) = V_0 \sin(\omega t)(\cosh(t/T_0))^{-1}, \quad \omega = \tfrac{1}{2},\ T_0 = 1,\ V_0 = 1.
\end{aligned}$$

We consider the initial condition

$$\psi(0) = (1, \ldots, 1)^T.$$

In Section 5.2.1 we give the local error and the deviations for the integrators introduced in Section 4.1 applied to the problem (5.6).

5.1.4 Cubic, nonlinear, nonautonomous Schrödinger equation

For this nonlinear, nonautonomous problem we merge two examples from [1, p.10] and [4, p.197]. We state the cubic, nonlinear, nonautonomous Schrödinger equation with time-dependent potential $t \mapsto V_\alpha(x,t) = (1-\alpha)\kappa|\psi_{\mathrm{ex}}(x,t)|^2$,

$$\tfrac{\partial}{\partial t}\psi(x,t) = \tfrac{\mathrm{i}}{2}\tfrac{\partial^2}{\partial x^2}\psi(x,t) - \mathrm{i}V_\alpha(x,t)\psi(x,t) - \mathrm{i}\alpha\kappa|\psi(x,t)|^2\psi(x,t), \quad x \in [-16,16], \quad t \geq 0. \tag{5.7}$$

The exact solution is given by

$$\begin{aligned}
\psi_{\mathrm{ex}}(x,t) &= \frac{2e^{\frac{3}{2}\mathrm{i}t - \mathrm{i}x}}{\cosh(2t+2x)},\\
u_0 := \psi_{ex}(x,0) &= \frac{2e^{-\mathrm{i}x}}{\cosh(2x)}.
\end{aligned}$$

We choose $\kappa = -1$, $\alpha = \frac{1}{2}$, final time $T = 1$ and impose periodic boundary conditions on the interval $[-16, 16]$. Spectral collocation at 1024 equidistant mesh points transforms (5.7) into a nonlinear, nonautonomous ODE system of the form (3.17).

Remark 5.1.1. This example is constructed, so that it represents the same problem with the same solution as the one from Section 5.1.1, however with an 'artificially' constructed nonlinear component. Therefore, one observes the solution in Figure 5.1. //

The evaluations of $Au(t)$ and $B(t)u(t)$ and their respective subflows work in the same way as in the purely linear cases above. The evaluation of $C(u(t)) = -\mathrm{i}\alpha\kappa|u(t)|^2u(t)$ works pointwise. For the problem (5.7) the subflow associated with $C(u(t))$ and its partial derivatives (cf. (3.20)) are known and stated in [4, pp.194,197]:

$$\begin{aligned}
\mathcal{E}_C(\tau, t_0, u_0) &= e^{-\mathrm{i}\alpha\kappa\tau|u_0|^2}u_0,\\
\partial_1\mathcal{E}_C(\tau, t_0, u_0) &= -\mathrm{i}\alpha\kappa|u_0|^2e^{-\mathrm{i}\alpha\kappa\tau|u_0|^2}u_0,\\
\partial_2\mathcal{E}_C(\tau, t_0, u_0) &= 0,\\
\partial_3\mathcal{E}_C(\tau, t_0, u_0)\cdot\phi &= e^{-\mathrm{i}\alpha\kappa\tau|u_0|^2}\big(\phi - \mathrm{i}\alpha\kappa\tau(|u_0|^2\phi + (u_0)^2\overline{\phi})\big).
\end{aligned}$$

In the subsequent Section 5.2 we present numerical results for the nonlinear splitting schemes introduced in Sections 4.5 and 4.6 applied to problem (5.7).

5.2 Empirical local errors and deviations

In this section we conclude this thesis by presenting the numerical data, that verify the expected local errors and deviations for the integrators introduced in Chapter 4. The Codes for the numerical experiments were written in the Julia Language Version 1.0.0, its first official release. The codes were run on a MacBook Air (13 inch, mid 2012) with 1,8 GHz Intel Core i5 processor and 8 GB 1600 MHz DDR3 ram.

5.2.1 Exponential midpoint scheme

We test the exponential midpoint scheme (4.2),

$$\mathcal{S}(\tau, t_0) = e^{\tau B(t_0+\frac{\tau}{2})},$$

of order $p = 2$ and its corresponding corrected schemes $\widehat{\mathcal{S}}_c$ and $\widehat{\mathcal{S}}_s$, introduced in (4.5) and (4.6), respectively (see Section 4.1), by applying them to the Rosen-Zener model from Section 5.1.3. Table 5.1 displays the local error and the deviations, as well as the empirical convergence rates.
Moreover, in Table 5.2 we display the results for the symmetrized corrected scheme $\widehat{\mathcal{S}}_s^{(4)}$ to the corrected scheme $\mathcal{S}^{(4)} = \widehat{\mathcal{S}}_s$, introduced in (4.8). According to the theory we expect $\widehat{\mathcal{S}}_s^{(4)}$ to be of order 5, which we verify. We remark that $\mathcal{S}, \mathcal{S}^{(4)}$ and $\widehat{\mathcal{S}}_s^{(4)}$ can be evaluated exactly, due to the absence of derivatives of the matrix exponential.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0\ -\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u-\mathcal{L}\,\psi_0\|_2$	order
1.00e+00	1.73e-01		4.83e-02		2.10e-02	
5.00e-01	2.79e-02	2.63	2.65e-03	4.19	9.24e-04	4.51
2.50e-01	3.74e-03	2.90	1.38e-04	4.26	3.19e-05	4.86
1.25e-01	4.76e-04	2.97	7.98e-06	4.11	1.02e-06	4.96
6.25e-02	5.98e-05	2.99	4.87e-07	4.03	3.22e-08	4.99
3.13e-02	7.48e-06	3.00	3.03e-08	4.01	1.01e-09	5.00
1.56e-02	9.35e-07	3.00	1.89e-09	4.00	3.15e-11	5.00
7.81e-03	1.17e-07	3.00	1.18e-10	4.00	9.83e-13	5.00
3.91e-03	1.46e-08	3.00	7.38e-12	4.00	3.07e-14	5.00

Table 5.1: Local error, deviations and empirical convergence rates for the exponential midpoint scheme (order $p = 2$) and its corrected schemes, applied to the Rosen-Zener model from Section 5.1.3.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s^{(4)}\,\psi_0\,u-\mathcal{L}\,\psi_0\|_2$	order
1.00e+00	2.10e-02		2.73e-03	
5.00e-01	9.24e-04	4.51	5.99e-05	5.51
2.50e-01	3.19e-05	4.86	1.02e-06	5.88
1.25e-01	1.02e-06	4.96	1.62e-08	5.97
6.25e-02	3.22e-08	4.99	2.54e-10	5.99
3.13e-02	1.01e-09	5.00	3.97e-12	6.00
1.56e-02	3.15e-11	5.00	6.25e-14	5.99

Table 5.2: Local error, deviations and empirical convergence rates for the scheme $\mathcal{S}^{(4)}$ (order $p = 4$) and its symmetrized corrected scheme, applied to the Rosen-Zener model from Section 5.1.3.

5.2.2 Strang splitting with exponential midpoint scheme

In this section we examine the numerical tests for the second-order integration scheme introduced in (4.14),

$$\mathcal{S}(\tau, t_0) = e^{\frac{\tau}{2}A} e^{\tau B(t_0+\frac{\tau}{2})} e^{\frac{\tau}{2}A},$$

as well as its corresponding corrected schemes $\widehat{\mathcal{S}}_c$ and $\widehat{\mathcal{S}}_s$ (see Section 4.2). We apply these schemes to both linear, nonautonomous Schrödinger equations in Sections 5.1.1 and 5.1.2: Table 5.3 displays the local errors and the deviations, as well as the empirical convergence rates for the problem in Section 5.1.1, while Table 5.4 displays the same quantities for the problem in Section 5.1.2. We see that the expected convergence rates can be verified.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0\,-\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u-\mathcal{L}\,\psi_0\|_2$	order
1.00e+00	1.94e+00		4.86e+00		1.43e+00	
5.00e-01	6.46e-01	1.59	9.91e-01	2.29	3.39e-01	2.08
2.50e-01	1.56e-01	2.05	1.64e-01	2.60	5.30e-02	2.68
1.25e-01	2.83e-02	2.46	1.92e-02	3.09	5.00e-03	3.41
6.25e-02	4.17e-03	2.76	1.63e-03	3.56	2.87e-04	4.12
3.13e-02	5.51e-04	2.92	1.14e-04	3.84	1.15e-05	4.64
1.56e-02	7.00e-05	2.98	7.33e-06	3.95	3.89e-07	4.89
7.81e-03	8.78e-06	2.99	4.62e-07	3.99	1.24e-08	4.97
3.91e-03	1.10e-06	3.00	2.89e-08	4.00	3.90e-10	4.99
1.95e-03	1.37e-07	3.00	1.81e-09	4.00	1.22e-11	5.00
9.77e-04	1.72e-08	3.00	1.13e-10	4.00	3.82e-13	5.00

Table 5.3: Local error, deviations and empirical convergence rates for the splitting scheme (4.14) of order $p = 2$ and its corrected schemes, applied to the evolution equation from Section 5.1.1.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0\,-\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u-\mathcal{L}\,\psi_0\|_2$	order
1.56e-01	6.85e-01	1.01	7.63e-01	6.74	4.04e-01	6.50
7.81e-02	1.09e-01	2.65	1.90e-02	5.32	8.38e-03	5.59
3.91e-02	1.43e-02	2.94	9.61e-04	4.31	1.49e-04	5.81
1.95e-02	1.81e-03	2.98	5.87e-05	4.03	2.98e-06	5.64
9.77e-03	2.26e-04	3.00	3.66e-06	4.00	7.41e-08	5.33
4.88e-03	2.83e-05	3.00	2.29e-07	4.00	2.14e-09	5.11
2.44e-03	3.54e-06	3.00	1.43e-08	4.00	6.54e-11	5.03
1.22e-03	4.43e-07	3.00	8.94e-10	4.00	2.03e-12	5.01
6.10e-04	5.53e-08	3.00	5.59e-11	4.00	6.32e-14	5.01
3.05e-04	6.91e-09	3.00	3.49e-12	4.00	1.99e-15	4.99

Table 5.4: Local error, deviations and empirical convergence rates for the splitting scheme (4.14) of order $p = 2$ and its corrected schemes, applied to the evolution equation from Section 5.1.2.

5.2.3 Triple Jump applied to Strang-midpoint-scheme

We continue our numerical experiments with the natural successor of the previous section, the triple jump introduced in (4.18) of order $p = 4$,

$$\mathcal{C}(\tau, t_0) = e^{\frac{\gamma_1}{2}\tau A} e^{\gamma_1 \tau B(t_0+(1-\frac{\gamma_1}{2})\tau)} e^{\frac{\gamma_1+\gamma_2}{2}\tau A} e^{\gamma_2 \tau B(t_0+\frac{1}{2}\tau)} e^{\frac{\gamma_1+\gamma_2}{2}\tau A} e^{\gamma_1 \tau B(t_0+\frac{\gamma_1}{2}\tau)} e^{\frac{\gamma_1}{2}\tau A},$$

with time steps

$$\gamma_1 = \gamma_3 = \frac{1}{2 - 2^{\frac{1}{3}}}, \quad \gamma_2 = 1 - 2\gamma_1 = -\frac{2^{\frac{1}{3}}}{2 - 2^{\frac{1}{3}}},$$

see Section 4.3. We apply the triple jump and its corrected schemes to both linear, nonautonomous Schrödinger equations in Sections 5.1.1 and 5.1.2: Table 5.5 displays the local error and the deviations, as well as the empirical convergence rates for the problem in Section 5.1.1,

while Table 5.6 displays the same quantities for the problem in Section 5.1.2. The tables verify the convergence rates expected from theory.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u - \mathcal{L}\,\psi_0\|_2$	order
1.00e+00	1.85e+00		6.07e+00		2.44e+00	
5.00e-01	6.29e-01	1.55	8.61e-01	2.82	4.11e-01	2.57
2.50e-01	8.20e-02	2.94	8.27e-02	3.38	3.41e-02	3.59
1.25e-01	6.29e-03	3.70	4.95e-03	4.06	1.58e-03	4.44
6.25e-02	3.14e-04	4.32	1.66e-04	4.90	3.59e-05	5.46
3.13e-02	1.18e-05	4.74	3.55e-06	5.55	4.54e-07	6.30
1.56e-02	3.88e-07	4.92	6.12e-08	5.86	4.18e-09	6.76
7.81e-03	1.23e-08	4.98	9.82e-10	5.96	3.42e-11	6.93
3.91e-03	3.86e-10	4.99	1.54e-11	5.99	2.70e-13	6.98
1.95e-03	1.21e-11	5.00	2.42e-13	6.00	5.30e-15	5.67
9.77e-04	3.77e-13	5.00	5.63e-15	5.42	4.21e-15	0.33

Table 5.5: Local error, deviations and empirical convergence rates for the triple jump (4.18) of order $p = 4$ and its corrected schemes, applied to the problem from Section 5.1.1.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u - \mathcal{L}\,\psi_0\|_2$	order
1.56e-01	7.59e-01	0.91	1.36e+01	3.62	6.42e+00	4.12
7.81e-02	2.83e-02	4.74	7.20e-03	10.88	4.04e-03	10.63
3.91e-02	8.68e-04	5.03	4.14e-05	7.44	1.56e-05	8.02
1.95e-02	2.69e-05	5.01	5.56e-07	6.22	1.15e-07	7.08
9.77e-03	8.40e-07	5.00	8.41e-09	6.05	8.85e-10	7.02
4.88e-03	2.63e-08	5.00	1.30e-10	6.01	6.89e-12	7.01
2.44e-03	8.20e-10	5.00	2.03e-12	6.00	5.38e-14	7.00
1.22e-03	2.56e-11	5.00	3.20e-14	5.99	2.19e-15	4.62

Table 5.6: Local error, deviations and empirical convergence rates for the triple jump (4.18) of order $p = 4$ and its corrected schemes, applied to the problem from Section 5.1.2.

5.2.4 Symplectic integrators with time dependent potential

We now apply the integrator (4.21),

$$\mathcal{S}(\tau, t_0) = e^{\frac{1}{6}\tau B(t_0+\tau)} e^{\frac{1}{2}\tau A} e^{\frac{2}{3}\tau \widetilde{B}(t_0+\frac{\tau}{2})} e^{\frac{1}{2}\tau A} e^{\frac{1}{6}\tau B(t_0)},$$

and its corresponding corrected schemes $\widehat{\mathcal{S}}_c$ and $\widehat{\mathcal{S}}_s$ (see Section 4.4) to the linear, nonautonomous Schrödinger equation in Section 5.1.1: Table 5.7 displays the local error and the deviations, as well as the empirical convergence rates for this problem. We verify the expected convergence rates of the integrators.

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u - \mathcal{L}\,\psi_0\|_2$	order
1.00e+00	1.12e+00		2.13e+00		9.12e-01	
5.00e-01	2.69e-01	2.06	3.38e-01	2.66	1.83e-01	2.32
2.50e-01	4.42e-02	2.61	4.44e-02	2.93	2.23e-02	3.04
1.25e-01	4.30e-03	3.36	3.25e-03	3.77	1.35e-03	4.04
6.25e-02	2.50e-04	4.11	1.25e-04	4.70	3.78e-05	5.16
3.13e-02	1.00e-05	4.64	2.92e-06	5.42	5.41e-07	6.12
1.56e-02	3.39e-07	4.89	5.22e-08	5.81	5.24e-09	6.69
7.81e-03	1.08e-08	4.97	8.47e-10	5.95	4.35e-11	6.91
3.91e-03	3.40e-10	4.99	1.34e-11	5.99	3.46e-13	6.98
1.95e-03	1.07e-11	5.00	2.09e-13	6.00	5.48e-15	5.98
9.77e-04	3.33e-13	5.00	5.19e-15	5.33	4.07e-15	0.43

Table 5.7: Local error, deviations and empirical convergence rates for the symplectic integration scheme (4.21) of order $p = 4$ and its corrected schemes, applied to the problem from Section 5.1.1.

5.2.5 Nonlinear Strang splitting combined with exponential midpoint scheme

To conclude this thesis we test the introduced nonlinear splitting schemes for the nonlinear problem (5.7), which we introduced in Section 5.1.4.

Table 5.8 displays the local error and the deviations, as well as the expected empirical convergence rates of the nonlinear Strang splitting scheme (4.36) and its corrected schemes from Section 4.5 applied to problem (5.7).

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u - \mathcal{L}\,\psi_0\|_2$	order
1.00e+00	1.52e+00		2.20e+00		1.03e+00	
5.00e-01	4.66e-01	1.71	5.46e-01	2.01	2.33e-01	2.14
2.50e-01	1.07e-01	2.12	1.01e-01	2.44	3.67e-02	2.67
1.25e-01	1.92e-02	2.48	1.20e-02	3.06	3.45e-03	3.41
6.25e-02	2.82e-03	2.77	1.03e-03	3.55	2.13e-04	4.02
3.13e-02	3.73e-04	2.92	7.57e-05	3.77	1.03e-05	4.37
1.56e-02	4.74e-05	2.98	5.10e-06	3.89	4.01e-07	4.69
7.81e-03	5.94e-06	2.99	3.26e-07	3.96	1.35e-08	4.90
3.91e-03	7.44e-07	3.00	2.05e-08	3.99	4.29e-10	4.97
1.95e-03	9.30e-08	3.00	1.29e-09	4.00	1.35e-11	4.99
9.77e-04	1.16e-08	3.00	8.04e-11	4.00	4.22e-13	5.00

Table 5.8: Local error, deviations and empirical convergence rates for the nonlinear splitting scheme (4.36) of order $p = 2$ and its corrected schemes, applied to the nonlinear problem from Section 5.1.4.

5.2.6 Nonlinear fourth-order splitting scheme

Table 5.9 displays the local error and the deviations, as well as the expected empirical convergence rates of the nonlinear splitting scheme AK 11-4 and its corrected schemes from Section 4.6 applied to problem (5.7).

t	$\|\mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_c\,\psi_0 - \mathcal{L}\,\psi_0\|_2$	order	$\|\widetilde{\mathcal{L}}_s\,\psi_0\,u - \mathcal{L}\,\psi_0\|_2$	order
1.00e+00	1.86e+00		8.68e+00		4.73e+00	
5.00e-01	4.04e-01	2.20	6.52e-01	3.73	3.14e-01	3.91
2.50e-01	5.13e-02	2.97	4.96e-02	3.72	2.28e-02	3.79
1.25e-01	4.27e-03	3.59	3.19e-03	3.96	1.16e-03	4.29
6.25e-02	2.19e-04	4.29	1.17e-04	4.76	2.72e-05	5.41
3.13e-02	7.88e-06	4.79	2.44e-06	5.59	2.60e-07	6.71
1.56e-02	2.51e-07	4.97	3.99e-08	5.93	1.59e-09	7.35
7.81e-03	7.85e-09	5.00	6.33e-10	5.98	1.19e-11	7.07
3.91e-03	2.45e-10	5.00	9.95e-12	5.99	9.47e-14	6.97
1.95e-03	7.67e-12	5.00	1.56e-13	5.99	5.90e-15	4.01

Table 5.9: Local error, deviations and empirical convergence rates for the nonlinear fourth-order splitting scheme AK 11-4 from Section 4.6 and its corrected schemes, applied to the nonlinear problem from Section 5.1.4.

Chapter 6

Appendix

We use the Appendix to list various well known definitions, theorems and methods, that would disrupt the reading flow, but are key parts of this thesis.

6.1 Definitions and theorems

Definition 6.1.1 (Commutator, [2]). *For two elements a, b of an associative algebra $\mathcal{A}$, the shared commutator is defined as*

$$[a, b] := ab - ba. \tag{6.1}$$

If $a, b \in \mathcal{A}$ commute, then $[a, b] = 0$.

Theorem 6.1.2 (Product rule for the Laplace operator). *For two functions $f, g : \mathbb{R}^n \supset \mathcal{U} \to \mathbb{R}$, with $f, g \in C^2(\mathcal{U})$ there holds the generalized product rule*

$$\Delta\big(f(x)g(x)\big) = f(x)\Delta g(x) + 2\nabla f(x) \cdot \nabla g(x) + g(x)\Delta f(x),\ x \in \mathcal{U}. \tag{6.2}$$

Here, $\cdot$ denotes the standard scalar product on $\mathbb{R}^n$.

Proof. (6.2) is an immediate consequence of the conventional product rule,

$$\tfrac{\partial^2}{\partial x_i^2}\big(f(x)g(x)\big) = f(x)\tfrac{\partial^2}{\partial x_i^2}g(x) + 2\tfrac{\partial}{\partial x_i}f(x)\tfrac{\partial}{\partial x_i}g(x) + g(x)\tfrac{\partial^2}{\partial x_i^2}f(x), \quad i = 1, \dots, n,$$

with $x = (x_1, \dots, x_n)$, since $\Delta = \frac{\partial^2}{\partial x_1^2} + \cdots + \frac{\partial^2}{\partial x_n^2}$. ■

6.2 Fréchet derivative of the matrix exponential

Throughout this thesis we encounter matrix exponentials of the form

$$t \mapsto e^{\Omega(t)}, \tag{6.3}$$

where the exponent is a time dependent operator. Differentiation of (6.3) with respect to t involves to know its Fréchet derivative $\frac{\mathrm{d}}{\mathrm{d}\Omega}e^{\Omega}\big|_{\Omega=\Omega(t)}(\cdot)$, which is not straightforward to compute. The key is the following theorem, which is presented in [12, p.238]. It provides us with an explicit representation of the Fréchet derivative of the matrix exponential.

Theorem 6.2.3. *The Fréchet derivative of the matrix exponential, i.e., $\frac{\mathrm{d}}{\mathrm{d}\Omega}e^{\Omega}(\cdot)$ has the explicit representation*

$$\frac{\mathrm{d}}{\mathrm{d}\Omega}e^{\Omega}(V) = \int_0^1 e^{s\Omega}Ve^{(1-s)\Omega}\,ds. \tag{6.4}$$

In this thesis we often abbreviate the operator (6.4) *by $\mathcal{R}(V)$.*

Proof. The reasoning for (6.4) is given in [12, p.238]. ■

6.2.1 The case $e^{\Omega(t)}$

We now wish to calculate $\frac{\mathrm{d}}{\mathrm{dt}}e^{\Omega(t)}$. With the help of Theorem 6.2.3 the time-derivative of the time dependent matrix exponential $t \mapsto e^{\Omega(t)}$ takes the form

$$\mathcal{R}(t)(\Omega'(t)) := \frac{\mathrm{d}}{\mathrm{d}\Omega}e^{\Omega}\big|_{\Omega=\Omega(t)}(\Omega'(t)) = \int_0^1 e^{s\Omega(t)}\Omega'(t)e^{(1-s)\Omega(t)}\,ds.$$

6.2.2 The case $e^{\Omega(\tau,t_0)}$

Here we apply our knowledge from the previous section to the generalized matrix exponential

$$\begin{pmatrix} t_0 \\ \tau \end{pmatrix} \mapsto e^{\Omega(\tau,t_0)}$$

that we introduced in Section 3.1. We want a representation of the partial derivatives $\frac{\partial}{\partial\tau}e^{\Omega(\tau,t_0)}$ and $\frac{\partial}{\partial t_0}e^{\Omega(\tau,t_0)}$. Again with the help of Theorem 6.2.3 we obtain:

$$\begin{aligned}\mathcal{R}(\tau,t_0)(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)) &:= \tfrac{\partial}{\partial\tau}e^{\Omega(\tau,t_0)}\\ &= \tfrac{\mathrm{d}}{\mathrm{d}\Omega}e^{\Omega}\big|_{\Omega=\Omega(\tau,t_0)}(\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)) = \int_0^1 e^{s\Omega(\tau,t_0)}\tfrac{\partial}{\partial\tau}\Omega(\tau,t_0)e^{(1-s)\Omega(\tau,t_0)}\,ds,\end{aligned}$$

$$\begin{aligned}\mathcal{R}(\tau,t_0)(\tfrac{\partial}{\partial t_0}\Omega(\tau,t_0)) &:= \tfrac{\partial}{\partial t_0}e^{\Omega(\tau,t_0)}\\ &= \tfrac{\mathrm{d}}{\mathrm{d}\Omega}e^{\Omega}\big|_{\Omega=\Omega(\tau,t_0)}(\tfrac{\partial}{\partial t_0}\Omega(\tau,t_0)) = \int_0^1 e^{s\Omega(\tau,t_0)}\tfrac{\partial}{\partial t_0}\Omega(\tau,t_0)e^{(1-s)\Omega(\tau,t_0)}\,ds.\end{aligned} \tag{6.5}$$

The formulas in (6.5) are not (always) analytically computable. In these cases one needs numerical approximations, which are also asymptotically correct for $t \to 0$ or $\tau \to 0$, respectively, with some sufficiently high order. Therefore, the next section discusses suitable quadrature formulas.

6.3 Quadrature formulas

To evaluate integrals of the form

$$\int_0^\tau F(\sigma;\tau)\,d\sigma, \tag{6.6}$$

with some integrable (matrix-valued) integrand $F(\sigma;\tau)$, we make use of the following quadrature formulas. These formulas are significant parts in the evaluation of the defects to integration schemes, where integrals of the form (6.6) occur, compare Sections 4.1–4.4.

6.3.1 Second-order trapezoidal quadrature

This second-order quadrature formula can be found in [15, p.9]:

$$\int_0^\tau F(\sigma;\tau)\,d\sigma \approx \tfrac{1}{2}\tau\big(F(0;\tau)+F(\tau;\tau)\big). \tag{6.7}$$

6.3.2 Fourth-order modified trapezoidal quadrature of Hermite-type

This fourth-order quadrature formula can also be found in [15, p.9]:

$$\int_0^\tau F(\sigma;\tau)\,d\sigma \approx \tfrac{1}{2}\tau\big(F(0;\tau)+F(\tau;\tau)\big) + \tfrac{1}{12}\tau^2\big(\tfrac{\partial}{\partial\sigma}F(\sigma;\tau)\big|_{\sigma=0} - \tfrac{\partial}{\partial\sigma}F(\sigma;\tau)\big|_{\sigma=\tau}\big). \tag{6.8}$$

Remark 6.3.4. For all integrators that have to make use of a quadrature formula when numerically evaluated, it is inevitable to consider quadrature formulas of a sufficiently high order, to obtain the asymptotically correct evaluation of its defects. Clearly, the order must be at least as high as the order of the considered integration scheme. //

6.4 Pseudospectral Fourier-type collocation

We devote this section to the realization of the numerical evaluation of the operator

$$\mathrm{i}\tfrac{\partial^2}{\partial x^2}\psi(x,t),$$

which takes the form $Au(t)$ after some spatial discretization,

$$\psi(x,t) \overset{\textbf{spat. discr.}}{\Longrightarrow} u(t).$$

The evaluation is effected by applying the method of pseudospectral Fourier method. For simplification we consider it in one dimension:

Consider the symmetric interval $[-L, L],\ L > 0$, with N interior points,

$$x_j = x_0 + jh, \quad h = \frac{2L}{N}, \quad k = 0, \ldots, N-1.$$

We introduce the space of L^2-functions on $[-L, L]$ with periodic boundary conditions:

$$L^2_{\mathrm{per}}([-L,L]) := \{u \in L^2([-L,L]) :\ u(-L) = u(L)\},$$

with inner product

$$\langle u, v\rangle := \frac{1}{N}\sum_{j=0}^{N-1} \overline{u(x_j)}v(x_j).$$

On $L^2_{\mathrm{per}}([-L, L])$ we introduce the Fourier basis, given by

$$\varphi_k(x) := \exp(\mathrm{i}\pi k\tfrac{x}{L}),\ k = 0, \ldots, N-1,$$

which satisfies $\langle\varphi_k, \varphi_\ell\rangle = \delta_{k,\ell}$. With it we can define the trigonometric interpolant $\widetilde{u}(x)$ of a function $u \in L^2_{\mathrm{per}}([-L, L])$:

$$\widetilde{u}(x) := \sum_{k=0}^{N-1} \gamma_k\varphi_k(x), \quad \gamma_k := \langle\varphi_k, u\rangle. \tag{6.9}$$

Due to $\langle \varphi_k, \varphi_\ell \rangle = \delta_{k,\ell}$, there holds for $\widetilde{u}(x) \approx u(x)$ the interpolation property $\widetilde{u}(x_j) = u(x_j)$, $j = 0, \ldots, N-1$. For notational reasons we abbreviate $u^j := u(x_j)$ and observe that the vector $(\gamma_0, \gamma_1, \ldots, \gamma_{N-1})$ is the discrete Fourier transform $\mathcal{F}$ of the vector $(u^0, u^1, \ldots, u^{N-1})$:

$$\boldsymbol{\gamma} := (\gamma_0, \gamma_1, \ldots, \gamma_{N-1}) = \mathcal{F}(u^0, u^1, \ldots, u^{N-1}).$$

Remark 6.4.5. We remark that

$$\tfrac{\mathrm{d}^2}{\mathrm{dx}^2}\varphi_k(x) = \varphi_k''(x) = -\Big(\frac{k\pi}{L}\Big)^2 \varphi_k(x),$$

i.e., the Fourier basis functions are eigenfunctions of the differential operator $\frac{\mathrm{d}^2}{\mathrm{dx}^2}$ on $L^2_{\mathrm{per}}([-L, L])$, while

$$-\Big(\frac{k\pi}{L}\Big)^2, \ k = 0, \ldots, N-1,$$

are the corresponding eigenvalues. //

Differentiation of (6.9) gives

$$\tfrac{\mathrm{d}^2}{\mathrm{dx}^2}\widetilde{u}(x) = \widetilde{u}''(x) = \sum_{k=0}^{N-1} -\Big(\frac{k\pi}{L}\Big)^2 \gamma_k \varphi_k(x), \tag{6.10}$$

where $\widetilde{u}''(x)$ is an approximation of $u''(x)$. A look at (6.10) shows that $(\widetilde{u}_0'', \widetilde{u}_1'', \ldots, \widetilde{u}_{N-1}'')$ represents exactly the inverse Fourier transform $\mathcal{F}^{-1}$ of

$$\big(0, -\big(\tfrac{\pi}{L}\big)^2, \ldots, -\big(\tfrac{(N-1)\pi}{L}\big)^2\big) \cdot \boldsymbol{\gamma}^T,$$

i.e.,

$$(\widetilde{u}_0'', \widetilde{u}_1'', \ldots, \widetilde{u}_{N-1}'') = \mathcal{F}^{-1}\Big(\big(0, -\big(\tfrac{\pi}{L}\big)^2, \ldots, -\big(\tfrac{(N-1)\pi}{L}\big)^2\big) \cdot \mathcal{F}(u^0, u^1, \ldots, u^{N-1})^T\Big). \tag{6.11}$$

In combination with spatial discretization, (6.11) is now applied to numerically evaluate the kinetic term

$$\mathrm{i}\tfrac{\partial^2}{\partial x^2}\psi(x,t),$$

in (5.1).

This approach also shows that the operator A is a diagonal matrix, whence the flow associated with problem (6.12) has the form $e^{tA}u(t)$. Consequently, its (approximated) evaluation is likewise done by pseudospectral Fourier-type method, which we show in the next section.

6.5 Pseudospectral Fourier-type approximation

We can proceed analogously to approximate the solution of

$$\frac{\partial}{\partial t}\psi(x,t) = \mathrm{i}\frac{\partial^2}{\partial x^2}\psi(x,t), \quad \psi_0(x) = \psi(x,0), \quad t \geq 0. \tag{6.12}$$

The solution to (6.12) is formally given by

$$\psi(x,t) = e^{\mathrm{i}t\frac{\partial^2}{\partial x^2}}\psi_0(x), \tag{6.13}$$

while the operator $e^{\mathrm{i}t\frac{\partial^2}{\partial x^2}}$ has the eigenvalues

$$e^{\mathrm{i}t\lambda_k}, \ k = 0, \ldots, N-1, \text{ with } \lambda_k = -\Big(\frac{k\pi}{L}\Big)^2. \tag{6.14}$$

With the insights that we got from the previous section we have

$$(\psi_1^0, \psi_1^1, \ldots, \psi_1^{N-1}) \approx \mathcal{F}^{-1}\Big(\big(1, e^{\mathrm{i}\tilde{t}\lambda_1}, \ldots, e^{\mathrm{i}\tilde{t}\lambda_{N-1}}\big) \cdot \mathcal{F}(\psi_0^0, \psi_0^1, \ldots, \psi_0^{N-1})^T\Big), \tag{6.15}$$

where $\psi_0(x) =: (\psi_0^0, \psi_0^1, \ldots, \psi_0^{N-1})$, while $\psi(x,\widetilde{t}) =: (\psi_1^0, \psi_1^1, \ldots, \psi_1^{N-1})$ is the solution after one time-step $\widetilde{t} \geq 0$.

List of Tables

List of Figures

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