Defect-based local error estimators for splitting methods, with application to Schrödinger equations Part III. The nonlinear case[1]

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Abstract

The present work is concerned with the efficient time integration of nonlinear evolution equations by exponential operator splitting methods. Defect-based local error estimators serving as a reliable basis for adaptive stepsize control are constructed and analyzed. In the context of time-dependent nonlinear Schrödinger equations, asymptotical correctness of the local error estimators associated with the first-order Lie–Trotter and second-order Strang splitting methods is proven. Numerical examples confirm the theoretical results and illustrate the performance of adaptive stepsize control.

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1. Introduction

Numerous contributions confirm the favorable behavior of exponential operator splitting methods for evolution equations of Schrödinger type, both linear and nonlinear; as a small selection, we mention [1, 2, 3] and refer to literature given therein. In the present work, we introduce and analyze a posteriori local error estimators serving as a reliable basis for adaptive time stepsize control. For this purpose, we extend techniques previously developed for linear evolution equations [5, 6] to the significantly more complex nonlinear case within a general setting of evolution equations on Banach spaces.

In order to construct a defect-based local error estimator associated with a splitting method, we determine the defect of the splitting solution and approximate a corresponding integral representation for the local error by means of a quadrature formula involving a single evaluation of the defect. We prove that the obtained local error estimator is asymptotically correct and confirm this theoretical result by a numerical experiment for the focusing cubic nonlinear Schrödinger equation. A further numerical example for the two-dimensional time-dependent Gross–Pitaevskii equation with additional rotation term illustrates the performance of adaptive time stepsize control based on a posteriori local error estimation. Compared to the approach exploited in [5, 6] for linear evolution equations, the treatment of the nonlinear case involves considerably more technicalities. For this reason, we include detailed calculations for the first-order Lie–Trotter method and describe the extension to the second-order Strang splitting method using automatic symbolic manipulations. The generalization to higher-order splitting methods is briefly indicated. As the a posteriori local error analysis requires a detailed investigation of the underlying error structures, we refrain from resorting to the formal calculus of Lie derivatives as this would imply the need to translate back to explicit representations anyway.

The manuscript is organized as follows. In Section 2, employing a framework of abstract nonlinear evolution equations, we state the defect-based local error estimators associated with a general splitting method. Section 3 is devoted to a detailed local error analysis of the Lie–Trotter splitting method in a general nonlinear setting. The extension to the Strang splitting method is described in Section 4. The specialization of our approach to time-dependent nonlinear Schrödinger equations is given in Section 5. Basic prerequisites and additional auxiliary results for the Strang splitting method are collected in

the appendix.

2. Defect-based local error estimators

2.1. Problem setting

We consider the initial value problem

$$\tfrac{\mathrm{d}}{\mathrm{d}t} u(t) = H(u(t)) = A(u(t)) + B(u(t))\,, \qquad t \in (0, T]\,, \tag{2.1a}$$

$$u(0) = u_0 \quad \text{given}\,, \tag{2.1b}$$

where $H \colon \mathcal{D}(H) \to \mathcal{B}$, $A \colon \mathcal{D}(A) \to \mathcal{B}$, and $B \colon \mathcal{D}(B) \to \mathcal{B}$ denote generally unbounded nonlinear operators on the underlying Banach space $\mathcal{B}$ such that $\mathcal{D}(A) \cap \mathcal{D}(B) = \mathcal{D}(H) \subset \mathcal{B}$. The exact flow associated with (2.1) is denoted by

$$u(t) = \mathcal{E}_H(t, u_0)\,, \qquad t \in [0, T]\,. \tag{2.1c}$$

By $\frac{\partial}{\partial t} \mathcal{E}_H(t, u_0)$ and $\partial_2 \mathcal{E}_H(t, u_0)$ we denote the Fréchet derivatives of $\mathcal{E}_H(t, u_0)$ with respect to t and u_0, respectively. By $\partial_2^k \mathcal{E}_H(t, u_0)$ we denote the k-th Fréchet derivative with respect to u_0. The same denotation is used for the flows $\mathcal{E}_A(t, u_0)$ and $\mathcal{E}_B(t, u_0)$.

Remark 1. Our theoretical considerations are valid under appropriate smoothness assumptions. This means that all relevant nonlinear operators and flows are assumed to be well-defined and sufficiently often continuously Fréchet differentiable. Then, all occurring higher Fréchet derivatives are symmetric functions of their arguments, and this is tacitly assumed in all formal calculations.

Since we are mainly interested in evolution equations of Schrödinger type, we restrict our general considerations to the time-reversible case. In particular, we use the variation-of-constants formula (A.2c) where reversibility in time is assumed. The extension to the non-reversible case requires suitable modifications, see for instance [7].

2.2. Splitting methods

For the time integration of (2.1) we study exponential operator splitting methods, see [8, 9] for detailed information. A single step of a splitting method is of the form

$$\mathcal{S}(t, u) = \mathcal{S}_s(t, \mathcal{S}_{s-1}(t, \ldots, \mathcal{S}_1(t, u))) \approx \mathcal{E}_H(t, u)\,,$$

$$\mathcal{S}_j(t, u) = \mathcal{E}_B(b_j\, t, \mathcal{E}_A(a_j\, t, u))\,,$$

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with time increment t, initial state u, and coefficients $(a_j, b_j)_{j=1}^s$; evidently, the relation $\mathcal{S}(0, u) = u$ is satisfied. In particular, a three-stage splitting method is given by

$$
\begin{aligned}
v_1 &= \mathcal{E}_A(a_1 t, u), & w_1 &= \mathcal{E}_B(b_1 t, v_1), \\
v_2 &= \mathcal{E}_A(a_2 t, w_1), & w_2 &= \mathcal{E}_B(b_2 t, v_2), \\
v_3 &= \mathcal{E}_A(a_3 t, w_2), & w_3 &= \mathcal{E}_B(b_3 t, v_3),
\end{aligned}
\tag{2.3}
$$
$$
\mathcal{S}(t, u) = \mathcal{S}_3(t, \mathcal{S}_2(t, \mathcal{S}_1(t, u))) = w_3.
$$

In view of the high amount of technicalities in the a posteriori local error analysis, we focus on the first-order Lie–Trotter and the second-order Strang splitting methods, defined by

$$
p = 1: \quad \mathcal{S}(t, u) = \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \approx \mathcal{E}_H(t, u), \tag{2.4}
$$

$$
p = 2: \quad \mathcal{S}(t, u) = \mathcal{E}_A(\tfrac{t}{2}, \mathcal{E}_B(t, \mathcal{E}_A(\tfrac{t}{2}, u))) \approx \mathcal{E}_H(t, u). \tag{2.5}
$$

Generally, for an approximation to the exact flow associated with the nonlinear evolution equation (2.1),

$$
\mathcal{S}^{(0)}(t, u) = \mathcal{S}(t, u) \approx \mathcal{E}_H(t, u), \qquad \mathcal{S}(0, u) = u, \tag{2.6a}
$$

we define its defect by

$$
\mathcal{S}^{(1)}(t, u) = \tfrac{\partial}{\partial t} \mathcal{S}(t, u) - H(\mathcal{S}(t, u)). \tag{2.6b}
$$

Higher-order defects such as the second- and third-order defects

$$
\mathcal{S}^{(2)}(t, u) = \tfrac{\partial}{\partial t} \mathcal{S}^{(1)}(t, u) - H'(\mathcal{S}(t, u)) \cdot \mathcal{S}^{(1)}(t, u), \tag{2.6c}
$$

$$
\begin{aligned}
\mathcal{S}^{(3)}(t, u) = {} & \tfrac{\partial}{\partial t} \mathcal{S}^{(2)}(t, u) - H'(\mathcal{S}(t, u)) \cdot \mathcal{S}^{(2)}(t, u) \\
& - H''(\mathcal{S}(t, u))(\mathcal{S}^{(1)}(t, u), \mathcal{S}^{(1)}(t, u)),
\end{aligned}
\tag{2.6d}
$$

occur in the local error analysis, see Lemma 1 below.

The local error of the approximation (2.6a) is denoted by

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

By means of the nonlinear variation-of-constants formula (A.3), the integral representation

$$
\mathcal{L}(t, u) = \int_0^t \mathcal{F}(\tau, t, u) \, \mathrm{d}\tau, \tag{2.7b}
$$

$$
\mathcal{F}(\tau, t, u) = \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(1)}(\tau, u), \tag{2.7c}
$$

involving the defect (2.6b) is obtained.

2.3. Error estimators

In order to construct a defect-based local error estimator associated with a splitting method of order $p \geq 1$, we approximate the local error on the basis of the following idea. Validity of the p-th order conditions ensures $\frac{\partial}{\partial t}\mathcal{L}(0, u) = \frac{\partial^2}{\partial t^2}\mathcal{L}(0, u) = \ldots = \frac{\partial^p}{\partial t^p}\mathcal{L}(0, u) = 0$, and due to (2.7b,c) this is equivalent to $\mathcal{S}^{(1)}(0, u) = \frac{\partial}{\partial t}\mathcal{S}^{(1)}(0, u) = \ldots = \frac{\partial^{p-1}}{\partial t^{p-1}}\mathcal{S}^{(1)}(0, u) = 0$. Thus, $\frac{\partial^{p+1}}{\partial t^{p+1}}\mathcal{L}(0, u) = \frac{\partial^p}{\partial t^p}\mathcal{S}^{(1)}(0, u)$, which implies

$$\mathcal{L}(t, u) = \frac{t^{p+1}}{(p+1)!} \frac{\mathrm{d}^p}{\mathrm{d}t^p} \mathcal{S}^{(1)}(0, u) + \mathcal{O}(t^{p+2}). \tag{2.8}$$

Here, $\frac{\mathrm{d}^p}{\mathrm{d}t^p} \mathcal{S}^{(1)}(0, u)$ is a linear combination of iterated commutators of A and B (see $(3.8), (4.5)$, and [4]) which would be rather cumbersome to evaluate, in particular for higher-order schemes. However, combining (2.8) with $\mathcal{S}^{(1)}(t, u) = \frac{t^p}{p!} \frac{\mathrm{d}^p}{\mathrm{d}t^p}\mathcal{S}^{(1)}(0, u) + \mathcal{O}(t^{p+1})$ we see that

$$\mathcal{P}(t, u) = \frac{1}{p+1} t \, \mathcal{S}^{(1)}(t, u) \approx \mathcal{L}(t, u) \tag{2.9a}$$

is expected to be an asymptotically correct local error estimator, i.e.,

$$\mathcal{P}(t, u) - \mathcal{L}(t, u) = \mathcal{O}(t^{p+2}). \tag{2.9b}$$

One of our main issues is to deduce a suitable representation for the defect and to give a rigorous proof of (2.9b), i.e., a precise estimate for the $\mathcal{O}(t^{p+2})$ term, for the schemes (2.4) and (2.5).

The estimator $\mathcal{P}(t, u)$ may also be interpreted as the evaluation of a Hermite quadrature formula for the local error integral (2.7b,c) (exploiting $\mathcal{S}^{(1)}(0, u) = \frac{\partial}{\partial t}\mathcal{S}^{(1)}(0, u) = \ldots = \frac{\partial^{p-1}}{\partial t^{p-1}}\mathcal{S}^{(1)}(0, u) = 0$, see [5, 6]). Our analysis will be based on a representation of the corresponding quadrature error.

In Section 3, we show that an explicit representation for the defect associated with the first-order Lie–Trotter splitting method is given by

$$\mathcal{S}^{(1)}(t, u) = \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \cdot A(\mathcal{E}_A(t, u)) - A(\mathcal{E}_B(t, \mathcal{E}_A(t, u))),$$

and deduce a representation implying (2.9b) with $p = 1$. As the analogous analysis for the second-order Strang splitting method, with defect $\mathcal{S}^{(1)}(t, u)$ represented by (C.1), involves a significantly higher amount of technicalities, we utilize automatic symbolic manipulations for verification of the results stated in Section 4, see also Appendix B and Appendix C.

For general multi-stage schemes, an explicit representation of the defect (2.6b) looks as follows. For a three-stage scheme we have

$$
\begin{aligned}
\mathcal{S}^{(1)}(t, u) = {}& \partial_2 \mathcal{E}_B(b_3\, t, v_3) \cdot \partial_2 \mathcal{E}_A(a_3\, t, w_2) \cdot \Big\{ a_3\, A(w_2) + b_2\, B(w_2) \\
& + \partial_2 \mathcal{E}_B(b_2\, t, v_2) \cdot \partial_2 \mathcal{E}_A(a_2\, t, w_1) \cdot \Big[a_2\, A(w_1) + b_1\, B(w_1) \\
& + \partial_2 \mathcal{E}_B(b_1\, t, v_1) \cdot \partial_2 \mathcal{E}_A(a_1\, t, u) \cdot (a_1\, A(u)) \Big] \Big\} \\
& - A(w_3) - (1 - b_3)\, B(w_3)\,,
\end{aligned} \tag{2.10}
$$

with the internal stages v_i and w_i from (2.3). Again, this does not contain explicit derivatives w.r.t. t and can be practically evaluated in typical applications, see Section 5. The proof of (2.10) is a routine calculation, where (2.6b) is rewritten by differentiating $\mathcal{S}(t)$ and making repeated use of the fundamental identity (A.7). The extension to the general case is now also obvious; however a rigorous analysis of $\mathcal{P}(t, u)$ based on (2.10) for the general case is out of the scope of this paper. For the linear case, see [6].

In view of our a posteriori local error analysis for the Lie–Trotter and Strang splitting methods, we next determine the first and second derivatives of the integrand in the local error representation (2.7) and express them in terms of defects.

Lemma 1 (Derivatives of $\mathcal{F}$). *The first and second derivatives of the function $\mathcal{F}$ defined in (2.7c) satisfy*

$$
\begin{aligned}
\tfrac{\partial}{\partial \tau} \mathcal{F}(\tau, t, u) = {}& \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(2)}(\tau, u) && \text{(2.11a)} \\
& + \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u))\,, \\
\tfrac{\partial^2}{\partial \tau^2} \mathcal{F}(\tau, t, u) = {}& \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(3)}(\tau, u) && \text{(2.11b)} \\
& + 3\, \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(2)}(\tau, u)) \\
& + \partial_2^3 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u))\,.
\end{aligned}
$$

PROOF. For notational simplicity, we meanwhile omit the arguments of $\mathcal{F}$ as well as $\mathcal{S}$, $\mathcal{S}^{(j)}$ and write $\mathcal{E}_H = \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))$ for short.

(i) Differentiation and an application of formula (A.13) proves (2.11a),

$$\frac{\partial}{\partial\tau}\mathcal{F} = \frac{\partial}{\partial\tau}\left(\partial_2\mathcal{E}_H \cdot \mathcal{S}^{(1)}\right)$$
$$= \left(\frac{\partial}{\partial\tau}\partial_2\mathcal{E}_H\right)\cdot\mathcal{S}^{(1)} + \partial_2\mathcal{E}_H \cdot \frac{\partial}{\partial\tau}\mathcal{S}^{(1)}$$
$$= -\partial_2\mathcal{E}_H \cdot H'(\mathcal{S})\cdot\mathcal{S}^{(1)} - \partial_2^2\mathcal{E}_H(H(\mathcal{S}),\mathcal{S}^{(1)}) + \partial_2^2\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S},\mathcal{S}^{(1)})$$
$$\qquad + \partial_2\mathcal{E}_H \cdot \frac{\partial}{\partial\tau}\mathcal{S}^{(1)}$$
$$= \partial_2\mathcal{E}_H \cdot \left(\frac{\partial}{\partial\tau}\mathcal{S}^{(1)} - H'(\mathcal{S})\cdot\mathcal{S}^{(1)}\right) + \partial_2^2\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S} - H(\mathcal{S}),\mathcal{S}^{(1)})$$
$$= \partial_2\mathcal{E}_H \cdot \mathcal{S}^{(2)} + \partial_2^2\mathcal{E}_H(\mathcal{S}^{(1)},\mathcal{S}^{(1)})\,.$$

(ii) We separately consider the contributions in

$$\frac{\partial^2}{\partial\tau^2}\mathcal{F} = \frac{\partial}{\partial\tau}\left(\partial_2\mathcal{E}_H \cdot \mathcal{S}^{(2)}\right) + \frac{\partial}{\partial\tau}\left(\partial_2^2\mathcal{E}_H(\mathcal{S}^{(1)},\mathcal{S}^{(1)})\right)\,.$$

For the first term we obtain

$$\frac{\partial}{\partial\tau}\left(\partial_2\mathcal{E}_H \cdot \mathcal{S}^{(2)}\right) = \left(\frac{\partial}{\partial\tau}\partial_2\mathcal{E}_H\right)\cdot\mathcal{S}^{(2)} + \partial_2\mathcal{E}_H\cdot\frac{\partial}{\partial\tau}\mathcal{S}^{(2)} \qquad\qquad (2.12a)$$
$$= -\partial_2\mathcal{E}_H \cdot H'(\mathcal{S})\cdot\mathcal{S}^{(2)} - \partial_2^2\mathcal{E}_H(H(\mathcal{S}),\mathcal{S}^{(2)})$$
$$\qquad + \partial_2^2\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S},\mathcal{S}^{(2)}) + \partial_2\mathcal{E}_H\cdot\frac{\partial}{\partial\tau}\mathcal{S}^{(2)}$$
$$= \partial_2\mathcal{E}_H \cdot \left(\frac{\partial}{\partial\tau}\mathcal{S}^{(2)} - H'(\mathcal{S})\cdot\mathcal{S}^{(2)}\right)$$
$$\qquad + \partial_2^2\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S} - H(\mathcal{S}),\mathcal{S}^{(2)})$$
$$= \partial_2\mathcal{E}_H \cdot \left(\frac{\partial}{\partial\tau}\mathcal{S}^{(2)} - H'(\mathcal{S})\cdot\mathcal{S}^{(2)}\right) + \partial_2^2\mathcal{E}_H(\mathcal{S}^{(1)},\mathcal{S}^{(2)})\,.$$

Applying (A.14) yields

$$\frac{\partial}{\partial\tau}\left(\partial_2^2\mathcal{E}_H(\mathcal{S}^{(1)},\mathcal{S}^{(1)})\right) \qquad\qquad (2.12b)$$
$$= \left(\frac{\partial}{\partial\tau}\partial_2^2\mathcal{E}_H\right)(\mathcal{S}^{(1)},\mathcal{S}^{(1)}) + 2\,\partial_2^2\mathcal{E}_H(\mathcal{S}^{(1)},\tfrac{\partial}{\partial\tau}\mathcal{S}^{(1)})$$
$$= -\partial_2\mathcal{E}_H\cdot H''(\mathcal{S})(\mathcal{S}^{(1)},\mathcal{S}^{(1)}) - 2\,\partial_2^2\mathcal{E}_H(H'(\mathcal{S})\cdot\mathcal{S}^{(1)},\mathcal{S}^{(1)})$$
$$\qquad - \partial_2^3\mathcal{E}_H(H(\mathcal{S}),\mathcal{S}^{(1)},\mathcal{S}^{(1)}) + \partial_2^3\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S},\mathcal{S}^{(1)},\mathcal{S}^{(1)})$$
$$\qquad + 2\,\partial_2^2\mathcal{E}_H(\mathcal{S}^{(1)},\tfrac{\partial}{\partial\tau}\mathcal{S}^{(1)})$$
$$= -\partial_2\mathcal{E}_H\cdot H''(\mathcal{S})(\mathcal{S}^{(1)},\mathcal{S}^{(1)}) + 2\,\partial_2^2\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S}^{(1)} - H'(\mathcal{S})\cdot\mathcal{S}^{(1)},\mathcal{S}^{(1)})$$
$$\qquad + \partial_2^3\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S} - H(\mathcal{S}),\mathcal{S}^{(1)},\mathcal{S}^{(1)})$$
$$= -\partial_2\mathcal{E}_H\cdot H''(\mathcal{S})(\mathcal{S}^{(1)},\mathcal{S}^{(1)}) + 2\,\partial_2^2\mathcal{E}_H(\tfrac{\partial}{\partial\tau}\mathcal{S}^{(1)} - H'(\mathcal{S})\cdot\mathcal{S}^{(1)},\mathcal{S}^{(1)})$$
$$\qquad + \partial_2^3\mathcal{E}_H(\mathcal{S}^{(1)},\mathcal{S}^{(1)},\mathcal{S}^{(1)})\,.$$

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Adding (2.12a) and (2.12b) leads to

$$\frac{\partial^2}{\partial \tau^2} \mathcal{F}(\tau, t, u) = \partial_2 \mathcal{E}_H \cdot \left(\frac{\partial}{\partial \tau} \mathcal{S}^{(2)} - H'(\mathcal{S}) \cdot \mathcal{S}^{(2)} \right) + \partial_2^2 (\mathcal{S}^{(1)}, \mathcal{S}^{(2)})$$
$$- \partial_2 \mathcal{E}_H \cdot H''(\mathcal{S})(\mathcal{S}^{(1)}, \mathcal{S}^{(1)})$$
$$+ 2\, \partial_2^2 \mathcal{E}_H \big(\tfrac{\partial}{\partial \tau} \mathcal{S}^{(1)} - H'(\mathcal{S}) \cdot \mathcal{S}^{(1)}, \mathcal{S}^{(1)} \big)$$
$$+ \partial_2^3 \mathcal{E}_H (\mathcal{S}^{(1)}, \mathcal{S}^{(1)}, \mathcal{S}^{(1)})$$
$$= \partial_2 \mathcal{E}_H \cdot \mathcal{S}^{(3)} + 3\, \partial_2^2 \mathcal{E}_H (\mathcal{S}^{(1)}, \mathcal{S}^{(2)}) + \partial_2^3 \mathcal{E}_H (\mathcal{S}^{(1)}, \mathcal{S}^{(1)}, \mathcal{S}^{(1)}),$$

which proves (2.11b). □

3. Lie–Trotter splitting method

In this section, we provide a local error analysis for the Lie–Trotter splitting method (2.4). In particular, we construct a defect-based local error estimator and prove asymptotical correctness. Our approach relies on the derivation of suitable evolution equations for the splitting operator and related quantities such as the defect and resulting integral representations. We note that the formal calculations are valid in a rigorous sense whenever the arising compositions of flows and Lie commutators are well-defined on the underlying Banach space. The specialization to a nonlinear Schrödinger equation is studied in Section 5.

3.1. Splitting operator and defect

We first state a nonlinear evolution equation satisfied by the splitting operator associated with the Lie–Trotter splitting method (2.4).

Lemma 2 (Evolution equation, Lie–Trotter splitting). *The splitting operator* $\mathcal{S}(t, u) = \mathcal{E}_B(t, \mathcal{E}_A(t, u))$ *satisfies the nonlinear Sylvester equation*

$$\frac{\partial}{\partial t} \mathcal{S}(t, u) = \partial_2 \mathcal{S}(t, u) \cdot A(u) + B(\mathcal{S}(t, u)), \tag{3.1}$$

where $\partial_2 \mathcal{S}(t, u) = \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \cdot \partial_2 \mathcal{E}_A(t, u).$

PROOF. Straightforward differentiation and an application of the fundamental identity (A.7) yields

$$\frac{\partial}{\partial t} \mathcal{S}(t, u) = \frac{\partial}{\partial t} \mathcal{E}_B(t, \mathcal{E}_A(t, u))$$
$$= B(\mathcal{E}_B(t, \mathcal{E}_A(t, u)) + \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \cdot A(\mathcal{E}_A(t, u))$$
$$= B(\mathcal{S}(t, u)) + \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \cdot A(\mathcal{E}_A(t, u))$$
$$= B(\mathcal{S}(t, u)) + \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \cdot \partial_2 \mathcal{E}_A(t, u) \cdot A(u),$$

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which proves (3.1). $\qquad\square$

The following auxiliary result provides a representation of the defect (2.6b).

Lemma 3 (Defect $\mathcal{S}^{(1)}(t,u)$, Lie–Trotter splitting).

(i) *The defect is given by*

$$\mathcal{S}^{(1)}(t,u) = \tilde{\mathcal{S}}^{(1)}(t, \mathcal{E}_A(t,u))\,, \tag{3.2a}$$

$$\tilde{\mathcal{S}}^{(1)}(t,v) = \partial_2 \mathcal{E}_B(t,v) \cdot A(v) - A(\mathcal{E}_B(t,v))\,. \tag{3.2b}$$

(ii) *The operator $\tilde{\mathcal{S}}^{(1)}$ satisfies the initial value problem*

$$\tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(1)}(t,v) = B'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1)}(t,v) + [B,A](\mathcal{E}_B(\tau,v))\,, \tag{3.3a}$$

$$\tilde{\mathcal{S}}^{(1)}(0,v) = 0\,. \tag{3.3b}$$

(iii) *The integral representations*

$$\tilde{\mathcal{S}}^{(1)}(t,v) = \partial_2 \mathcal{E}_B(t,v) \cdot \tag{3.4a}$$
$$\int_0^t \partial_2 \mathcal{E}_B(-\tau, \mathcal{E}_B(\tau,v)) \cdot [B,A](\mathcal{E}_B(\tau,v))\,\mathrm{d}\tau\,,$$

$$\mathcal{S}^{(1)}(t,u) = \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t,u)) \cdot \tag{3.4b}$$
$$\int_0^t \partial_2 \mathcal{E}_B(-\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(t,u))) \cdot [B,A](\mathcal{E}_B(\tau, \mathcal{E}_A(t,u)))\,\mathrm{d}\tau\,,$$

are valid.

PROOF.

(i) From (3.1) we obtain

$$\begin{aligned}
\mathcal{S}^{(1)}(t,u) &= \tfrac{\partial}{\partial t}\mathcal{S}(t,u) - H(\mathcal{S}(t,u)) \\
&= \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t,u)) \cdot A(\mathcal{E}_A(t,u)) + B(\mathcal{E}_B(t, \mathcal{E}_A(t,u))) \\
&\quad - H(\mathcal{S}(t,u)) \\
&= \partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t,u)) \cdot A(\mathcal{E}_A(t,u)) - A(\mathcal{S}(t,u))\,,
\end{aligned}$$

which proves (3.2).

(ii) Equation (3.3a) follows by differentiation, see (A.8a).

(iii) The integral representation (3.4a) for $\tilde{\mathcal{S}}^{(1)}$ follows from (A.2). Substituting $v = \mathcal{E}_A(t, u)$ yields the integral representation (3.4b) for the defect $\mathcal{S}^{(1)}$. $\qquad\square$

Remark 2. In view of Lemma 4 below, we next deduce a representation for $\partial_2 \tilde{\mathcal{S}}^{(1)}$. Using (3.2b), we obtain

$$\partial_2 \tilde{\mathcal{S}}^{(1)}(t, v) = \partial_2^2 \mathcal{E}_B(t, v)(A(v), \cdot) \tag{3.5a}$$
$$+ \big(\partial_2 \mathcal{E}_B(t, v) \cdot A'(v) - A'(\mathcal{E}_B(t, v)) \cdot \partial_2 \mathcal{E}_B(t, v)\big), \tag{3.5b}$$

where $\partial_2 \tilde{\mathcal{S}}^{(1)}(0, v) = 0$. Differentiating (3.5a) and inserting (3.3a) yields

$$\frac{\partial}{\partial t}\big(\partial_2 \tilde{\mathcal{S}}^{(1)}(t, v)\big) = \partial_2\big(\tfrac{\partial}{\partial t}\tilde{\mathcal{S}}^{(1)}(t, v)\big)$$
$$= \partial_2\big(B'(\mathcal{E}_B(t, v)) \cdot \tilde{\mathcal{S}}^{(1)}(t, v) + [B, A](\mathcal{E}_B(t, v))\big)$$
$$= B'(\mathcal{E}_B(t, v)) \cdot \partial_2 \tilde{\mathcal{S}}^{(1)}(t, v) \tag{3.5c}$$
$$+ B''(\mathcal{E}_B(t, v))(\tilde{\mathcal{S}}^{(1)}(t, v), \partial_2 \mathcal{E}_B(t, v) \cdot)$$
$$+ [B, A]'(\mathcal{E}_B(t, v)) \cdot \partial_2 \mathcal{E}_B(t, v).$$

By means of (A.2) the integral representation

$$\partial_2 \tilde{\mathcal{S}}^{(1)}(t, v) = \partial_2 \mathcal{E}_B(t, v) \cdot \int_0^t \partial_2 \mathcal{E}_B(-\tau, \mathcal{E}_B(\tau, v)) \cdot \tag{3.5d}$$
$$\Big\{ B''(\mathcal{E}_B(\tau, v))(\tilde{\mathcal{S}}^{(1)}(\tau, v), \partial_2 \mathcal{E}_B(\tau, v) \cdot)$$
$$+ [B, A]'(\mathcal{E}_B(\tau, v)) \cdot \partial_2 \mathcal{E}_B(\tau, v) \Big\} \, \mathrm{d}\tau$$

follows.

3.2. A priori local error analysis

Inserting the integral representation (3.4b) for the defect into (2.7) leads to a representation for the local error which implies

$$\mathcal{L}(t, u) = \mathscr{O}(t^2), \tag{3.6}$$

provided that the integrand remains bounded on the underlying Banach space. The resulting local error representation corresponds to the integral representation deduced in [10].

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Theorem 1 (Local error, Lie–Trotter splitting). *The local error of the Lie–Trotter splitting method satisfies*

$$\mathcal{L}(t,u) = \int_0^t \int_0^{\tau_1} \partial_2 \mathcal{E}_H(t - \tau_1, \mathcal{S}(\tau_1, u)) \cdot \tag{3.7}$$
$$\partial_2 \mathcal{E}_B(\tau_1, \mathcal{E}_A(\tau_1, u)) \cdot \partial_2 \mathcal{E}_B(-\tau_2, \mathcal{E}_B(\tau_2, \mathcal{E}_A(\tau_1, u))) \cdot$$
$$[B, A](\mathcal{E}_B(\tau_2, \mathcal{E}_A(\tau_1, u)))\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,.$$

Remark 3. The leading term after Taylor expansion of $\mathcal{L}(t,u)$ is given by

$$\tfrac{t^2}{2} \tfrac{\mathrm{d}^2}{\mathrm{d}t^2} \mathcal{L}(0, u) = \tfrac{t^2}{2} \tfrac{\mathrm{d}}{\mathrm{d}t} \mathcal{S}^{(1)}(0, u) = \tfrac{t^2}{2} \mathcal{S}^{(2)}(0, u) = \tfrac{t^2}{2} [B, A](u)\,, \tag{3.8}$$

which exactly corresponds with the linear case, see [5].

3.3. Second-order defect

The following considerations serve as a preparation for the analysis of the a posteriori local error estimator provided in Section 3.4.

Lemma 4 (Second-order defect $\mathcal{S}^{(2)}(t, u)$, Lie–Trotter splitting).

(i) *The second-order defect defined in (2.6c) is given by*

$$\mathcal{S}^{(2)}(t, u) = \tilde{\mathcal{S}}^{(2)}(t, \mathcal{E}_A(t, u))\,, \tag{3.9a}$$
$$\tilde{\mathcal{S}}^{(2)}(t, v) = \partial_2 \tilde{\mathcal{S}}^{(1)}(t, v) \cdot A(v) - A'(\mathcal{E}_B(t, v)) \cdot \tilde{\mathcal{S}}^{(1)}(t, v) \tag{3.9b}$$
$$+ [B, A](\mathcal{E}_B(t, v))\,.$$

(ii) *The operator $\tilde{\mathcal{S}}^{(2)}$ satisfies the initial value problem*

$$\tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(2)}(t, v) = B'(\mathcal{E}_B(t, v)) \cdot \tilde{\mathcal{S}}^{(2)}(t, v) \tag{3.10a}$$
$$+ B''(\mathcal{E}_B(t, v)(\tilde{\mathcal{S}}^{(1)}(t, v), \tilde{\mathcal{S}}^{(1)}(t, v))$$
$$+ [[B, A], A](\mathcal{E}_B(t, v)) + [[B, A], B](\mathcal{E}_B(t, v))$$
$$+ 2 [B, A]'(\mathcal{E}_B(t, v)) \cdot \tilde{\mathcal{S}}^{(1)}(t, v)\,,$$
$$\tilde{\mathcal{S}}^{(2)}(0, v) = [B, A](v)\,. \tag{3.10b}$$

(iii) *The representations*

$$\tilde{\mathcal{S}}^{(2)}(t,v) = \tilde{\mathcal{S}}^{(2,0)}(t,v) + \tilde{\mathcal{S}}^{(2,1)}(t,v)\,, \tag{3.11a}$$

$$\tilde{\mathcal{S}}^{(2,0)}(t,v) = \partial_2\mathcal{E}_B(t,v) \cdot [B,A](v)\,, \tag{3.11b}$$

$$\tilde{\mathcal{S}}^{(2,1)}(t,v) = \partial_2\mathcal{E}_B(t,v) \cdot \int_0^t \partial_2\mathcal{E}_B(-\tau,\mathcal{E}_B(\tau,v)) \cdot \tag{3.11c}$$
$$\Big\{ B''(\mathcal{E}_B(\tau,v)(\tilde{\mathcal{S}}^{(1)}(\tau,v),\tilde{\mathcal{S}}^{(1)}(\tau,v))$$
$$+ [[B,A],A](\mathcal{E}_B(\tau,v)) + [[B,A],B](\mathcal{E}_B(\tau,v))$$
$$+ 2\,[B,A]'(\mathcal{E}_B(\tau,v)) \cdot \tilde{\mathcal{S}}^{(1)}(\tau,v) \Big\}\,\mathrm{d}\tau\,,$$

and

$$\mathcal{S}^{(2)}(t,u) = \mathcal{S}^{(2,0)}(t,u) + \mathcal{S}^{(2,1)}(t,u) \tag{3.11d}$$
$$= \tilde{\mathcal{S}}^{(2,0)}(t,\mathcal{E}_A(t,u)) + \tilde{\mathcal{S}}^{(2,1)}(t,\mathcal{E}_A(t,u))$$

are valid.

PROOF.

(i) We recall that the second-order defect is defined in (2.6c). From (3.2b) and (3.3a) we have

$$\tfrac{\partial}{\partial t}\mathcal{S}^{(1)}(t,u) = \tfrac{\partial}{\partial t}\tilde{\mathcal{S}}^{(1)}(t,\mathcal{E}_A(t,u))$$
$$= B'(\mathcal{E}_B(t,\mathcal{E}_A(t,u))) \cdot \tilde{\mathcal{S}}^{(1)}(t,\mathcal{E}_A(t,u))$$
$$+ [B,A](\mathcal{E}_B(t,\mathcal{E}_A(t,u)))$$
$$+ \partial_2\tilde{\mathcal{S}}^{(1)}(t,\mathcal{E}_A(t,u)) \cdot A(\mathcal{E}_A(t,u))\,.$$

Consequently, this yields

$$\tilde{\mathcal{S}}^{(2)}(t,v) = B'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1)}(t,v) + [B,A](\mathcal{E}_B(t,v))$$
$$+ \partial_2\tilde{\mathcal{S}}^{(1)}(t,v) \cdot A(v) - H'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1)}(t,v)$$
$$= \partial_2\tilde{\mathcal{S}}^{(1)}(t,v) \cdot A(v) - A'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1)}(t,v) + [B,A](\mathcal{E}_B(t,v))\,,$$

which proves (3.9b).

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(ii) Evaluation of (3.9b) at $t = 0$ implies (3.10b). In the proof of (3.10a), we meanwhile suppress the argument to simplify notation. Proceeding from

$$\tilde{\mathcal{S}}^{(2)} = \partial_2 \tilde{\mathcal{S}}^{(1)} \cdot A(v) - A'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} + [B, A](\mathcal{E}_B) \,,$$

see (3.9b), differentiation yields

$$\begin{aligned}
\tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(2)} &= \left(\tfrac{\partial}{\partial t} \partial_2 \tilde{\mathcal{S}}^{(1)} \right) \cdot A(v) - \tfrac{\partial}{\partial t} \left(A'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} \right) + \tfrac{\partial}{\partial t} \left([B, A](\mathcal{E}_B) \right) \\
&= \left(\tfrac{\partial}{\partial t} \partial_2 \tilde{\mathcal{S}}^{(1)} \right) \cdot A(v) - A'(\mathcal{E}_B) \cdot \tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(1)} \\
&\quad - A''(\mathcal{E}_B)(\tfrac{\partial}{\partial t} \mathcal{E}_B, \tilde{\mathcal{S}}^{(1)}) + [B, A]'(\mathcal{E}_B) \cdot \tfrac{\partial}{\partial t} \mathcal{E}_B \\
&= \left(\tfrac{\partial}{\partial t} \partial_2 \tilde{\mathcal{S}}^{(1)} \right) \cdot A(v) - A'(\mathcal{E}_B) \cdot \tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(1)} \\
&\quad - A''(\mathcal{E}_B)(B(\mathcal{E}_B), \tilde{\mathcal{S}}^{(1)}) + [B, A]'(\mathcal{E}_B) \cdot B(\mathcal{E}_B) \,.
\end{aligned}$$

From (3.5c) we obtain

$$\begin{aligned}
\left(\tfrac{\partial}{\partial t} \partial_2 \tilde{\mathcal{S}}^{(1)} \right) \cdot A(v) = {}& B'(\mathcal{E}_B) \cdot \partial_2 \tilde{\mathcal{S}}^{(1)} \cdot A(v) + B''(\mathcal{E}_B)(\tilde{\mathcal{S}}^{(1)}, \partial_2 \mathcal{E}_B \cdot A(v)) \\
& + [B, A]'(\mathcal{E}_B) \cdot \partial_2 \mathcal{E}_B \cdot A(v) \,,
\end{aligned}$$

and from (3.3a) we have

$$A'(\mathcal{E}_B) \cdot \tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(1)} = A'(\mathcal{E}_B) \cdot B'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} + A'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \,.$$

In this manner, we determine the occurring time derivatives and obtain

$$\begin{aligned}
\tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(2)} = {}& B'(\mathcal{E}_B) \cdot \partial_2 \tilde{\mathcal{S}}^{(1)} \cdot A(v) + B''(\mathcal{E}_B)(\partial_2 \mathcal{E}_B \cdot A(v), \tilde{\mathcal{S}}^{(1)}) \\
& + [B, A]'(\mathcal{E}_B) \cdot \partial_2 \mathcal{E}_B \cdot A(v) \\
& - A'(\mathcal{E}_B) \cdot B'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} - A'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \\
& - A''(\mathcal{E}_B)(B(\mathcal{E}_B), \tilde{\mathcal{S}}^{(1)}) + [B, A]'(\mathcal{E}_B) \cdot B(\mathcal{E}_B) \,.
\end{aligned}$$

Recombination gives

$$\begin{aligned}
\tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(2)} = {}& B'(\mathcal{E}_B) \cdot \partial_2 \tilde{\mathcal{S}}^{(1)} \cdot A(v) - B'(\mathcal{E}_B) \cdot A'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} \\
& + B'(\mathcal{E}_B) \cdot [B, A] \, \mathcal{E}_B \\
& - A''(\mathcal{E}_B)(B(\mathcal{E}_B), \tilde{\mathcal{S}}^{(1)}) - A'(\mathcal{E}_B) \cdot B'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} \\
& + B'(\mathcal{E}_B) \cdot A'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} + B''(\mathcal{E}_B)(\partial_2 \mathcal{E}_B \cdot A(v), \tilde{\mathcal{S}}^{(1)}) \\
& + [B, A]'(\mathcal{E}_B) \cdot B(\mathcal{E}_B) - A'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \\
& + [B, A]'(\mathcal{E}_B) \cdot \partial_2 \mathcal{E}_B \cdot A(v) - B'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \,,
\end{aligned}$$

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where, due to (3.2b), we use

$$\partial_2 \mathcal{E}_B \cdot A(v) = \tilde{\mathcal{S}}^{(1)} + A(\mathcal{E}_B)\,.$$

As a consequence, we obtain

$$
\begin{aligned}
\tfrac{\partial}{\partial t} \tilde{\mathcal{S}}^{(2)} =\ & B'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(2)} + B''(\mathcal{E}_B)(\tilde{\mathcal{S}}^{(1)}, \tilde{\mathcal{S}}^{(1)}) \\
& - A''(\mathcal{E}_B)(B(\mathcal{E}_B), \tilde{\mathcal{S}}^{(1)}) - A'(\mathcal{E}_B) \cdot B'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} \\
& + B''(\mathcal{E}_B)(A(\mathcal{E}_B), \tilde{\mathcal{S}}^{(1)}) + B'(\mathcal{E}_B) \cdot A'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} \\
& + [B, A]'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(1)} + [B, A]'(\mathcal{E}_B) \cdot B(\mathcal{E}_B) \\
& - A'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) + [B, A]'(\mathcal{E}_B) \cdot A(\mathcal{E}_B) \\
& - B'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \\
=\ & B'(\mathcal{E}_B) \cdot \tilde{\mathcal{S}}^{(2)} + B''(\mathcal{E}_B)(\tilde{\mathcal{S}}^{(1)}, \tilde{\mathcal{S}}^{(1)}) \\
& + [B, A]'(\mathcal{E}_B) \cdot B(\mathcal{E}_B) - A'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \\
& + [B, A]'(\mathcal{E}_B) \cdot A(\mathcal{E}_B) - B'(\mathcal{E}_B) \cdot [B, A](\mathcal{E}_B) \\
& + \big\{ - A''(\mathcal{E}_B)(B(\mathcal{E}_B), \cdot) - A'(\mathcal{E}_B) \cdot B'(\mathcal{E}_B) + B'(\mathcal{E}_B) \cdot A'(\mathcal{E}_B) \\
& \quad + B''(\mathcal{E}_B)(A(\mathcal{E}_B), \cdot) + [B, A]'(\mathcal{E}_B) \big\} \cdot \tilde{\mathcal{S}}^{(1)}\,.
\end{aligned}
$$

This expression simplifies to (3.10a).

(iii) The integral representations (3.11) for $\tilde{\mathcal{S}}^{(2)}$ and $\mathcal{S}^{(2)}$ follow from an application of the variation-of-constants formula (A.2). $\qquad \square$

3.4. A posteriori local error analysis

For the construction of a defect-based local error estimator we approximate the integral representation (2.7b) by the trapezoidal rule. Applying $\mathcal{F}(0, t, u) = \mathcal{S}^{(1)}(0, u) = 0$, see also (2.7c) and (3.4b), and the representation of the defect provided by Lemma 3, we obtain

$$
\begin{aligned}
\mathcal{P}(t, u) &= \tfrac{1}{2}\, t\, \big(\mathcal{F}(0, t, u) + \mathcal{F}(t, t, u) \big) = \tfrac{1}{2}\, t\, \mathcal{F}(t, t, u)\ = \tfrac{1}{2}\, t\, \mathcal{S}^{(1)}(t, u) \\
&= \tfrac{1}{2}\, t\, \big(\partial_2 \mathcal{E}_B(t, \mathcal{E}_A(t, u)) \cdot A(\mathcal{E}_A(t, u)) - A(\mathcal{E}_B(t, \mathcal{E}_A(t, u))) \big)\,. \quad \text{(3.12a)}
\end{aligned}
$$

Practical evaluation of the a posteriori local error estimator is discussed in Section 5.

Our aim is to show that the local error estimator is asymptotically correct, that is, its deviation satisfies

$$\mathcal{P}(t, u) - \mathcal{L}(t, u) = \mathcal{O}(t^3)\,. \tag{3.13}$$

For this purpose, we analyze the quadrature error employing the first- and second-order Peano kernels

$$K_1(\tau, t) = \tau - \tfrac{1}{2} t = \mathscr{O}(t) \,, \qquad K_2(\tau, t) = \tfrac{1}{2} \tau(t - \tau) = \mathscr{O}(t^2) \,;$$

(note that $K_1(\tau, t) = -\frac{\partial}{\partial \tau} K_2(\tau, t)$). Recalling the representations for the first- and second-order defect terms provided by Lemma 3 and Lemma 4, the following result implies (3.13), provided that the integrand remains bounded.

Theorem 2 (Deviation, Lie–Trotter splitting). *For the deviation of the a posteriori local error estimator, the integral representation*

$$\mathcal{P}(t, u) - \mathcal{L}(t, u) = \int_0^t \big(K_1(\tau, t)\, \mathcal{G}_1(\tau, t, u) - K_2(\tau, t)\, \mathcal{G}_2(\tau, t, u) \big)\, \mathrm{d}\tau \,, \quad \text{(3.14a)}$$

$$\mathcal{G}_1(\tau, t, u) = \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(2,1)}(t, u) \hspace{3cm} \text{(3.14b)}$$
$$\hspace{2cm} + \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u)) \,,$$

$$\mathcal{G}_2(\tau, t, u) = \Big\{ \partial_2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, v)) \cdot \partial_2 \tilde{\mathcal{S}}^{(1)}(t, v) \cdot [B, A](v) \hspace{1cm} \text{(3.14c)}$$
$$\hspace{1cm} + \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, v))(\tilde{\mathcal{S}}^{(1)}(\tau, v), \partial_2 \mathcal{E}_B(\tau, v) \cdot [B, A](v))$$
$$\hspace{1cm} + \partial_2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, v)) \cdot \partial_2 \mathcal{E}_B(\tau, v) \, \cdot \, [[B, A], A](v) \Big\}\Big|_{v = \mathcal{E}_A(\tau, u)}$$

holds.

PROOF. We start from the first-order Peano representation

$$\mathcal{P}(t, u) - \mathcal{L}(t, u) = \int_0^t K_1(\tau, t)\, \tfrac{\partial}{\partial \tau} \mathcal{F}(\tau, t, u)\, \mathrm{d}\tau \,.$$

From (2.11a) in Lemma 1 we have

$$\tfrac{\partial}{\partial \tau} \mathcal{F}(\tau, t, u) = \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(2)}(\tau, u)$$
$$\hspace{2cm} + \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u)) \,.$$

Lemma 3 implies $\mathcal{S}^{(1)}(\tau, u) = \mathscr{O}(\tau)$, which results in an $\mathscr{O}(\tau^2)$ contribution to $\frac{\partial}{\partial \tau} \mathcal{F}(\tau, t, u)$. Furthermore, due to Lemma 4, $\mathcal{S}^{(2)}$ splits into

$$\mathcal{S}^{(2)}(\tau, u) = \mathcal{S}^{(2,0)}(\tau, u) + \mathcal{S}^{(2,1)}(\tau, u) = \mathscr{O}(1) + \mathscr{O}(\tau) \,.$$

Consequently, we have

$$\tfrac{\partial}{\partial \tau}\mathcal{F}(\tau,t,u) = \mathcal{G}_1(\tau,t,u) + \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(2,0)}(\tau,u)\,,$$

with $\mathcal{G}_1$ from (3.14b), which gives an $\mathscr{O}(\tau^2)$ contribution to $\tfrac{\partial}{\partial \tau}\mathcal{F}$. The remaining contribution to the quadrature error influenced by $\mathcal{S}^{(2,0)}(\tau) = \mathscr{O}(1)$ is now analyzed in detail. Using integration by parts, we convert it into second-order Peano form

$$\int_0^t K_1(\tau,t)\,\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(2,0)}(\tau,u)\,\mathrm{d}\tau$$

$$= \int_0^t K_2(\tau,t)\,\tfrac{\partial}{\partial \tau}\big(\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(2,0)}(\tau,u)\big)\,\mathrm{d}\tau\,,$$

involving

$$\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\mathcal{S}^{(2,0)}(\tau,u)$$
$$= \partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot\partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot[B,A](\mathcal{E}_A(\tau,u))\,,$$

see (3.11). The derivatives of these three factors evaluate to

$$\tfrac{\partial}{\partial \tau}\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))$$
$$= -\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot H'(\mathcal{S}(\tau,u))$$
$$\quad - \partial_2^2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))(H(\mathcal{S}(\tau,u)),\cdot)$$
$$\quad + \partial_2^2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))(\tfrac{\partial}{\partial \tau}\mathcal{S}(\tau,u),\cdot)$$
$$= -\partial_2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))\cdot H'(\mathcal{S}(\tau,u))$$
$$\quad + \partial_2^2\mathcal{E}_H(t-\tau,\mathcal{S}(\tau,u))(\mathcal{S}^{(1)}(\tau,u),\cdot)$$
$$= \Big\{ -\partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))\cdot H'(\mathcal{E}_B(\tau,v))$$
$$\quad + \partial_2^2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1)}(\tau,v),\cdot)\Big\}\Big|_{v=\mathcal{E}_A(\tau,u)}\,,$$

and

$$\tfrac{\partial}{\partial \tau}\partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))$$
$$= \partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot B'(\mathcal{E}_A(t,u))$$
$$\quad + \partial_2^2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))(\tfrac{\partial}{\partial \tau}\mathcal{E}_A(\tau,u)+B(\mathcal{E}_A(\tau,u)),\cdot)$$
$$= \partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))\cdot B'(\mathcal{E}_A(t,u)) + \partial_2^2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))(H(\mathcal{E}_A(\tau,u)),\cdot)$$
$$= \Big\{\partial_2\mathcal{E}_B(\tau,v)\cdot B'(v) + \partial_2^2\mathcal{E}_B(\tau,v)(H(v),\cdot)\Big\}\Big|_{v=\mathcal{E}_A(\tau,u)}\,,$$

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and

$$\frac{\partial}{\partial \tau}\big([B,A](\mathcal{E}_A(\tau,u))\big) = [B,A]'(\mathcal{E}_A(\tau,u)) \cdot \frac{\partial}{\partial \tau}\mathcal{E}_A(\tau,u)$$
$$= [B,A]'(\mathcal{E}_A(\tau,u)) \cdot A(\mathcal{E}_A(\tau,u))$$
$$= \Big\{[B,A]'(v) \cdot A(v)\Big\}\Big|_{v=\mathcal{E}_A(\tau,u)}.$$

Altogether,

$$\frac{\partial}{\partial \tau}\partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u))) \cdot \partial_2\mathcal{E}_B(\tau,\mathcal{E}_A(\tau,u)) \cdot [B,A](\mathcal{E}_A(\tau,u))$$

$$= \Big\{ -\partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot H'(\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot [B,A](v)$$

$$+ \partial_2^2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1)}(\tau,v),\partial_2\mathcal{E}_B(\tau,v) \cdot [B,A](v))$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot B'(v) \cdot [B,A](v)$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2^2\mathcal{E}_B(\tau,v)(H(v),[B,A](v))$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot [B,A]'(v) \cdot A(v) \Big\}\Big|_{v=\mathcal{E}_A(\tau,u)},$$

which can be rewritten as

$$\Big\{ -\partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot H'(\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot [B,A](v)$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot H'(v) \cdot [B,A](v)$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot (-A'(v)) \cdot [B,A](v)$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v) \cdot [B,A]'(v) \cdot A(v)$$

$$+ \partial_2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v)) \cdot \partial_2^2\mathcal{E}_B(\tau,v)(H(v),[B,A](v))$$

$$+ \partial_2^2\mathcal{E}_H(t-\tau,\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1)}(\tau,v),\partial_2\mathcal{E}_B(\tau,v) \cdot [B,A](v)) \Big\}\Big|_{v=\mathcal{E}_A(\tau,u)}.$$

Now we recombine terms. Consider

$$\partial_2^2\mathcal{E}_B(\tau,v)(H(v),\cdot) + \partial_2\mathcal{E}_B(\tau,v) \cdot H'(v) - H'(\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v)$$

$$= \partial_2^2\mathcal{E}_B(\tau,v)(A(v),\cdot) + \partial_2\mathcal{E}_B(\tau,v) \cdot A'(v) - A'(\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v)$$

$$+ \partial_2^2\mathcal{E}_B(\tau,v)(B(v),\cdot) + \partial_2\mathcal{E}_B(\tau,v) \cdot B'(v) - B'(\mathcal{E}_B(\tau,v)) \cdot \partial_2\mathcal{E}_B(\tau,v).$$

Here, the term in the first line equals $\partial_2\tilde{\mathcal{S}}^{(1)}(t,v)$, see (3.5a), and the other term vanishes because it is the Fréchet derivative with respect to v of

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$\partial_2 \mathcal{E}_B(t,v) \cdot B(v) - B(\mathcal{E}_B(t,v)) = 0$, see (A.7). With this observation we finally obtain

$$\frac{\partial}{\partial \tau} \big(\partial_2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tau, u))) \cdot \partial_2 \mathcal{E}_B(\tau, \mathcal{E}_A(\tau, u)) \cdot [B, A](\mathcal{E}_A(\tau, u)) \big)$$

$$= \Big\{ \partial_2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, v)) \cdot \partial_2 \tilde{\mathcal{S}}^{(1)}(t, v) \cdot [B, A](v)$$

$$+ \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, v))(\tilde{\mathcal{S}}^{(1)}(\tau, v), \partial_2 \mathcal{E}_B(\tau, v) \cdot [B, A](v))$$

$$+ \partial_2 \mathcal{E}_H(t - \tau, \mathcal{E}_B(\tau, v)) \cdot \partial_2 \mathcal{E}_B(\tau, v) \cdot$$

$$(-A' \cdot [B, A] + [B, A]' \cdot A)(v) \Big\} \Big|_{v = \mathcal{E}_A(\tau, u)} ,$$

which is identical to $\mathcal{G}_2(\tau, t, u)$ from (3.14c). This completes the proof of Theorem 2. $\qquad \square$

4. Strang splitting method

In this section, we construct a defect-based local error estimator for the Strang splitting method (2.5) and prove its asymptotical correctness. Compared to the local error analysis for the Lie–Trotter splitting method, the calculations are significantly more involved. Suitable representations for the defects $\mathcal{S}^{(1)}, \mathcal{S}^{(2)}, \mathcal{S}^{(3)}$ defined in (2.6) are provided by Lemmas 5–7 in Appendix C. These have been verified by automatic symbolic manipulations, see Appendix B. The specialization to a nonlinear Schrödinger equation is described in Section 5.

4.1. A priori local error analysis

Inserting the integral representation (3.4b) for the defect into (2.7) yields a representation for the local error. The proof of the following theorem is based on a further expansion leading to an integral representation which implies

$$\mathcal{L}(t, u) = \mathcal{O}(t^3) , \tag{4.1}$$

provided that the integrand remains bounded.

Theorem 3 (Local error, Strang splitting). *The local error of the Strang splitting method satisfies*

$$\mathcal{L}(t, u) = \int_0^t \int_0^{\tau_1} \Big\{ \partial_2 \mathcal{E}_H(t_2 - \tau, \mathcal{S}(\tau_2, u)) \cdot \mathcal{S}^{(2)}(\tau_2, u) \tag{4.2}$$

$$+ \partial_2^2 \mathcal{E}_H(t - \tau_2, \mathcal{S}(\tau_2, u))(\mathcal{S}^{(1)}(\tau_2, u), \mathcal{S}^{(1)}(\tau_2, u)) \Big\} \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 ,$$

with $\mathcal{S}^{(1)}, \mathcal{S}^{(2)}$ given in Lemmas 5 and 6, see Appendix C.

PROOF. We perform a twofold expansion of the local error integral (2.7b). Due to $\mathcal{F}(0, t, u) = \mathcal{S}^{(1)}(0, u) = 0$,

$$\mathcal{L}(t, u) = \int_0^t \mathcal{F}(\tau_1, t, u) \, \mathrm{d}\tau_1 = \int_0^t \int_0^{\tau_1} \tfrac{\mathrm{d}}{\mathrm{d}\tau_2} \mathcal{F}(\tau_2, t, u) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1 \,, \qquad (4.3\text{a})$$

where, according to (2.11a) in Lemma 1,

$$\begin{aligned}
\tfrac{\partial}{\partial \tau} \mathcal{F}(\tau, t, u) &= \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(2)}(\tau, u) \qquad\qquad (4.3\text{b}) \\
&\quad + \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u)) \,.
\end{aligned}$$

From Lemma 5 in Appendix C below we see that $\mathcal{S}^{(1)}(\tau, u) = \mathcal{O}(\tau)$ holds due to the homogeneous initial conditions (C.2b) and (C.2d), provided that the respective integrands remain bounded. Furthermore, from Lemma 6 we obtain with the help of the generalized fundamental identity (A.9):

$$\begin{aligned}
\mathcal{S}^{(2)}(\tau, u) &= \left\{ \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot \mathcal{S}^{(2,1)}(\tau, v) + \mathcal{S}^{(2,2)}(\tau, w) \right\}\Big|_{\substack{v = \mathcal{E}_A(\frac{1}{2}\tau, u) \\ w = \mathcal{E}_B(\tau, \mathcal{E}_A(\frac{1}{2}\tau, u))}} \\
&= \left\{ \tfrac{1}{2} \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot \left(\partial_2 \mathcal{E}_B(\tau, v) \cdot [B, A](v) - [B, A](\mathcal{E}_B(\tau, v)) \right) \right\}\Big|_{\substack{v = \mathcal{E}_A(\frac{1}{2}\tau, u) \\ w = \mathcal{E}_B(\tau, \mathcal{E}_A(\frac{1}{2}\tau, u))}} \\
&\quad + \mathcal{O}(\tau) \\
&= \Big\{ \tfrac{1}{2} \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot \partial_2 \mathcal{E}_B(\tau, v) \cdot \\
&\qquad \int_0^t \partial_2 \mathcal{E}_B(-\tau, \mathcal{E}_B(\tau, v)) \cdot [B, [B, A]](\mathcal{E}_B(\tau, v)) \Big\}\Big|_{\substack{v = \mathcal{E}_A(\frac{1}{2}\tau, u) \\ w = \mathcal{E}_B(\tau, \mathcal{E}_A(\frac{1}{2}\tau, u))}} + \mathcal{O}(\tau) \\
&= \mathcal{O}(\tau) \,,
\end{aligned}$$

provided that all integrands involved remain bounded. $\qquad\qquad\qquad\square$

Remark 4. We note that for $\tau = 0$ we have

$$\begin{aligned}
&\mathcal{S}^{(2)}(0, u) \\
&= \tfrac{1}{2} \partial_2 \mathcal{E}_A(0, u) \cdot \left(\partial_2 \mathcal{E}_B(0, v) \cdot [B, A](v) - [B, A](\mathcal{E}_B(0, v)) \right)\big|_{\substack{v = \mathcal{E}_A(0, u) \\ w = \mathcal{E}_B(0, \mathcal{E}_A(0, u))}} \\
&= \tfrac{1}{2}[B, A](u) - \tfrac{1}{2}[B, A](u) = 0 \,, \qquad\qquad\qquad\qquad\qquad (4.4)
\end{aligned}$$

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which corresponds with the second-order condition satisfied by the Strang splitting method.

The leading term after Taylor expansion of $\mathcal{L}(t,u)$ is given by

$$
\begin{aligned}
\tfrac{t^3}{6}\tfrac{\mathrm{d}^3}{\mathrm{d}t^3}\mathcal{L}(0,u) &= \tfrac{t^3}{6}\tfrac{\mathrm{d}^2}{\mathrm{d}t^2}\mathcal{S}^{(1)}(0,u) = \tfrac{t^3}{6}\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{S}^{(2)}(0,u) = \tfrac{t^3}{6}\mathcal{S}^{(3)}(0,u) \\
&= \tfrac{t^3}{6}\left(\tfrac{1}{4}\left[[A,B],A\right](u) + \tfrac{1}{2}\left[[A,B],B\right](u)\right),
\end{aligned}
\tag{4.5}
$$

which exactly corresponds with the linear case, see [5].

4.2. A posteriori local error analysis

The error estimator is defined as the approximation of the local error integral (2.7b) by a third-order Hermite quadrature formula, exploiting $\mathcal{F}(0,t,u) = \mathcal{S}^{(1)}(0,u) = 0$ (see (2.7c), Lemma 5), and $\frac{\partial}{\partial\tau}\mathcal{F}(0,t,u) = 0$ (see (2.11a), (4.4)):

$$
\begin{aligned}
\mathcal{P}(t,u) &= t\left(\tfrac{2}{3}\,\mathcal{F}(0,t,u) + \tfrac{1}{6}\,t\,\tfrac{\partial}{\partial\tau}\mathcal{F}(0,t,u) + \tfrac{1}{3}\,\mathcal{F}(t,t,u)\right) \\
&= \tfrac{1}{3}\,t\,\mathcal{F}(t,t,u) = \tfrac{1}{3}\,t\,\mathcal{S}^{(1)}(t,u).
\end{aligned}
\tag{4.6a}
$$

By means of the representation of $\mathcal{S}^{(1)}(t,u)$ provided by Lemma 5 we have

$$
\mathcal{P}(t,u) = \tfrac{1}{3}\,t\left\{\partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\cdot\tilde{\mathcal{S}}^{(1,1)}(t,v) + \tilde{\mathcal{S}}^{(1,2)}(t,w)\right\}\Big|_{\substack{v=\mathcal{E}_A(\frac{1}{2}t,u)\\ w=\mathcal{E}_B(t,\mathcal{E}_A(\frac{1}{2}t,u))}},
\tag{4.6b}
$$

with

$$
\tilde{\mathcal{S}}^{(1,1)}(t,v) = \tfrac{1}{2}\left(\partial_2\mathcal{E}_B(t,v)\cdot A(v) - A(\mathcal{E}_B(t,v))\right),
\tag{4.6c}
$$

$$
\tilde{\mathcal{S}}^{(1,2)}(t,w) = \partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\cdot B(w) - B(\mathcal{E}_A(\tfrac{1}{2}t,w)).
\tag{4.6d}
$$

Our aim is to show that the local error estimator $\mathcal{P}(t,u)$ is asymptotically correct, i.e., that its deviation, the error of the Hermite quadrature rule applied to (2.7b), satisfies

$$
\mathcal{P}(t,u) - \mathcal{L}(t,u) = \mathcal{O}(t^4).
\tag{4.7}
$$

In the following, this quadrature error is analyzed on the basis of its Peano representation, with the second- and third-order Peano kernels

$$
K_2(\tau,t) = \tfrac{1}{6}\,(3\tau - t)(t - \tau) = \mathcal{O}(t^2),
$$
$$
K_3(\tau,t) = \tfrac{1}{6}\,\tau(t - \tau)^2 = \mathcal{O}(t^3)
$$

(note that $K_2(\tau,t) = -\frac{\partial}{\partial\tau}K_3(\tau,t)$). For the following theorem we recall the representations for the first-, second-, and third-order defect terms provided in Lemmas 5–7.

Theorem 4 (Deviation, Strang splitting). *The deviation $\mathcal{P} - \mathcal{L}$ of the a posteriori local error estimator admits an integral representation which implies* (4.7).

PROOF. We start from the second-order Peano representation

$$\mathcal{P}(t, u) - \mathcal{L}(t, u) = \int_0^t K_2(\tau, t) \, \tfrac{\partial^2}{\partial \tau^2} \, \mathcal{F}(\tau, t, u) \, \mathrm{d}\tau \, .$$

From (2.11b) in Lemma 1 we conclude

$$\begin{aligned}
\tfrac{\partial^2}{\partial \tau^2} \, \mathcal{F}(\tau, t, u) = {} & \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(3)}(\tau, u) \\
& + 3 \, \partial_2^2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(2)}(\tau, u)) \\
& + \partial_2^3 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u))(\mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u), \mathcal{S}^{(1)}(\tau, u)) \, .
\end{aligned}$$

Lemmas 5 and 6 imply $\mathcal{S}^{(1)}(\tau, u) = \mathcal{O}(\tau)$ and $\mathcal{S}^{(2)}(\tau, u) = \mathcal{O}(1)$, which result in a $\mathcal{O}(\tau)$ contribution to $\tfrac{\partial^2}{\partial \tau^2} \, \mathcal{F}(\tau, t, u)$. Thus,

$$\tfrac{\partial^2}{\partial \tau^2} \mathcal{F}(\tau, t, u) = \partial_2 \mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \mathcal{S}^{(3)}(\tau, u) + \mathcal{O}(\tau) \, ,$$

where $\mathcal{S}^{(3)}(\tau, u)$ is represented by (C.7a) from Lemma 7. Together with (see Appendix C)

$$\begin{aligned}
\tilde{\mathcal{S}}^{(1,1)}(\tau, v) &= \mathcal{O}(\tau) \, , \quad \tilde{\mathcal{S}}^{(2,1)}(\tau, v) = \mathcal{O}(1) \, , \\
\partial_2 \tilde{\mathcal{S}}^{(1,2)}(\tau, w) &= \mathcal{O}(\tau) \, , \quad \partial_2 \tilde{\mathcal{S}}^{(2,2)}(\tau, w) = \mathcal{O}(1) \, , \quad \text{and} \quad \partial_2^2 \tilde{\mathcal{S}}^{(1,2)}(\tau, w) = \mathcal{O}(\tau) \, ,
\end{aligned}$$

we obtain

$$\mathcal{S}^{(3)}(t, u) = \left\{ \partial_2 \mathcal{E}_A(\tfrac{1}{2} t, w) \cdot \tilde{\mathcal{S}}^{(3,1)}(t, v) + \tilde{\mathcal{S}}^{(3,2)}(t, w) \right\}\Big|_{\substack{v = \mathcal{E}_A(\frac{1}{2} t, u) \\ w = \mathcal{E}_B(t, \mathcal{E}_A(\frac{1}{2} t, u))}} + \mathcal{O}(t) \, ,$$

and due to representations (C.9a) and (C.9b) for $\tilde{\mathcal{S}}^{(3,1)}(t, v)$ and $\tilde{\mathcal{S}}^{(3,2)}(t, w)$ this yields

$$\begin{aligned}
\mathcal{S}^{(3)}(t, u) = \Big\{ & \partial_2 \mathcal{E}_A(\tfrac{1}{2} t, w) \cdot \partial_2 \mathcal{E}_B(t, v) \cdot \big(- \tfrac{1}{2} [B, [B, A]](v) - \tfrac{1}{2} [A, [B, A](v)) \\
& + \partial_2 \mathcal{E}_A(\tfrac{1}{2} t, w) \cdot \big([B, [B, A]](w) + \tfrac{3}{4} [A, [B, A](w)) \big) \Big\}\Big|_{\substack{v = \mathcal{E}_A(\frac{1}{2} t, u) \\ w = \mathcal{E}_B(t, \mathcal{E}_A(\frac{1}{2} t, u))}} + \mathcal{O}(t) \, .
\end{aligned}$$

It remains to show that

$$\int_0^t K_2(\tau, t)\, \partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$\partial_2\mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u)) \cdot [B, [B, A]](\mathcal{E}_A(\tfrac{1}{2}\tau, u))\, \mathrm{d}\tau = \mathscr{O}(t^4)\,,$$

$$\int_0^t K_2(\tau, t)\, \partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$\partial_2\mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u)) \cdot [A, [B, A]](\mathcal{E}_A(\tfrac{1}{2}\tau, u))\, \mathrm{d}\tau = \mathscr{O}(t^4)\,,$$

$$\int_0^t K_2(\tau, t)\, \partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$[B, [B, A]](\mathcal{E}_B(\tau, (\mathcal{E}_A(\tfrac{1}{2}\tau, u))))\, \mathrm{d}\tau = \mathscr{O}(t^4)\,,$$

$$\int_0^t K_2(\tau, t)\, \partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$[A, [B, A]](\mathcal{E}_B(\tau, (\mathcal{E}_A(\tfrac{1}{2}\tau, u))))\, \mathrm{d}\tau = \mathscr{O}(t^4)\,,$$

are satisfied. Using integration by parts we convert these integrals into third-order Peano form. For the first integral this yields

$$\int_0^t K_3(\tau, t)\, \tfrac{\partial}{\partial\tau}\big(\partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$\partial_2\mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u)) \cdot [B, [B, A]](\mathcal{E}_A(\tfrac{1}{2}\tau, u))\big)\, \mathrm{d}\tau\,,$$

and analogously for the other integrals. Thus, we have to show

$$\tfrac{\partial}{\partial\tau}\big(\partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$\partial_2\mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u)) \cdot [B, [B, A]](\mathcal{E}_A(\tfrac{1}{2}\tau, u))\big) = \mathscr{O}(1)\,, \quad (4.8\text{a})$$

$$\tfrac{\partial}{\partial\tau}\big(\partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$\partial_2\mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u)) \cdot [A, [B, A]](\mathcal{E}_A(\tfrac{1}{2}\tau, u))\big) = \mathscr{O}(1)\,, \quad (4.8\text{b})$$

$$\tfrac{\partial}{\partial\tau}\big(\partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$[B, [B, A]](\mathcal{E}_B(\tau, (\mathcal{E}_A(\tfrac{1}{2}\tau, u)))) = \mathscr{O}(1)\,, \quad (4.8\text{c})$$

$$\tfrac{\partial}{\partial\tau}\big(\partial_2\mathcal{E}_H(t - \tau, \mathcal{S}(\tau, u)) \cdot \partial_2\mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot$$
$$[A, [B, A]](\mathcal{E}_B(\tau, (\mathcal{E}_A(\tfrac{1}{2}\tau, u)))) = \mathscr{O}(1)\,. \quad (4.8\text{d})$$

Relations (4.8a) and (4.8b) are valid because for each smooth operator F and thus in particular for $F = [B, [B, A]]$ and $F = [A, [B, A]]$, the respective

derivative can be evaluated as

$$
\frac{\partial}{\partial \tau} \big(\partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot \partial_2 \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u)) \cdot F(\mathcal{E}_A(\tfrac{1}{2}\tau, u)))
$$
$$
= \Big\{ -\tfrac{1}{2}\, \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot \partial_2 \mathcal{E}_B(\tau, v) \cdot [A, F](v)
$$
$$
+ \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \tilde{\mathcal{S}}^{(1,2)}(\tau, w) \cdot \partial_2 \mathcal{E}_B(\tau, v) \cdot F(v)
$$
$$
+ \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot \partial_2 \tilde{\mathcal{S}}^{(1,1)}(\tau, v) \cdot F(v)
$$
$$
+ \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2^2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \big(\tilde{\mathcal{S}}^{(1,1)}(\tau, v), \partial_2 \mathcal{E}_B(\tau, v) \cdot F(v) \big)
$$
$$
+ \partial_2^2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \big(S^{(1)}(\tau, u), \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot \partial_2 \mathcal{E}_B(\tau, v) \cdot F(v) \big) \Big\} \Big|_{\substack{v=\mathcal{E}_A(\frac{1}{2}t,u) \\ w=\mathcal{E}_B(t,\mathcal{E}_A(\frac{1}{2}t,u))}} .
$$

Relations (4.8c) and (4.8d)) are valid because for each smooth operator F and thus in particular for $F = [B, [B, A]]$ and $F = [A, [B, A]]$, the respective derivative can be computed as

$$
\frac{\partial}{\partial \tau} \big(\partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, \mathcal{E}_B(\tau, \mathcal{E}_A(\tfrac{1}{2}\tau, u))) \cdot F(\mathcal{E}_B(\tau, (\mathcal{E}_A(\tfrac{1}{2}\tau, u))))
$$
$$
= \Big\{ -\partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot [B, F](w)
$$
$$
+ \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \tilde{\mathcal{S}}^{(1,2)}(\tau, w) \cdot F(w)
$$
$$
- \tfrac{1}{2}\, \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot [A, F](w)
$$
$$
+ \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot F'(w) \cdot \tilde{\mathcal{S}}^{(1,1)}(\tau, v)
$$
$$
+ \partial_2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \cdot \partial_2^2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \big(\tilde{\mathcal{S}}^{(1,1)}(\tau, v), F(w) \big)
$$
$$
+ \partial_2^2 \mathcal{E}_H(t-\tau, \mathcal{S}(\tau, u)) \big(\mathcal{S}^{(1)}(\tau, u), \partial_2 \mathcal{E}_A(\tfrac{1}{2}\tau, w) \cdot F(w) \big) \Big\} \Big|_{\substack{v=\mathcal{E}_A(\frac{1}{2}t,u) \\ w=\mathcal{E}_B(t,\mathcal{E}_A(\frac{1}{2}t,u))}} .
$$

The manipulations leading to these representations are analogous to those performed in the proof of Theorem 2, but are too lengthy to carry out here in detail. The given result concludes the proof of Theorem 4. $\qquad\square$

5. Application to Schrödinger equations

In this section, we study the application of our local error analysis to time-dependent nonlinear Schrödinger equations. We state regularity requirements sufficient the formal bounds in Theorems 1–4 to hold in a rigorous sense and illustrate the theoretical results by numerical examples. As a

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model problem, we consider the time-dependent Schrödinger equation

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = -\frac{1}{2}\,\Delta\psi(x,t) + \kappa\,|\psi(x,t)|^2\,\psi(x,t)\,, \\ \psi(x,0) = \psi_0(x)\,, \qquad x \in \mathbb{R}^3\,, \quad t > 0\,, \end{cases} \tag{5.1}$$

involving a cubic nonlinearity[2], where $\kappa \in \mathbb{R}$. Incorporation of an additional multiplicative potential W acting by $\psi(x) \mapsto \mathrm{i}\,W(x)\,\psi(x)$ is already covered by the analysis given in [5].

5.1. Semi-discretization in time

In the following, we deduce regularity requirements on the exact solution to the time-dependent nonlinear Schrödinger equation (5.1) which ensure that the compositions of operators and their Lie commutators appearing in

---

[2]The nonlinearity in (5.1) is not complex Fréchet differentiable. This is merely a formal problem which can be circumvented by considering ψ and $\overline{\psi}$ as separate variables and considering the system

$$\begin{aligned} \mathrm{i}\,\partial_t \psi(x,t) &= -\tfrac{1}{2}\Delta\psi + \overline{\psi(x,t)}\,\psi(x,t)^2\,, \\ -\mathrm{i}\,\partial_t \overline{\psi}(x,t) &= -\tfrac{1}{2}\Delta\overline{\psi} + \psi(x,t)\,\overline{\psi(x,t)}^2\,. \end{aligned} \tag{5.2}$$

More generally, an operator $\mathcal{X}(\psi)$ involving terms depending on $\overline{\psi}$ can be identified with an operator $\hat{\mathcal{X}}(\hat{\psi}) \equiv \big(\mathcal{X}(\psi), \overline{\mathcal{X}}(\psi)\big)$, with $\hat{\psi} = (\psi, \overline{\psi})$. If $\hat{\mathcal{X}}(\hat{\psi})$ is Fréchet differentiable, then

$$\hat{\mathcal{X}}(\hat{\psi} + \hat{\phi}) = \hat{\mathcal{X}}(\hat{\psi}) + \hat{\mathcal{X}}'(\hat{\psi}) \cdot \hat{\phi} + o(\|\hat{\phi}\|)\,.$$

Here, evaluation of the Fréchet derivative $\hat{\mathcal{X}}'(\hat{\psi}) \cdot \hat{\phi}$ is identical with the Gâteaux derivative

$$\lim_{\delta \to 0} \tfrac{1}{\delta}\big(\hat{\mathcal{X}}(\hat{\psi} + \delta\hat{\phi}) - \hat{\mathcal{X}}(\hat{\psi})\big)\,,$$

and the first component is given by

$$\lim_{\delta \to 0} \tfrac{1}{\delta}\big(\mathcal{X}(\psi + \delta\phi) - \mathcal{X}(\psi)\big) =: \mathcal{X}'(\psi) \cdot \phi\,.$$

In this sense, the Fréchet derivative of the dilated operator $\hat{\mathcal{X}}(\hat{\psi})$ can be expressed by the Gâteaux derivative of $\mathcal{X}(\psi)$. For example, the cubic complex function $f(z) = |z|^2\,z = \bar{z}z^2$ has the derivative $f'(z)w = \bar{z}zw + z^2\bar{w}$ which is only real linear but which can be identified with the Fréchet derivative of its dilated version $\hat{f}(\hat{z}) = \hat{f}(z,\bar{z}) = (\bar{z}z^2, z\bar{z}^2)$.

In the following, we refrain from explicitly referring to (5.2) and all its corresponding Fréchet differentiable dilations. All differentiation processes can be expressed in terms of equivalent Gâteaux linearizations. This applies to all nonlinear operators involved, including corresponding flows and subflows.

the a priori and a posteriori local error representations given in Theorems 1–4 are well–defined and bounded. We point out that the regularity of the initial state is inherited by all flows and subflows. For the subflow associated with the linear kinetic part

$$A = T := \tfrac{1}{2}\,\mathrm{i}\,\Delta$$

this has been demonstrated in [5]. For simplicity, for the nonlinear part we meanwhile set $\kappa = 1$ such that

$$B(\psi) := V(\psi) = -\mathrm{i}\,|\psi|^2\psi\,.$$

For the associated flow

$$\mathcal{E}_V(t,\psi)(x) = \mathrm{e}^{-\mathrm{i}\,t\,|\psi(x)|^2}\psi(x)\,, \quad x \in \mathbb{R}^3 \tag{5.3}$$

we conclude differentiability in the sense of the remark above.

We next collect the relevant Lie commutators and Fréchet derivatives arising in Theorems 1–4.

- Theorem 1: $[T,V]$

- Theorem 2: additionally $[T,[T,V]]$, $[V,[T,V]]$, $[T,V]'$, V''

- Theorem 3 only involves Lie commutators and Fréchet derivatives arising in Theorems 1 and 2.

- Theorem 4: additionally[3] $[V,[V,[V,T]]]$, $[T,[V,[V,T]]] = [V,[T,[V,T]]]$, $[V,[V,[V,T]]]$, $[T,[V,T]]'$, $[V,[V,T]]'$, $[V,T]''$, $T'' = 0, T''' = 0$, V'''

For those quantities which have been estimated in our previous work [11], we only quote the necessary regularity requirements, see also [12, 13]. For a bound that depends on the respective norm of ψ, possibly in a nonlinear way, we write $\mathcal{C} = \mathcal{C}(\|\psi\|_{H^m})$. The symbol $\sim$ indicates that the term on the right-hand side is the dominant term in the expression, in the sense that other terms that are omitted can be estimated under milder regularity assumptions.

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[3]$[T,[V,[V,T]]] = [V,[T,[V,T]]]$ follows from the Jacobi identity (A.1c).

- According to [11], the first Lie commutator is equal to

$$[T, V](\psi) = \overline{\Delta\psi}\,\psi^2 + 2\,\psi\,\overline{\nabla\psi}\cdot\nabla\psi + \overline{\psi}\,\nabla\psi\cdot\nabla\psi\,, \qquad (5.4)$$

  and satisfies the estimate

$$\|[T, V](\psi)\|_{L^2} \leq \mathcal{C}(\|\psi\|_{H^2})\,.$$

- The estimate
$$\|[T, [T, V]](\psi)\|_{L^2} \leq \mathcal{C}(\|\psi\|_{H^4})$$
  also follows by the analysis given in [11].

- Calculating $[V, [T, V]](\psi)$ it is found that the result consists of products of five instances of ψ or its derivatives, where the sum of the derivatives equals two. Thus it is sufficient to estimate terms of either of the following two forms,

$$\begin{aligned}
\|\psi^3(\nabla\psi)^2\|_{L^2} &\leq \mathcal{C}\|\psi\|_{L^\infty}^3\|(\nabla\psi)^2\|_{L^2} \\
&\leq \mathcal{C}\|\psi\|_{H^2}^3\|\nabla\psi\|_{H^1}^2 \leq \mathcal{C}\|\psi\|_{H^2}^5 = \mathcal{C}(\|\psi\|_{H^2})\,, \\
\|\psi^4\Delta\psi\|_{L^2} &\leq \mathcal{C}\|\psi\|_{L^\infty}^4\|\Delta\psi\|_{L^2} \leq \mathcal{C}\|\psi\|_{H^2}^5 = \mathcal{C}(\|\psi\|_{H^2})\,,
\end{aligned}$$

  where the bounds follow from $\|\psi_1\,\psi_2\|_{L^2} \leq \|\psi_1\|_\infty\|\psi_2\|_{L^2}$ and the Sobolev embedding of $H^2(\mathbb{R}^3)$ in $L^\infty(\mathbb{R}^3)$.

- From (5.4) we can compute and estimate the derivative

$$\begin{aligned}
[T, V]'(\psi)\cdot\phi = {}& \overline{\Delta\phi}\,\psi^2 + 2\,\overline{\Delta\psi}\,\psi\,\phi + 2\,\phi\,\overline{\nabla\psi}\cdot\nabla\psi \\
& + 2\,\psi\,\overline{\nabla\phi}\cdot\nabla\psi + 2\,\psi\,\overline{\nabla\psi}\cdot\nabla\phi \\
& + \overline{\phi}\,\nabla\psi\cdot\nabla\psi + 2\,\overline{\psi}\,\nabla\psi\cdot\nabla\phi\,,
\end{aligned}$$

$$\|[T, V]'(\psi)\cdot\phi\|_{L^2} \leq \mathcal{C}(\|\psi\|_{H^2}, \|\phi\|_{H^2})\,,$$

  using additionally the Hölder inequalities $\|\psi_1\,\psi_2\|_{L^2} \leq \|\psi_1\|_{L^4}\|\psi_2\|_{L^4}$ and $\|\psi_1\,\psi_2\,\psi_3\|_{L^2} \leq \|\psi_1\|_{L^6}\|\psi_2\|_{L^6}\|\psi_3\|_{L^6}$ and the Sobolev embeddings of $H^1(\mathbb{R}^3)$ in $L^4(\mathbb{R}^3)$ and in $L^6(\mathbb{R}^3)$.

- The first and second Fréchet derivatives of V evaluate to

$$\begin{aligned}
V'(\psi)\cdot\phi &= -\mathrm{i}\left(2\,\psi^2\,\overline{\phi} + \overline{\psi}\,\psi\,\phi\right)\,, \\
V''(\psi)(\phi_1, \phi_2) &= -2\,\mathrm{i}\left(\psi\,(\overline{\phi_1}\,\phi_2 + \phi_1\,\overline{\phi_2}) + \overline{\psi}\,\phi_1\,\phi_2\right)\,,
\end{aligned}$$

resulting in the bound

$$\|V''(\psi)(\phi_1, \phi_2)\|_{L^2} \le \mathcal{C}(\|\psi\|_{H^1})\|\phi_1\|_{H^1}\|\phi_2\|_{H^1} \,.$$

- It has been shown in [11] that

$$\|[T, [T, [T, V]]](\psi)\|_{L^2} \le \mathcal{C}(\|\psi\|_{H^6}) \,.$$

- The Fréchet derivative of $[T, [T, V]]$ can be estimated by realizing that the critical term in $[T, [T, V]]$ is equal to (see [11])

$$[T, [T, V]](\psi) \sim \psi^2 \, \overline{\Delta^2 \psi} \,,$$

and thus

$$[T, [T, V]]'(\psi) \cdot \phi \sim 2\, \phi \, \psi \, \overline{\Delta^2 \psi} + \psi^2 \, \overline{\Delta^2 \phi} \,,$$
$$\|[T, [T, V]]'(\psi) \cdot \phi\|_{L^2} \le \mathcal{C}(\|\psi\|_{H^4}, \|\phi\|_{H^4}) \,.$$

- The second Fréchet derivative of the first Lie commutator, $[V, T]''(\psi)(\phi_1, \phi_2)$ contains products of three functions, and is thus computed similarly as V'', resulting in

$$\|[V, T]''(\psi)(\phi_1, \phi_2)\|_{L^2} \le \mathcal{C}(\|\psi\|_{H^2}, \|\phi_1\|_{H^2}, \|\phi_2\|_{H^2}) \,,$$

where we have used

$$\|\psi \, \phi_1 \, \overline{\Delta\phi_2}\|_{L^2} \le \|\psi\phi_1\|_{L^\infty}\|\overline{\Delta\phi_2}\|_{L^2} \le \mathcal{C} \, \|\psi\|_{H^2}\|\phi_1\|_{H^2}\|\phi_2\|_{H^2} \,,$$
$$\|\psi \, \nabla\phi_1 \cdot \overline{\nabla\phi_2}\|_{L^2} \le \mathcal{C}\|\psi\|_{L^6}\|\nabla\phi_1\|_{L^6}\|\nabla\phi_2\|_{L^6} \le \mathcal{C}\,(\|\psi\|_{H^1}, \|\phi_1\|_{H^2}, \|\phi_2\|_{H^2}) \,.$$

- The third Fréchet derivative V''' satisfies

$$V'''(\psi)(\phi_1, \phi_2, \phi_3) = -2\,\mathrm{i}\,\left(\overline{\phi_1}\,\phi_2\,\phi_3 + \phi_1\,\overline{\phi_2}\,\phi_3 + \phi_1\,\phi_2\,\overline{\phi_3}\right) \,,$$

and thus

$$\|V'''(\psi)(\phi_1, \phi_2, \phi_3)\|_{L^2} \le \mathcal{C}(\|\phi_1\|_{H^1}, \|\phi_2\|_{H^1}, \|\phi_3\|_{H^1}) \,.$$

- The Fréchet derivative of the second Lie commutator $[V, [V, T]]'$ can be analyzed by the following reasoning: The Lie commutator consists of products of five functions or their derivatives, where the sum of the orders of the derivatives equals two. Thus, the same holds for the Fréchet derivative, and accordingly

$$\|[V, [V, T]]'(\psi) \cdot \phi\|_{L^2} \le \mathcal{C}(\|\psi\|_{H^2}, \|\phi\|_{H^2}) \,.$$

- A Lie commutator of the form $[V, [V, [V, T]]]$ consists of products of seven functions or their derivatives, where the sum of derivatives equals two. Thus,
$$\|[V, [V, [V, T]]](\psi)\|_{L^2} \leq \mathcal{C}(\|\psi\|_{H^2}).$$

- To analyze the Lie commutator $[V, [T, [V, T]]]$ we note that the critical term in $[T, [V, T]](\psi)$ is $J := \overline{\psi^{(4)}} \psi^2$, and therefore we need to estimate the Lie commutator of the corresponding operator with the operator V. First, we compute $J'(\psi) \cdot \phi = \overline{\phi^{(4)}} \psi^2 + \overline{\psi^{(4)}} \phi^2$ and $V'(\psi) \cdot \phi = -\mathrm{i}\left(\overline{\phi}\psi^2 + 2|\psi|^2 \phi\right)$. Thus, both $J'(\psi) \cdot V(\psi)$ and $V'(\psi) \cdot (\overline{\psi^{(4)}} \psi^2)$ consist of products of five functions, which allow bounds

$$\|J'(\psi) \cdot V(\psi)\|_{L^2} \leq \mathcal{C}(\|\psi\|_{H^4}), \quad \|V'(\psi) \cdot (\overline{\psi^{(4)}} \psi^2)\|_{L^2} \leq \mathcal{C}(\|\psi\|_{H^4}).$$

With these considerations we can now formulate the error bounds for the local errors and their estimators for the Lie–Trotter and Strang splitting methods.

Theorem 5 (Error bounds, Lie–Trotter and Strang splitting). *The Lie–Trotter splitting method (2.4) applied to the nonlinear Schrödinger equation (5.1) satisfies the following local error estimates.*

(i) *A priori: If $\|\psi_0\|_{H^2} \leq M_2$, then*

$$\|\mathcal{L}(t, \psi_0)\|_{L^2} \leq \mathcal{C}\, t^2, \tag{5.5}$$

   with a constant $\mathcal{C} > 0$ depending in particular on M_2.

(ii) *A posteriori: If $\|\psi_0\|_{H^4} \leq M_4$, then $\mathcal{P}(t, \psi_0)$ is well-defined in $L^2(\mathbb{R}^3)$ and there holds*

$$\|\mathcal{P}(t, \psi_0) - \mathcal{L}(t, \psi_0)\|_{L^2} \leq \mathcal{C}\, t^3, \tag{5.6}$$

   with a constant $\mathcal{C} > 0$ depending in particular on M_4.

The Strang splitting method (2.5) applied to the nonlinear Schrödinger equation (5.1) satisfies the following local error estimates.

(iii) *A priori: If $\|\psi_0\|_{H^4} \leq M_4$, then*

$$\|\mathcal{L}(t, \psi_0)\|_{L^2} \leq \mathcal{C}\, t^3, \tag{5.7}$$

   with a constant $\mathcal{C} > 0$ depending in particular on M_4.

(iv) *A posteriori: If $\|\psi_0\|_{H^6} \leq M_6$, then $\mathcal{P}(t, \psi_0)$ is well-defined in $L^2(\mathbb{R}^3)$ and there holds*

$$\|\mathcal{P}(t, \psi_0) - \mathcal{L}(t, \psi_0)\|_{L^2} \leq \mathcal{C}\, t^4, \tag{5.8}$$

with a constant $\mathcal{C} > 0$ depending in particular on M_6.

By the stability analysis given in [10, 11, 13] it is clear that the a priori local error estimates in Theorem 5 reproduce the convergence result therein. The a posteriori local error estimators relevant for adaptive time-stepping are applied only locally and do not require additional stability properties.

5.2. Full discretization

In the following, we briefly discuss the effect of an additional spatial discretization error resulting from an application of a spectral method; see also [14, 15].

In particular, in the context of the cubic nonlinear Schrödinger equation (5.1) the numerical resolution of the linear subproblem involving the Laplace operator typically relies on the Fourier spectral method. The operator $\mathrm{i}\,T = -\frac{1}{2}\Delta$ is selfadjoint with a complete orthonormal system of eigenfunctions $(\mathcal{B}_m)_{m \in \mathcal{M}}$. By $(\lambda_m)_{m \in \mathcal{M}}$ we denote the eigenvalues associated with T. As a detailed analysis is not in the scope of the present work, we indicate the arguments for the least technical case of the Lie–Trotter splitting method

$$\mathcal{S}(t, u) = \mathcal{E}_T\big(t, \mathcal{E}_V(t, u)\big)\,, \quad \mathcal{E}_T(t, u) = \mathrm{e}^{tT} u = \sum_{m \in \mathcal{M}} \mathrm{e}^{t\lambda_m}\, c_m(u)\, \mathcal{B}_m\,,$$

$$\mathcal{P}(t, u) = \tfrac{1}{2}\, t\left(\mathrm{e}^{tT}\, V\big(\mathcal{E}_V(t, u)\big) - V\big(\mathrm{e}^{tT}\mathcal{E}_V(t, u)\big)\right), \tag{5.9}$$

where $\mathcal{P}$ is given in (3.12a) and with $\mathcal{E}_V$ as specified in (5.3). With $\mathcal{Q}_M$ denoting the spectral interpolation operator which involves the restriction to a finite index set $\mathcal{M}_M \subset \mathcal{M}$ with $|\mathcal{M}_M| = M$ and a quadrature approximation of the spectral coefficients $\tilde{c}_m(u) \approx c_m(u)$ for $m \in \mathcal{M}_M$, the numerical realization of (5.9) can be cast into the form

$$\mathcal{P}_{\mathrm{full}}(t, u) = \tfrac{1}{2}\, t\left(\mathrm{e}^{tT}\mathcal{Q}_M\, V\big(\mathcal{E}_V(t, u)\big) - V\big(\mathrm{e}^{tT}\mathcal{Q}_M\, \mathcal{E}_V(t, u)\big)\right).$$

The additional approximation error induced by a spectral space discretization is thus given by

$$\mathcal{P}_{\mathrm{full}}(t, u) - \mathcal{P}(t, u) = \tfrac{1}{2}\, t\left(\mathrm{e}^{tT}\mathcal{Q}_M\, V\big(\mathcal{E}_V(t, u)\big) - V\big(\mathrm{e}^{tT}\mathcal{Q}_M\, \mathcal{E}_V(t, u)\big)\right)$$

$$- \tfrac{1}{2}\, t\left(\mathrm{e}^{tT}\, V\big(\mathcal{E}_V(t, u)\big) - V\big(\mathrm{e}^{tT}\mathcal{E}_V(t, u)\big)\right).$$

Aiming for a suitable representation in terms of the spectral interpolation error $\mathcal{Q}_M - I$, we employ the reformulation

$$\mathcal{P}_{\text{full}}(t,u) - \mathcal{P}(t,u) = \tfrac{1}{2}\,t\,\Big(e^{tT}\big(\mathcal{Q}_M - I\big)\,V\big(\mathcal{E}_V(t,u)\big)$$

$$- \int_0^1 V'\big(\sigma\,e^{tT}\mathcal{Q}_M\,\mathcal{E}_V(t,u) + (1-\sigma)\,e^{tT}\mathcal{E}_V(t,u)\big)\,\mathrm{d}\sigma\,\cdot$$

$$e^{tT}\big(\mathcal{Q}_M - I\big)\,\mathcal{E}_V(t,u)\Big)\,.$$

Auxiliary estimates for $\|\mathcal{Q}_M\,\mathcal{E}_V(t,u)\|_{H^2}$ and $\|\mathcal{Q}_M - I\|_{L^2}$ are provided by [15, Lemma 4]. Altogether this leads to the estimate

$$\|\mathcal{P}_{\text{full}}(t,u) - \mathcal{P}(t,u)\|_{L^2} \leq \mathcal{C}\,t\,\|\mathcal{Q}_M - I\|_{L^2}\,,$$

with a constant $\mathcal{C} > 0$ depending in particular on bounds for $\|u\|_{H^2}$ and $\|\mathcal{Q}_M\,\mathcal{E}_V(t,u)\|_{H^2}$.

Finally, we obtain the following proposition. A similar estimate is valid for the Strang splitting method. These investigations can also be extended, for instance, to the Hermite and the generalized Laguerre–Fourier–Hermite spectral methods on the basis of the analysis given in [16, 14].

Proposition 1 (Convergence of spectral discretization). *The error of the fully discretized a posteriori local error estimator associated with the Lie–Trotter splitting method satisfies an estimate of the form*

$$\|\mathcal{P}_{\text{full}}(t,u) - \mathcal{P}(t,u)\|_{L^2} \leq \mathcal{C}\,t\,M^{-q}\,,$$

where the exponent $q > 0$ in particular depends on the space dimension, the regularity of u, and the underlying spectral method.

5.3. Practical realization

It is straightforward to realize our defect-based local error estimators algorithmically. As in Section 5.1, we set $A = T = \tfrac{1}{2}\,\mathrm{i}\,\Delta$ and $B(\psi) = V(\psi) = -\mathrm{i}\,|\psi|^2\,\psi$. The numerical resolution of the subproblem involving the Laplace operator relies on the application of the Fourier spectral method, and the solution to the subproblem involving the cubic nonlinearity can be computed by the pointwise multiplication (5.3). The Fréchet derivative of the evolution operator $\mathcal{E}_V$ with respect to ψ is given by

$$\big(\partial_2\mathcal{E}_V(t,\psi)\cdot\phi\big)(x) = e^{-\mathrm{i}\,t\,|\psi(x)|^2}\big(\phi(x) - \mathrm{i}\,t\,(|\psi(x)|^2\,\phi(x) + (\psi(x))^2\,\overline{\phi(x)})\big)\,.$$

This enters the evaluation of the error estimators (3.12a) and (4.6). For higher-order schemes, evaluation according to (2.10) works in an analogous way.

Δt	err (Lie–Trotter)	p	$\mathrm{err}_{\mathrm{est}}$	p_{est}
2^{-8}	$1.5556 \cdot 10^{-4}$	2.00	$4.0136 \cdot 10^{-6}$	2.99
2^{-9}	$3.8903 \cdot 10^{-5}$	2.00	$5.0266 \cdot 10^{-7}$	3.00
2^{-10}	$9.7265 \cdot 10^{-6}$	2.00	$6.2862 \cdot 10^{-8}$	3.00
2^{-11}	$2.4317 \cdot 10^{-6}$	2.00	$7.8587 \cdot 10^{-9}$	3.00
2^{-12}	$6.0792 \cdot 10^{-7}$	2.00	$9.8237 \cdot 10^{-10}$	3.00
2^{-13}	$1.5198 \cdot 10^{-7}$	2.00	$1.2280 \cdot 10^{-10}$	3.00

Δt	err (Strang)	p	$\mathrm{err}_{\mathrm{est}}$	p_{est}
2^{-8}	$5.9464 \cdot 10^{-7}$	3.00	$1.2514 \cdot 10^{-8}$	3.98
2^{-9}	$7.4344 \cdot 10^{-8}$	3.00	$7.8448 \cdot 10^{-10}$	4.00
2^{-10}	$9.2935 \cdot 10^{-9}$	3.00	$4.9067 \cdot 10^{-11}$	4.00
2^{-11}	$1.1617 \cdot 10^{-9}$	3.00	$3.0672 \cdot 10^{-12}$	4.00
2^{-12}	$1.4521 \cdot 10^{-10}$	3.00	$1.9157 \cdot 10^{-13}$	4.00
2^{-13}	$1.8152 \cdot 10^{-11}$	3.00	$1.1867 \cdot 10^{-14}$	4.01

Table 1: Local errors (err) and deviation of error estimates ($\mathrm{err}_{\mathrm{est}}$) and corresponding observed orders p, p_{est} for the Lie–Trotter (top) and Strang (bottom) splitting methods applied to (5.1) with soliton solution. Δt is the stepsize used.

5.4. Numerical examples

In this section we give some numerical support for our theoretical convergence results given in Theorem 5 and Proposition 1 for (5.1) in the semi-discrete and fully discrete settings.

1. Firstly, to verify the convergence order, we consider (5.1) in 1D with $\kappa = -1$ and the initial condition chosen such that the problem solution is a soliton given by

$$\psi(x,t) = \frac{2\,\mathrm{e}^{\frac{3}{2}\mathrm{i}t - \mathrm{i}x}}{\cosh(2t + 2x)}\,, \qquad x \in [-16, 16]\,.$$

For the spatial discretization we use 512 Fourier modes. Table 1 gives the local error of one step of the Lie–Trotter and the Strang splitting method and of the errors of the local error estimates as compared to the exact errors. As predicted by Proposition 1, the local error has order two for the Lie–Trotter and order three for the Strang splitting, and the error estimators are asymptotically correct.

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2. Finally, we demonstrate that our error estimates may serve as a reliable basis for adaptive time–stepping to enhance the efficiency of a split-step time integrator. For this purpose, we consider the Gross–Pitaevskii equation for a rotating Bose–Einstein condensate in 2D, see [2, Ex. 1 (iii)] and also [14],

$$\mathrm{i}\,\partial_t\psi(x,y,t) = \left(-\tfrac{1}{2}\,\Delta + V_{ext}(x,y) - \Omega\,L_z + \kappa\,|\psi(x,y,t)|^2 \right)\psi(x,y,t)\,,$$
$$\psi(x,y,0) = \frac{x+\mathrm{i}\,y}{\sqrt{\pi}}\,e^{-(x^2+y^2)/2}\,,$$

with an external potential consisting of a scaled harmonic part and a regular potential W,

$$V_{ext}(x,y) = \tfrac{\gamma}{2}\,(x^2+y^2) + W(x,y)\,, \quad W(x,y) = \tfrac{1}{2}\,(\gamma_y^2 - \gamma_x^2)\,y^2\,,$$

and a rotation term $\Omega\,L_z$ defined in terms of a given angular velocity Ω and the angular momentum operator $L_z = -\mathrm{i}\,(x\,\partial_y - y\,\partial_x)$.
For the application of splitting schemes, we proceed as in [14], with

$$A\,\psi(x,y,\cdot) = \left(-\tfrac{1}{2}\,\Delta + \tfrac{\gamma}{2}\,(x^2+y^2) - \Omega\,L_z \right)\psi(x,y,\cdot)\,,$$
$$B(\psi)(x,y,\cdot) = \left(W(x,y) + \kappa\,|\psi(x,y)|^2 \right)\psi(x,y,\cdot)\,.$$

Spectral discretization of the linear A-part is performed by a generalized Laguerre–Fourier–Hermite pseudospectral method which was proposed in [2] and has been recently analyzed in [14].
Problem parameters are chosen as in [2, Ex. 1 (iii)]: $\Omega = 0.5$, $\kappa = 100$, $\gamma_x = 0.8$, $\gamma_y = 1.2$. In Figure 1 we plot the functional "condensate width",

$$\sigma_r^2 = \sigma_x^2 + \sigma_y^2\,, \quad \text{with} \quad \sigma_\alpha^2 = \int_{\mathbb{R}^2} \alpha^2\,|\psi(x,y,t)|^2\,\mathrm{d}(x,y)\,, \quad \alpha = x,y\,,$$

together with the sequence of stepsizes chosen by a standard local error control [17] on the basis of our error estimators for both the Lie–Trotter and Strang splitting. Both stepsize sequences show a qualitatively similar behavior which is in line with the local smoothness of the solution according to the plotted functional. This example demonstrates that our results are also applicable to problems from a wider class than (5.1) which feature a more challenging dynamical behavior as a test for adaptive time-stepping.
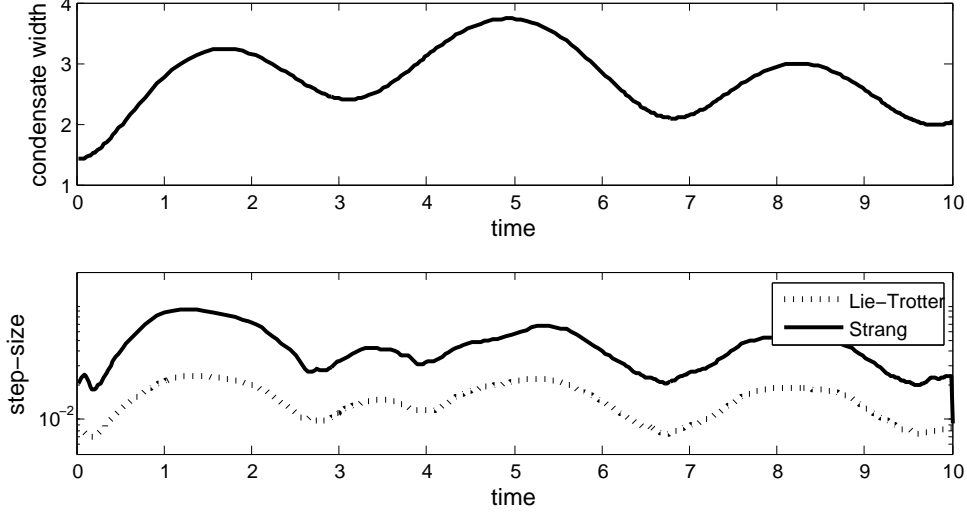
Figure 1: Condensate width (top) and stepsizes (bottom) for the Lie-Trotter and Strang splittings applied to the GPE for a rotating Bose–Einstein condensate.

Appendix A. Auxiliary notations and results

First and second iterated Lie-commutators. The first and second nested Lie-brackets of smooth vector fields are defined in terms of the first and second iterated Lie-commutators

$$[F, G](v) = F'(v) \cdot G(v) - G'(v) \cdot F(v) = -[G, F](v) \,, \qquad (A.1a)$$

$$[[F, G], H](v) = [F, G]'(v) \cdot H(v) - H'(v) \cdot [F, G](v) \,, \qquad (A.1b)$$

where

$$[F, G]'(v) \cdot w$$
$$= F''(v)(G(v), w) + F'(v) \cdot G'(v) \cdot w - G'(v) \cdot F'(v) \cdot w - G''(v)(F(v), w) \,.$$

For the Lie commutator, the Jacobi identity is valid:

$$[F, [G, H]] + [G, [H, F]] + [H, [F, G]] = 0 \,. \qquad (A.1c)$$

Variation-of-constants formulae. The solution to the initial value problem

$$\frac{\partial}{\partial t} \mathcal{X}(t, u) = F'(\mathcal{E}_F(t, u)) \cdot \mathcal{X}(t, u) + \mathcal{R}(t, u) \,, \qquad (A.2a)$$

$$\mathcal{X}(0, u) = \mathcal{X}_0(u) \,, \qquad (A.2b)$$

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has the representation by the linear variation-of-constants formula

$$\mathcal{X}(t, u) = \partial_2 \mathcal{E}_F(t, u) \cdot \left(\mathcal{X}_0(u) + \int_0^t \partial_2 \mathcal{E}_F(-\tau, \mathcal{E}_F(\tau, u)) \cdot \mathcal{R}(\tau, u) \, \mathrm{d}\tau \right). \quad \text{(A.2c)}$$

This follows from the fact that $\partial_2 \mathcal{E}_F(t, u)$ is a fundamental system for the associated homogeneous equation together with the identity $\partial_2 \mathcal{E}_F(\tau, u)^{-1} = \partial_2 \mathcal{E}_F(-\tau, \mathcal{E}_F(\tau, u))$, which is verified by differentiating both sides of the relations $\mathcal{E}_F(-t, \mathcal{E}_F(t, u)) = u$ and $\mathcal{E}_F(t, \mathcal{E}_F(-t, u)) = u$ with respect to u.

For the initial value problems

$$\frac{\mathrm{d}}{\mathrm{d}t} v(t) = F(v(t)), \qquad \frac{\mathrm{d}}{\mathrm{d}t} w(t) = F(w(t)) + r(t),$$
$$v(0) = w(0),$$

an application of the nonlinear variation-of-constants formula (Gröbner–Alekseev Lemma) implies

$$w(t) - v(t) = \int_0^t \partial_2 \mathcal{E}_F(t - \tau, w(\tau)) \cdot r(\tau) \, \mathrm{d}\tau. \quad \text{(A.3)}$$

First- and second-order variational equations. By differentiating the evolution equation

$$\frac{\partial}{\partial t} \mathcal{E}_F(t, u) = F(\mathcal{E}_F(t, u)), \quad \text{(A.4a)}$$
$$\mathcal{E}_F(0, u) = u, \quad \text{(A.4b)}$$

and interchanging the order of derivatives leads to the first- and second-order variational equations

$$\frac{\partial}{\partial t} \partial_2 \mathcal{E}_F(t, u) = F'(\mathcal{E}_F(t, u)) \cdot \partial_2 \mathcal{E}_F(t, u), \quad \text{(A.5a)}$$
$$\partial_2 \mathcal{E}_F(0, u) = I, \quad \text{(A.5b)}$$

and

$$\frac{\partial}{\partial t} (\partial_2^2 \mathcal{E}_F(t, u))(\cdot, \cdot) = F'(\mathcal{E}_F(t, u)) \cdot \partial_2^2 \mathcal{E}_F(t, u)(\cdot, \cdot) \quad \text{(A.6a)}$$
$$+ F''(\mathcal{E}_F(t, u))(\partial_2 \mathcal{E}_F(t, u) \cdot, \partial_2 \mathcal{E}_F(t, u) \cdot),$$
$$\partial_2^2 \mathcal{E}_F(0, u) = 0. \quad \text{(A.6b)}$$

Due to (A.2c), the solution of (A.6) is given by

$$\partial_2^2 \mathcal{E}_F(t, u)(\cdot, \cdot) = \partial_2 \mathcal{E}_F(t, u) \cdot \int_0^t \partial_2 \mathcal{E}_F(-\tau, \mathcal{E}_F(\tau, u)) \cdot \quad \text{(A.6c)}$$
$$F''(\mathcal{E}_F(\tau, u))(\partial_2 \mathcal{E}_F(\tau, u) \cdot \partial_2 \mathcal{E}_F(\tau, u) \cdot) \, \mathrm{d}\tau.$$

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Fundamental identities. For our considerations, it is essential to employ the fundamental identity

$$\partial_2 \mathcal{E}_F(t, u) \cdot F(u) - F(\mathcal{E}_F(t, u)) = 0 \,, \tag{A.7}$$

which is a consequence of (A.5). Furthermore, by differentiation it is verified that $\mathcal{X}(t, u) = \partial_2 \mathcal{E}_F(t, u) \cdot G(u) - G(\mathcal{E}_F(t, u))$ satisfies the initial value problem

$$\tfrac{\partial}{\partial t} \mathcal{X}(t, u) = F'(\mathcal{E}_F(t, u)) \cdot \mathcal{X}(t, u) + [F, G](\mathcal{E}_F(\tau, u)) \,, \tag{A.8a}$$
$$\mathcal{X}(0, u) = 0 \,, \tag{A.8b}$$

which implies the generalized fundamental identity

$$\partial_2 \mathcal{E}_F(t, u) \cdot G(u) - G(\mathcal{E}_F(t, u)) \tag{A.9}$$
$$= \partial_2 \mathcal{E}_F(t, u) \cdot \int_0^t \partial_2 \mathcal{E}_F(-\tau, \mathcal{E}_F(\tau, u)) \cdot [F, G](\mathcal{E}_F(\tau, u)) \, \mathrm{d}\tau \,.$$

A fundamental identity involving the second derivative $\partial_2^2 \mathcal{E}_F$ reads

$$\partial_2^2 \mathcal{E}_F(t, u)(F(u), v) + \partial_2 \mathcal{E}_F(t, u) \cdot F'(u) \cdot v = F'(\mathcal{E}_F(t, u)) \cdot \partial_2 \mathcal{E}_F(t, u) \cdot v \,, \tag{A.10}$$

which follows by differentiation of (A.7) with respect to u.

Reformulation of variational equations. An alternative formulation of the first-order variational equation (A.5a) in the form

$$\tfrac{\partial}{\partial t} \partial_2 \mathcal{E}_F(t, u) = \partial_2 \mathcal{E}_F(t, u) \cdot F'(u) + \partial_2^2 \mathcal{E}_F(t, u)(F(u), \cdot) \tag{A.11}$$

is obtained by interchanging the order of differentiation and applying relations (A.4a) and (A.7),

$$\tfrac{\partial}{\partial t} \partial_2 \mathcal{E}_F(t, u) = \partial_2\big(\tfrac{\partial}{\partial t} \mathcal{E}_F(t, u)\big) = \partial_2\big(\partial_2 \mathcal{E}_F(t, u) \cdot F(u)\big)$$
$$= \partial_2 \mathcal{E}_F(t, u) \cdot F'(u) + \partial_2^2 \mathcal{E}_F(t, u)(F(u), \cdot) \,.$$

Furthermore, the second-order variational equation (A.6a) can be rewritten in the form

$$\tfrac{\partial}{\partial t} \partial_2^2 \mathcal{E}_F(t, u)(v, \cdot) \tag{A.12}$$
$$= \partial_2 \mathcal{E}_F(t, u) \cdot F''(u)(v, \cdot) + 2\, \partial_2^2 \mathcal{E}_F(t, u)(F'(u) \cdot v, \cdot) + \partial_2^3 \mathcal{E}_F(t, u)(F(u), v, \cdot) \,.$$

This follows by interchanging the order of differentiation and using (A.11),

$$
\begin{aligned}
\tfrac{\partial}{\partial t} \partial_2^2 \mathcal{E}_F(t,u)(v,\cdot) &= \tfrac{\partial}{\partial t}\big(\partial_2^2 \mathcal{E}_F(t,u)\cdot v\big) = \partial_2\big(\tfrac{\partial}{\partial t}\partial_2 \mathcal{E}_F(t,u)\cdot v\big) \\
&= \partial_2\big(\partial_2 \mathcal{E}_F(t,u)\cdot F'(u)\cdot v + \partial_2^2 \mathcal{E}_F(t,u)(F(u),v)\big) \\
&= \partial_2 \mathcal{E}_F(t,u)\cdot F''(u)(v,\cdot) + \partial_2^2 \mathcal{E}_F(t,u)(F'(u)\cdot v,\cdot) \\
&\quad + \partial_2^2 \mathcal{E}_F(t,u)(F'(u)\cdot v,\cdot) + \partial_2^3 \mathcal{E}_F(t,u)(F(u),v,\cdot)\,.
\end{aligned}
$$

Reformulation of the variational equations with time-dependent arguments.
In a similar manner, an application of the chain rule yields the following generalization of (A.11) and (A.12), respectively, for explicitly time-dependent arguments

$$
\begin{aligned}
\tfrac{\partial}{\partial t}\partial_2 \mathcal{E}_F(t,G(t,u)) &= \partial_2 \mathcal{E}_F(t,G(t,u))\cdot F'(G(t,u)) \qquad\qquad\quad \text{(A.13)} \\
&\quad + \partial_2^2 \mathcal{E}_F(t,G(t,u))(\tfrac{\partial}{\partial t}G(t,u) + F(G(t,u)),\cdot)\,,
\end{aligned}
$$

and

$$
\begin{aligned}
\tfrac{\partial}{\partial t}\big(\partial_2^2 \mathcal{E}_F(t,G(t,u))\big)(v,w) &= \partial_2 \mathcal{E}_F(t,G(t,u))\cdot F''(G(t,u))(v,w) \qquad \text{(A.14)} \\
&\quad + 2\,\partial_2^2 \mathcal{E}_F(t,G(t,u))(F'(G(t,u))\cdot v,w) \\
&\quad + \partial_2^3 \mathcal{E}_F(t,G(t,u))(\tfrac{\partial}{\partial t}G(t,u) + F(G(t,u)),v,w)\,.
\end{aligned}
$$

Appendix B. Automatic manipulations of flows

For the analysis of the error estimator for the Lie–Trotter splitting in Section 3 all calculations have been carried out explicitly. Additionally, the results have been verified by a tool for automatic formula manipulation which we implemented in the Perl programming language. For the Strang splitting method, the manipulations of flows are too intricate for calculation by hand. Although the general structure of the arising terms could be inferred theoretically in principle, we restricted ourselves to the verification of educated guesses for these terms by our tool for formula manipulation.

This computer implementation is based on appropriate definitions of classes representing expressions composed of operators, flows, and higher derivatives of flows. Methods were implemented for instance for

- collecting and expanding terms,

- substitution of variables by sub-expressions,

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- symbolic differentiation with respect to time and space variables.

Additionally, a method was implemented realizing the substitution of expressions of the form $\partial_2 \mathcal{E}_F(t, u) \cdot F(u)$ by $F(\mathcal{E}_F(t, u))$ according to the fundamental identity (A.7). In the same way, the highest derivative appearing after differentiation of (A.7) with respect to u is substituted by terms of lower differentiation order.

Appendix C. Defect representations, Strang splitting

In this section we collect the precise details involved in the representation of the defect $\mathcal{S}^{(1)}(t, u)$ and the higher-order defects $\mathcal{S}^{(2)}(t, u)$ and $\mathcal{S}^{(3)}(t, u)$ for the Strang splitting method. These form the basis for the analysis in Section 4.

The results collected in Lemmas 5–7 have been verified by means of automated symbolic manipulation, see Appendix B.

Lemma 5 (Defect $\mathcal{S}^{(1)}(t, u)$, Strang splitting).

(i) *The defect* $\mathcal{S}^{(1)}(t, u) = \frac{\partial}{\partial t} \mathcal{S}(t, u) - H(\mathcal{S}(t, u))$ *has the form*

$$\mathcal{S}^{(1)}(t, u) = \frac{\partial}{\partial t} \mathcal{S}(t, u) - H(\mathcal{S}(t, u)) \tag{C.1a}$$
$$= \partial_2 \mathcal{E}_A(\tfrac{1}{2}t, \mathcal{E}_B(t, \mathcal{E}_A(\tfrac{1}{2}t, u))) \cdot \tilde{\mathcal{S}}^{(1,1)}(t, \mathcal{E}_A(\tfrac{1}{2}t, u))$$
$$+ \mathcal{S}^{(1,2)}(t, \mathcal{E}_B(t, \mathcal{E}_A(\tfrac{1}{2}t, u)))$$
$$= \left\{ \partial_2 \mathcal{E}_A(\tfrac{1}{2}t, w) \cdot \tilde{\mathcal{S}}^{(1,1)}(t, v) + \tilde{\mathcal{S}}^{(1,2)}(t, w) \right\}\Big|_{\substack{v = \mathcal{E}_A(\tfrac{1}{2}t, u) \\ w = \mathcal{E}_B(t, \mathcal{E}_A(\tfrac{1}{2}t, u))}},$$

with

$$\tilde{\mathcal{S}}^{(1,1)}(t, v) = \tfrac{1}{2} \left(\partial_2 \mathcal{E}_B(t, v) \cdot A(v) - A(\mathcal{E}_B(t, v)) \right), \tag{C.1b}$$

and

$$\tilde{\mathcal{S}}^{(1,2)}(t, w) = \partial_2 \mathcal{E}_A(\tfrac{1}{2}t, w) \cdot B(w) - B(\mathcal{E}_A(\tfrac{1}{2}t, w)). \tag{C.1c}$$

(ii) $\tilde{\mathcal{S}}^{(1,1)}(t, v)$ *and* $\tilde{\mathcal{S}}^{(1,2)}(t, w)$ *satisfy the initial value problems*

$$\frac{\partial}{\partial t} \tilde{\mathcal{S}}^{(1,1)}(t, v) = B'(\mathcal{E}_B(t, v)) \cdot \tilde{\mathcal{S}}^{(1,1)}(t, v) + \tfrac{1}{2}[B, A](\mathcal{E}_B(t, v)), \tag{C.2a}$$
$$\tilde{\mathcal{S}}^{(1,1)}(0, v) = 0, \tag{C.2b}$$

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and

$$\tfrac{\partial}{\partial t}\tilde{\mathcal{S}}^{(1,2)}(t,w) = A'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(1,2)}(t,w) + \tfrac{1}{2}[A,B](\mathcal{E}_A(\tfrac{1}{2}t,w)), \quad \text{(C.2c)}$$

$$\tilde{\mathcal{S}}^{(1,2)}(0,w) = 0. \quad \text{(C.2d)}$$

(iii) *For $\tilde{\mathcal{S}}^{(1,1)}(t,v)$ and $\tilde{\mathcal{S}}^{(1,2)}(t,w)$ the following integral representations are valid:*

$$\tilde{\mathcal{S}}^{(1,1)}(t,v) = \tfrac{1}{2}\partial_2 \mathcal{E}_B(t,v) \cdot \quad \text{(C.3a)}$$
$$\int_0^t \partial_2 \mathcal{E}_B(-\tau, \mathcal{E}_B(\tau,v)) \cdot [B,A](\mathcal{E}_B(\tau,v))\,\mathrm{d}\tau,$$

and

$$\tilde{\mathcal{S}}^{(1,2)}(t,w) = \tfrac{1}{2}\partial_2 \mathcal{E}_A(\tfrac{1}{2}t,w) \cdot \quad \text{(C.3b)}$$
$$\int_0^t \partial_2 \mathcal{E}_A(-\tfrac{1}{2}\tau, \mathcal{E}_A(\tfrac{1}{2}\tau,w)) \cdot [A,B](\mathcal{E}_A(\tfrac{1}{2}\tau,w))\,\mathrm{d}\tau.$$

Remark 5. Integral representations for $\partial_2\tilde{\mathcal{S}}^{(1,1)}(t,v)$, $\partial_2\tilde{\mathcal{S}}^{(1,2)}(t,w)$ and $\partial_2^2\tilde{\mathcal{S}}^{(1,1)}(t,v)$, $\partial_2^2\tilde{\mathcal{S}}^{(1,2)}(t,w)$ are obtained in an analogous way as for $\partial_2\tilde{\mathcal{S}}^{(1)}(t,v)$, see the Remark following Lemma 3.

Lemma 6 (Second-order defect $\mathcal{S}^{(2)}(t,u)$, Strang splitting).

(i) *The second-order defect $\mathcal{S}^{(2)}(t,u)$ (see (2.6c)) has the form*

$$\mathcal{S}^{(2)}(t,u) = \tfrac{\partial}{\partial t}\mathcal{S}^{(1)}(t,u) - H'(\mathcal{S}(t,u)) \cdot \mathcal{S}^{(1)}(t,u) \quad \text{(C.4a)}$$
$$= \Big\{ \partial_2 \mathcal{E}_A(\tfrac{1}{2}t,w) \cdot \tilde{\mathcal{S}}^{(2,1)}(t,v) + \tilde{\mathcal{S}}^{(2,2)}(t,w)$$
$$+ \partial_2^2 \mathcal{E}_A(\tfrac{1}{2}t,w)(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v))$$
$$+ 2\,\partial_2\tilde{\mathcal{S}}^{(1,2)}(t,w) \cdot \tilde{\mathcal{S}}^{(1,1)}(t,v) \Big\}\Big|_{\substack{v=\mathcal{E}_A(\tfrac{1}{2}t,u) \\ w=\mathcal{E}_B(t,\mathcal{E}_A(\tfrac{1}{2}t,u))}},$$

with

$$\tilde{\mathcal{S}}^{(2,1)}(t,v) = \tfrac{1}{2}\partial_2\tilde{\mathcal{S}}^{(1,1)}(t,v) \cdot A(v) - \tfrac{1}{2}A'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1,1)}(t,v)$$
$$+ \tfrac{1}{2}[B,A](\mathcal{E}_B(t,v)), \quad \text{(C.4b)}$$

and

$$\tilde{\mathcal{S}}^{(2,2)}(t,w) = \partial_2\tilde{\mathcal{S}}^{(1,2)}(t,w) \cdot H(w) - H'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(1,2)}(t,w)$$
$$- \tfrac{1}{2}\partial_2 \mathcal{E}_A(\tfrac{1}{2}t,w) \cdot [B,A](w). \quad \text{(C.4c)}$$

(ii) $\tilde{\mathcal{S}}^{(2,1)}(t,v)$ and $\tilde{\mathcal{S}}^{(2,2)}(t,w)$ satisfy the initial value problems

$$\frac{\partial}{\partial t}\tilde{\mathcal{S}}^{(2,1)}(t,v) = B'(\mathcal{E}_B(t,v))\cdot\tilde{\mathcal{S}}^{(2,1)}(t,v) \tag{C.5a}$$
$$+ B''(\mathcal{E}_B(t,v))(\tilde{\mathcal{S}}^{(1,1)}(t,v),\tilde{\mathcal{S}}^{(1,1)}(t,v))$$
$$+ [B,A]'(\mathcal{E}_B(t,v))\cdot\tilde{\mathcal{S}}^{(1,1)}(t,v)$$
$$- \tfrac{1}{2}[B,[B,A]](\mathcal{E}_B(t,v)) - \tfrac{1}{4}[A,[B,A]](\mathcal{E}_B(t,v))\,,$$
$$\tilde{\mathcal{S}}^{(2,1)}(0,v) = \tfrac{1}{2}[B,A](v)\,, \tag{C.5b}$$

and

$$\frac{\partial}{\partial t}\tilde{\mathcal{S}}^{(2,2)}(t,w) = \tfrac{1}{2}A'(\mathcal{E}_A(\tfrac{1}{2}t,w))\cdot\tilde{\mathcal{S}}^{(2,2)}(t,w) \tag{C.5c}$$
$$+ \tfrac{1}{2}A''(\mathcal{E}_A(\tfrac{1}{2}t,w))(\tilde{\mathcal{S}}^{(1,2)}(t,w),\tilde{\mathcal{S}}^{(1,2)}(t,w))$$
$$- [B,A]'(\mathcal{E}_A(\tfrac{1}{2}t,w))\cdot\tilde{\mathcal{S}}^{(1,2)}(t,w)$$
$$+ \tfrac{1}{2}[B,[B,A]](\mathcal{E}_A(\tfrac{1}{2}t,w)) + \tfrac{1}{2}[A,[B,A]](\mathcal{E}_A(\tfrac{1}{2}t,w))\,,$$
$$\tilde{\mathcal{S}}^{(2,2)}(0,w) = -\tfrac{1}{2}[B,A](w)\,. \tag{C.5d}$$

(iii) For $\tilde{\mathcal{S}}^{(2,1)}(t,v)$ and $\tilde{\mathcal{S}}^{(2,2)}(t,w)$ the following integral representations are valid:

$$\tilde{\mathcal{S}}^{(2,1)}(t,v) = \tfrac{1}{2}\,\partial_2\mathcal{E}_B(t,v)\cdot[B,A](v) \tag{C.6a}$$
$$+ \partial_2\mathcal{E}_B(t,v)\,\cdot\,\int_0^t \partial_2\mathcal{E}_B(-\tau,\mathcal{E}_B(\tau,v))\,\cdot$$
$$\Big\{ B''(\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1,1)}(\tau,v),\tilde{\mathcal{S}}^{(1,1)}(\tau,v))$$
$$- \tfrac{1}{2}[B,[B,A]](\mathcal{E}_B(\tau,v)) - \tfrac{1}{4}[A,[B,A]](\mathcal{E}_B(\tau,v))$$
$$+ [B,A]'(\mathcal{E}_B(\tau,v))\cdot\tilde{\mathcal{S}}^{(1,1)}(\tau,v)\Big\}\,d\tau\,,$$

and

$$\tilde{\mathcal{S}}^{(2,2)}(t,w) = -\tfrac{1}{2}\,\partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\cdot[B,A](w) \tag{C.6b}$$
$$+ \partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\,\cdot\,\int_0^t \partial_2\mathcal{E}_A(-\tfrac{1}{2}\tau,\mathcal{E}_A(\tfrac{1}{2}\tau,w))\,\cdot$$
$$\Big\{ \tfrac{1}{2}A''(\mathcal{E}_A(\tfrac{1}{2}\tau,w))(\tilde{\mathcal{S}}^{(1,2)}(\tau,w),\tilde{\mathcal{S}}^{(1,2)}(\tau,w))$$
$$+ \tfrac{1}{2}[B,[B,A]](\mathcal{E}_A(\tfrac{1}{2}\tau,w)) + \tfrac{1}{2}[A,[B,A]](\mathcal{E}_A(\tfrac{1}{2}\tau,w))$$
$$- [B,A]'(\mathcal{E}_A(\tfrac{1}{2}\tau,w))\cdot\tilde{\mathcal{S}}^{(1,2)}(\tau,w)\Big\}\,d\tau\,.$$

Remark 6. Integral representations for $\partial_2 \tilde{\mathcal{S}}^{(2,1)}(t,v)$ and $\partial_2 \tilde{\mathcal{S}}^{(2,2)}(t,w)$ are obtained in an analogous way as for $\partial_2 \tilde{\mathcal{S}}^{(1)}(t,v)$, see the remark following Lemma 3.

Lemma 7 (Third-order defect $\mathcal{S}^{(3)}(t,u)$, Strang splitting).

(i) *The third-order defect $\mathcal{S}^{(3)}(t,u)$ (see (2.6d)) has the form*

$$
\begin{aligned}
\mathcal{S}^{(3)}(t,u) = {}& \tfrac{\partial}{\partial t}\mathcal{S}^{(2)}(t,u) - H'(\mathcal{S}(t,u)) \cdot \mathcal{S}^{(2)}(t,u) \\
& \qquad - H''(\mathcal{S}(t,u))(\mathcal{S}^{(1)}(t,u), \mathcal{S}^{(1)}(t,u)) \\
= {}& \Big\{ \partial_2 \mathcal{E}_A(\tfrac{1}{2}t,w) \cdot \tilde{\mathcal{S}}^{(3,1)}(t,v) + \tilde{\mathcal{S}}^{(3,2)}(t,w) && \text{(C.7a)} \\
& + 3\,\partial_2^2 \mathcal{E}_A(\tfrac{1}{2}t,w)(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(2,1)}(t,v)) \\
& + \partial_2^3 \mathcal{E}_A(\tfrac{1}{2}t,w)(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v)) \\
& + 3\,\partial_2 \tilde{\mathcal{S}}^{(1,2)}(t,w) \cdot \tilde{\mathcal{S}}^{(2,1)}(t,v) + 3\,\partial_2 \tilde{\mathcal{S}}^{(2,2)}(t,w) \cdot \tilde{\mathcal{S}}^{(1,1)}(t,v) \\
& + 3\,\partial_2^2 \tilde{\mathcal{S}}^{(1,2)}(t,w)(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v)) \Big\}\Big|_{\substack{v=\mathcal{E}_A(\frac{1}{2}t,u) \\ w=\mathcal{E}_B(t,\mathcal{E}_A(\frac{1}{2}t,u))}},
\end{aligned}
$$

with

$$
\begin{aligned}
\tilde{\mathcal{S}}^{(3,1)}(t,v) = {}& \tfrac{1}{2}\partial_2 \tilde{\mathcal{S}}^{(2,1)}(t,v) \cdot A(v) - \tfrac{1}{2}A'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(2,1)}(t,v) && \text{(C.7b)} \\
& - \tfrac{1}{2}A''(\mathcal{E}_B(t,v))(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v)) \\
& - \tfrac{1}{2}[B,[B,A]](\mathcal{E}_B(t,v)) - \tfrac{1}{4}[A,[B,A]](\mathcal{E}_B(t,v)) \\
& + [B,A]'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1,1)}(t,v),
\end{aligned}
$$

and

$$
\begin{aligned}
\tilde{\mathcal{S}}^{(3,2)}(t,w) = {}& \partial_2 \tilde{\mathcal{S}}^{(2,2)}(t,w) \cdot H(w) - H'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(2,2)}(t,w) && \text{(C.7c)} \\
& - H''(\mathcal{E}_A(\tfrac{1}{2}t,w))(\tilde{\mathcal{S}}^{(1,2)}(t,w), \tilde{\mathcal{S}}^{(1,2)}(t,w)) \\
& + \tfrac{1}{2}\partial_2 \mathcal{E}_A(\tfrac{1}{2}t,w) \cdot [B,[B,A]](w) + \tfrac{1}{4}\partial_2 \mathcal{E}_A(\tfrac{1}{2}t,w) \cdot [A,[B,A]](w) \\
& - \partial_2 \tilde{\mathcal{S}}^{(1,2)}(t,w) \cdot [B,A](w).
\end{aligned}
$$

(ii) $\tilde{\mathcal{S}}^{(3,1)}(t,v)$ *and* $\tilde{\mathcal{S}}^{(3,2)}(t,w)$ *satisfy the initial value problems*

$$\frac{\partial}{\partial t}\tilde{\mathcal{S}}^{(3,1)}(t,v) = B'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(3,1)}(t,v) \tag{C.8a}$$
$$+ 3\,B''(\mathcal{E}_B(t,v))(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(2,1)}(t,v))$$
$$+ B'''(\mathcal{E}_B(t,v))(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v))$$
$$+ \tfrac{1}{8}[A,[A,[B,A]]](\mathcal{E}_B(t,v)) + \tfrac{1}{2}[A,[B,[B,A]]](\mathcal{E}_B(t,v))$$
$$+ \tfrac{1}{2}[B,[B,[B,A]]](\mathcal{E}_B(t,v))$$
$$- \tfrac{3}{4}[A,[B,A]]'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1,1)}(t,v)$$
$$- \tfrac{3}{2}[B,[B,A]]'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(1,1)}(t,v)$$
$$+ \tfrac{3}{2}[B,A]'(\mathcal{E}_B(t,v)) \cdot \tilde{\mathcal{S}}^{(2,1)}(t,v)$$
$$+ \tfrac{3}{2}[B,A]''(\mathcal{E}_B(t,v))(\tilde{\mathcal{S}}^{(1,1)}(t,v), \tilde{\mathcal{S}}^{(1,1)}(t,v))\,,$$
$$\tilde{\mathcal{S}}^{(3,1)}(0,v) = -\tfrac{1}{2}[B,[B,A]](v) - \tfrac{1}{2}[A,[B,A]](v)\,, \tag{C.8b}$$

and

$$\frac{\partial}{\partial t}\tilde{\mathcal{S}}^{(3,2)}(t,w) = \tfrac{1}{2}A'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(3,2)}(t,w) \tag{C.8c}$$
$$+ \tfrac{3}{2}A''(\mathcal{E}_A(\tfrac{1}{2}t,w))(\tilde{\mathcal{S}}^{(1,2)}(t,w), \tilde{\mathcal{S}}^{(2,2)}(t,w))$$
$$+ \tfrac{1}{2}A'''(\mathcal{E}_A(\tfrac{1}{2}t,w))(\tilde{\mathcal{S}}^{(1,2)}(t,w), \tilde{\mathcal{S}}^{(1,2)}(t,w), \tilde{\mathcal{S}}^{(1,2)}(t,w))$$
$$- \tfrac{1}{2}[A,[A,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}t,w)) - [A,[B,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}\tau,w))$$
$$- \tfrac{1}{2}[B,[B,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}t,w))$$
$$+ \tfrac{3}{2}[A,[B,A]]'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(1,2)}(t,w)$$
$$+ \tfrac{3}{2}[B,[B,A]]'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(1,2)}(t,w)$$
$$- \tfrac{3}{2}[B,A]'(\mathcal{E}_A(\tfrac{1}{2}t,w)) \cdot \tilde{\mathcal{S}}^{(2,1)}(t,w)$$
$$- \tfrac{3}{2}[B,A]''(\mathcal{E}_A(\tfrac{1}{2}t,w))(\tilde{\mathcal{S}}^{(1,2)}(t,w), \tilde{\mathcal{S}}^{(1,2)}(t,w))\,,$$
$$\tilde{\mathcal{S}}^{(3,2)}(0,w) = [B,[B,A]](w) + \tfrac{3}{4}[A,[B,A]](w)\,. \tag{C.8d}$$

(iii) *For* $\tilde{\mathcal{S}}^{(3,1)}(t,v)$ *and* $\tilde{\mathcal{S}}^{(3,2)}(t,w)$ *the following integral representations are*

valid:

$$\tilde{\mathcal{S}}^{(3,1)}(t,v) = -\tfrac{1}{2}\,\partial_2\mathcal{E}_B(t,v)\cdot[B,[B,A]](v) - \tfrac{1}{2}\,\partial_2\mathcal{E}_B(t,v)\cdot[A,[B,A]](v)$$

$$+\,\partial_2\mathcal{E}_B(t,v)\,\cdot\int_0^t\partial_2\mathcal{E}_B(-\tau,\mathcal{E}_B(\tau,v))\cdot \qquad\qquad (\text{C.9a})$$

$$\left\{3\,B''(\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1,1)}(\tau,v),\tilde{\mathcal{S}}^{(2,1)}(\tau,v))\right.$$

$$+\,B'''(\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1,1)}(\tau,v),\tilde{\mathcal{S}}^{(1,1)}(\tau,v),\tilde{\mathcal{S}}^{(1,1)}(\tau,v))$$

$$+\,\tfrac{1}{8}[A,[A,[B,A]]](\mathcal{E}_B(\tau,v)) + \tfrac{1}{2}[A,[B,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}\tau,w))$$

$$+\,\tfrac{1}{2}[B,[B,[B,A]]](\mathcal{E}_B(\tau,v))$$

$$-\,\tfrac{3}{4}[A,[B,A]]'(\mathcal{E}_B(\tau,v))\cdot\tilde{\mathcal{S}}^{(1,1)}(\tau,v)$$

$$-\,\tfrac{3}{2}[B,[B,A]]'(\mathcal{E}_B(\tau,v))\cdot\tilde{\mathcal{S}}^{(1,1)}(\tau,v)$$

$$+\,\tfrac{3}{2}[B,A]'(\mathcal{E}_B(\tau,v))\cdot\tilde{\mathcal{S}}^{(2,1)}(\tau,v)$$

$$+\,\tfrac{3}{2}[B,A]''(\mathcal{E}_B(\tau,v))(\tilde{\mathcal{S}}^{(1,1)}(\tau,v),\tilde{\mathcal{S}}^{(1,1)}(\tau,v))\Big\}\,\mathrm{d}\tau\,,$$

and

$$\tilde{\mathcal{S}}^{(3,2)}(t,w) = \partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\cdot[B,[B,A]](w) + \tfrac{3}{4}\,\partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\cdot[A,[B,A]](w)$$

$$+\,\partial_2\mathcal{E}_A(\tfrac{1}{2}t,w)\,\cdot\int_0^t\partial_2\mathcal{E}_A(-\tfrac{1}{2}\tau,\mathcal{E}_A(\tfrac{1}{2}\tau,w))\cdot \qquad (\text{C.9b})$$

$$\left\{\tfrac{3}{2}A''(\mathcal{E}_A(\tfrac{1}{2}\tau,w))(\tilde{\mathcal{S}}^{(1,2)}(\tau,w),\tilde{\mathcal{S}}^{(2,2)}(\tau,w))\right.$$

$$+\,\tfrac{1}{2}A'''(\mathcal{E}_A(\tfrac{1}{2}\tau,w))(\tilde{\mathcal{S}}^{(1,2)}(\tau,w),\tilde{\mathcal{S}}^{(1,2)}(\tau,w),\tilde{\mathcal{S}}^{(1,2)}(\tau,w))$$

$$-\,\tfrac{1}{2}[A,[A,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}\tau,w)) - [A,[B,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}\tau,w))$$

$$-\,\tfrac{1}{2}[B,[B,[B,A]]](\mathcal{E}_A(\tfrac{1}{2}\tau,w))$$

$$+\,\tfrac{3}{2}[A,[B,A]]'(\mathcal{E}_A(\tfrac{1}{2}\tau,w))\cdot\tilde{\mathcal{S}}^{(1,2)}(\tau,w)$$

$$+\,\tfrac{3}{2}[B,[B,A]]'(\mathcal{E}_A(\tfrac{1}{2}\tau,w))\cdot\tilde{\mathcal{S}}^{(1,2)}(\tau,w)$$

$$-\,\tfrac{3}{2}[B,A]'(\mathcal{E}_A(\tfrac{1}{2}\tau,w))\cdot\tilde{\mathcal{S}}^{(2,1)}(\tau,w)$$

$$-\,\tfrac{3}{2}[B,A]''(\mathcal{E}_A(\tfrac{1}{2}\tau,w))(\tilde{\mathcal{S}}^{(1,2)}(\tau,w),\tilde{\mathcal{S}}^{(1,2)}(\tau,w))\Big\}\,\mathrm{d}\tau\,.$$

Acknowledgements

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