FRACTIONAL ERROR ESTIMATES OF SPLITTING SCHEMES FOR THE NONLINEAR SCHRÖDINGER EQUATION

JOHANNES EILINGHOFF, ROLAND SCHNAUBELT, AND KATHARINA SCHRATZ

Abstract. We investigate the Lie and the Strang splitting for the cubic nonlinear Schrödinger equation on the full space and on the torus in up to three spatial dimensions. We prove that the Strang splitting converges in L^2 with order $1+\theta$ for initial values in $H^{2+2\theta}$ with $\theta \in (0,1)$ and that the Lie splitting converges with order one for initial values in H^2.

1. Introduction

Semilinear Schrödinger equations naturally split into the free linear Schrödinger equation and a nonlinear ordinary differential equation. For both subsystems one has explicit analytical solution formulas, which allow us to solve them very efficiently on a computer (at least on the torus). This observation makes splitting approaches very attractive for the time integration. In this paper we study the (semi-discrete) Strang and Lie splitting schemes for the cubic nonlinear Schrödinger equation in up to three space dimensions. The first main goal is a new fractional error estimate for initial values in appropriate fractional Sobolev spaces. With our approach we can then establish first order convergence of the Lie splitting for initial values in H^2.

Let $d \in \{1,2,3\}$, $\mu \in \{-1,1\}$ and Ω be either the full space $\mathbb{R}^d$ or the d-dimensional torus $\mathbb{T}^d$. We consider the cubic nonlinear Schrödinger equation

$$\begin{aligned} \partial_t u(t) &= i\Delta u(t) - i\mu \left|u(t)\right|^2 u(t), \quad t \geq 0, \\ u(0) &= u_0 \in H^2(\Omega). \end{aligned} \tag{1.1}$$

In the *focusing* case $\mu = -1$ the problem (1.1) has blow-up solutions for $d \geq 2$, see e.g. Theorem 6.5.10 in [5], whereas in *defocusing* case $\mu = 1$ the solutions are global in time by e.g. Corollary 6.1.2 in [5]. We look at this problem as an equation in $L^2(\Omega)$ and thus require that the initial value belongs to $H^2(\Omega)$, at least. We fix a number $T > 0$ such that the solution exists on $[0,T]$.

Nonlinear Schrödinger equations arise in nonlinear optics or in the theory of shallow water waves as amplitude equations that approximatively determine the

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2000 *Mathematics Subject Classification.* Primary: 65J15. Secondary: 35Q55, 65M12, 65M15.

Key words and phrases. Nonlinear Schrödinger equation, Strang splitting, Lie splitting, error analysis, stability, fractional convergence order, interpolation.

We gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) through CRC 1173.

evolution of wave packets. A variant of (1.1) with a potential term (the Gross–Pitaevskii equation) governs Bose–Einstein condensates. Further information on the physical background can be found in [18] and [19]. Semilinear Schrödinger equations are investigated in the monograph [5] in great detail and generality.

The cubic nonlinearity in (1.1) is the most important one for the applications, but can also be considered as a model case. Actually, our analysis can be extended to nonlinearities of the type $i\varphi(|u|^2)u$ for smooth $\varphi : \mathbb{R} \to \mathbb{R}$ with $\varphi(0) = 0$. However, to avoid technicalities in the context of fractional Sobolev spaces we restrict ourselves to the cubic case. To treat higher dimensions, we would have to work in higher order Sobolev spaces to ensure Sobolev embeddings into L^∞. In the case of one or two spatial dimensions some simplifications of the proofs are possible, which we do not discuss.

One can easily solve the nonlinear ordinary differential equation

$$\partial_t u(t) = -i\mu \, |u(t)|^2 \, u(t)$$

by a simple formula and the linear equation

$$\partial_t u(t) = i\Delta u(t)$$

by means of the Fourier transform, which can numerically be approximated efficiently on the torus. This observation is exploited in the following splitting schemes for (1.1). In the Lie scheme the numerical solution after one time step $\tau > 0$ starting at $u_0 \in H^2(\Omega)$ is given by

$$\Phi_\tau(u_0) := \exp\bigl(-i\mu\tau \, |\widetilde{u}|^2\bigr)\widetilde{u} \quad \text{with} \quad \widetilde{u} := T(\tau)u_0, \tag{1.2}$$

and in the Strang splitting scheme by

$$\begin{gathered} \Psi_\tau(u_0) := T(\tau/2)u^{**} \\ \text{with} \quad u^{**} := \exp\bigl(-i\mu\tau \, |u^*|^2\bigr)u^* \quad \text{with} \quad u^* := T(\tau/2)u_0, \end{gathered} \tag{1.3}$$

where $T(\cdot)$ denotes the free Schrödinger group.

Second-order convergence of the Strang splitting scheme for initial values in $H^4(\mathbb{R}^d)$ was shown by C. Lubich in [16] based on the theory of Lie derivatives (see also [13] for linear Schrödinger equations). More precisely, there exists a time step size $\tau_0 \in (0, T]$ such that for all $u_0 \in H^4(\mathbb{R}^d)$, $\tau \in (0, \tau_0]$ and $n \in \mathbb{N}$ with $n\tau \in [0, T]$ we have

$$\|u(n\tau) - \Psi_\tau^n(u_0)\|_{L^2} \le C\tau^2$$

with a constant $C \ge 0$ depending only on the norm of u in $C([0, T], H^4(\mathbb{R}^d))$ and on T, see Theorem 7.1 in [16]. The time step size restriction was elaborated in Section 5 in [11], where a similar result for PDEs with Burgers' nonlinearity was shown. The earlier paper [3] contains a convergence result for the case $d = 2$ and a general globally Lipschitz nonlinearity. Our considerations take place on a fixed time interval $[0, T]$ within the maximal existence interval. The long-time behavior of numerical (splitting) schemes for a spectral semi-discretization of nonlinear Schrödinger equations was investigated in [8] and [9], see also [6]. For a quasilinear Schrödinger equation and solutions in H^7, the paper [15] provides error estimates in H^1 of the Strang splitting combined with a frequency cut-off.

For smooth solutions a Taylor series expansion shows that the Lie and the Strang splitting are of classical order one and two, respectively. Hence, more regular initial data will not lead to a higher order of convergence. Higher-order splitting methods for Schrödinger equations were investigated in [20], and in [21] for the Gross–Pitaevskii equation.

In our first Theorem 3.1 we reduce the level of regularity of the solutions to $H^{2+2\theta}$ with $\theta \in (0,1)$ and show an error estimate in L^2 of the Strang splitting with the corresponding fractional convergence order $1+\theta$. We then use an analogous fractional convergence result to show a first order error estimate in L^2 for the Lie splitting with initial values in H^2, see Theorem 3.8. Results for the Lie splitting in the case of the cubic NLS have been known so far only in spaces of functions on the torus with summable Fourier coefficients. See Proposition IV.6 of [6], where the calculus of Lie derivatives was used. Moreover, for nonlinearities of the type $i\lambda|u|^p u$ with $p < 4/3$ in [12] first order convergence of the Lie splitting in L^2 was shown for initial values in H^2 by different methods than ours. In this paper we focus on the time integration and do not treat the space discretization (which was studied in e.g. [6]).

We first prove a local error bound and that the numerical solution after one time step $\tau > 0$ is a Lipschitz function of the initial value. To iterate this stability estimate, the Lipschitz constant has to be of the form $e^{c\tau}$. One then obtains a Lipschitz bound on time intervals $[0, n\tau]$ with constant $e^{cn\tau}$. Because of the nonlinearity, c depends on the (so far uncontrolled) H^s–norm of the numerical solution on $[0, n\tau]$, cf. Lemmas 3.3 and 3.10. Here we take $s = 2$ for the Strang splitting and $s = 7/4$ in the Lie case. By means of a telescoping sum, see e.g. [10] or [16], we then deduce a global error bound in our Theorems 3.1 and 3.8. Here the error is measured in L^2, but one can bound it also in H^s (with a smaller fractional convergence order). Since the solution itself is bounded in H^s, the needed a priori estimate on the numerical solution in H^s follows under an additional step size restriction, see [11] or our Lemmas 3.5 and 3.11.

In contrast to [6] or [16], we do not use Lie derivatives and commutators to show the local error estimate. Instead we employ an error formula which is derived by iterating Duhamel's formula for the solution and by replacing the exponential function in the numerical scheme by a Taylor expansion, see [4] for a similar procedure. We split the error formula into a quadrature error and several remainder terms as in e.g. [4] or [7]. The main novelty of our approach is the use of fractional convergence results. They allow us to treat initial values in spaces larger than H^4 (which was taken in [16]). Moreover, for the Lie splitting the fractional convergence in $H^{7/4}$ is crucial for the necessary a priori bound in $H^{7/4}$ of the numerical solution. The needed estimates involving fractional orders are established by various interpolation arguments, e.g. when controlling quadrature errors.

This paper is organised as follows. In Section 2 we describe the functional analytic framework and recall a few facts about the cubic nonlinear Schrödinger equation. The two convergence theorems and various lemms are presented in Section 3. Section 4 is devoted to the proof of the claims in $H^2(\Omega)$ for the Strang splitting, while the statements in $L^2(\Omega)$ for the Strang splitting are shown in

Section 5. The proof of the convergence theorem for the Lie splitting is presented in Section 6.

2. Functional analytic setting

Throughout this paper, I denotes the identity operator and c a generic constant (possibly depending on d). We work on the spatial domain $\Omega \in \{\mathbb{R}^d, \mathbb{T}^d\}$ for $d \in \{1, 2, 3\}$. We use the fractional Sobolev spaces

$$H^s(\Omega) := \{f \in L^2(\Omega) \mid \mathcal{F}^{-1}\big((1 + |\xi|^2)^{s/2}\mathcal{F}f\big) \in L^2(\Omega)\}$$

for $s \geq 0$ equipped with the norms

$$\|f\|_{H^s} := \left\|\mathcal{F}^{-1}\big((1 + |\xi|^2)^{s/2}\mathcal{F}f\big)\right\|_{L^2} = \left\|(1 + |\xi|^2)^{s/2}\mathcal{F}f\right\|_{L^2},$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ denote the unitary Fourier transform and its inverse, both on $\mathbb{R}^d$ and $\mathbb{T}^d$. On the torus one actually has the norm of $\ell^2(\mathbb{Z}^d)$ on the right-hand side of the above identity. We abbreviate $H^s := H^s(\Omega)$ with $H^0 = L^2(\Omega)$. Since $d \leq 3$, we have the Sobolev embedding $H^s \hookrightarrow L^p$ for $\frac{1}{p} \geq \frac{1}{2} - \frac{s}{3}$ and $p \in (2, \infty)$, see e.g. in Corollary 2.2 of [1]. For $s > 3/2$, one further has $H^s \hookrightarrow L^\infty$ since

$$\|f\|_\infty \leq c\,\|\mathcal{F}f\|_1 \leq c\,\|(1 + |\cdot|^2)^{-s/2}\|_2\, \|f\|_{H^s} \leq c\,\|f\|_{H^s}.$$

We define the operators

$$A : H^2 \to L^2;\quad Au := i\Delta u, \qquad \text{and} \qquad B : H^2 \to L^2;\quad B(u) := -i\mu\,|u|^2.$$

The free Schrödinger group generated by A is designated by $T(\cdot)$. We observe that $I - \Delta : H^{s+2} \to H^s$ is an isomorphism and that $T(\cdot)$ induces a unitary C_0–group on H^s generated by $i\Delta$ on H^{s+2} for all $s \geq 0$, which we also denote by $T(\cdot)$. With this notation problem (1.1) takes the form

$$\begin{aligned} \partial_t u(t) &= Au(t) + B(u(t))u(t), \quad t \geq 0, \\ u(0) &= u_0 \in H^2. \end{aligned} \tag{2.1}$$

We look at the two "subproblems"

$$\begin{aligned} \partial_t v(t) &= Av(t) = i\Delta v(t), \quad t \geq 0, \\ v(0) &= v_0 \in H^2, \end{aligned}$$

and

$$\begin{aligned} \partial_t w(t) &= B(w(t))w(t) = -i\mu\,|w(t)|^2\, w(t), \quad t \geq 0, \\ w(0) &= w_0 \in H^2. \end{aligned}$$

The first subproblem is uniquely solved by $v(t) = T(t)v_0$ and the second one by $w(t) = e^{tB(w_0)}w_0$. For both systems we thus have explicit analytical solution formulas. A fully discrete numerical approximation to the solution of the first subproblem can effectively be computed at least for the torus using the fast Fourier transform, see e.g. [6]. The solution of the second subproblem can quickly be calculated by means of the solution formula. Therefore splitting methods like (1.2) and (1.3) are very attractive for the numerical treatment of (1.1). With the above notations the Lie splitting (1.2) reads

$$\Phi_\tau(u_0) := \exp\big(\tau B(\widetilde{u})\big)\widetilde{u} \quad \text{with} \quad \widetilde{u} := T(\tau)u_0 \tag{2.2}$$

and the Strang splitting (1.3) becomes

$$\Psi_\tau(u_0) := T(\tau/2)u^{**} \tag{2.3}$$
$$\text{with}\quad u^{**} := \exp\big(\tau B(u^*)\big)u^* \quad\text{and}\quad u^* := T(\tau/2)u_0.$$

We recall the well-known fact that the space H^s is an algebra if $s > 3/2$ and several related properties which are crucial for our analysis.

Lemma 2.1. (a) *For $s \in [s_0, s_1] \subseteq (3/2, \infty)$, the product of functions $f, g \in H^s$ also belongs to H^s and satisfies*

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

(b) *For $s \in [s_0, s_1] \subseteq (3/2, \infty)$, $t \ge 0$, and $v, w \in H^s$ with $\|v\|_{H^s} \le r$ and $\|w\|_{H^s} \le r$, we have*

$$\|B(v)\|_{H^s} \le cr^2,$$
$$\|B(v) - B(w)\|_{H^s} \le cr\,\|v - w\|_{H^s}\,,$$
$$\left\|e^{tB(v)}\right\|_{H^s} \le e^{ctr^2}.$$

The constants only depend on s_0 and s_1.

Proof. (a): Let $s > 3/2$ and $f, g \in H^s$. From the estimate

$$\big(1 + |\xi|^2\big)^{s/2} \le c\Big(\big(1 + |\xi - \eta|^2\big)^{s/2} + \big(1 + |\eta|^2\big)^{s/2}\Big)$$

and $\mathcal{F}(fg) = c(\mathcal{F}f) * (\mathcal{F}g)$ we derive that

$$\begin{aligned}\big(1 + |\xi|^2\big)^{s/2}\,|\mathcal{F}(fg)(\xi)| &= c\int_{\mathbb{R}^d}\big(1 + |\xi|^2\big)^{s/2}(|\mathcal{F}f)(\xi - \eta)(\mathcal{F}g)(\eta)|\,\mathrm{d}\eta\\ &\le c\Big(\Big|\big(1 + |\cdot|^2\big)^{s/2}\mathcal{F}f\Big| * |\mathcal{F}g|\Big)(\xi) + c\Big(|\mathcal{F}f| * \Big|\big(1 + |\cdot|^2\big)^{s/2}\mathcal{F}g\Big|\Big)(\xi).\end{aligned}$$

Young's inequality and the Sobolev embedding thus yield

$$\begin{aligned}\|fg\|_{H^s} &\le c\big(\|f\|_{H^s}\,\|\mathcal{F}g\|_{L^1} + \|\mathcal{F}f\|_{L^1}\,\|g\|_{H^s}\big)\\ &\le c\big(\|f\|_{H^s}\,\|g\|_{L^\infty} + \|f\|_{L^\infty}\,\|g\|_{H^s}\big) \le c\,\|f\|_{H^s}\,\|g\|_{H^s}\,.\end{aligned}$$

(b): The first two estimates follow directly from part (a). For $t \ge 0$ and $v \in H^s$ with $s > 3/2$ and $\|v\|_{H^s} \le r$ we calculate

$$\left\|e^{tB(v)}\right\|_{H^s} \le \sum_{n=0}^{\infty}\frac{t^n}{n!}\,\|B(v)\|_{H^s}^n \le \sum_{n=0}^{\infty}\frac{t^n(cr^2)^n}{n!} = e^{ctr^2}. \qquad \square$$

Remark 2.2. In the rest of this paper we only deal with the case $s \in [7/4, 4]$, so that the constant c in the previous lemma can be chosen independently of s.

Additionally, for $f \in L^2$ and $g \in H^2$ the Sobolev embedding yields

$$\|fg\|_{L^2} \le \|f\|_{L^2}\,\|g\|_{L^\infty} \le c\,\|f\|_{L^2}\,\|g\|_{H^2}\,. \tag{2.4}$$

Theorem 4.1 in [14] shows that for $u_0 \in H^s$ with $s \ge 2$ the problem (2.1) is locally wellposed; i.e., there exists a time $T > 0$ such that there exists a unique solution $u = u(\cdot, u_0) \in C([0, T], H^s)$ of (2.1). Throughout the paper T is chosen in this way. (In the defocusing case $\mu = 1$ one obtains a global solution on $\mathbb{R}_+$, but we will not need this fact.) The solution is given by Duhamel's formula

$$u(t) = T(t)u_0 - i\mu \int_0^t T(t-r)\big(|u(r)|^2 u(r)\big)\,\mathrm{d}r. \tag{2.5}$$

Since H^s is an algebra, the function $|u|^2 u$ belongs to $C([0,T], H^s)$. Hence, u is also contained in $C^1([0,T], H^{s-2})$ and solves (2.1) in H^{s-2} by standard semigroup theory. Below, we use the quantities

$$M_s := \sup_{t\in[0,T]} \|u(t)\|_{H^s} \quad \text{for } s \geq 0, \qquad M_{2,\theta} := \sup_{t\in[0,T]} \|u(t)\|_{H^{2+2\theta}} \quad \text{for } \theta \in [0,1),$$

whenever these expressions are finite. We remark that M_s and $M_{2,\theta}$ depend only on u_0, s, θ and T, and that we have $M_s \leq M_2 \leq M_{2,\theta}$ for all $\theta \in (0,1)$ and $s \in [0,2)$. We next state several important regularity properties of the free Schrödinger group and the solutions to (2.1).

Lemma 2.3. *Let $\eta \in (0,1)$ and $s \geq 0$.*

(a) *For $f \in H^{2\eta}$ and $g \in H^2$, we have $fg \in H^{2\eta}$ and*

$$\|fg\|_{H^{2\eta}} \leq c\,\|f\|_{H^{2\eta}}\,\|g\|_{H^2}\,.$$

(b) *For each $y \in H^{s+2\eta}$, the mapping $T(\cdot)y : [0,\infty) \to H^s$ is η-Hölder continuous with*

$$\|T(t_1)y - T(t_2)y\|_{H^s} \leq c\,|t_1 - t_2|^\eta\,\|y\|_{H^{s+2\eta}}$$

for all $t_1, t_2 \geq 0$.

(c) *Let $s > 3/2$. For each $y \in H^{s+2\eta}$ the solution $u(\cdot, y) : [0,T] \to H^s$ of (2.1) is η-Hölder continuous with*

$$\begin{aligned}\|u(t_1,y) - u(t_2,y)\|_{H^s} &\leq c\big(M_{s+2\eta} + M_s^3 T^{1-\eta} + T M_{s+2\eta}^3\big)\,|t_1 - t_2|^\eta \\ &=: C(M_{s+2\eta}, T)\,|t_1 - t_2|^\eta\end{aligned}$$

for all $t_1, t_2 \in [0,T]$.

The above constants c do not depend on η.

Proof. Let $\eta \in (0,1)$. We first recall that $H^{s+2\eta}$ is an interpolation space between H^s and H^{s+2} by Theorem 5.4.1 in [2] in combination with the Fourier transform. (See also Theorems 6.2.4 and 6.4.4 in [2] for $\mathbb{R}^d$.) We observe that the involved constants can be chosen independently of η.

(a) Let $g \in H^2$. The norms of the linear operators $V_1 : L^2 \to L^2$ and $V_2 : H^2 \to H^2$ given by $V_j f := fg$ are bounded by $c\,\|g\|_{H^2}$ due to (2.4) and Lemma 2.1. Assertion (a) then follows by interpolation.

(b) Let $t_1, t_2 \geq 0$ with $t_1 \neq t_2$ be fixed. We look at the linear mapping $\widetilde{T}_{t_1,t_2} : H^s \to H^s$; $\widetilde{T}_{t_1,t_2} y := T(t_1)y - T(t_2)y$, which is bounded by 2. We also use its restriction $\widetilde{T}_{t_1,t_2} : H^{s+2} \to H^s$. For $y \in H^s$, we have $\frac{\mathrm{d}}{\mathrm{d}t}T(t)y = T(t)Ay$ and hence

$$\Big\|\widetilde{T}_{t_1,t_2} y\Big\|_{H^s} \leq \sup_{t\in[t_1,t_2]} \|T(t)Ay\|_{H^s}\,|t_1 - t_2| \leq |t_1 - t_2|\,\|y\|_{H^{s+2}}\,.$$

Interpolation then yields assertion (b).

(c) The representation (2.5), part (b) and Lemma 2.1 imply

$$
\begin{aligned}
&\|u(t_1,y)-u(t_2,y)\|_{H^s}\\
&\le \|T(t_1)y-T(t_2)y\|_{H^s}+\int_{t_1}^{t_2}\left\|T(t_2-s)[u(s)\,|u(s)|^2]\right\|_{H^s}\mathrm{d}s\\
&\quad+\int_0^{t_1}\left\|\big(T(t_2-t_1)-\mathbb{1}\big)T(t_1-s)[u(s)\,|u(s)|^2]\right\|_{H^s}\mathrm{d}s\\
&\le c\,|t_1-t_2|^\eta\,\|y\|_{H^{s+2\eta}}+cM_s^3\,|t_1-t_2|^\eta\,T^{1-\eta}+c\,|t_1-t_2|^\eta\,TM_{s+2\eta}^3
\end{aligned}
$$

for $0\le t_1\le t_2\le T$. □

3. Statement of the results

The first main result of this paper is the following fractional convergence theorem for the Strang splitting.

Theorem 3.1. *For all $\theta\in(0,1)$ and $u_0\in H^{2+2\theta}$, there exists a maximal time step size $\tau_0>0$ such that for all $\tau\in(0,\tau_0]$ and $n\in\mathbb{N}$ with $n\tau\in[0,T]$, we have*

$$\|u(n\tau)-\Psi_\tau^n(u_0)\|_{L^2}\le C\tau^{1+\theta}$$

with a constant $C\ge 0$ that depends only on u_0 and T. More precisely, C depends only on T and $M_{2,\theta}$. The number $\tau_0=\tau_0(M_{2,\theta},M_2,\theta,T)$ is given by Lemma 3.5.

In Remark 3.12 we comment on a variant of the maximal step size which does not depend on θ itself. The strategy of the proof of the theorem is similar as in [16] for the case $\theta=1$. We first show that the local error in H^2 is of order $1+\theta$.

Lemma 3.2. *For all $\theta\in(0,1)$ and $u_0\in H^{2+2\theta}$, we have*

$$\|u(\tau)-\Psi_\tau(u_0)\|_{H^2}\le C_1\tau^{1+\theta}$$

with a constant $C_1\ge 0$ depending only on T and $M_{2,\theta}$.

This local error bound will be combined with the following stability result for the scheme in H^2.

Lemma 3.3. *Let $M\ge 0$ and $u_0,v_0\in H^2$ with $\|u_0\|_{H^2}\le M$ and $\|v_0\|_{H^2}\le M$. There exists a constant $C_2\ge 0$, only depending on T and M, such that*

$$\|\Psi_\tau(u_0)-\Psi_\tau(v_0)\|_{H^2}\le e^{C_2\tau}\,\|u_0-v_0\|_{H^2}$$

for all $\tau\in(0,T]$.

Here the precise form of the constant in the estimate is crucial since its n-th power will enter in the proof of the main result. The next property of the numerical approximation will also be needed in this proof.

Definition 3.4. *Let $T>0$, $\tau_0\in(0,T]$, u be a solution of (1.1) defined on $[0,T]$ and ϕ_τ be a time integration scheme. For an initial value $u_0\in H^s$ we call the numerical solution $\phi_\tau^n(u_0)$* strongly bounded *in H^s if there exists a constant $\widehat{C}\ge 0$, only depending on u_0 and T, such that for all $\tau\in(0,\tau_0]$, $n\in\mathbb{N}$ with $n\tau\in[0,T]$ and $k\in\{0,\dots,n\}$ we have $\left\|\phi_\tau^{n-k}(u(k\tau))\right\|_{H^s}\le\widehat{C}$.*

Our numerical solutions are strongly bounded in H^2.

Lemma 3.5. *Let $\theta \in (0,1)$ and $u_0 \in H^{2+2\theta}$. There exists a maximal time step size $\tau_0 > 0$ given by*

$$\tau_0 := \min\left\{ \left(\frac{M_2}{T e^{TC_2} C_1} \right)^{1/\theta}, T \right\}$$

with C_1 from Lemma 3.2 and C_2 from Lemma 3.3, such that the following two statements hold true.

(a) *For all $\tau \in (0, \tau_0]$ and $n \in \mathbb{N}$ with $n\tau \in [0,T]$, we have*

$$\|\Psi_\tau^n(u_0) - u(n\tau)\|_{H^2} \leq C\tau^\theta$$

with a constant $C \geq 0$ depending only on T and $M_{2,\theta}$; i.e., the Strang splitting converges in H^2 with order θ.

(b) *Ψ_τ is strongly bounded; i.e., there exists a constant $\widehat{C} \geq 0$, only depending on M_2, such that $\left\|\Psi_\tau^{n-k}(u(k\tau))\right\|_{H^2} \leq \widehat{C}$ for all $\tau \in (0, \tau_0]$ and $n \in \mathbb{N}$ with $n\tau \in [0,T]$ and $k \in \{0, \dots, n\}$. In particular, the numerical solution is bounded in H^2 (choose $k = 0$).*

The above lemmas are proved in Section 4. In the next lemma we show that the local error in L^2 is of order $2 + \theta$, instead of order $1 + \theta$ as in H^2.

Lemma 3.6. *For all $\theta \in (0,1)$, $u_0 \in H^{2+2\theta}$ and $\tau \in (0,T]$, we have*

$$\|u(\tau) - \Psi_\tau(u_0)\|_{L^2} \leq C_3 \tau^{2+\theta}$$

with a constant $C_3 \geq 0$ depending only on T and $M_{2,\theta}$.

Because of the nonlinearity, in L^2 we only obtain a weaker stability property than in Lemma 3.3, which we call H^2-conditional stability. For this reason we have to invoke the strong boundedness in H^2. It is used to apply Lady Windermere's fan, see [10], in the proof of Theorem 3.1.

Lemma 3.7. *Let $M \geq 0$ and $u_0, v_0 \in H^2$ with $\|u_0\|_{H^2} \leq M$ and $\|v_0\|_{H^2} \leq M$. Then there exists a constant $C_4 \geq 0$, only depending on T and M, such that*

$$\|\Psi_\tau(u_0) - \Psi_\tau(v_0)\|_{L^2} \leq e^{C_4 \tau} \|u_0 - v_0\|_{L^2}$$

for all $\tau \in (0,T]$.

The preceding two lemmas and Theorem 3.1 are shown in Section 5. The convergence theorem for the Lie splitting is established in an analogous way, but using strong boundedness in $H^{7/4}$. Due to this choice of s, we still have the embedding into L^∞ and a local error estimate of order greater than one.

Theorem 3.8. *For all $u_0 \in H^2$, there exists a maximal time step size $\tau_0 > 0$ such that for all $\tau \in (0, \tau_0]$ and $n \in \mathbb{N}$ with $n\tau \in [0,T]$, we have*

$$\|u(n\tau) - \Phi_\tau^n(u_0)\|_{L^2} \leq C\tau$$

with a constant $C \geq 0$ that depends only on u_0 and T. More precisely, C depends only on T and M_2. The number $\tau_0 = \tau_0(M_2, T)$ is given by Lemma 3.11.

For the Lie splitting we again have local error bounds, stability estimates and strong boundedness.

Lemma 3.9. *For all $u_0 \in H^2$ and $\tau \in (0,T]$, we have*

$$\|u(\tau) - \Phi_\tau(u_0)\|_{H^{7/4}} \le C_5 \tau^{9/8},$$
$$\|u(\tau) - \Phi_\tau(u_0)\|_{L^2} \le C_7 \tau^2$$

with constants $C_5, C_7 \ge 0$ depending only on T and M_2.

Lemma 3.10. *Let $M \ge 0$ and $u_0, v_0 \in H^2$ with $\|u_0\|_{H^{7/4}} \le M$ and $\|v_0\|_{H^{7/4}} \le M$. Then there are constants $C_6, C_8 \ge 0$, only depending on T and M, such that*

$$\|\Phi_\tau(u_0) - \Phi_\tau(v_0)\|_{H^{7/4}} \le e^{C_6 \tau} \|u_0 - v_0\|_{H^{7/4}},$$
$$\|\Phi_\tau(u_0) - \Phi_\tau(v_0)\|_{L^2} \le e^{C_8 \tau} \|u_0 - v_0\|_{L^2}$$

for all $\tau \in (0,T]$.

Lemma 3.11. *Let $u_0 \in H^2$. There exists a maximal time step size $\tau_0 > 0$, which is given by*

$$\tau_0 := \min \left\{ \left(\frac{M_2}{T e^{T C_6} C_5} \right)^8, T \right\}$$

with C_5 from Lemma 3.9 and C_6 from Lemma 3.10, such that the following two statements hold true.

(a) *For all $\tau \in (0, \tau_0]$ and $n \in \mathbb{N}$ with $n\tau \in [0,T]$, we have*

$$\|\Phi_\tau^n(u_0) - u(n\tau)\|_{H^{7/4}} \le C \tau^{1/8}$$

with a constant $C \ge 0$ depending only on T and M_2; i.e., the Lie splitting converges in $H^{7/4}$ with order $1/8$.

(b) *Φ_τ is strongly bounded in $H^{7/4}$; i.e., there exists a constant $\widehat{C} \ge 0$, only depending on M_2, such that $\left\|\Phi_\tau^{n-k}(u(k\tau))\right\|_{H^{7/4}} \le \widehat{C}$ for all $\tau \in (0, \tau_0]$ and $n \in \mathbb{N}$ with $n\tau \in [0,T]$ and $k \in \{0, \dots, n\}$. In particular, the numerical solution is bounded in $H^{7/4}$ (choose $k = 0$).*

The proof of these lemmas and of Theorem 3.8 is given in Section 6.

Remark 3.12. Let $u_0 \in H^2$. One can show the assertions of Lemmas 3.9 and 3.10 also for the Strang splitting by similar arguments. Arguing as in Lemma 3.11, one then obtains the strong boundedness of the Strang splitting in $H^{7/4}$ for a maximal step size τ_0'. In this way it is possible to extend Theorem 3.1 to the case $\theta = 0$; i.e., one derives first order convergence in L^2 of the Strang scheme for $u_0 \in H^2$. Of course, this fact is not interesting since already the simpler Lie splitting has this property due to Theorem 3.8. However, using the Strang variants of Lemmas 3.9 and 3.10 one can also prove Theorem 3.1 with $u_0 \in H^{2+2\theta}$ and order $1+\theta$, but replacing τ_0 by the maximal step size τ_0' which does not depend on θ. We omit the details of the proof of these claims.

4. Proof of the strong boundedness in H^2

We prove Lemmas 3.2 and 3.3 and combine them to show Lemma 3.5.

4.1. **Proof of Lemma 3.2.** We start with an auxiliary lemma that we need later to apply interpolation theory.

Lemma 4.1. *Let $(X, \|\cdot\|)$ be a Banach space, $T > 0$ and $\tau \in (0, T]$. We define the linear operators*

$$V_1 : C([0,T], X) \to X, \quad V_2 : C^1([0,T], X) \to X \quad \text{and} \quad V_3 : C^2([0,T], X) \to X$$

by

$$V_j f := \int_0^\tau f(s)\,\mathrm{d}s - \tau f(\tau/2)$$

for $j \in \{1,2,3\}$. These operators are bounded with

$$\|V_1 f\| \le c\tau \|f\|_C, \quad \|V_2 f\| \le c\tau^2 \|f\|_{C^1} \quad \text{and} \quad \|V_3 f\| \le c\tau^3 \|f\|_{C^2}.$$

The proof of this lemma transfers directly from the known scalar-valued case to our situation.

Proof of Lemma 3.2. Let $\theta > 0$, $u_0 \in H^{2+2\theta}$ and $\tau > 0$. By (2.5), the solution of (2.1) at time τ is given by

$$u(\tau) = T(\tau)u_0 + \int_0^\tau T(\tau - s)B(u(s))u(s)\,\mathrm{d}s.$$

Plugging this formula into itself, we derive the representation

$$\begin{aligned} u(\tau) = T(\tau)u_0 &+ \int_0^\tau T(\tau - s)B(u(s))T(s)u_0\,\mathrm{d}s \\ &+ \int_0^\tau T(\tau - s)B(u(s)) \int_0^s T(s-\sigma)B(u(\sigma))u(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \end{aligned} \tag{4.1}$$

in H^2. To show a corresponding formula for the numerical approximation, we use the Taylor expansion

$$e^{\tau x} = I + \tau x + \int_0^\tau x^2 e^{sx}(\tau - s)\,\mathrm{d}s.$$

Applying this identity to $u^{**} = \exp\big(\tau B(u^*)\big)u^*$, we infer

$$u^{**} = u^* + \tau B(u^*)u^* + \int_0^\tau (\tau - s)B(u^*)^2 e^{sB(u^*)}u^*\,\mathrm{d}s.$$

Since $\Psi_\tau(u_0) = T(\tau/2)u^{**}$ and $u^* = T(\tau/2)u_0$, see (2.3), the numerical solution after one time step is then given by

$$\Psi_\tau(u_0) = T(\tau)u_0 + \tau T(\tfrac{\tau}{2})B(u^*)T(\tfrac{\tau}{2})u_0 + \int_0^\tau (\tau - s)T(\tfrac{\tau}{2})B(u^*)^2 e^{sB(u^*)}T(\tfrac{\tau}{2})u_0\,\mathrm{d}s.$$

This equation and (4.1) yield the expression

$$\begin{aligned} u(\tau) - \Psi_\tau(u_0) = &\left(\int_0^\tau T(\tau - s)B(u(s))T(s)u_0\,\mathrm{d}s - \tau T(\tfrac{\tau}{2})B(u^*)T(\tfrac{\tau}{2})u_0\right) \\ &+ \left(\int_0^\tau T(\tau - s)B(u(s)) \int_0^s T(s-\sigma)B(u(\sigma))u(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \right. \\ &\left. \quad - \int_0^\tau (\tau - s)T(\tfrac{\tau}{2})B(u^*)^2 e^{sB(u^*)}T(\tfrac{\tau}{2})u_0\,\mathrm{d}s\right) \end{aligned}$$

$$=: I_1 + I_2. \tag{4.2}$$

1) *Bound on* I_1: We look at the function $w : [0,T] \to H^2$;

$$w(s) := T(\tau - s)B(u(s))T(s)u_0,$$

and estimate

$$\begin{aligned} \|I_1\|_{H^2} &\le \Big\| \int_0^\tau w(s)\,\mathrm{d}s - \tau w(\tau/2) \Big\|_{H^2} + \|\tau w(\tau/2) - \tau T(\tau/2)B(u^*)T(\tau/2)u_0\|_{H^2} \\ &=: S_1 + S_2. \end{aligned} \tag{4.3}$$

For each $y \in H^{2+2\theta}$, the maps $t \mapsto T(t)y$ and $t \mapsto u(t,y)$ are θ-Hölder continuous on $[0,T]$ by Lemma 2.3. Taking into account Lemma 2.1, we infer that w belongs to $C^{0,\theta}([0,T],H^2)$ and

$$\|w(s_1) - w(s_2)\|_{H^2} \le c\big(M_{2,\theta}^3 + M_2^2 C(M_{2,\theta},T) + M_2^2 M_{2,\theta}\big)\,|s_1 - s_2|^\theta \tag{4.4}$$

for all $s_1, s_2 \in [0,T]$. The Hölder space $C^{0,\theta}([0,T],H^2)$ is the real interpolation space $\big(C([0,T],H^2), C^1([0,T],H^2)\big)_{\theta,\infty}$. This can be proved as in the scalar case, see e.g. Examples 1.8 and 1.9 in [17]. An inspection of this proof shows that the occuring constants can be chosen independently of $\theta \in (0,1)$. We can thus interpolate in Lemma 4.1 to derive

$$S_1 \le \tau^{1+\theta} c\big(M_{2,\theta}^3 + M_2^2 C(M_{2,\theta},T) + M_2^2 M_{2,\theta}\big) \le C_{1,1}\tau^{1+\theta}, \tag{4.5}$$

where $C_{1,1}$ only depends on T and $M_{2,\theta}$. To deal with S_2 in (4.3), we set

$$f(t) := \big(B(u(t/2)) - B(T(t/2)u_0)\big)T(t/2)u_0$$

for $0 \le t \le T$. Lemmas 2.1 and 2.3 yield

$$\begin{aligned} \|f(t_1) - f(t_2)\|_{H^2} &\le cM_2^2\,\big\|T(\tfrac{t_1}{2})u_0 - T(\tfrac{t_2}{2})u_0\big\|_{H^2} + cM_2^2\,\big\|u(\tfrac{t_1}{2}) - u(\tfrac{t_2}{2})\big\|_{H^2} \\ &\le cM_2^2\,|t_1 - t_2|^\theta\,\|u_0\|_{H^{2+2\theta}} + cM_2^2 C(M_{2,\theta},T)\,|t_1 - t_2|^\theta \\ &\le C_{1,2}\,|t_1 - t_2|^\theta \end{aligned} \tag{4.6}$$

for $t_1, t_2 \in [0,T]$, where $C_{1,2}$ only depends on T and $M_{2,\theta}$. Using $f(0) = 0$ and

$$S_2 = \|\tau T(\tau/2)f(\tau)\|_{H^2}$$

in (4.3), we derive from (4.6) that

$$S_2 \le C_{1,2}\tau^{1+\theta}. \tag{4.7}$$

2) *Bound on* I_2: By means of Lemma 2.1, we estimate the two summands of I_2 by

$$\Big\| \int_0^\tau T(\tau - s)B(u(s)) \int_0^s T(s-\sigma)B(u(\sigma))u(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \Big\|_{H^2} \le c\tau^2 M_2^5,$$

$$\Big\| \int_0^\tau T(\tau/2)B(u^*)^2 e^{sB(u^*)}(\tau - s)u^*\,\mathrm{d}s \Big\|_{H^2} \le cM_2^3 \exp\big(cTM_2^2\big)\tau^2.$$

The assertion follows if we combine the above two inequalities with (4.2), (4.3), (4.5) and (4.7). □

4.2. **Proof of Lemma 3.3.** Let $M \geq 0$ and $z_0, w_0 \in H^2$ with $\|z_0\|_{H^2} \leq M$ and $\|w_0\|_{H^2} \leq M$. We first look at the initial value problem

$$\partial_t z(t) = -i\mu \, |z(t)|^2 \, z(t), \quad z(0) = z_0.$$

It is solved by $z(t) = \exp(-i\mu t \, |z_0|^2) z_0$. We also set $w(t) = \exp(-i\mu t \, |w_0|^2) w_0$. By a straightforward calculation employing also the Sobolev embedding $H^1 \hookrightarrow L^4$, we estimate

$$\|z(t)\|_{H^2} \leq c\Big(\|z_0\|_{H^2} + t \, \|z_0\|_{H^2}^3 + t^2 \, \|z_0\|_{H^2}^5\Big). \tag{4.8}$$

(If one simply applies Lemma 2.1 here, one obtains worse constants below.) This inequality implies

$$\begin{aligned} \|\partial_t z(t) - \partial_t w(t)\|_{H^2} &= \Big\| |z_0|^2 \, z(t) - |w_0|^2 \, w(t) \Big\|_{H^2} \qquad (4.9) \\ &\leq c\big(\|z_0\|_{H^2} + \|w_0\|_{H^2}\big)\big(\|z_0\|_{H^2} + t \, \|z_0\|_{H^2}^3 + t^2 \, \|z_0\|_{H^2}^5\big) \, \|z_0 - w_0\|_{H^2} \\ &\quad + c \, \|w_0\|_{H^2}^2 \, \|z(t) - w(t)\|_{H^2} \, . \end{aligned}$$

Integrating from 0 to τ, we derive

$$\begin{aligned} \|z(\tau) - w(\tau)\|_{H^2} &= \Big\| z_0 - w_0 + \int_0^\tau \partial_t (z(t) - w(t)) \, \mathrm{d}t \Big\|_{H^2} \\ &\leq \|z_0 - w_0\|_{H^2} + cM\tau\big(M + \tau M^3 + \tau^2 M^5\big) \, \|z_0 - w_0\|_{H^2} \\ &\quad + cM^2 \int_0^\tau \|z(t) - w(t)\|_{H^2} \, \mathrm{d}t. \end{aligned}$$

The Gronwall inequality now yields

$$\begin{aligned} \|z(\tau) - w(\tau)\|_{H^2} &\leq \big(1 + cM^2\tau + (cM^2)^2 \tfrac{\tau^2}{2} + (cM^2)^3 \tfrac{\tau^3}{6}\big) \, \|z_0 - w_0\|_{H^2} \, e^{cM^2\tau} \\ &\leq e^{c\tau M^2} \, \|z_0 - w_0\|_{H^2} \, . \end{aligned} \tag{4.10}$$

Let $u_0, v_0 \in H^2$ with $\|u_0\|_{H^2} \leq M$ and $\|v_0\|_{H^2} \leq M$. Since $T(\tau/2)$ is unitary, (4.10) leads to

$$\begin{aligned} &\|\Psi_\tau(u_0) - \Psi_\tau(v_0)\|_{H^2} \\ &= \Big\| T(\tfrac{\tau}{2}) \exp\big(-i\mu\tau \, |T(\tfrac{\tau}{2})u_0|^2\big) T(\tfrac{\tau}{2}) u_0 - T(\tfrac{\tau}{2}) \exp\big(-i\mu\tau \, |T(\tfrac{\tau}{2})v_0|^2\big) T(\tfrac{\tau}{2}) v_0 \Big\|_{H^2} \\ &= \Big\| \exp\big(-i\mu\tau \, |T(\tau/2)u_0|^2\big) T(\tau/2) u_0 - \exp\big(-i\mu\tau \, |T(\tau/2)v_0|^2\big) T(\tau/2) v_0 \Big\|_{H^2} \\ &\leq e^{cM^2\tau} \, \|T(\tau/2)u_0 - T(\tau/2)v_0\|_{H^2} = e^{cM^2\tau} \, \|u_0 - v_0\|_{H^2} \, . \end{aligned}$$

The result follows with $C_2 := cM^2$. □

4.3. **Proof of Lemma 3.5.** Let $\theta \in (0,1)$. We denote by $u(s, y_0)$ the solution to (2.1) at time $s \geq 0$ with initial value $y_0 \in H^{2+2\theta}$. Let $u_0 \in H^{2+2\theta}$ and define

$$\tau_0 := \min\left\{ \left(\frac{M_2}{T e^{TC_2} C_1} \right)^{1/\theta}, T \right\}. \tag{4.11}$$

We prove part (b) and a stronger version of part (a) by one induction argument. For all $\tau \in (0, \tau_0]$, $n \in \mathbb{N}_0$ with $n\tau \in [0, T]$ and $k \in \{0, \dots, n\}$ we claim that

$$\left\| \Psi_\tau^{n-k}(u(k\tau, u_0)) - u(n\tau, u_0) \right\|_{H^2} \le T e^{TC_2} C_1 \tau^\theta \tag{4.12}$$

with C_1 from Lemma 3.2 and C_2 from Lemma 3.3 (with $M := 2M_2$) and that

$$\left\| \Psi_\tau^{n-k}(u(k\tau, u_0)) \right\|_{H^2} \le 2M_2 =: \widehat{C}. \tag{4.13}$$

We first note that (4.11) and (4.12) yield

$$\left\| \Psi_\tau^{n-k}(u(k\tau, u_0)) - u(n\tau, u_0) \right\|_{H^2} \le M_2$$

for $0 < \tau \le \tau_0$, so that (4.13) will follow from (4.12).

We fix $\tau \in (0, \tau_0]$ and establish (4.12) by induction. The case $n = 0$ is trivial. Let the induction hypothesis

$$\left\| \Psi_\tau^{n-k}(u(k\tau, u_0)) - u(n\tau, u_0) \right\|_{H^2} \le T e^{TC_2} C_1 \tau^\theta \le M_2$$

hold for all $k \in \{0, \dots, n\}$ and some $n \in \mathbb{N}_0$ with $(n+1)\tau \le T$. Hence, (4.13) is valid for all $k \in \{0, \dots, n\}$. We now show (4.12) with $n+1$ instead of n. For $k = n+1$ the estimate (4.12) is clear. Let $k \in \{0, \dots, n\}$. Estimate (4.13) for n and Lemmas 3.3 and 3.2 imply

$$\begin{aligned}
&\left\| \Psi_\tau^{n+1-k}(u(k\tau, u_0)) - u((n+1)\tau, u_0) \right\|_{H^2} \\
&\le \sum_{j=0}^{n-k} \left\| \Psi_\tau^{n-k-j}\big(\Psi_\tau\big(u((k+j)\tau, u_0)\big)\big) - \Psi_\tau^{n-k-j}\big(u((k+j+1)\tau, u_0)\big) \right\|_{H^2} \\
&= \sum_{j=0}^{n-k} \left\| \Psi_\tau\big(\Psi_\tau^{n-k-j}\big(u((k+j)\tau, u_0)\big)\big) - \Psi_\tau\big(\Psi_\tau^{n-k-j-1}\big(u((k+j+1)\tau, u_0)\big)\big) \right\|_{H^2} \\
&\le \sum_{j=0}^{n-k} e^{(n-k-j)C_2\tau} \left\| \Psi_\tau\big(u((k+j)\tau, u_0)\big) - u\big(\tau, u((k+j)\tau, u_0)\big) \right\|_{H^2} \\
&\le \sum_{j=0}^{n-k} e^{(n-k-j)C_2\tau} C_1 \tau^{1+\theta} \le T e^{TC_2} C_1 \tau^\theta,
\end{aligned}$$

using that $n\tau \le T$. Estimate (4.12) is thus shown. □

5. Proof of the convergence theorem for the Strang splitting

We first prove Lemma 3.6 and Lemma 3.7. Then we combine them with Lemma 3.5 to derive Theorem 3.1.

5.1. **Proof of Lemma 3.6.** The proof of Lemma 3.6 is similar to the one of Lemma 3.2, but we need a Taylor expansion of second order instead of first order. Besides Lemma 4.1 we use here the following fact about a quadrature formula on a two-dimensional simplex.

Lemma 5.1. *Let* $(X, \|\cdot\|)$ *be a Banach space,* $\tau > 0$ *and*

$$S_\tau := \{(x,y) \in \mathbb{R}^2 \mid 0 \le y \le x \le \tau\}.$$

We define the linear operators

$$U_1 : C(S_\tau, X) \to X \quad \text{and} \quad U_2 : C^1(S_\tau, X) \to X$$

by

$$U_j f := \int_{S_\tau} f(x,y)\,\mathrm{d}(x,y) - \frac{\tau^2}{8}\big(f(0,0) + f(\tau,0) + f(\tau,\tau) + f(2\tau/3, \tau/3)\big).$$

These operators are bounded and we have

$$\|U_1 f\| \le \tau^2 \|f\|_C \quad \text{and} \quad \|U_2 f\| \le c\tau^3 \|f\|_{C^1}.$$

The first estimate in the lemma is clear. To see the second one, we write

$$f(x,y) - f(a,b) = -\int_0^1 f'(x + r(a-x), y + r(b-y)) \cdot (a-x, b-y)\,\mathrm{d}r$$

for $(a,b) \in \{(0,0), (\tau,0), (\tau,\tau), (2\tau/3, \tau/3)\}$.

Proof of Lemma 3.6. Let $\theta \in (0,1)$, $u_0 \in H^{2+2\theta}$ and $\tau \in (0,T]$. We use the Taylor expansion

$$e^{\tau x} = I + \tau x + \frac{\tau^2}{2}x^2 + \frac{1}{2}\int_0^\tau (\tau - s)^2 x^3 e^{sx}\,\mathrm{d}s$$

for $u^{**} = \exp\big(\tau B(u^*)\big)u^*$ and obtain

$$u^{**} = u^* + \tau B(u^*)u^* + \frac{\tau^2}{2}B(u^*)^2 u^* + \frac{1}{2}\int_0^\tau (\tau - s)^2 B(u^*)^3 e^{sB(u^*)}u^*\,\mathrm{d}s. \tag{5.1}$$

Recall that $\Psi_\tau(u_0) = T(\tau/2)u^{**}$ with $u^* = T(\tau/2)u_0$, see (2.3). We apply $T(\tau/2)$ to (5.1) and insert $u^* = T(\tau/2)u_0$ thrice, arriving at

$$\begin{aligned}\Psi_\tau(u_0) = T(\tau)u_0 + \tau T(\tau/2)B(u^*)T(\tau/2)u_0 + \frac{\tau^2}{2}T(\tau/2)B(u^*)^2 T(\tau/2)u_0 \\ + \frac{1}{2}\int_0^\tau (\tau - s)^2 T(\tau/2)B(u^*)^3 e^{sB(u^*)}u^*\,\mathrm{d}s.\end{aligned}$$

Subtracting this identity from (4.1), we derive the error formula

$$\begin{aligned}
&u(\tau) - \Psi_\tau(u_0) \\
&\quad = \left(\int_0^\tau T(\tau - s)B(u(s))T(s)u_0\,\mathrm{d}s - \tau T(\tau/2)B(u^*)T(\tau/2)u_0\right) \qquad (5.2)\\
&\qquad + \left(\int_0^\tau T(\tau - s)B(u(s))\int_0^s T(s-\sigma)B(u(\sigma))u(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s\right. \\
&\qquad\quad \left. - \frac{\tau^2}{2}T(\tau/2)B(u^*)^2 T(\tau/2)u_0\right) \\
&\qquad - \frac{1}{2}\int_0^\tau (\tau - s)^2 T(\tau/2)B(u^*)^3 e^{sB(u^*)}u^*\,\mathrm{d}s \\
&\quad =: I_1 + I_2 + I_3.
\end{aligned}$$

1) *Bound on* I_1: For I_1 in (5.2), we employ again the function $w : [0,T] \to H^s$;

$$w(s) = T(\tau - s)B(u(s))T(s)u_0,$$

and estimate

$$\begin{aligned}\|I_1\|_{L^2} \leq &\left\| \int_0^\tau T(\tau - s)B(u(s))T(s)u_0 \,\mathrm{d}s - \tau w(\tau/2) \right\|_{L^2} \\ &+ \|\tau w(\tau/2) - \tau T(\tau/2)B(u^*)T(\tau/2)u_0\|_{L^2} .\end{aligned} \tag{5.3}$$

The first summand on the right-hand side will by controlled by interpolation. First observe that

$$w'(s) = -Aw(s) - 2i\mu T(t-s)\operatorname{Re}(\overline{u}(s)Au(s))T(s)u_0 + T(t-s)B(u(s))T(s)Au_0.$$

Estimates (4.4) and (2.4) and Lemmas 2.1 and 2.3 imply that

$$\left\|w'(s_1) - w'(s_2)\right\|_{L^2} \leq C_{3,1} \left|s_1 - s_2\right|^\theta \quad \text{and} \quad \left\|w'(s_1)\right\|_{L^2} \leq C_{3,1} \tag{5.4}$$

for $s_1, s_2 \in [0,T]$ where $C_{3,1}$ only depends on T and $M_{2,\theta}$. So, w belongs to $C^{1,\theta}([0,T],L^2)$ which is the interpolation space $\big(C^1([0,T],L^2), C^2([0,T],L^2)\big)_{\theta,\infty}$, cf. again Examples 1.8 and 1.9 in [17]. Lemma 4.1 and interpolation then yield

$$\left\| \int_0^\tau T(\tau - s)B(u(s))T(s)u_0 \,\mathrm{d}s - \tau w(\tau/2) \right\|_{L^2} \leq c\tau^{2+\theta} C_{3,1}. \tag{5.5}$$

To treat the second summand in (5.3), as before we look at the function $f : [0,T] \to L^2$ given by

$$f(t) = \big(B(u(t/2)) - B(T(t/2)u_0)\big)T(t/2)u_0.$$

We want to check that f belongs to $C^{1,\theta}([0,T], L^2)$. Observe that

$$\begin{aligned}2f'(t) = &-i\mu\Big(\operatorname{Re}\big(\overline{u}(t/2)Au(t/2)\big) - \operatorname{Re}\big(\overline{T(t/2)u_0}\big(T(t/2)Au_0\big)\big)\Big)T(t/2)u_0 \\ &+ \big(B(u(t/2)) - B(T(t/2)u_0)\big)T(t/2)Au_0.\end{aligned}$$

As above we deduce that

$$\begin{aligned}\left\|f'(t_1) - f'(t_2)\right\|_{L^2} &\leq cM_2^2 C(M_{2,\theta}, T) \left|t_1 - t_2\right|^\theta + cM_2^2 \left|t_1 - t_2\right|^\theta \|u_0\|_{H^{2+2\theta}} \\ &\leq C_{3,2} \left|t_1 - t_2\right|^\theta\end{aligned}$$

for all $t_1, t_2 \in [0,T]$ with a constant $C_{3,2}$ only depending on T and $M_{2,\theta}$. Since $f(0) = 0$ and $f'(0) = 0$, it follows

$$\|f(\tau)\|_{L^2} = \left\| \int_0^\tau \big(f'(s) - f'(0)\big) \,\mathrm{d}s \right\|_{L^2} \leq C_{3,2}\tau^{1+\theta}.$$

We then conclude

$$\|\tau w(\tau/2) - \tau T(\tau/2)B(u^*)T(\tau/2)u_0\|_{L^2} = \|\tau T(\tau/2)f(\tau)\|_{L^2} \leq C_{3,2}\tau^{2+\theta}. \tag{5.6}$$

The expressions (5.3), (5.5) and (5.6) yield $\|I_1\|_{H^2} \leq \widetilde{C}_3\tau^{2+\theta}$ with a constant $\widetilde{C}_3$ that only depends on T and $M_{2,\theta}$.

2) *Bound on* I_2: We now tackle the summand I_2 in (5.2). We define

$$v(s,\sigma) := T(\tau - s)B(u(s))T(s - \sigma)B(u(\sigma))u(\sigma)$$

for $(s,\sigma) \in [0,T] \times [0,T]$ and split

$$\|I_2\|_{L^2} \le Q + R \tag{5.7}$$

with the abbreviations

$$\begin{aligned} Q :&= \bigg\| \int_0^\tau \int_0^s T(\tau - s) B(u(s)) T(s-\sigma) B(u(\sigma)) u(\sigma)\,\mathrm{d}\sigma\,\mathrm{d}s \\ &\qquad - \frac{\tau^2}{8}\big(v(0,0) + v(\tau,0) + v(\tau,\tau) + v(2\tau/3, \tau/3)\big)\bigg\|_{L^2}, \\ R :&= \bigg\| \frac{\tau^2}{8}\big(v(0,0) + v(\tau,0) + v(\tau,\tau) + v(2\tau/3,\tau/3)\big) \\ &\qquad - \frac{\tau^2}{2} T(\tau/2) B(u^*)^2 T(\tau/2) u_0 \bigg\|_{L^2}. \end{aligned}$$

For all $(s_1,\sigma_1),(s_2,\sigma_2) \in S_\tau$, Lemmas 2.1 and 2.3 imply

$$\begin{aligned} \|v(s_1,\sigma_1) - v(s_2,\sigma_2)\|_{L^2} &\le c\Big(M_2^3 M_0 C(M_{2,\theta},T) + M_2^5\Big) \left| \begin{pmatrix} s_1 - s_2 \\ \sigma_1 - \sigma_2 \end{pmatrix} \right|^\theta \\ &\le C_{4,1} \left| \begin{pmatrix} s_1 - s_2 \\ \sigma_1 - \sigma_2 \end{pmatrix} \right|^\theta \end{aligned}$$

where $C_{4,1}$ only depends on T and $M_{2,\theta}$. Interpolating in Lemma 5.1, we infer

$$Q \le c\tau^{2+\theta} C_{4,1}. \tag{5.8}$$

To estimate R, we introduce the function $g : [0,T] \to L^2$ by

$$\begin{aligned} g(t) :&= T(t)B(u_0)^2 u_0 + B(u(t))T(t)B(u_0)u_0 \\ &\quad + B(u(t))^2 u(t) + T(t/3)B(u(2t/3))T(t/3)B(u(t/3))u(t/3) \\ &\quad - 4T(t/2)B(T(t/2)u_0)^2 T(t/2)u_0. \end{aligned}$$

For all $t_1, t_2 \in [0,T]$, we derive from Lemmas 2.1 and 2.3 that

$$\|g(t_1) - g(t_2)\|_{L^2} \le c\big(M_2^5\,|t_1 - t_2|^\theta + M_2^4 C(M_{2,\theta},T)\,|t_1 - t_2|^\theta\big).$$

Since $g(0) = 0$ and $R = \left\|\frac{\tau^2}{8} g(\tau)\right\|_{L^2}$, this inequality leads to

$$R = \left\| \frac{\tau^2}{8} g(\tau) \right\|_{L^2} \le C_{4,2}\tau^{2+\theta} \tag{5.9}$$

with $C_{4,2}$ only depending on T and $M_{2,\theta}$. From (5.7), (5.8) and (5.9) we conclude

$$\|I_2\|_{L^2} \le cC_{4,1}\tau^{2+\theta} + C_{4,2}\tau^{2+\theta} =: \widetilde{C}_4 \tau^{2+\theta}$$

where $\widetilde{C}_4$ only depends on T and $M_{2,\theta}$.

3) *Bound on* I_3: The summand I_3 of (5.2) can directly be controlled using Lemma 2.1 so that I_3 is bounded by $\widetilde{C}_5 \tau^{2+\theta}$ for a constant $\widetilde{C}_5$ that only depends on T and M_2. □

5.2. **Proof of Lemma 3.7.** Let $u_0, v_0 \in H^2$ with $\|u_0\|_{H^2} \le M$ and $\|v_0\|_{H^2} \le M$. For $z_0, w_0 \in H^2$, we look at the solutions of the initial value problems

$$\partial_t z(t) = -i\mu \, |z(t)|^2 \, z(t), \quad z(0) = z_0,$$
$$\partial_t w(t) = -i\mu \, |w(t)|^2 \, w(t), \quad w(0) = w_0.$$

As in (4.9) one shows the estimate

$$\begin{aligned}\|\partial_t z(t) - \partial_t w(t)\|_{L^2} \le c\big(\|z_0\|_{H^2} + \|w_0\|_{H^2}\big)\big(\|z_0\|_{H^2} + t\,\|z_0\|_{H^2}^3 \\ + t^2\,\|z_0\|_{H^2}^5\big)\,\|z_0 - w_0\|_{L^2} + c\,\|w_0\|_{H^2}^2\,\|z(t) - w(t)\|_{L^2}.\end{aligned}$$

From this fact we conclude as in (4.10) that

$$\left\| \exp(-i\mu\tau\,|z_0|^2) z_0 - \exp(-i\mu\tau\,|w_0|^2) w_0 \right\|_{L^2} \le e^{C_4\tau}\,\|z_0 - w_0\|_{L^2}$$

for a constant C_4 that only depends on T, $\|z_0\|_{H^2}$ and $\|w_0\|_{H^2}$. As in the proof of Lemma 3.3 we then arrive at

$$\|\Psi_\tau(u_0) - \Psi_\tau(v_0)\|_{L^2} \le e^{C_4\tau}\,\|u_0 - v_0\|_{L^2}. \qquad \square$$

5.3. **Proof of Theorem 3.1.** Let $\theta > 0$ and $u_0 \in H^{2+2\theta}$. Take $\tau \in (0, \tau_0]$ with τ_0 from Lemma 3.5 and $n \in \mathbb{N}$ with $n\tau \in [0, T]$. We have

$$u(n\tau) - \Psi_\tau^n(u_0) = \sum_{k=0}^{n-1} \Psi_\tau^k\big(u((n-k)\tau)\big) - \Psi_\tau^{k+1}\big(u((n-k-1)\tau)\big).$$

In view of Lemma 3.5, the expressions $\Psi_\tau^l\big(u((n-1-l)\tau)\big)$ with $l \in \{0, \dots, n-1\}$ are bounded in H^2 by a constant $\widehat{C}$ that only depends on M_2. Iteratively, Lemma 3.7 with $M := \widehat{C}$ can thus be applied to all summands appearing in the second line of the following calculation. Together with Lemma 3.6 we derive

$$\begin{aligned}&\|u(n\tau) - \Psi_\tau^n(u_0)\|_{L^2} \\ &\quad \le \sum_{k=0}^{n-1} \left\| \Psi_\tau\big(\Psi_\tau^{k-1}\big(u((n-k)\tau)\big)\big) - \Psi_\tau\big(\Psi_\tau^k\big(u((n-k-1)\tau)\big)\big) \right\|_{L^2} \\ &\quad \le \sum_{k=0}^{n-1} e^{kC_4\tau} \big\| u\big(\tau, u((n-k-1)\tau)\big) - \Psi_\tau\big(u((n-k-1)\tau)\big) \big\|_{L^2} \\ &\quad \le \sum_{k=0}^{n-1} e^{kC_4\tau} C_3 \tau^{2+\theta} \le T e^{TC_4} C_3 \tau^{1+\theta},\end{aligned}$$

where we use again $n\tau \le T$. $\square$

6. Proof of the convergence theorem for the Lie spliting

We first prove the Lemmas 3.9 and 3.10. Using them, we then establish Lemma 3.11 and Theorem 3.8.

6.1. **Proof of Lemma 3.9.** We again start with a lemma needed for an interpolation argument. The very simple proof is omitted.

Lemma 6.1. *Let $T > 0$ and $\tau \in (0, T]$. We define the Banach space $Z := C^1([0,T], L^2) \cap C([0,T], H^2)$ with norm*

$$\|f\|_Z := \|f\|_{C^1([0,T],L^2)} + \|f\|_{C([0,T],H^2)}$$

and the linear operators

$$V_1 : Z \to H^2 \quad \text{and} \quad V_2 : Z \to L^2 \quad \text{by} \quad V_j f := \int_0^\tau f(s)\,\mathrm{d}s - \tau f(0).$$

These operators are bounded and we have

$$\|V_1 f\|_{H^2} \le 2\tau \|f\|_Z \quad \text{and} \quad \|V_2 f\|_{L^2} \le \tau^2 \|f\|_Z.$$

Proof of Lemma 3.9. Let $u_0 \in H^2$ and $\tau > 0$. By (2.5), the solution of (2.1) at time τ is given by

$$u(\tau) = T(\tau)u_0 + \int_0^\tau T(\tau - s)B(u(s))u(s)\,\mathrm{d}s.$$

Applying the Taylor expansion

$$e^{\tau x} = I + \tau x + \int_0^\tau (\tau - s)x^2 e^{\tau x}\,\mathrm{d}s$$

to $\Phi_\tau(u_0) = \exp\big(\tau B(\widetilde{u})\big)\widetilde{u}$ with $\widetilde{u} = T(\tau)u_0$, see (2.2), we determine the numerical solution after one time step as

$$\Phi_\tau(u_0) = T(\tau)u_0 + \tau B(\widetilde{u})\widetilde{u} + \int_0^\tau (\tau - s)B(\widetilde{u})^2 e^{sB(\widetilde{u})}\widetilde{u}\,\mathrm{d}s. \tag{6.1}$$

The difference of (2.5) and (6.1) is

$$\begin{aligned} u(\tau) - \Phi_\tau(u_0) &= \left(\int_0^\tau T(\tau - s)B(u(s))u(s)\,\mathrm{d}s - \tau B(\widetilde{u})\widetilde{u}\right) \\ &\quad - \int_0^\tau (\tau - s)B(\widetilde{u})^2 e^{sB(\widetilde{u})}\widetilde{u}\,\mathrm{d}s \\ &=: I_1 + I_2. \end{aligned} \tag{6.2}$$

1) *Bound on I_1*: To estimate I_1, we again look at the function $w : [0,T] \to H^2$;

$$w(s) := T(\tau - s)B(u(s))u(s),$$

and write

$$\begin{aligned} I_1 &= \left(\int_0^\tau T(\tau - s)B(u(s))u(s)\,\mathrm{d}s - \tau w(0)\right) + \Big(\tau w(0) - \tau B(\widetilde{u})\widetilde{u}\Big) \\ &=: S_1 + S_2. \end{aligned} \tag{6.3}$$

As in (5.4) we see that w belongs $C^1([0,T], L^2) \cap C([0,T], H^2)$ and that its norm in this space is bounded by a constant $\widetilde{C}_{1,1}$ only depending on M_2. Lemma 6.1 then yields

$$\|S_1\|_{L^2} \le C_{1,1}\tau^2 \quad \text{and} \quad \|S_1\|_{H^2} \le 2C_{1,1}\tau,$$

so that

$$\|S_1\|_{H^{7/4}} \le cC_{1,1}\tau^{9/8}$$

by interpolation. For S_2 we note that $w(0) = T(\tau)B(u_0)u_0$ and

$$\begin{aligned} T(\tau)B(u_0)u_0 - B(T(\tau)u_0)T(\tau)u_0 = \Big(&T(\tau)B(u_0)u_0 - B(u_0)u_0\Big) \\ &+ \Big(B(u_0)(u_0 - T(\tau)u_0)\Big) \\ &+ \Big(\big(B(u_0) - B(T(\tau)u_0)\big)T(\tau)u_0\Big). \end{aligned} \tag{6.4}$$

To treat the first term on the right-hand side, we define $f_1 : [0,T] \to H^2$ by $f_1(t) := T(t)B(u_0)u_0 - B(u_0)u_0$. Since $f_1(0) = 0$, Lemma 2.3 yields

$$\begin{aligned} \|f_1(\tau)\|_{H^{7/4}} &\le c\,\|u_0\|_{H^2}^3\,\tau^{1/8}, \\ \|f_1(\tau)\|_{L^2} &\le \int_0^\tau \|f'(s)\|_{L^2}\,\mathrm{d}s \le c\,\|u_0\|_{H^2}^3\,\tau. \end{aligned}$$

For the other two terms in (6.4) one obtains analogous estimates. So we can bound

$$\|S_2\|_{H^{7/4}} \le C_{1,2}\tau^{9/8} \quad \text{and} \quad \|S_2\|_{L^2} \le C_{1,2}\tau^2$$

with a constant $C_{1,2}$ only depending on M_2. In view of (6.3) we obtain

$$\|I_1\|_{H^{7/4}} \le \widetilde{C}_1\tau^{9/8} \quad \text{and} \quad \|I_1\|_{L^2} \le \widetilde{C}_1\tau^2$$

where $\widetilde{C}_1$ only depends on M_2.

2) *Bound on* I_2: Lemma 2.1 allows to estimate the second term in (6.2) by

$$\begin{aligned} \|I_2\|_{H^{7/4}} &\le cM_2^4 e^{cTM_2^2} T^{7/8}\tau^{9/8} \le \widetilde{C}_2\tau^{9/8}, \\ \|I_2\|_{L^2} &\le cM_2^4 e^{cTM_2^2}\tau^2 \le \widetilde{C}_2\tau^2 \end{aligned}$$

with a constant $\widetilde{C}_2$ only depending on T and M_2. □

Proof of Lemma 3.10, Lemma 3.11 and Theorem 3.8. One shows Lemma 3.10 in the same way as Lemmas 3.3 and 3.7, using instead of (4.8) only Lemma 2.1 to estimate $z(t)$ in $H^{7/4}$. Based on Lemmas 3.9 and 3.10, one proves Lemma 3.11 as Lemma 3.5 with $\theta = 1/8$ and $M_{7/4}$ instead of M_2. Finally Lemmas 3.9, 3.10 and 3.11 imply Theorem 3.8 as in the proof of Theorem 3.1. □

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J. Eilinghoff, Department of Mathematics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany.
E-mail address: `johannes.eilinghoff@kit.edu`

R. Schnaubelt, Department of Mathematics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany.
E-mail address: `schnaubelt@kit.edu`

K. Schratz, Department of Mathematics, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany.
E-mail address: `katharina.schratz@kit.edu`