Superconvergence of Strang splitting for NLS in T^d

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Abstract

In this paper we investigate the convergence properties of semi-discretized approximations by Strang splitting method applied to fast-oscillating nonlinear Schrödinger equations. In a first step and for further use, we briefly adapt a known convergence result for Strang method in the context of NLS on $\mathbb{T}^d$ for a large class of nonlinearities. In a second step, we examine how errors depend on the length of the period ε, the solutions being considered on intervals of fixed length (independent of the period). Our main contribution is to show that Strang splitting with constant step-sizes is unexpectedly more accurate by a factor ε as compared to established results when the step-size is chosen as an integer fraction of the period, owing to an averaging effect.

Keywords: highly-oscillatory systems, averaging, partial differential equation, Schrödinger equation, nonlinear, Strang splitting, splitting schemes.

MSC numbers: 34K33, 37L05, 35Q55.

1 Introduction

In this work, we analyze the convergence of *Strang splitting* method for nonlinear Schrödinger equations of the form

$$i\partial_t u^\varepsilon = -\frac{1}{\varepsilon}\Delta u^\varepsilon + f(|u^\varepsilon|^2)u^\varepsilon, \quad u^\varepsilon(0) = u_0 \in H^\sigma(\mathbb{T}^d), \quad t \le T, \tag{1}$$

where Δ is the Laplacian operator acting on the Hilbert space H^σ of functions on $\mathbb{T}^d = [0, 2\pi]^d$ with derivatives up to order σ and f is a C^∞-function from $\mathbb{R}$ into itself such that $f(0) = 0$.[1] The operator Δ being self-adjoint, Stone's theorem asserts that it generates a strongly continuous one-parameter unitary group $e^{i\tau\Delta}$ which, here, is in addition 1-periodic

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[1]The assumption $\mathbb{T}^d = [0, 2\pi]^d$ can be relaxed, provided the corresponding spectrum of Δ remains a subset of $\omega\mathbb{N}$ for some $\omega > 0$.

in the variable $\tau = t/\varepsilon$, so that on a fixed interval of time, the number of oscillations tend to $+\infty$ as ε goes to zero, thus making the problem highly-oscillatory. It is customary for the ease of analysis to reparametrize the time and consider the evolution in the variable τ. In this language (but denoting again by t the new variable τ), the equation reads

$$i\partial_t u^\varepsilon = -\Delta u^\varepsilon + \varepsilon f(|u^\varepsilon|^2)u^\varepsilon, \quad u^\varepsilon(0) = u_0 \in H^\sigma(\mathbb{T}^d), \quad t \leq T/\varepsilon, \tag{2}$$

the period of the group $e^{it\Delta}$ is 1, and the equation must be solved on the interval $[0, T/\varepsilon]$ (where interesting dynamics of the solutions appear). Of course, the number of oscillations $\lfloor T/\varepsilon \rfloor$ over the interval of resolution still goes to ∞ for vanishing ε. Albeit the occurrence of ε in front of the nonlinearity, we insist that (2) is **not** a perturbation problem, owing to the length of the interval of time which scales like $1/\varepsilon$. In the sequel, we give convergence results for semi-discretized numerical schemes applied to (2), keeping in mind that they are straightforwardly transferred to the original format (as stated in the Abstract). Accordingly, we assume in the **whole paper** the following:

Hypothesis (H) There exist $T > 0$ and $\varepsilon_0 > 0$, such that, for any $0 < \varepsilon < \varepsilon_0$, equation (2) has a unique solution $u^\varepsilon(t, \cdot) \in C^1([0, T/\varepsilon]; H^\sigma(\mathbb{T}^d))$ with $\sigma > d/2 + 2$ and $\sigma \geq 4$. Furthermore, there exists a positive constant K such that

$$\forall 0 < \varepsilon < \varepsilon_0, \quad \forall 0 \leq t \leq T/\varepsilon, \qquad \|u^\varepsilon(t)\|_{H^\sigma} \leq K\|u_0\|_{H^\sigma}. \tag{3}$$

For convenience, we shall denote in the sequel, $R = 2K\|u_0\|_{H^\sigma}$ and

$$B^s_\rho = \{u \in H^s, \|u\|_{H^s} \leq \rho\},$$

so that under previous hypothesis, the solution $u^\varepsilon(t) \equiv u^\varepsilon(t, \cdot)$ remains in $B^\sigma_{R/2}$ for all $t \in [0, T/\varepsilon]$. Note that in our context, the validity of this assumption can be rigorously established (see for instance [3]).

In this paper, we study the approximation properties of a semi-discretization in time. The numerical scheme that we consider is Strang splitting method, yielding approximations

$$\Phi^h(u) = \varphi_T^{h/2} \circ \varphi_V^h \circ \varphi_T^{h/2}(u),$$

where h is the step size and φ_T^h and φ_V^h are the exact flows of respectively

$$i\partial_t u = -\Delta u \quad \text{and} \quad i\partial_t u = \varepsilon f(|u|^2)u. \tag{4}$$

By Stone's theorem and the gauge invariance, they can be written for all $u \in H^s$ and all $h \in \mathbb{R}$ as

$$\varphi_T^h(u) = e^{ih\Delta}u \quad \text{and} \quad \varphi_V^h(u) = e^{-ih\varepsilon f(|u|^2)}u.$$

Note that both maps are isometries of L^2, that is, one has for all $u \in L^2$, $\|\varphi_T^h(u)\|_{L^2} = \|u\|_{L^2}$ and $\|\varphi_V^h(u)\|_{L^2} = \|u\|_{L^2}$. It is perfectly clear that the first map is also an isometry in H^s for all $0 \leq s \leq \sigma$.

In agreement with the results of [9] derived for NLS in $\mathbb{R}^3$ and $f(u) = u$, the sequence of approximations $(\Phi^h)^n(u_0)$ are expected to converge on $[0, T/\varepsilon]$ with second-order error estimates of the form

$$\|(\Phi^h)^n(u_0) - u(t_n)\|_{H^{\sigma-4}} \leq \text{Const } h^2$$

for $t_n = nh \leq T/\varepsilon$ and sufficiently small h. Note that here σ and d are arbitrary with the only constraint that $\sigma > d/2 + 2$ and that the convergence is uniform in ε. The aim of this paper is to show that, somehow unexpectedly at first glance, this error estimate can be refined to obtain

$$\|(\Phi^h)^n(u_0) - u(t_n)\|_{H^{\sigma-2m}} \leq \text{Const } (\varepsilon h^2 + h^m)$$

where $2 \leq m \leq \lfloor \sigma/2 \rfloor$ depends on the smoothness of the initial value u_0, provided the step size h is chosen in such a way that $1/h$ is an integer.[2] The precise formulation of this result is given in Theorem 5.5.

The paper is organized more or less along the following inclusions:

$$\underbrace{B^{\sigma}_{R/2}}_{exact\, solution} \left(\subset \underbrace{B^{\sigma}_{R} \subset B^{\sigma-2}_{R}}_{functional\ bounds} \right) \subset \underbrace{B^{\sigma-2}_{3R/4}}_{h^1-error,\, H^s-stability} \subset \underbrace{H^{\sigma-4}}_{h^2-error} \subset \underbrace{H^{\sigma-2m}}_{h^2\varepsilon-error}$$

In Section 2, we consider the two functions $u \mapsto F(u) = -if(|u|^2)u$ and $(\tau, u) \mapsto F_\tau(u) = e^{-i\tau\Delta}F\left(e^{i\tau\Delta}u\right)$ which are essential ingredients of further proofs and derive bounds of their derivatives with respect to both u and τ. In addition, we give a Lipschitz estimate for F, which lies at the core of stability estimates derived in Section 3. In the spirit of [9] again, stability holds in H^s-norms for $0 \leq s \leq \sigma - 2$ provided the numerical solutions remain in $H^{\sigma-2}$. Bounds on derivatives of F and F_τ are then used in Section 4 to analyze the local truncation errors. In Section 5, we first briefly (re)-derive the (uniform in ε) convergence results of [9] (though without resorting to Lie-derivatives) and then analyze in great details the accumulation of errors in the case where $1/h \in \mathbb{N}$. The final result is then obtained in two steps, by first studying the errors over one period (see Theorem 5.4) where an averaging effect essentially kills the main error term and then extending the so-obtained estimates to the whole interval (see Theorem 5.5) . Finally, Section 7 presents numerical experiments confirming the occurrence of an additional ε-factor in error bounds. A few more technical results are exposed in Appendix.

2 Bounds on F, F_τ and their derivatives

The embeddings of H^σ and $H^{\sigma-2}$ into L^∞ implies that H^σ and $H^{\sigma-2}$ are algebras: there exists a constant $A > 1$ such that for $s = \sigma$ and $s = \sigma - 2$, one has

$$\forall (u, v) \in H^s \times H^s, \quad \|uv\|_{H^s} \leq A\|u\|_{H^s}\|v\|_{H^s}.$$

[2] Such step sizes are said to be resonant and can lead to exponential error growth (see Weideman and Herbst [12]). However, this possible very long-time instability does not contradict the convergence results given. Instabilities are indeed typically observed on intervals of length T/ε^2 in this scaling.

In this context, any C^∞-function G from $\mathbb{C}$ to itself, such that $G(0)=0$, satisfies a so-called *tame* estimate (see [1]): there exists a non-decreasing function χ_G from $\mathbb{R}^+$ into $\mathbb{R}^+$, such that for $s=\sigma$ and $s=\sigma-2$, one has

$$\forall u \in H^s, \quad \|G(u)\|_{H^s} \leq \chi_G(\|u\|_{L^\infty})\|u\|_{H^s} \leq \chi_G(c\|u\|_{H^s})\|u\|_{H^s}, \tag{5}$$

where we have used in the second part of the inequalities the continuous embedding of $H^{\sigma-2}$ and H^σ into L^∞ and denoted c the corresponding constant $\|\cdot\|_{L^\infty} \leq c\|\cdot\|_{H^{\sigma-2}} \leq c\|\cdot\|_{H^\sigma}$. More generally, when $G(0)$ is not assumed to vanish, we may consider $\tilde{G}(u) = G(u) - G(0)$ and assert that there exists again a non-decreasing function χ_G from $\mathbb{R}^+$ into $\mathbb{R}^+$, such that for $s=\sigma$ and $s=\sigma-2$, one has

$$\forall u \in H^s, \quad \|G(u)\|_{H^s} \leq (2\pi)^{d/2}|G(0)| + \chi_G(\|u\|_{L^\infty})\|u\|_{H^s}. \tag{6}$$

In the sequel, the following functions will play an important role:

$$\begin{array}{rccl} F: & H^\sigma & \to & H^\sigma \\ & u & \mapsto & -if(|u|^2)u \end{array}$$

and

$$\begin{array}{rccl} F_\tau: & [0,1]\times H^\sigma & \to & H^\sigma \\ & (\tau,u) & \mapsto & e^{-i\tau\Delta}F(e^{i\tau\Delta}u). \end{array}$$

Let us notice that $F \equiv F_0$, so that we will mostly concentrate on estimates for F_τ.

A Lipschitz inequality for F_τ. Regarding F as a function of $H^{\sigma-2}$ into itself, it is not difficult to show that it a Lipschitz continuous function. Owing to Lemma 7.3 in Appendix, it is also a Lipschitz continuous function in H^s-norm for all $0 \leq s \leq \sigma-2$, provided u and v lie in $B_R^{\sigma-2}$. We have indeed

$$\begin{aligned}
\|F(u)-F(v)\|_{H^s} &= \|f(|u|^2)u - f(|u|^2)v + f(|u|^2)v - f(|v|^2)v\|_{H^s} \\
&= \|f(|u|^2)(u-v)\|_{H^s} + \|(f(|u|^2)-f(|v|^2))v\|_{H^s} \\
&\leq \kappa\|f(|u|^2)\|_{H^{\sigma-2}}\|u-v\|_{H^s} + \kappa\|v\|_{H^{\sigma-2}}\|f(|u|^2)-f(|v|^2)\|_{H^s} \\
&\leq \kappa\, A\chi_f(c^2\|u\|^2_{H^{\sigma-2}})\|u\|^2_{H^{\sigma-2}}\|u-v\|_{H^s} + \alpha\|v\|_{H^{\sigma-2}}\alpha(f,AR^2)\||u|^2-|v|^2\|_{H^s} \\
&\leq \kappa\, A\chi_f(c^2R^2)R^2\|u-v\|_{H^s} + \kappa\, R\,\alpha(f,AR^2)\|u\bar{u} - u\bar{v} + u\bar{v} - v\bar{v}\|_{H^s} \\
&\leq \kappa\, A\chi_f(c^2R^2)R^2\|u-v\|_{H^s} + 2\,\kappa^2\, R^2\,\alpha(f,AR^2)\|u-v\|_{H^s} \\
&\leq L\,\|u-v\|_{H^s}
\end{aligned}$$

with[3] $L = \kappa\, R^2(A\chi_f(c^2R^2) + 2\,\kappa\,\alpha(f,AR^2))$. The map $e^{ih\Delta}$ being an isometry of H^s for all s, it is clear that F_τ is also Lipschitz continuous with the same constant L.

Derivatives with respect to u. Let $s=\sigma$ or $s=\sigma-2$. Function F_τ is C^∞ w.r.t. u from H^s into itself, and we have for instance

$$F'_\tau(u)(v) = e^{-i\tau\Delta}F'(e^{i\tau\Delta}u)(e^{i\tau\Delta}v)$$

[3]Constants κ and $\alpha(f,AR^2)$ are defined in Lemma 7.3 in Appendix.

where $F'(u)(v) = -if(|u|^2)v - if'(|u|^2)(\bar{u}v + \bar{v}u)u$. From (6) for f and f' and the identity $\|e^{i\tau\Delta}u\|_{H^s} = \|u\|_{H^s}$, we get the estimates for all $\tau \in [0,1]$, all $u \in B_R^s$ and all $v \in H^s$

$$\|F_\tau(u)\|_{H^s} \le A^2 \chi_f(c^2\|u\|_{H^s}^2)\|u\|_{H^s}^3 \le M_0$$

and

$$\begin{aligned}\|F'_\tau(u)(v)\|_{H^s} &\le A^3\|f'(|e^{i\tau\Delta}u|^2)\|_{H^s}\|u\|_{H^s}^2\|v\|_{H^s} + A\|f(|e^{i\tau\Delta}u|^2)\|_{H^s}\|v\|_{H^s}\\ &\le M_1\|v\|_{H^s}\end{aligned}$$

for some constants M_0 and M_1. The second derivative of F takes the form

$$F''(u)(v,w) = -if''(|u|^2)u(\bar{u}v + \bar{v}u)(\bar{u}w + \bar{w}u) - 2if'(|u|^2)(\bar{u}vw + \bar{v}uw + \bar{w}uv),$$

so that by similar arguments, we obtain

$$\forall u \in B_R^s, \forall (v,w) \in H^s \times H^s, \quad \|F''_\tau(u)(v,w)\|_{H^s} \le M_2\|v\|_{H^s}\|w\|_{H^s}.$$

Note that the constants M_0, M_1 and M_2 depend on f and R. These estimates can be easily generalized to higher derivatives $F_\tau^{(l)}$, $l = 3, \dots, \lfloor \sigma/2 \rfloor$ for some constants M_l.

Derivatives with respect to τ. The first derivative of F_τ w.r.t. τ can be computed as follows:

$$\frac{dF_\tau(u)}{d\tau} = -ie^{-i\tau\Delta}\Delta F(e^{i\tau\Delta}u) + e^{-i\tau\Delta}F'(e^{i\tau\Delta}u)(ie^{i\tau\Delta}\Delta u) = -i\Delta F_\tau(u) + F'_\tau(u)(i\Delta u).$$

Note that here, $iF'_\tau(u)(\Delta u) - F'_\tau(u)(i\Delta u) \ne 0$, so that the function $u \mapsto \frac{dF_\tau(u)}{d\tau}$ is a function from H^σ to $H^{\sigma-2}$. The $H^{\sigma-2}$-norm of $F_\tau(u)$ for $u \in B_R^\sigma$ can be estimated as follows

$$\left\|\frac{dF_\tau(u)}{d\tau}\right\|_{H^{\sigma-2}} \le \|\Delta F_\tau(u)\|_{H^{\sigma-2}} + \|F'_\tau(u)(i\Delta u)\|_{H^{\sigma-2}} \le M_0 + M_1 R.$$

More generally, the j-th derivative w.r.t. τ reads[4]

$$\frac{d^jF_\tau(u)}{d\tau^j} = \sum_{l=0}^{j}\begin{pmatrix} j \\ l \end{pmatrix}(-i)^{j-l}\Delta^{j-l}F_\tau^{(l)}(u)(i\Delta u)^l$$

and is a function from H^σ into $H^{\sigma-2j}$, provided $\sigma \ge 2j$. Its $H^{\sigma-2j}$-norm can be bounded as follows

$$\begin{aligned}\left\|\frac{d^jF_\tau(u)}{d\tau^j}\right\|_{H^{\sigma-2j}} &\le \sum_{l=0}^{j}\begin{pmatrix} j \\ l \end{pmatrix}\|F_\tau^{(l)}(u)(i\Delta u)^l\|_{H^{\sigma-2l}}\\ &\le \|F_\tau(u)\|_{H^\sigma} + \sum_{l=1}^{j}\begin{pmatrix} j \\ l \end{pmatrix}\|F_\tau^{(l)}(u)(i\Delta u)^l\|_{H^{\sigma-2}}\\ &\le (1+R)^j \max_{l=0,\dots,j} M_l.\end{aligned}$$

[4]We sometimes use the notation $F^{(l)}(u)(w^j)$ as a shorthand for $F^{(l)}(u)\underbrace{(w,\dots,w)}_{j \text{ times}}$.

The bounds of local truncation errors will finally require to estimate

$$\frac{d}{d\tau}F'_\tau(u)(v) = -i\Delta F'_\tau(u)(v) + F'_\tau(u)(i\Delta v) + F''_\tau(u)(v, i\Delta u).$$

For u and v in B_R^σ, the following bound stems directly from previous inequalities

$$\left\|\frac{dF'_\tau(u)}{d\tau}\right\|_{H^{\sigma-2}} \leq 2M_1R + M_2R^2.$$

H^σ-H^s inequality for derivatives of F_τ. Proceeding as for F_τ, it is straightforward to show that derivatives of F_τ w.r.t. to u satisfy a Lipschitz estimate on B_R^σ: there exists a constant $\mathcal{L} > 0$ such that, for all $0 \leq 2j \leq \sigma$,

$$\forall w \in B_R^{\sigma-2}, \quad \forall (u,v) \in B_R^\sigma \times B_R^\sigma, \quad \|F^{(j)}(u)(w^j) - F^{(j)}(v)(w^j)\|_{H^{\sigma-2}} \leq \mathcal{L}\|u-v\|_{H^{\sigma-2}}.$$

It then follows that

$$\forall (u,v) \in B_R^\sigma \times B_R^\sigma, \quad \left\|\frac{d^jF_\tau(u)}{d\tau^j} - \frac{d^jF_\tau(v)}{d\tau^j}\right\|_{H^{\sigma-2j}} \leq L_2\|u-v\|_{H^\sigma}$$

for some constant L_2. We finally collect in next proposition the findings of this Section.

Proposition 2.1. *Let $m = \lfloor \sigma/2 \rfloor$. For $s \in \{\sigma, \sigma-2\}$, the function $(\tau, u) \mapsto F_\tau(u) = e^{-i\tau\Delta}F(e^{i\tau\Delta}u)$ is a well-defined function from $[0,1] \times H^s$ into H^s, is C^∞ w.r.t. u, and for all $0 \leq j \leq m$, it is j-times differentiable with values in $H^{\sigma-2j}$. Moreover, there exists a positive constant M such that for all $\tau \in [0,1]$, all $u \in B_R^s$ and all $(v_1, v_2) \in (H^s)^2$ one has*

$$\|F_\tau(u)\|_{H^s} \leq M, \ \|F'_\tau(u)(v_1)\|_{H^s} \leq M\|v_1\|_{H^s}, \ \|F''_\tau(u)(v_1,v_2)\|_{H^s} \leq M\|v_1\|_{H^s}\|v_2\|_{H^s}, \tag{7}$$

and for all $\tau \in [0,1]$ and all $(u,v) \in (B_R^\sigma)^2$, one has

$$\left\|\frac{d^jF_\tau(u)}{d\tau^j}\right\|_{H^{\sigma-2j}} \leq M \quad \text{and} \quad \left\|\frac{dF'_\tau(u)}{d\tau}\right\|_{H^{\sigma-2}} \leq M. \tag{8}$$

Finally, there exist positive constants L and L_2 such that for all $\tau \in [0,1]$

$$\forall 0 \leq s \leq \sigma - 2, \quad \forall (u,v) \in B_R^{\sigma-2} \times B_R^{\sigma-2}, \quad \|F_\tau(u) - F_\tau(v)\|_{H^s} \leq L\|u-v\|_{H^s}, \tag{9}$$

and for all $0 \leq j \leq m$, all $\tau \in [0,1]$

$$\forall (u,v) \in B_R^\sigma \times B_R^\sigma, \quad \left\|\frac{d^jF_\tau(u)}{d\tau^j} - \frac{d^jF_\tau(v)}{d\tau^j}\right\|_{H^{\sigma-2j}} \leq L_2\|u-v\|_{H^\sigma}. \tag{10}$$

The constants M, L and L_2 depend on f, R and σ.

3 Stability estimates

In order to estimate local errors in a neighborhood of the exact solution, we need to ensure that the numerical solutions lie in $B_R^{\sigma-2}$. Besides, stability estimates in various norms are required in the study of the error accumulation. These points are addressed in next lemma.

Lemma 3.1. *Consider the map $u \mapsto A_1^h(u) := \Phi^h(u) - e^{ih\Delta}u$ and let $h_0 = \frac{\log(4/3)}{L\varepsilon_0}$. If v and w are two functions of $B_{3R/4}^{\sigma-2}$, then for all $0 \leq h < h_0$, $\Phi^h(v)$ and $\Phi^h(w)$ are in $B_R^{\sigma-2}$ and the following statements hold for all $0 \leq s \leq \sigma - 2$*

$$\|\Phi^h(v) - \Phi^h(w)\|_{H^s} \leq e^{\varepsilon Lh}\|v - w\|_{H^s} \quad \textit{and} \quad \|A_1^h(v) - A_1^h(w)\|_{H^s} \leq \varepsilon h e^{\varepsilon Lh}\|v - w\|_{H^s}.$$

Proof. Denoting $v(t) = \varphi_V^t(v)$ and $w(t) = \varphi_V^t(w)$, we have

$$\dot{w}(t) = \varepsilon F(w(t)) \text{ and } \dot{v}(t) = \varepsilon F(v(t))$$

so that

$$\|v(t) - w(t)\|_{H^s} \leq \|v - w\|_{H^s} + \varepsilon \int_0^t \Big\|F(v(\tau)) - F(w(\tau))\Big\|_{H^s} d\tau.$$

As long as $w(t)$ and $v(t)$ remain in $B_R^{\sigma-2}$, we have, according to (9)

$$\Big\|F(v(\tau)) - F(w(\tau))\Big\|_{H^s} \;\leq\; L\|v(\tau) - w(\tau)\|_{H^s}$$

so that, by Gronwall lemma

$$\|v(t) - w(t)\|_{H^s} \leq e^{\varepsilon Lt}\|v - w\|_{H^s}.$$

In particular, taking $w = 0$, we have $\|v(h)\|_{H^{\sigma-2}} \leq \frac{3R}{4}e^{\varepsilon Lh} \leq R$. Now, we immediately get

$$\|\varphi_V^h(v) - v - \varphi_V^h(w) + w\|_{H^s} \leq \varepsilon\, L\, h\, e^{\varepsilon Lh}\|v - w\|_{H^s},$$

and both statements then follow from the fact that $e^{i\frac{h}{2}\Delta}$ is an isometry of H^s. $\square$

4 Local truncation errors

Denoting $t_n = nh \leq T/\varepsilon$ and $u_n^\varepsilon = u^\varepsilon(t_n)$, we define the local truncation errors as follows

$$\delta^n(\varepsilon, h) = \Phi^h(u_n^\varepsilon) - u_{n+1}^\varepsilon.$$

Comparing the Taylor expansions of $u^\varepsilon(t_n + h)$ and $\Phi^h(u_n^\varepsilon)$ and using Proposition 2.1, we can now derive bounds for $\delta^n(\varepsilon, h)$.

4.1 Expansion of the exact solution

The exact solution at time $t+h$ can be written with the Duhamel formula as

$$u^\varepsilon(t+h) = e^{ih\Delta}u^\varepsilon(t) + \varepsilon e^{ih\Delta}\int_0^h F_\tau(e^{-i\tau\Delta}u^\varepsilon(t+\tau))d\tau,$$

or equivalently for $v^\varepsilon(t) = e^{-it\Delta}u^\varepsilon(t)$

$$v^\varepsilon(t+h) = v^\varepsilon(t) + \varepsilon\int_0^h F_{t+\tau}(v^\varepsilon(t+\tau))d\tau. \tag{11}$$

We then use the following expansion of $F_\tau(\tilde{u}+\tilde{v})$

$$F_\tau(\tilde{u}+\tilde{v}) = F_\tau(\tilde{u}) + F'_\tau(\tilde{u})(\tilde{v}) + \int_0^1 (1-\xi)F''_\tau(\tilde{u}+\xi\tilde{v})(\tilde{v}^2)d\xi.$$

Inserting the expression of $v^\varepsilon(t+h)$ into the right-hand side of (11) and denoting $v = v^\varepsilon(t)$ for the sake of brevity, we obtain

$$\begin{aligned}
v^\varepsilon(t+h) &= v + \varepsilon\int_0^h F_{t+\tau}\Big(v + \varepsilon\int_0^\tau F_{t+\tau_1}(v^\varepsilon(t+\tau_1))d\tau_1\Big)d\tau \\
&= v + \varepsilon\int_0^h F_{t+\tau}(v)d\tau + \varepsilon^2\int_0^h\int_0^\tau F'_{t+\tau}(v)F_{t+\tau_1}(v^\varepsilon(t+\tau_1))d\tau_1 d\tau \\
&+ \varepsilon^3\int_0^h\int_0^1 (1-\xi)F''_{t+\tau}\Big((1-\xi)v + \xi v^\varepsilon(t+\tau)\Big)d\xi\Big(\int_0^\tau F_{t+\tau_1}(v^\varepsilon(t+\tau_1))d\tau_1\Big)^2 d\tau.
\end{aligned}$$

The second-order term in ε can be further expanded as

$$\begin{aligned}
&\int_0^h\int_0^\tau F'_{t+\tau}(v)F_{t+\tau_1}(v)d\tau_1 d\tau \\
&+\varepsilon\int_0^h\int_0^\tau F'_{t+\tau}(v)\int_0^1 F'_{t+\tau_1}\Big((1-\xi)v + \xi v^\varepsilon(t+\tau_1)\Big)d\xi\Big(\int_0^{\tau_1} F_{t+\tau_2}(v^\varepsilon(t+\tau_2))d\tau_2\Big)d\tau_1 d\tau.
\end{aligned}$$

Finally, we have with $u = u^\varepsilon(t)$

$$u^\varepsilon(t+h) = e^{ih\Delta}u + \varepsilon e^{ih\Delta}\int_0^h F_\tau(u)d\tau + \varepsilon^2 e^{ih\Delta}\int_0^h\int_0^\tau F'_\tau(u)F_{\tau_1}(u)d\tau_1 d\tau + \varepsilon^3 e^{ih\Delta}\mathcal{E}_3(u,\varepsilon,h),$$

with $\mathcal{E}_3(u,\varepsilon,h) = \mathcal{E}_{3,a}(u,\varepsilon,h) + \mathcal{E}_{3,b}(u,\varepsilon,h)$ where

$$\mathcal{E}_{3,a}(u,\varepsilon,h) = \int_0^h\int_0^1 (1-\xi)F''_\tau\Big((1-\xi)u + \xi e^{-i\tau\Delta}u^\varepsilon(t+\tau)\Big)d\xi\Big(\int_0^\tau F_{\tau_1}(e^{-i\tau_1\Delta}u^\varepsilon(t+\tau_1))d\tau_1\Big)^2 d\tau,$$

$$\mathcal{E}_{3,b}(u,\varepsilon,h) = \int_0^h\int_0^\tau F'_\tau(u)\int_0^1 F'_{\tau_1}\Big((1-\xi)u + \xi e^{-i\tau_1\Delta}u^\varepsilon(t+\tau_1)\Big)d\xi\Big(\int_0^{\tau_1} F_{\tau_2}(e^{-i\tau_2\Delta}u^\varepsilon(t+\tau_2))d\tau_2\Big)d\tau_1 d\tau.$$

Since $u^\varepsilon(t)$ remains in $B^\sigma_{R/2} \subset B^\sigma_R \subset B^{\sigma-2}_R$, we have by Proposition 2.1

$$\|\mathcal{E}_3(u^\varepsilon(t),\varepsilon,h)\|_{H^{\sigma-2}} \leq \frac{1}{3}M^3h^3. \tag{12}$$

4.2 Expansion of numerical solutions

Assume here that $u \in B^{\sigma-2}_{3R/4}$ and $0 < h \leq h_0$ where h_0 is defined in Lemma 3.1. Using that

$$\frac{d}{dh}\varphi_V^h(u) = \varepsilon F(\varphi_V^h(u))$$

we get immediately

$$\begin{aligned}\varphi_V^h(u) &= u + \varepsilon h F(u) + \frac{1}{2}(\varepsilon h)^2 F'(u)F(u) + \\ &\quad \varepsilon^3 \int_0^h \frac{(h-\tau)^2}{2}\Big(F''(\varphi_V^\tau(u))(F(\varphi_V^\tau(u)))^2 + F'(\varphi_V^\tau(u))F'(\varphi_V^\tau(u))F(\varphi_V^\tau(u))\Big)d\tau,\end{aligned}$$

which we may write as

$$\varphi_V^h(u) = u + \varepsilon h F(u) + \frac{1}{2}(\varepsilon h)^2 F'(u)F(u) + \varepsilon^3 \mathcal{E}_{3,V}(u,\varepsilon,h) \tag{13}$$

with

$$\mathcal{E}_{3,V}(u,\varepsilon,h) = \int_0^h \frac{(h-\tau)^2}{2}\Big(F''(\varphi_V^\tau(u))(F(\varphi_V^\tau(u)))^2 + F'(\varphi_V^\tau(u))F'(\varphi_V^\tau(u))F(\varphi_V^\tau(u))\Big)d\tau.$$

The Strang splitting solution can then be expanded as

$$\begin{aligned}\Phi^h(u) &= e^{ih/2\Delta}\Big(e^{ih/2\Delta}u + \varepsilon h F(e^{ih/2\Delta}u) + \frac{1}{2}(\varepsilon h)^2 F'(e^{ih/2\Delta}u)F(e^{ih/2\Delta}u) + \varepsilon^3\mathcal{E}_{3,V}(e^{ih/2\Delta}u,\varepsilon,h)\Big) \\ &= e^{ih\Delta}\Big(u + \varepsilon h F_{h/2}(u) + \frac{1}{2}(\varepsilon h)^2 F'_{h/2}(u)F_{h/2}(u)\Big) + \varepsilon^3 e^{ih/2\Delta}\mathcal{E}_{3,V}(e^{ih/2\Delta}u,\varepsilon,h). \qquad (14)\end{aligned}$$

Note that owing to Lemma 3.1, $\varphi_V^\tau(u)$ remains in $B_R^{\sigma-2}$ for $0 \leq \tau \leq h$ so that, by using Proposition 2.1,

$$\forall u \in B^{\sigma-2}_{3R/4}, \quad \forall 0 < h \leq h_0, \quad \|\mathcal{E}_{3,V}(u,\varepsilon,h)\|_{H^{\sigma-2}} \leq \frac{M^3}{3}h^3. \tag{15}$$

4.3 Bounds of local truncation errors

The local truncation error finally reads

$$\begin{aligned}\delta^n(\varepsilon,h) &= \varepsilon e^{ih\Delta}\Big(hF_{h/2}(u_n^\varepsilon) - \int_0^h F_\tau(u_n^\varepsilon)d\tau\Big) \\ &+ \varepsilon^2 e^{ih\Delta}\Big(\frac{1}{2}h^2 F'_{h/2}(u_n^\varepsilon)F_{h/2}(u_n^\varepsilon) - \int_0^h\int_0^\tau F'_\tau(u_n^\varepsilon)F_{\tau_1}(u_n^\varepsilon)d\tau_1 d\tau\Big) \\ &+ \varepsilon^3\Big(e^{ih/2\Delta}\mathcal{E}_{3,V}(e^{ih/2\Delta}u_n^\varepsilon,\varepsilon,h) - e^{ih\Delta}\mathcal{E}_3(u_n^\varepsilon,\varepsilon,h)\Big) \qquad (16)\end{aligned}$$

and we have to estimate each term individually.

First-order term in ε. We use the second-order Peano kernel κ_2 of the midpoint rule

$$hF_{h/2}(u) - \int_0^h F_\tau(u)d\tau = h^3\int_0^1 \kappa_2(\tau)\,\frac{d^2}{d\theta^2}F_\theta(u)\Big|_{\theta=\tau h}\,d\tau$$

where κ_2 is a scalar continuous function, so that, owing to (8) (note that $\sigma \geq 4$)

$$\left\| hF_{h/2}(u) - \int_0^h F_\tau(u)d\tau \right\|_{H^{\sigma-4}} \leq M\Big(\int_0^1 |\kappa_2(\tau)|d\tau\Big)\, h^3. \tag{17}$$

Second-order term in ε. We here use that

$$F_{\tau_1}(u) = F_{h/2}(u) + \int_{h/2}^{\tau_1} \frac{d}{d\theta} F_\theta(u)d\theta \quad \text{ and } \quad F'_\tau(u) = F'_{h/2}(u) + \int_{h/2}^{\tau} \frac{d}{d\theta} F'_\theta(u)d\theta$$

and insert these expressions into the double integral term to get

$$\int_0^h \int_0^\tau F'_\tau(u)F_{\tau_1}(u)d\tau_1 d\tau = \frac{h^2}{2} F'_{h/2}(u)F_{h/2}(u) + r_1$$

where

$$\begin{aligned} r_1 &= \int_0^h \int_0^\tau F'_{h/2}(u) \int_{h/2}^{\tau_1} \frac{d}{d\theta} F_\theta(u)d\theta d\tau_1 d\tau + \int_0^h \int_0^\tau \int_{h/2}^{\tau} \frac{d}{d\theta} F'_\theta(u)d\theta F_{h/2}(u)d\tau_1 d\tau \\ &+ \int_0^h \int_0^\tau \int_{h/2}^{\tau} \frac{d}{d\theta} F_\theta(u)d\theta \int_{h/2}^{\tau_1} \frac{d}{d\theta} F_\theta(u)d\theta d\tau_1 d\tau \end{aligned}$$

so that

$$\|r_1\|_{H^{\sigma-2}} \leq \frac{1}{4} M^2 h^3 + \frac{1}{32} M^2 h^4 \leq \frac{1}{4} M^2 h^3 (1 + h_0/8).$$

Third-order term in ε. Collecting previous estimates of this section and estimates (15) and (12), we obtain

$$\exists C > 0, \quad \forall 0 < h \leq h_0, \quad \|\delta^n(\varepsilon, h)\|_{H^{\sigma-4}} \leq C\varepsilon h^3. \tag{18}$$

We end up this section by noticing that the following bound also holds (using the first-order Peano kernel)

$$\exists \tilde{C} > 0, \quad \forall 0 < h \leq h_0, \quad \|\delta^n(\varepsilon, h)\|_{H^{\sigma-2}} \leq \tilde{C}\varepsilon h^2, \tag{19}$$

and for later use in our refined analysis of errors, we observe that

$$\delta^n(\varepsilon, h) \quad = \quad \varepsilon e^{ih\Delta} \Lambda_h(u_n^\varepsilon) + \varepsilon^2 R_h(u_n^\varepsilon) \tag{20}$$

with

$$\Lambda_h(u_n^\varepsilon) = hF_{h/2}(u_n^\varepsilon) - \int_0^h F_\tau(u_n^\varepsilon)d\tau, \tag{21}$$

and

$$\forall 0 < h \leq h_0, \quad \|\Lambda_h(u_n^\varepsilon)\|_{H^{\sigma-4}} \leq Ch^3 \quad \text{ and } \quad \|R_h(u_n^\varepsilon)\|_{H^{\sigma-2}} \leq Ch^3.$$

5 Global error estimates

The basic ingredient of the proofs of this section is the following telescopic identity

$$(\Phi^h)^n(u_0) - u_n^\varepsilon = \sum_{l=1}^{n} \Big((\Phi^h)^{n-l} \circ \Phi^h(u_{l-1}^\varepsilon) - (\Phi^h)^{n-l}(u_l^\varepsilon) \Big).$$

We proceed in two steps: in the first one, we obtain ε-independent error estimates on the whole interval $[0, T/\varepsilon]$ (in agreement with [9]) and in the second one we use these estimates in a more refined analysis, on one period and then on the whole interval.

5.1 $H^{\sigma-4}$-convergence

The following theorem is the formulation in our context of a result from [9].

Theorem 5.1. *Let $h_1 = \min(h_0, \frac{RL}{4\tilde{C}(e^{LT}-1)})$ where h_0 is defined in Lemma 3.1. The numerical solution given by the Strang splitting scheme for equation (2) with $0 \le h \le h_1$ satisfies a second-order error bound in $H^{\sigma-4}$*

$$\exists C > 0, \quad \|(\Phi^h)^n(u_0) - u^\varepsilon(t_n)\|_{H^{\sigma-4}} \le C \frac{e^{LT}-1}{L} h^2 \text{ for } t_n = nh \le T/\varepsilon. \tag{22}$$

The constants L and C depend on σ, R and f, but are independent of ε.

Proof. As long as the numerical approximations $(\Phi^h)^j(u^\varepsilon(t_k))$ remain in $B^{\sigma-2}_{3R/4}$ for $1 \le j+k \le n$, stability estimates of Lemma 3.1 hold and the telescopic identity leads to

$$\|(\Phi^h)^n(u_0) - u^\varepsilon(t_n)\|_{H^{\sigma-2}} \le \sum_{l=1}^{n} e^{\varepsilon L h(n-l)} \|\delta^{l-1}(\varepsilon, h)\|_{H^{\sigma-2}}$$

where $\|\delta^{l-1}(\varepsilon, h)\|_{H^{\sigma-2}}$ can be bounded by $\varepsilon\tilde{C}h^2$ (see (19)). Hence, since $nh \le T/\varepsilon$, we have straightforwardly

$$\|(\Phi^h)^n(u_0) - u^\varepsilon(t_n)\|_{H^{\sigma-2}} \le \tilde{C}\, \frac{e^{n\varepsilon L h} - 1}{L}\, h \le \tilde{C}\, \frac{e^{LT}-1}{L}\, h.$$

The boundedness in $H^{\sigma-2}$ required by the stability lemma is ensured by induction by the previous error bound provided $\tilde{C}\frac{e^{LT}-1}{L}\, h \le \frac{R}{4}$. Now, Lemma 3.1 applies and gives stability in $H^{\sigma-4}$, so that owing to estimate (18), we get the second-order convergence in $H^{\sigma-4}$. $\square$

5.2 $H^{\sigma-2m}$-convergence on one period

We now examine more closely the errors after one period. Let us first notice that, according to Theorem 5.1, $(\Phi^h)^l \in B^{\sigma-2}_{3R/4}$ for all $0 \le l \le n$ with $nh \le T/\varepsilon$ and hence $(\Phi^h)^l \in B^s_{3R/4}$ for all $0 \le s \le \sigma - 2$.

Lemma 5.2. *The following estimate holds*

$$\forall 0 \le t \le 1, \quad \|u^\varepsilon(t) - e^{it\Delta}u_0\|_{H^\sigma} \le \varepsilon M. \tag{23}$$

Proof. The terms $u^\varepsilon(t)$ and $e^{it\Delta}u_0$ are the exact solutions of the differential equations

$$\dot{u}^\varepsilon = i\Delta u^\varepsilon + \varepsilon F(u^\varepsilon), \quad u^\varepsilon(0) = u_0 \quad \text{and} \quad \dot{v}^\varepsilon = i\Delta v^\varepsilon, \quad v^\varepsilon(0) = u_0.$$

By Duhamel formula and Proposition 2.1, we have immediately

$$\|u^\varepsilon(t) - v^\varepsilon(t)\|_{H^\sigma} = \varepsilon\Big\| \int_0^t e^{i(t-\tau)\Delta} F(u^\varepsilon(\tau))d\tau \Big\|_{H^\sigma} \le \varepsilon t M \le \varepsilon M.$$

□

Lemma 5.3. *Given u and v, assume that both sequences $\big((\Phi^h)^l(u)\big)_l$ and $\big((\Phi^h)^l(v)\big)_l$ lie in $B^{\sigma-2}_{3R/4}$ for all $0 \le l \le n$ with $nh \le 1$ and $0 < h \le h_1$ where h_1 is defined in Theorem 5.1. Then the map $u \mapsto A^h_l(u) := (\Phi^h)^l(u) - e^{ilh\Delta}u$ satisfies a Lipschitz condition for all $0 \le s \le \sigma - 2$ of the form*

$$\|A^h_l(u) - A^h_l(v)\|_{H^s} \le \varepsilon L e^{\varepsilon L}\|u - v\|_{H^s}.$$

Proof. A telescopic identity gives

$$(\Phi^h)^l(u) - e^{ilh\Delta}u \;=\; \sum_{k=1}^{l} e^{ih(l-k)\Delta}\left(\Phi^h - e^{ih\Delta}\right) \circ \left((\Phi^h)^{(k-1)}(u)\right).$$

Hence,

$$\|A^h_l(u) - A^h_l(v)\|_{H^s} \le \sum_{k=1}^{l} \left\| A^h_1((\Phi^h)^{(k-1)}(u) - A^h_1((\Phi^h)^{(k-1)}(v)) \right\|_{H^s}$$

and according to Lemma 3.1 , we have

$$\begin{aligned}
\|A^l_h(u) - A^l_h(v)\|_{H^s} &\le \sum_{k=1}^{l} \varepsilon L h e^{L\varepsilon h} \left\| (\Phi^h)^{(k-1)}(u)) - (\Phi^h)^{(k-1)}(v) \right\|_{H^s} \\
&\le \sum_{k=1}^{l} \varepsilon L h e^{kL\varepsilon h}\|u - v\|_{H^s} \le \varepsilon L e^{\varepsilon L}\|u - v\|_{H^s}.
\end{aligned}$$

□

Theorem 5.4. *Let $m = \lfloor \sigma/2 \rfloor$. The numerical solution given by the Strang splitting scheme for equation (2) with step size $0 < h \le h_1$ where h_1 is defined in Theorem 5.1, has a second-order error bound in $H^{\sigma-2m}$ of the form*

$$\exists \hat{C} > 0, \quad \|(\Phi^h)^n(u_0) - u^\varepsilon(1)\|_{H^{\sigma-2m}} \le \hat{C}(\varepsilon^2 h^2 + \varepsilon h^m) \text{ for } nh = 1. \tag{24}$$

The constant $\hat{C}$ depends on σ, R and f, but is independent of ε.

Proof. The proof proceeds in two steps.

Identification of the ε-error term. Replacing $(\Phi^h)^{(n-l)}$ by $e^{ih(n-l)\Delta}$ in the telescopic identity we get

$$(\Phi^h)^n(u_0) - u^\varepsilon(1) = \sum_{l=1}^{n} e^{ih(n-l)\Delta}\delta^{l-1}(\varepsilon, h) + r$$

where

$$r = \sum_{l=1}^{n} \left(A_{n-l}^h \left(\Phi^h(u_{l-1}^\varepsilon) \right) - A_{n-l}^h \left(u_l^\varepsilon \right) \right).$$

According to previous lemma and using (18), we can estimate r as follows:

$$\|r\|_{H^{\sigma-4}} \le \varepsilon L e^{\varepsilon L} \sum_{l=1}^{n} \|\delta^{l-1}(\varepsilon, h)\|_{H^{\sigma-4}} \le \varepsilon^2 L e^{\varepsilon L} C h^2.$$

In addition, according to (20), we have

$$\sum_{l=1}^{n} e^{ih(n-l)\Delta}\delta^{l-1}(\varepsilon, h) = \varepsilon \sum_{l=1}^{n} e^{ih(n-l+1)\Delta}\Lambda_h(u_{l-1}^\varepsilon) + \tilde{r}$$

where

$$\tilde{r} = \varepsilon^2 \sum_{l=1}^{n} e^{ih(n-l)\Delta} R_h(u_{l-1}^\varepsilon)$$

can again be bounded by $C\varepsilon^2 h^2$ in $H^{\sigma-2}$-norm. Finally, taking into account that (see Lemma 5.2)

$$\|u_{l-1}^\varepsilon - e^{i(l-1)h\Delta}u_0\|_{H^\sigma} \le M\varepsilon$$

and that Λ_h is Lipschitz continuous with a Lipschitz constant of the form $h^3 \tilde{L}_2$ (see (21-17) and Proposition 2.1) we have

$$\left\| (\Phi^h)^n(u_0) - u^\varepsilon(1) - \varepsilon \sum_{l=1}^{n} e^{i(n-l+1)h\Delta}\Lambda_h(e^{i(l-1)h\Delta}u_0) \right\|_{H^{\sigma-4}} \le \text{ Const } \varepsilon^2 h^2.$$

Estimate of the ε-error term. From previous analysis, the main error is concentrated in the term

$$\sum_{l=1}^{n} e^{i(n-l+1)h\Delta}\Lambda_h(e^{i(l-1)h\Delta}u_0)$$

which is of order εh^2. For a finer estimation, we now proceed as follows:

$$\begin{aligned}
\sum_{l=1}^{n} e^{i(n-l+1)h\Delta}\Lambda_h(e^{i(l-1)h\Delta}u_0) &= \sum_{l=0}^{n-1} hF_{(lh+h/2)}(u_0) - \int_0^1 F_\tau(u_0)d\tau \\
&= \sum_{l=0}^{n-1} hF_{(lh+h/2)}(u_0) - \int_0^1 F_{(\tau+h/2)}(u_0)d\tau \\
&= e^{-ih/2\Delta}E_{Rie}(e^{ih/2\Delta}u_0, h)
\end{aligned}$$

where E_{Rie} denotes the error in the approximation by Riemann sums according to Lemma 7.1 and where we have right away taken into account that $e^{inh\Delta}$ is the identity operator and that $\tau \mapsto F_\tau(u_0)$ is 1-periodic. From Lemma 7.1, we thus have

$$\Big\| \sum_{l=1}^{n} e^{i(n-l+1)h\Delta}\Lambda_h(e^{i(l-1)h\Delta}u_0)\Big\|_{H^{\sigma-2m}} \leq C_m^{Rie} \, \Big\| \frac{d^j}{d\tau^j}F_\tau \Big\|_{H^{\sigma-2m}} \, h^m$$

with $C_m^{Rie} = 2\frac{\zeta(m)}{(2\pi)^m}$. Together with estimate (8) of Proposition 2.1, this completes the proof. □

5.3 $H^{\sigma-2m}$-convergence on the whole interval

It is now straightforward to get error estimates on the whole interval by considering $\hat{\Phi}(u) = (\Phi^h)^n(u)$ as an integrator with step size 1, for which the "local error" is of size $\hat{C}\varepsilon(\varepsilon h^2 + h^m)$ and which is obviously Lipschitz continuous. A telescopic identity with $\hat{\Phi}$ iterated $N = \lfloor T/\varepsilon \rfloor$ times then leads to an error of size $\hat{C}T(\varepsilon h^2 + h^m)$. Finally, the solution at intermediate points (i.e. within an interval $[n, n+1]$ or $[N, T/\varepsilon]$) can then be obtained by composing $\hat{\Phi}$ and Φ^h.

Theorem 5.5. *Let $m = \lfloor \sigma/2) \rfloor$. The numerical solution given by the Strang splitting scheme for equation (2) with step size $h > 0$ such that $1/h \in \mathbb{N}$ has a second-order error bound in $H^{\sigma-2m}$ of the form*

$$\exists \hat{C} > 0, \quad \|(\Phi^h)^n(u_0) - u^\varepsilon(1)\|_{H^{\sigma-2m}} \leq \hat{C}T(\varepsilon h^2 + h^m) \text{ for } nh \leq T/\varepsilon. \tag{25}$$

The constant $\hat{C}$ depends on σ, R and f, but is independent of ε.

6 Extension to general splitting methods

Assume now that

$$\Phi^h(u) = e^{ih\alpha_1\Delta} \circ \varphi_V^{\beta_1 h} \circ \cdots \circ e^{ih\alpha_r\Delta} \circ \varphi_V^{\beta_r h},$$

is a general splitting method of order p. More precisely, suppose that

$$\delta^n(\varepsilon, h) = \Phi^h(u_n^\varepsilon) - u_{n+1}^\varepsilon$$

can be written as in (20)

$$\delta^n(\varepsilon, h) = \varepsilon e^{ih\Delta}\Lambda_h(u_n^\varepsilon) + \varepsilon^2 R_h(u_n^\varepsilon)$$

with

$$\|\Lambda_h(u_n^\varepsilon)\|_{H^{\sigma-2p}} \leq Ch^{p+1} \quad \text{and} \quad \|R_h(u_n^\varepsilon)\|_{H^{\sigma-2p+2}} \leq Ch^{p+1}.$$

Then, it is possible to identify through an ε-expansion the term Λ_h. One has indeed

$$\Lambda_h(u) = \sum_{j=1}^{r} \beta_j h e^{ih(\gamma_j-1)\Delta} F\left(e^{ih(1-\gamma_j)\Delta}u\right) - \int_0^h F_\tau(u)d\tau,$$

where $\gamma_j = \sum_{k=1}^{j} \alpha_k$ and $\gamma_r = 1$ by a first-order condition on the splitting method. By consistency again, $\sum_{j=1}^{s} \beta_j = 1$, and one has

$$\Lambda_h(u) = \sum_{j=1}^{r} \beta_j \left(hF_{(\gamma_j-1)h}(u) - \int_0^h F_\tau(u)\right)$$

so that

$$\begin{aligned}
\sum_{l=1}^{n} e^{i(n-l+1)h\Delta}\Lambda_h(e^{i(l-1)h\Delta}u_0) &= \sum_{j=1}^{r} \beta_j \left(\sum_{l=0}^{n-1} hF_{(lh+\gamma_j h)}(u_0) - \int_0^1 F_\tau(u_0)d\tau\right) \\
&= \sum_{j=1}^{r} \beta_j \left(e^{-i\gamma_j h\Delta} E_{Rie}(e^{i\gamma_j h\Delta}u_0, h)\right)
\end{aligned}$$

Higher-order conditions on the splitting method then lead to the following expression

$$\Lambda_h(u) = h^{p+1} \int_0^1 \kappa_p(\tau) \left.\frac{d^p F_\theta}{d\theta^p}\right|_{\theta=\tau h} (u)d\tau$$

so that Λ_h is Lipschitz continuous with a Lipschitz constant of the $\tilde{L}_2 h^{p+1}$. The proof derived for Strang splitting can then be readily adapted leading to the estimate

$$\exists \hat{C} > 0, \quad \|(\Phi^h)^n(u_0) - u^\varepsilon(1)\|_{H^{\sigma-2m}} \leq \hat{C}T(\varepsilon h^p + h^m) \text{ for } nh \leq T/\varepsilon,$$

under the additional assumption that $\sigma \geq 2p$.

7 Numerical experiments

In this section, we present numerical results of Strang and another fourth-order splitting methods when applied to NLS equation with initial conditions as follows:

$$i\partial_t u^\varepsilon = -\partial_{xx}u^\varepsilon + \varepsilon\, 2\cos(2x)|u^\varepsilon|^2 u^\varepsilon, \qquad 0 \leq t \leq T/\varepsilon, \quad x \in \mathbb{T}_{2\pi} \tag{26}$$

$$u^\varepsilon(0, x) = u_0(x) = \cos(x) + \sin(x), \qquad x \in \mathbb{T}_{2\pi}. \tag{27}$$

Given that the wave function is enforced to be periodic in space for all positive times, it is in practice discretized by Fourier series as $u^\varepsilon(t,x) = \sum_{-N_x/2+1}^{N_x/2} \widehat{u}_k^\varepsilon(t) e^{ikx}$, with $N_x = 256$, such that errors originating from space discretization can be considered as negligible. The final time is taken here as $T = \pi/4$. The reference solution u^{ref} used to assess numerical accuracy is obtained by a fourth-order time splitting method [11] with a very small time-step $\Delta t = 2\pi/10^4$. The time-step for the Strang splitting is always taken under the form $2\pi/N$, where $N \in \mathbb{N}^*$ (note that in contrast with the assumption of the rest of the paper, the time-period is here 2π and not 1. This is obviously of no consequence, since a simple rescaling of time would lead to a period 1). Numerical errors are computed in discrete H^s-norm of the wave function

$$error = \|u^{ref} - u^{num}\|_{H^s} := \left(\sum_{k=-N_x/2+1}^{N_x/2} (1+|k|^2)^s |(\widehat{u^{ref}})_k - (\widehat{u^{num}})_k|^2 \right)^{1/2},$$

where u^{num} is the numerical solution.

Strang splitting scheme

Figure 1 presents the errors as a function of step size h in L^2-norm (left) and H^1-norm (right) for $\varepsilon = 2^{-6}, 2^{-7}, \ldots, 2^{-12}$ (from top to bottom). A line of slope 2 (black circle line) is drawn as reference. One can clearly observe that for fixed ε, the error scales like h^2. On the other hand, for fixed h, the error scales like ε. The contribution to the error of the term εh^2 is perfectly apparent in Table 1.

Fourth order splitting scheme

Figure 2 now presents the errors as a function of step size h in L^2 norm (left) and H^1 norm (right) for $\varepsilon = 2^{-3}, 2^{-4}, \ldots, 2^{-9}$ (from top to bottom) for the fourth-order splitting method of [11]. Again, a line of slope 4 (black circle line) is given as a reference. Essentially the same conclusions as for Strang can be drawn, confirming the estimates of Section 6. The contribution to the error of the term εh^4 is made perfectly clear in Table 2.

Appendix.

An elementary result on Riemann sums for periodic functions

Lemma 7.1. *For the function $(\tau, u) \in [0,1] \times H^\sigma \mapsto F_\tau(u) \in H^\sigma$ and given $h > 0$ and $n \geq 1$ such that $nh = 1$, consider the error*

$$E_{Rie}(u,h) := \frac{1}{n} \sum_{l=0}^{n-1} F_{lh}(u) - \int_0^1 F_\tau(u) d\tau \tag{28}$$

in the approximation of the integral by its Riemann sum. Then the following statement hold for $m = \lfloor \sigma/2 \rfloor$

$$\|E_{Rie}(u,h)\|_{H^{\sigma-2m}} \leq \left(2\frac{\zeta(m)}{(2\pi)^m} \right) \sup_{\tau \in [0,1]} \left\| \frac{d^m}{d\tau^m} F_\tau(u) \right\|_{H^{\sigma-2m}} h^m. \tag{29}$$

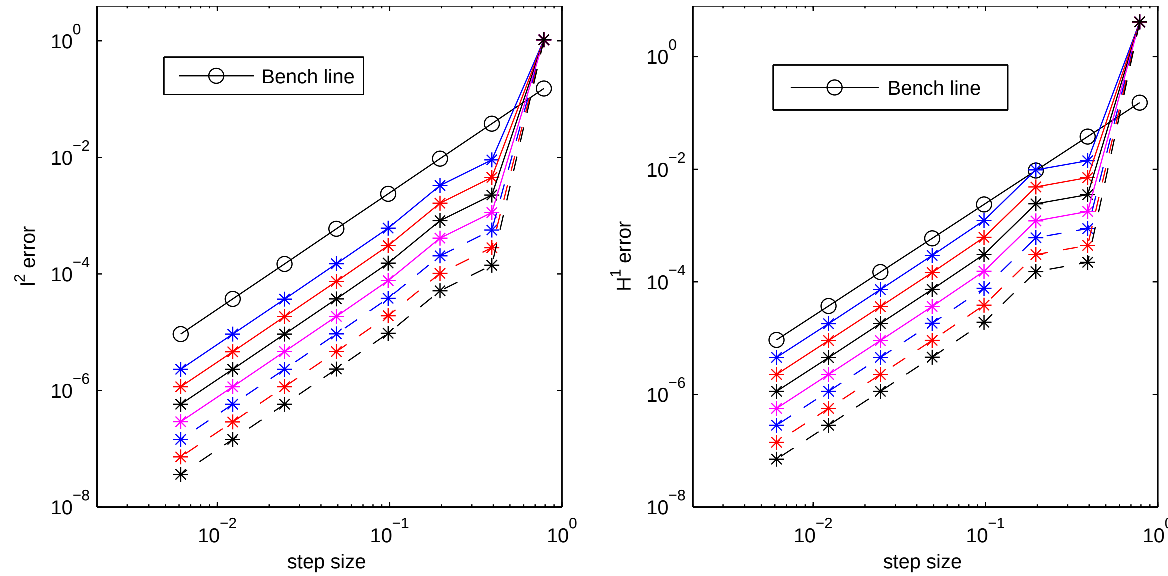

Figure 1: Numerical errors for Strang splitting at time T/ε in L^2-norm and H^1-norm for $\varepsilon = 2^{-6}, 2^{-7}, \ldots, 2^{-12}$ (from top to bottom). Slope 2 in indicated as the black circle line.

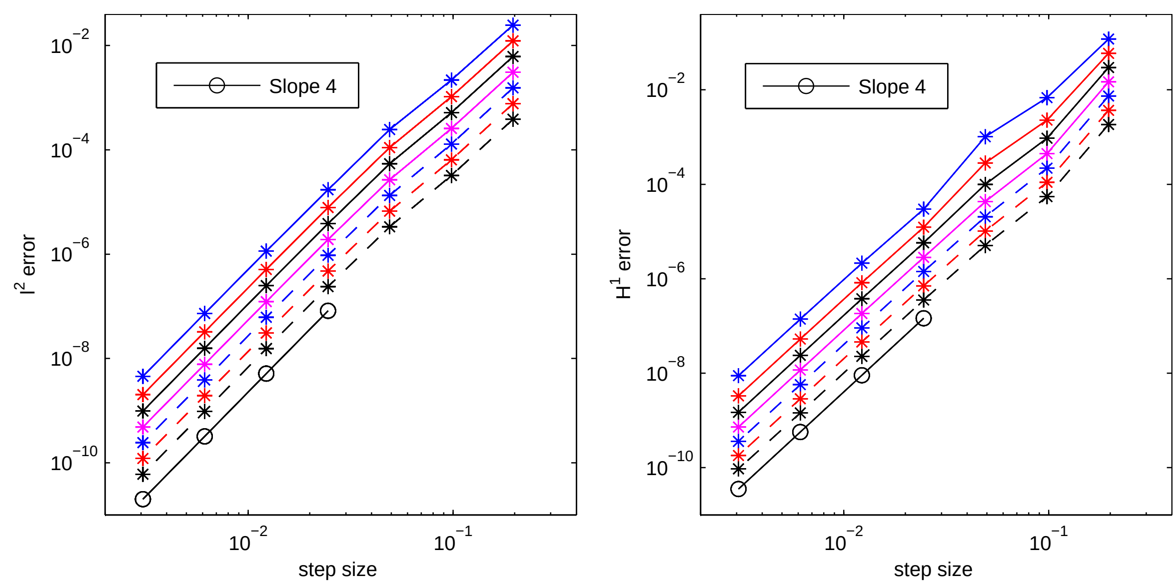

Figure 2: Numerical errors for Yoshida splitting at time T/ε in L^2-norm and H^1-norm for $\varepsilon = 2^{-6}, 2^{-7}, \ldots, 2^{-12}$ (from top to bottom). Slope 4 in indicated as the black circle line.

Table 1: Errors of Strang splitting for NLS on $\mathbb{T}_{2\pi}$ in L^2 norm (upper) and H^1 norm.

	$h = 2\pi/2^4$	$h = 2\pi/2^5$	$h = 2\pi/2^6$	$h = 2\pi/2^7$	$h = 2\pi/2^8$
$\varepsilon = 2^{-6}$	9.037E-03	3.279E-03	6.121E-04	1.489E-04	3.700E-05
$\varepsilon = 2^{-7}$	4.519E-03	1.639E-03	3.060E-04	7.444E-05	1.850E-05
$\varepsilon = 2^{-8}$	2.259E-03	8.196E-04	1.530E-04	3.722E-05	9.249E-06
$\varepsilon = 2^{-9}$	1.130E-03	4.098E-04	7.648E-05	1.861E-05	4.624E-06
$\varepsilon = 2^{-10}$	5.648E-04	2.049E-04	3.824E-05	9.304E-06	2.312E-06
$\varepsilon = 2^{-6}$	1.415E-02	9.691E-03	1.230E-03	2.930E-04	7.244E-05
$\varepsilon = 2^{-7}$	7.077E-03	4.845E-03	6.142E-04	1.464E-04	3.621E-05
$\varepsilon = 2^{-8}$	3.538E-03	2.423E-03	3.071E-04	7.319E-05	1.810E-05
$\varepsilon = 2^{-9}$	1.769E-03	1.211E-03	1.535E-04	3.660E-05	9.052E-06
$\varepsilon = 2^{-10}$	8.846E-04	6.056E-04	7.676E-05	1.830E-05	4.526E-06

Table 2: Errors of Yoshida splitting for NLS on $\mathbb{T}_{2\pi}$ in L^2 norm (upper) and H^1 norm.

	$h = 2\pi/2^4$	$h = 2\pi/2^5$	$h = 2\pi/2^6$	$h = 2\pi/2^7$	$h = 2\pi/2^8$	$h = 2\pi/2^9$	$h = 2\pi/2^{10}$
$\varepsilon = 2^{-3}$	4.777E-02	2.463E-02	2.193E-03	2.452E-04	1.719E-05	1.141E-06	7.255E-08
$\varepsilon = 2^{-4}$	2.375E-02	1.231E-02	1.048E-03	1.108E-04	7.854E-06	5.112E-07	3.230E-08
$\varepsilon = 2^{-5}$	1.186E-02	6.153E-03	5.180E-04	5.390E-05	3.834E-06	2.481E-07	1.564E-08
$\varepsilon = 2^{-6}$	5.926E-03	3.076E-03	2.582E-04	2.676E-05	1.905E-06	1.231E-07	7.758E-09
$\varepsilon = 2^{-7}$	2.963E-03	1.538E-03	1.290E-04	1.336E-05	9.511E-07	6.143E-08	3.871E-09
$\varepsilon = 2^{-8}$	1.481E-03	7.691E-04	6.449E-05	6.676E-06	4.754E-07	3.070E-08	1.934E-09
$\varepsilon = 2^{-9}$	7.407E-04	3.846E-04	3.224E-05	3.338E-06	2.377E-07	1.535E-08	9.670E-10
$\varepsilon = 2^{-3}$	2.14E-01	1.19E-01	6.80E-03	1.02E-03	2.98E-05	2.13E-06	1.40E-07
$\varepsilon = 2^{-4}$	1.06E-01	5.92E-02	2.28E-03	2.83E-04	1.23E-05	8.23E-07	5.27E-08
$\varepsilon = 2^{-5}$	5.30E-02	2.96E-02	9.49E-04	9.92E-05	5.79E-06	3.77E-07	2.39E-08
$\varepsilon = 2^{-6}$	2.65E-02	1.48E-02	4.47E-04	4.29E-05	2.85E-06	1.84E-07	1.16E-08
$\varepsilon = 2^{-7}$	1.32E-02	7.38E-03	2.20E-04	2.05E-05	1.42E-06	9.15E-08	5.76E-09
$\varepsilon = 2^{-8}$	6.62E-03	3.69E-03	1.10E-04	1.02E-05	7.09E-07	4.57E-08	2.87E-09
$\varepsilon = 2^{-9}$	3.31E-03	1.85E-03	5.48E-05	5.06E-06	3.55E-07	2.28E-08	1.44E-09

Proof. Let

$$(\tau, u) \in [0,1] \times H^\sigma \mapsto \sum_{k\in\mathbb{Z}} e^{i2\pi k\tau} \hat{F}_k(u)$$

be the Fourier expansion of F_τ. By definition of Fourier coefficients, $\int_0^1 F_\tau(u)d\theta = \hat{F}_0(u)$. As for the numerical counterpart of this integral, one has

$$\frac{1}{n}\sum_{l=0}^{n-1} F_{lh}(u) \quad = \quad \frac{1}{n}\sum_{l=0}^{n-1}\sum_{k\in\mathbb{Z}} e^{i2\pi lkh}\hat{F}_k(u) = \sum_{k\in\mathbb{Z}}\frac{1}{n}\sum_{l=0}^{n-1} e^{i2\pi klh}\hat{F}_k(u) = \sum_{q\in\mathbb{Z}}\hat{F}_{nq}(u)$$

Hence, we have

$$\|E_{Rie}(u,h)\|_{H^{\sigma-2m}} \leq \sum_{q\in\mathbb{Z}^*}\|\hat{F}_{nq}(u)\|_{H^{\sigma-2m}}.$$

Besides, owing to the regularity of F_τ

$$\forall k\in\mathbb{Z}^*, \quad \|\hat{F}_k(u)\|_{H^{\sigma-2m}} \leq \sup_{\tau\in[0,1]}\frac{\|\frac{d^m}{d\tau^m}F_\tau(u)\|_{H^{\sigma-2m}}}{(2\pi|k|)^m}$$

and it follows that

$$\|E_{Rie}(u,h)\|_{H^{\sigma-2m}} \leq 2\sup_{\tau\in[0,1]}\left\|\frac{d^m}{d\tau^m}F_\tau(u)\right\|_{H^{\sigma-2m}}\sum_{q\in\mathbb{N}^*}(2\pi nq)^{-m} = 2\sup_{\tau\in[0,1]}\left\|\frac{d^m}{d\tau^m}F_\tau(u)\right\|_{H^{\sigma-2m}}\frac{\zeta(m)}{(2\pi n)^m}$$

□

Two lemmas on products and functions in Sobolev spaces

Let us first recall the fractional Leibniz rule:

Lemma 7.2. *For all $s>0$ and $1<p<+\infty$, we have*

$$\|uv\|_{W^{s,p}(\mathbb{T}^d)} \leq \alpha\|u\|_{L^{p_1}(\mathbb{T}^d)}\|v\|_{W^{s,q_1}(\mathbb{T}^d)} + \alpha\|u\|_{W^{s,q_2}(\mathbb{T}^d)}\|v\|_{L^{p_2}(\mathbb{T}^d)} \tag{30}$$

provided

$$\frac{1}{p}=\frac{1}{p_1}+\frac{1}{q_1}=\frac{1}{p_2}+\frac{1}{q_2}, \quad q_1,\, q_2\in(1,+\infty), \quad p_1,\, p_2\in(1,+\infty].$$

Proof. This inequality can be deduced from the standard fractional Leibniz rule stated in Sobolev spaces on $\mathbb{R}^d$. □

Now we are in a position to prove the following lemma, where all functional spaces are implicitly defined on the torus $\mathbb{T}^d$.

Lemma 7.3. *Let $s\geq 0$ and $\sigma>\frac{d}{2}$, with $s\leq\sigma$. Then*

(i) for all $u\in H^s$ and $v\in H^\sigma$, we have

$$\|uv\|_{H^s} \leq \kappa\|u\|_{H^s}\,\|v\|_{H^\sigma}\,, \tag{31}$$

(ii) for all $u, v \in H^\sigma$ with $\|u\|_{H^\sigma} \le R$, $\|v\|_{H^\sigma} \le R$ and for all smooth function f from $\mathbb{R}$ to $\mathbb{R}$, we have

$$\|f(u) - f(v)\|_{H^s} \le \alpha(f, R)\, \|u - v\|_{H^s}\,. \tag{32}$$

Proof. Recall that, by $\sigma > \frac{d}{2}$, we have the Sobolev embedding $H^\sigma \hookrightarrow L^\infty$ with $\|v\|_{L^\infty} \le C_\sigma \|v\|_{H^\sigma}$. Hence, in the case $s = 0$, the result is obvious since we have

$$\|uv\|_{L^2} \le \|u\|_{L^2}\, \|v\|_{L^\infty} \le c\|u\|_{L^2}\, \|v\|_{H^\sigma}$$

and

$$\|f(u) - f(v)\|_{L^2} \le \max_{|w| \le cR} |f'(w)|\, \|u - v\|_{L^2}\,.$$

Consider now the case $s > 0$ and let us prove (31). If $s > \frac{d}{2}$, the result is well-known since H^s is an algebra. If $0 < s < \frac{d}{2}$, we apply (30) with the admissible set of coefficients

$$p = 2, \qquad p_1 = \frac{2d}{d - 2s}, \qquad q_1 = \frac{d}{s}, \qquad p_2 = +\infty, \qquad q_2 = 2$$

and use the Sobolev embeddings $H^\sigma \hookrightarrow L^\infty$, $H^s \hookrightarrow L^{p_1}$ and $H^\sigma \hookrightarrow W^{s,q_1}$. We have then

$$\|uv\|_{H^s} \le \alpha\|u\|_{L^{p_1}}\|v\|_{W^{s,q_1}} + \alpha\|u\|_{H^s}\|v\|_{L^\infty} \le \alpha\|u\|_{H^s}\, \|v\|_{H^\sigma}$$

which proves (31). If $s = \frac{d}{2}$, we obtain the same estimate by applying (30) with

$$p = 2, \qquad p_1 = \frac{1}{\mu}, \qquad q_1 = \frac{2}{1 - 2\mu}, \qquad p_2 = +\infty, \qquad q_2 = 2$$

for $\mu > 0$ small enough such that we also have the embeddings $H^s \hookrightarrow L^{p_1}$ and $H^\sigma \hookrightarrow W^{s,q_1}$.

Next, to prove (32), we consider the Taylor formula

$$f(u) - f(v) = \int_0^1 f'(tu + (1-t)v)(u - v)dt$$

and use a tame estimate in H^σ (see (5)). Hence, applying *(i)* yields

$$\begin{aligned}
\|f(u) - f(v)\|_{H^s} &\le \int_0^1 \left\|f'(tu + (1-t)v)(u - v)\right\|_{H^s} dt \\
&\le \int_0^1 \|f'(tu + (1-t)v)\|_{H^\sigma} \|u - v\|_{H^s} dt \\
&\le \big(\|f'(0)\|_{H^\sigma} + \chi_{f'}(cR)\, R\big)\, \|u - v\|_{H^s}.
\end{aligned}$$

The proof of the lemma is complete. □

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