

# Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations

Philippe Chartier, Florian Méhats, Mechthild Thalhammer, Yong Zhang

### ▶ To cite this version:

Philippe Chartier, Florian Méhats, Mechthild Thalhammer, Yong Zhang. Improved error estimates for splitting methods applied to highly-oscillatory nonlinear Schrödinger equations. Mathematics of Computation, American Mathematical Society, 2016, 85 (302), pp.2863-2885. 10.1090/mcom/3088 . hal-01373280

## HAL Id: hal-01373280 https://hal.archives-ouvertes.fr/hal-01373280

Submitted on 28 Sep 2016

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés. MATHEMATICS OF COMPUTATION Volume 00, Number 0, Pages 000-000 S 0025-5718(XX)0000-0

#### IMPROVED ERROR ESTIMATES FOR SPLITTING METHODS APPLIED TO HIGHLY-OSCILLATORY NONLINEAR SCHRÖDINGER EQUATIONS

#### PHILIPPE CHARTIER, FLORIAN MÉHATS, MECHTHILD THALHAMMER, AND YONG ZHANG

ABSTRACT. In this work, the error behavior of operator splitting methods is analyzed for highly-oscillatory differential equations. The scope of applications includes time-dependent nonlinear Schrödinger equations, where the evolution operator associated with the principal linear part is highly-oscillatory and periodic in time. In a first step, a known convergence result for the second-order Strang splitting method applied to the cubic Schrödinger equation is adapted to a wider class of nonlinearities. In a second step, the dependence of the global error on the decisive parameter  $0 < \varepsilon \ll 1$ , defining the length of the period, is examined. The main result states that, compared to established error estimates, the Strang splitting method is more accurate by a factor  $\varepsilon$ , provided that the time stepsize is chosen as an integer fraction of the period. This improved error behavior over a time interval of fixed length, which is independent of the period, is due to an averaging effect. The extension of the convergence result to higher-order splitting methods and numerical illustrations complement the investigations.

*Keywords*: Highly-oscillatory differential equations, Time-dependent nonlinear Schrödinger equations, Operator splitting methods, Strang splitting method, Error estimate, Convergence result, Averaging.

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

#### 1. INTRODUCTION

**Highly-oscillatory nonlinear Schrödinger equations.** In this work, we study time-dependent nonlinear Schrödinger equations of the form

(1.1) 
$$\begin{cases} i\partial_t u^{\varepsilon}(x,t) = -\frac{1}{\varepsilon}\Delta u^{\varepsilon}(x,t) + f(|u^{\varepsilon}(x,t)|^2)u^{\varepsilon}(x,t), \\ u^{\varepsilon}(x,0) = u_0(x), \qquad (x,t) \in \mathbb{T}^d \times [0,T]. \end{cases}$$

Here, *i* denotes the imaginary unit,  $0 < \varepsilon \ll 1$  the decisive small parameter, and  $\Delta$  the Laplace operator with respect to the spatial variables. The function defining the nonlinearity is supposed to fulfill the conditions  $f \in C^{\infty}(\mathbb{R}, \mathbb{R})$  and f(0) = 0. As underlying Hilbert space, we consider the Lebesgue-space of square integrable complex-valued functions on a *d*-dimensional torus of the form  $\mathbb{T}^d = [0, a]^d$  with a > 0. More generally, our considerations apply to situations where the spectrum of  $\Delta$  remains a subset of  $\omega \mathbb{N}$  for some  $\omega > 0$ . A fundamental assumption is that the exact

Received by the editor March 24, 2015.

Corresponding author: Philippe Chartier.

solution to (1.1) is sufficiently regular, that is, we choose the initial value in the Sobolev space  $H^{\sigma}(\mathbb{T}^d)$ , requiring the exponent  $\sigma > 0$  to be sufficiently large (see below).

Under the stated requirements, Stone's theorem asserts that the selfadjoint operator  $\Delta : H^2(\mathbb{T}^d) \to L^2(\mathbb{T}^d)$  generates a unitary strongly continuous one-parameter group  $(e^{it\Delta/\varepsilon})_{t\in\mathbb{R}}$  on  $L^2(\mathbb{T}^d)$ . Moreover, the operator  $e^{it\Delta/\varepsilon} : L^2(\mathbb{T}^d) \to L^2(\mathbb{T}^d)$  is periodic with respect to the time variable  $t \in \mathbb{R}$ . The (minimal) period is of the form  $\varepsilon T_0$ , where  $T_0 > 0$  depends on a. For the theoretical analysis, we may assume  $T_0 = 1$ , since this can be achieved by a simple rescaling of time.

On any finite time interval, the number of oscillations tends to infinity as the decisive parameter tends to zero, which renders the differential equation highly-oscillatory.

Equivalent formulation as long-term problem. For the ease of analysis, it is customary to reparametrize the time variable t as  $t/\varepsilon$ , which leads to the long-term problem

(1.2) 
$$\begin{cases} i\partial_t u^{\varepsilon}(x,t) = -\Delta u^{\varepsilon}(x,t) + \varepsilon f(|u^{\varepsilon}(x,t)|^2)u^{\varepsilon}(x,t), \\ u^{\varepsilon}(x,0) = u_0(x), \quad (x,t) \in \mathbb{T}^d \times [0,T/\varepsilon]. \end{cases}$$

Employing this equivalent formulation, the evolution operator associated with the principal linear part,  $e^{it\Delta} : L^2(\mathbb{T}^d) \to L^2(\mathbb{T}^d)$ , is periodic with periode  $T_0 = 1$ . We point out that the length of the time interval is proportional to  $1/\varepsilon$  and thus (1.2) *cannot* be considered as a small perturbation of the free linear Schrödinger equation. Indeed, closeness of the solutions to (1.2) and the free linear Schrödinger equation is ensured over a single period (see Lemma 5.2), but not on the whole time interval  $[0, T/\varepsilon]$ .

Throughout, we rely on the following regularity result, see [2] and references given therein. For the practically relevant case  $d \in \{1, 2, 3\}$  and in view of a detailed error analysis of the second-order Strang splitting method, i.e. p = 2, we shall employ the regularity requirement  $u_0 \in H^{\sigma}(\mathbb{T}^d)$  with  $\sigma \geq 2p = 4$ .

**Theorem 1.1** (See [2]). Assume  $\sigma > d/2+2$  and K > 1. There exists a constant T > 0 such that, for any  $\varepsilon > 0$  and  $u_0 \in H^{\sigma}(\mathbb{T}^d)$ , the time-dependent nonlinear Schrödinger equation (1.2) has a unique solution satisfying

$$u^{\varepsilon} \in C^{0}([0, T/\varepsilon]; H^{\sigma}(\mathbb{T}^{d})) \cap C^{1}([0, T/\varepsilon]; H^{\sigma-2}(\mathbb{T}^{d})),$$
  
$$\forall t \in [0, T/\varepsilon]: \quad \|u^{\varepsilon}(\cdot, t)\|_{H^{\sigma}} \leq K \|u_{0}\|_{H^{\sigma}}.$$

**Splitting methods.** In this work, we analyze the error behavior of (multiplicative) operator splitting methods for the time integration of (1.2), based on the solution of the subproblems

(1.3)  
$$\begin{cases} i\partial_t v(x,t) = -\Delta v(x,t), \\ v(x,0) = v_0(x), \quad (x,t) \in \mathbb{T}^d \times \mathbb{R}, \\ \\ i\partial_t w(x,t) = \varepsilon f(|w(x,t)|^2)w(x,t), \\ w(x,0) = w_0(x), \quad (x,t) \in \mathbb{T}^d \times \mathbb{R} \end{cases}$$

The associated evolution operators are given by

$$v(\cdot,t) = \varphi_T^t(v_0) = e^{it\Delta}v_0, \qquad t \in \mathbb{R},$$
$$w(x,t) = \left(\varphi_V^t(w_0)\right)(x) = e^{-i\varepsilon t f(|w_0(x)|^2)}w_0(x), \qquad (x,t) \in \mathbb{T}^d \times \mathbb{R},$$

and satisfy the isometry relations

$$\begin{aligned} \|\varphi_T^t(v_0)\|_{H^s} &= \|v_0\|_{H^s}, \quad t \in \mathbb{R}, \quad s \ge 0, \\ \|\varphi_V^t(w_0)\|_{L^2} &= \|w_0\|_{L^2}, \quad t \in \mathbb{R}. \end{aligned}$$

We consider splitting methods that can be cast into the format

(1.4) 
$$\Phi^{h}(u_{0}) = \varphi_{T}^{\alpha_{1}h} \circ \varphi_{V}^{\beta_{1}h} \circ \cdots \circ \varphi_{T}^{\alpha_{r}h} \circ \varphi_{V}^{\beta_{r}h}(u_{0}) \approx u_{1}^{\varepsilon} = u^{\varepsilon}(h)$$

for a time stepsize h > 0 and certain real coefficients  $(\alpha_j, \beta_j)_{j=1}^r$ . In accordance with the preservation of the  $L^2$ -norm of the exact solution to (1.2), the identity

$$\|(\Phi^h)^n(u_0)\|_{L^2} = \|u_0\|_{L^2}, \qquad t_n = nh \le T/\varepsilon,$$

follows at once from the stated isometry relations. Henceforth, we focus on the widely used second-order Strang splitting method, yielding an approximation to the solution through

(1.5) 
$$p = 2:$$
  $\Phi^h(u_0) = \varphi_T^{h/2} \circ \varphi_V^h \circ \varphi_T^{h/2}(u_0) \approx u_1^\varepsilon = u^\varepsilon(h).$ 

**Global error estimate (Strang splitting).** In agreement with the analysis given in [4] for the three-dimensional cubic Schrödinger equations, i.e. f(x) = x, we shall prove that the sequence of approximations satisfies a second-order error estimate for sufficiently small time stepsizes h > 0

$$p = 2: \qquad \|(\Phi^h)^n(u_0) - u^{\varepsilon}(t_n)\|_{H^{\sigma-2p}} \le Ch^p, \qquad t_n = nh \le T/\varepsilon.$$

We note that here the convergence is uniform in  $\varepsilon > 0$ .

Our main objective is to show that under the additional condition that the time stepsize h > 0 is chosen in such a way that  $T_0/h$  is an integer number, this error estimate can be refined to obtain

$$p = 2: \qquad \|(\Phi^h)^n(u_0) - u^{\varepsilon}(t_n)\|_{H^{\sigma-2m}} \le C(\varepsilon h^p + h^m), \qquad t_n = nh \le T/\varepsilon,$$

where  $m = \lfloor \sigma/2 \rfloor$  depends on the Sobolev regularity of the initial value  $u_0$ . The precise formulation of this result, which is somehow unexpectedly at first glance, is given in Theorem 5.5, see also Theorem 6.1 for the generalization to higher-order splitting methods.

Time stepsizes h > 0 such that  $T_0/h \in \mathbb{N}$  are said to be resonant and can lead to exponential error growth, see [6]. However, this possible instability over very long times does not contradict the convergence results given, since in this scaling instabilities are indeed observed, typically on intervals of length  $T/\varepsilon^2$ .

Our convergence analysis of splitting methods applies to highly-oscillatory nonlinear Schrödinger equations of arbitrary space dimension, with the constriction that the evolution operator associated with the principal linear part is periodic in time. However, as the practical realisation of the time-splitting approach requires the numerical solution of the subproblems in (1.3), we consider low-dimensional nonlinear Schrödinger equations to be relevant applications. For instance, for the cubic Schrödinger equation on a torus, the solutions to the linear and nonlinear subproblems are given by a spectral decomposition into Fourier basis functions, realized numerically by Fast Fourier techniques, and pointwise multiplications. Moreover, a fundamental presumption is that the solution to (1.2) is sufficiently regular. Otherwise, due to the encountered order reduction and the fact that a high number of basis functions is required for an adequate spatial resolution, the use of time-splitting spectral methods is less favourable.

We expect that our error analysis for splitting methods extends to other situations, where the principal linear part defines a selfadjoint operator and a decomposition with respect to the associated countable complete orthonormal system can be utilised, see for instance [3] for the study of a timesplitting Hermite spectral method.

Notations and outline. In the sequel, it is convenient to employ the abbreviations

$$R = 2K \|u_0\|_{H^{\sigma}}, \qquad B^s_{\rho} = \{ u \in H^s(\mathbb{T}^d), \|u\|_{H^s} \le \rho \}.$$

The stated regularity result thus ensures

$$\forall t \in [0, T/\varepsilon] : \qquad u^{\varepsilon}(t, \cdot) \in B^{\sigma}_{R/2}.$$

Furthermore, we do not distinguish in notation the solution  $u^{\varepsilon}$  :  $\mathbb{T}^d \times [0, T/\varepsilon] \to \mathbb{C}$  :  $(x, t) \mapsto u^{\varepsilon}(x, t)$  and the corresponding abstract function  $u^{\varepsilon} : [0, T/\varepsilon] \to L^2(\mathbb{T}^d) : t \mapsto u^{\varepsilon}(\cdot, t).$ 

0

Our work basically follows the inclusions

exa

$$\underbrace{B_{R/2}^{\sigma}}_{\text{act solution}} \subset \underbrace{B_{R}^{\sigma} \subset B_{R}^{\sigma-2}}_{\text{functional bounds}} \\
\subset \underbrace{B_{3R/4}^{\sigma-2}}_{\text{stability in } H^{s}(\mathbb{T}^{d})}_{\text{Global error} = \mathcal{O}(h)} \\
\subset \underbrace{H^{\sigma-4}}_{\text{global error} = \mathcal{O}(h^{2})} \\
\subset \underbrace{H^{\sigma-2m}}_{\text{global error} = \mathcal{O}(\varepsilon h^{2})}$$

In Section 2, we deduce auxiliary results for the functions

(1.6) 
$$F = F_0 : H^s(\mathbb{T}^d) \longrightarrow H^s(\mathbb{T}^d) : u \longmapsto -if(|u|^2)u,$$
$$F_\tau : H^s(\mathbb{T}^d) \longrightarrow H^s(\mathbb{T}^d) : u \longmapsto e^{-i\tau\Delta}F(e^{i\tau\Delta}u), \qquad \tau \in (0,1],$$

where  $s \in \{\sigma - 2, \sigma\}$ , needed as essential ingredients in our convergence analysis. A Lipschitz estimate for  $F_{\tau}$  lies at the core of a stability bound for the Strang splitting method, stated in Section 3. In the spirit of [4], stability in ensured with respect to the  $H^s$ -norm for  $s \in [0, \sigma - 2]$ , provided that the time-discrete solution remains bounded in  $H^{\sigma-2}(\mathbb{T}^d)$ . For further use, we also deduce a stability estimate for the difference between the Strang splitting solution and the solution to the free Schrödinger equation

(1.7) 
$$A_n^h(u_0) = (\Phi^h)^n(u_0) - e^{inh\Delta}u_0.$$

Auxiliary estimates for derivatives of  $F_{\tau}$  are utilised in Section 4 to analyze the local truncation error of the Strang splitting method

(1.8) 
$$\delta^{n-1}(\varepsilon,h) = \Phi^h(u_{n-1}^{\varepsilon}) - u_n^{\varepsilon}, \qquad u_n^{\varepsilon} = u^{\varepsilon}(t_n).$$

In Section 5, we first sketch the proof of a second-order convergence estimate that is uniform in the small parameter  $\varepsilon > 0$ , see [4]. Afterwards, we study in detail the accumulation of errors in the special case  $T_0/h \in \mathbb{N}$ . Our main result, proving the occurrence of an additional factor  $\varepsilon > 0$  under this assumption, is obtained in two steps: Theorem 5.4 provides an estimate for the error over a single period, showing that the principal error term is not present, due to an averaging effect. Theorem 5.5 then extends the error estimate to the whole interval. The extension of our analysis to higherorder splitting methods is indicated in Section 6. In Section 7, we present numerical experiments for the second-order Strang splitting method and a fourth-order splitting by Yoshida that confirm the improved error behavior. On account of the computation of a highly accurate reference solution, a one-dimensional model problem is considered. Additional technical results are exposed in an appendix.

#### 2. Auxiliary estimates

In the following proposition, we collect basic auxiliary estimates for the functions in (1.6). The remainder of this section is devoted to their derivation.

**Proposition 2.1.** (i) Let  $s \in \{\sigma, \sigma - 2\}$ . For any  $\tau \in [0, 1]$ , the function  $F_{\tau} : H^{s}(\mathbb{T}^{d}) \to H^{s}(\mathbb{T}^{d})$  is  $C^{\infty}$ . There exists a constant M > 0such that for all  $\tau \in [0, 1]$  and  $(u, v, w) \in B^{s}_{R} \times H^{s}(\mathbb{T}^{d}) \times H^{s}(\mathbb{T}^{d})$  the estimates

(2.1)  
$$\begin{aligned} \|F_{\tau}(u)\|_{H^{s}} \leq M, \\ \|F_{\tau}'(u)(v)\|_{H^{s}} \leq M \|v_{1}\|_{H^{s}}, \\ \|F_{\tau}''(u)(v,w)\|_{H^{s}} \leq M \|v\|_{H^{s}} \|w\|_{H^{s}} \end{aligned}$$

hold. Moreover, for  $\tau \in [0,1]$ , integer  $j \in [0,\sigma/2]$ , and  $(u,v) \in B_R^{\sigma} \times B_R^{\sigma}$ , the derivatives with respect to  $\tau$  satisfy the bounds

(2.2) 
$$\begin{aligned} \|\partial_{\tau}^{j} F_{\tau}(u)\|_{H^{\sigma-2j}} &\leq M, \\ \|\partial_{\tau} F_{\tau}'(u)(v)\|_{H^{\sigma-2}} &\leq M. \end{aligned}$$

(ii) Let  $s \in [0, \sigma - 2]$ . There exists a constant L > 0 such that for all  $\tau \in [0, 1]$  and  $(u, v) \in B_R^{\sigma-2} \times B_R^{\sigma-2}$  the Lipschitz estimate

(2.3) 
$$\|F_{\tau}(u) - F_{\tau}(v)\|_{H^s} \le L \|u - v\|_{H^s}$$

is valid. Furthermore, there exists a constant  $L_2 > 0$  such that for all  $\tau \in [0, 1]$ , integer  $j \in [0, \sigma/2]$ , and  $(u, v) \in B_R^{\sigma} \times B_R^{\sigma}$  the relation

(2.4) 
$$\|\partial_{\tau}^{j}F_{\tau}(u) - \partial_{\tau}^{j}F_{\tau}(v)\|_{H^{\sigma-2j}} \leq L_{2}\|u - v\|_{H^{\sigma}}$$

holds.

The arising constants depend on f, R and  $\sigma$ .

**Tame estimates.** Let  $s \in \{\sigma - 2, \sigma\}$ . The continuous embedding of the Sobolev space  $H^s(\mathbb{T}^d)$  into  $L^{\infty}(\mathbb{T}^d)$  implies that  $H^s(\mathbb{T}^d)$  forms an algebra. Thus, there exists a constant A > 1 such that

$$\forall (u, v) \in H^{s}(\mathbb{T}^{d}) \times H^{s}(\mathbb{T}^{d}) : \qquad ||uv||_{H^{s}} \leq A ||u||_{H^{s}} ||v||_{H^{s}}.$$

In this context, any function  $G \in C^{\infty}(\mathbb{C}, \mathbb{C})$  with G(0) = 0 satisfies a socalled *tame estimate*, see [1]. That is, there exists a non-decreasing function  $\chi_G : \mathbb{R}^+ \to \mathbb{R}^+$  such that

(2.5) 
$$\forall u \in H^{s}(\mathbb{T}^{d}) : \qquad \|G(u)\|_{H^{s}} \leq \chi_{G}(\|u\|_{L^{\infty}})\|u\|_{H^{s}} \\ \leq \chi_{G}(c\|u\|_{H^{s}})\|u\|_{H^{s}}.$$

Here, the relation  $\|\cdot\|_{L^{\infty}} \leq c \|\cdot\|_{H^{\sigma-2}} \leq c \|\cdot\|_{H^{\sigma}}$ , valid for some constant c > 0, is used. More generally, whenever  $G(0) \neq 0$ , considering  $\widetilde{G}(u) = G(u) - G(0)$  yields

(2.6) 
$$\forall u \in H^{s}(\mathbb{T}^{d}): \qquad \|G(u)\|_{H^{s}} \leq (2\pi)^{d/2} |G(0)| + \chi_{G}(\|u\|_{L^{\infty}}) \|u\|_{H^{s}}.$$

**Lipschitz estimate.** A straightforward calculation shows that the function  $F : H^{\sigma-2}(\mathbb{T}^d) \to H^{\sigma-2}(T^d)$  is Lipschitz continuous. Moreover, owing to Lemma A.3, a Lipschitz estimate is obtained with respect to the  $H^s$ -norm for any exponent  $s \in [0, \sigma - 2]$ . Indeed, for all elements  $u, v \in B_R^{\sigma-2}$ , we have

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

with positive constants  $\kappa, \alpha(f, AR^2)$  defined in Lemma A.3 and Lipschitz constant

$$L = \kappa R^2 (A\chi_f(c^2 R^2) + 2 \kappa \alpha(f, A R^2)).$$

Due to the fact that the evolution operator  $e^{it\Delta}$ ,  $t \in \mathbb{R}$ , defines an isometry, the function  $F_{\tau} : H^s(\mathbb{T}^d) \to H^s(T^d), \tau \in (0, 1]$ , satisfies a Lipschitz estimate with the same constant L.

**Derivatives.** Let  $s \in \{\sigma - 2, \sigma\}$  and  $\tau \in [0, 1]$ . We note that  $F_{\tau} : H^s(\mathbb{T}^d) \to H^s(\mathbb{T}^d)$  is arbitrarily often differentiable. For instance, we have

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

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

Applying the tame estimate (2.6) with f as well as f' and the identity  $\|e^{i\tau\Delta}u\|_{H^s} = \|u\|_{H^s}$ , for all  $u \in B^s_R$  and  $v \in H^s(\mathbb{T}^d)$ , we get

$$\begin{split} \|F_{\tau}(u)\|_{H^{s}} &\leq A^{2}\chi_{f}(c^{2}\|u\|_{H^{s}}^{2})\|u\|_{H^{s}}^{3} \\ &\leq M_{0}, \\ \|F_{\tau}'(u)(v)\|_{H^{s}} &\leq A^{3}\|f'(|e^{i\tau\Delta}u|^{2})\|_{H^{s}}\|u\|_{H^{s}}^{2}\|v\|_{H^{s}} \\ &\quad + A\|f(|e^{i\tau\Delta}u|^{2})\|_{H^{s}}\|v\|_{H^{s}} \\ &\leq M_{1}\|v\|_{H^{s}}, \end{split}$$

with some constants  $M_0, M_1$  that depend on f and R. The second derivative of F takes the form

 $F''(u)(v,w) = -if''(|u|^2)u(\bar{u}v + \bar{v}u)(\bar{u}w + \bar{w}u) - 2if'(|u|^2)(\bar{u}vw + \bar{v}uw + \bar{w}uv),$ and, as a consequence, for all  $u \in B_R^s$  and  $(v,w) \in H^s(\mathbb{T}^d) \times H^s(\mathbb{T}^d)$ , we have

$$\|F_{\tau}''(u)(v,w)\|_{H^s} \le M_2 \|v\|_{H^s} \|w\|_{H^s}.$$

Estimates for higher derivatives are obtained in a similar manner.

The first derivative of  $F_{\tau}$  with respect to  $\tau$  is given by

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

We note that, in general, the highest derivatives do not cancel, and thus we have to consider  $\partial_{\tau} F_{\tau}(u) : H^{\sigma}(\mathbb{T}^d) \to H^{\sigma-2}(\mathbb{T}^d)$ , which yields

$$\begin{aligned} \|\partial_{\tau}F_{\tau}(u)\|_{H^{\sigma-2}} &\leq \|\Delta F_{\tau}(u)\|_{H^{\sigma-2}} + \|F_{\tau}'(u)(i\Delta u)\|_{H^{\sigma-2}} \leq M_{0} + M_{1}R. \end{aligned}$$
As for the second derivative,  $\partial_{\tau}^{2}F_{\tau}(u) :H^{\sigma}(\mathbb{T}^{d}) \to H^{\sigma-4}(\mathbb{T}^{d}),$  it comes
$$\partial_{\tau}^{2}F_{\tau}(u) &= (-i\Delta)^{2}e^{-i\tau\Delta}F(e^{i\tau\Delta}u) + 2(-i\Delta)e^{-i\tau\Delta}F'(e^{i\tau\Delta}u)((i\Delta)e^{i\tau\Delta}u) \\ &+ e^{-i\tau\Delta}F''(e^{i\tau\Delta}u)((i\Delta)e^{i\tau\Delta}u)^{2} + e^{-i\tau\Delta}F'(e^{i\tau\Delta}u)((i\Delta)^{2}e^{i\tau\Delta}u) \\ &= (-i\Delta)^{2}F_{\tau}(u) + 2(-i\Delta)F_{\tau}'(u)(i\Delta u) + F_{\tau}'(u)((i\Delta)^{2}u) \\ &+ F_{\tau}''(u)(i\Delta u, i\Delta u). \end{aligned}$$

More generally, the *j*-th derivative with respect to  $\tau$ ,  $\partial_{\tau}^{j}F_{\tau}(u): H^{\sigma}(\mathbb{T}^{d}) \to H^{\sigma-2j}(\mathbb{T}^{d})$ , reads

$$\begin{aligned} \partial_{\tau}^{j} F_{\tau}(u) \\ &= (-i\Delta)^{j} F_{\tau}(u) \\ &+ \sum_{\substack{1 \leq k, \ell \leq j, \\ 1 \leq m_{1} \leq \ldots \leq m_{k}, \\ m_{1} + \ldots + m_{k} = \ell}} \alpha_{k\ell \mathbf{m}} (-i\Delta)^{j-\ell} F_{\tau}^{(k)}(u) ((i\Delta)^{m_{1}} u, \ldots, (i\Delta)^{m_{k}} u) \end{aligned}$$

with some nonnegative coefficients  $\alpha_{k\ell \mathbf{m}}$ , and satisfies the bound

$$\begin{aligned} \|\partial_{\tau}^{j}F_{\tau}(u)\|_{H^{\sigma-2j}} \\ &\leq \|F_{\tau}(u)\|_{H^{\sigma}} \\ &+ \sum_{\substack{1 \leq k, \ell \leq j, \\ 1 \leq m_{1} \leq \ldots \leq m_{k}, \\ m_{1} + \ldots + m_{k} = \ell}} \alpha_{k\ell \mathbf{m}} \|F_{\tau}^{(k)}(u)\big((i\Delta)^{m_{1}}u, \ldots, (i\Delta)^{m_{k}}u\big)\|_{H^{\sigma-2\ell}}, \end{aligned}$$

provided that  $\sigma \geq 2j$ .

In regard to the estimation of the local truncation error of the Strang splittig method, we consider

$$\partial_{\tau} F_{\tau}'(u)(v) = -i\Delta F_{\tau}'(u)(v) + F_{\tau}'(u)(i\Delta v) + F_{\tau}''(u)(v, i\Delta u).$$

Provided that  $u, v \in B_R^{\sigma}$ , the previous bounds imply

$$\|\partial_{\tau} F_{\tau}'(u)(v)\|_{H^{\sigma-2}} \le 2M_1 R + M_2 R^2.$$

**Lipschitz estimates for derivatives.** Proceeding as for  $F_{\tau}$ , it is straightforward to show that derivatives of  $F_{\tau}$  satisfy a Lipschitz estimate on  $B_R^{\sigma}$ . That is, there exists a constant L > 0 such that, for any integer  $j \in [0, \sigma/2]$  and all elements  $(u, v, w) \in B_R^{\sigma} \times B_R^{\sigma-2} \times B_R^{\sigma-2}$  the relation

$$\|F^{(j)}(u)(w^{j}) - F^{(j)}(v)(w^{j})\|_{H^{\sigma-2}} \le L \|u - v\|_{H^{\sigma-2}}$$

holds. Here, we use the short notation  $F^{(j)}(u)(w^j) = F^{(j)}(u)(w, \ldots, w)$ . Consequently, for  $(u, v) \in B_R^{\sigma} \times B_R^{\sigma}$  we obtain the Lipschitz estimate

$$\|\partial_{\tau}^{j}F_{\tau}(u) - \partial_{\tau}^{j}F_{\tau}(v)\|_{H^{\sigma-2j}} \le L_{2}\|u - v\|_{H^{\sigma}},$$

valid for some constant  $L_2 > 0$ .

#### 3. Stability estimate

The purpose of the following stability result is a twofold: On the one hand, in view of Section 4, where we provide a local error estimate for the Strang splitting method, we have to ensure that the time-discrete solution remains in  $B_R^{\sigma-2}$ . On the other hand, stability estimates in various norms are needed in the study of the error accumulation. We recall the abbreviations (1.5) and (1.7).

**Lemma 3.1.** Assume  $s \in [0, \sigma - 2]$  as well as  $v, w \in B^{\sigma-2}_{3R/4}$ , and set  $h_0 = \log(4/3)/(\varepsilon_0 L)$ . Then, for any  $0 < \varepsilon < \varepsilon_0$  and  $0 < h < h_0$ , the time-discrete solutions associated with the Strang splitting method satisfy  $\Phi^h(v), \Phi^h(w) \in B^{\sigma-2}_B$ . In addition, the stability estimates

$$\begin{aligned} \|\Phi^{h}(v) - \Phi^{h}(w)\|_{H^{s}} &\leq e^{\varepsilon Lh} \|v - w\|_{H^{s}}, \\ \|A_{1}^{h}(v) - A_{1}^{h}(w)\|_{H^{s}} &\leq \varepsilon h e^{\varepsilon Lh} \|v - w\|_{H^{s}}, \end{aligned}$$

hold.

*Proof.* Due to the fact that the operator  $e^{it\Delta} : H^s(\mathbb{T}^d) \to H^s(\mathbb{T}^d), t \in \mathbb{R}$ , is an isometry, it suffices to study the evolution operator associated with the nonlinear subproblem. Denoting  $v(t) = \varphi_V^t(v_0)$  and  $w(t) = \varphi_V^t(w_0)$ , we have

$$w'(t) = \varepsilon F(w(t)), \qquad v'(t) = \varepsilon F(v(t)).$$

Employing (2.3), we obtain

$$\|v(t) - w(t)\|_{H^{s}} \leq \|v_{0} - w_{0}\|_{H^{s}} + \varepsilon \int_{0}^{t} \|F(v(\zeta)) - F(w(\zeta))\|_{H^{s}} d\zeta$$
$$\leq \|v_{0} - w_{0}\|_{H^{s}} + \varepsilon L \int_{0}^{t} \|v(\zeta) - w(\zeta)\|_{H^{s}} d\zeta,$$

as long as  $v(\zeta), w(\zeta) \in B_R^{\sigma-2}$  for  $\zeta \in [0, t]$ , so that, by Gronwall's lemma

$$||v(t) - w(t)||_{H^s} \le e^{\varepsilon Lt} ||v_0 - w_0||_{H^s}.$$

Setting in particular t = h and  $w_0 = 0$  implies  $||v(h)||_{H^{\sigma-2}} \leq \frac{3R}{4}e^{\varepsilon Lh} \leq R$ . A straightforward estimation further yields

$$\|\varphi_V^h(v_0) - \varphi_V^h(w_0) - (v_0 - w_0)\|_{H^s} \le \varepsilon L h e^{\varepsilon L h} \|v_0 - w_0\|_{H^s}.$$

Altogether, the stated result follows.

#### 4. Local error estimate

Employing suitable expansions of the exact and time-discrete solutions, an estimate for the local truncation error is obtained by means of Proposition 2.1, see also (1.8). In addition to the basic requirement  $\sigma > d/2+2$ , see Theorem 1.1, we henceforth assume  $\sigma \ge 2p = 4$  so that the nonstiff order of convergence is retained for the second-order Strang splitting method.

**Expansion of exact solution.** An application of the Duhamel formula leads to the following representation of the exact solution value at time t+h

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

Equivalently, for  $v^{\varepsilon}(t) = e^{-it\Delta}u^{\varepsilon}(t)$ , we have

$$v^{\varepsilon}(t+h) = v^{\varepsilon}(t) + \varepsilon \int_{0}^{h} F_{t+\tau}(v^{\varepsilon}(t+\tau))d\tau.$$

We use the expansion

$$F_{\tau}(w_1 + w_2) = F_{\tau}(w_1) + F_{\tau}'(w_1)(w_2) + \int_0^1 (1 - \zeta) F_{\tau}''(w_1 + \zeta w_2)(w_2^2) d\zeta$$

to arrive at

$$\begin{aligned} v^{\varepsilon}(t+h) &= v^{\varepsilon}(t) + \varepsilon \int_{0}^{h} F_{t+\tau} \left( v^{\varepsilon}(t) + \varepsilon \int_{0}^{\tau} F_{t+\tau_{1}} (v^{\varepsilon}(t+\tau_{1})) d\tau_{1} \right) d\tau \\ &= v^{\varepsilon}(t) + \varepsilon \int_{0}^{h} F_{t+\tau} (v^{\varepsilon}(t)) d\tau \\ &+ \varepsilon^{2} \int_{0}^{h} \int_{0}^{\tau} F_{t+\tau}' (v^{\varepsilon}(t)) F_{t+\tau_{1}} (v^{\varepsilon}(t+\tau_{1})) d\tau_{1} d\tau \\ &+ \varepsilon^{3} \int_{0}^{h} \int_{0}^{1} (1-\xi) F_{t+\tau}' \left( (1-\xi) v^{\varepsilon}(t) + \xi v^{\varepsilon}(t+\tau) \right) \\ &\qquad \left( \int_{0}^{\tau} F_{t+\tau_{1}} (v^{\varepsilon}(t+\tau_{1})) d\tau_{1} \right)^{2} d\xi d\tau. \end{aligned}$$

A further expansion of the second-order term with respect to  $\varepsilon$  yields

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

Finally, we obtain

$$u^{\varepsilon}(t+h) = e^{ih\Delta}u^{\varepsilon}(t) + \varepsilon e^{ih\Delta} \int_{0}^{h} F_{\tau}(u^{\varepsilon}(t))d\tau + \varepsilon^{2}e^{ih\Delta} \int_{0}^{h} \int_{0}^{\tau} F_{\tau}'(u^{\varepsilon}(t))F_{\tau_{1}}(u^{\varepsilon}(t))d\tau_{1}d\tau + \varepsilon^{3}e^{ih\Delta}E_{3}(u^{\varepsilon}(t),\varepsilon,h),$$

involving

$$\begin{split} E_{3}(u^{\varepsilon}(t),\varepsilon,h) &= E_{3,a}(u^{\varepsilon}(t),\varepsilon,h) + E_{3,b}(u^{\varepsilon}(t),\varepsilon,h),\\ E_{3,a}(u^{\varepsilon}(t),\varepsilon,h) &= \int_{0}^{h} \int_{0}^{1} (1-\xi) F_{\tau}'' \left( (1-\xi) u^{\varepsilon}(t) + \xi e^{-i\tau\Delta} u^{\varepsilon}(t+\tau) \right) \\ & \left( \int_{0}^{\tau} F_{\tau_{1}}(e^{-i\tau_{1}\Delta} u^{\varepsilon}(t+\tau_{1})) d\tau_{1} \right)^{2} d\xi d\tau,\\ E_{3,b}(u^{\varepsilon}(t),\varepsilon,h) &= \int_{0}^{h} \int_{0}^{\tau} \int_{0}^{1} F_{\tau}'(u^{\varepsilon}(t)) \\ & F_{\tau_{1}}' \left( (1-\xi) u^{\varepsilon}(t) + \xi e^{-i\tau_{1}\Delta} u^{\varepsilon}(t+\tau_{1}) \right) \\ & \left( \int_{0}^{\tau_{1}} F_{\tau_{2}}(e^{-i\tau_{2}\Delta} u^{\varepsilon}(t+\tau_{2})) d\tau_{2} \right) d\xi d\tau_{1} d\tau \end{split}$$

As  $u^{\varepsilon}(t)$  remains in  $B_{R/2}^{\sigma} \subset B_R^{\sigma} \subset B_R^{\sigma-2}$ , by Proposition 2.1, the estimate

(4.1) 
$$||E_3(u^{\varepsilon}(t),\varepsilon,h)||_{H^{\sigma-2}} \le \frac{1}{3}M^3h^3$$

follows.

**Expansion of time-discrete solution.** In the sequel, in regard to Lemma 3.1, we suppose  $0 < h < h_0 = \log(4/3)/(\varepsilon_0 L)$  and  $u \in B^{\sigma-2}_{3R/4}$ . Using that  $v(t) = \varphi^t_V(u)$  satisfies  $v'(t) = \varepsilon F(v(t))$ , we get

$$\varphi_V^h(u) = u + \varepsilon h F(u) + \frac{1}{2} \varepsilon^2 h^2 F'(u) F(u) + \frac{1}{2} \varepsilon^3 \int_0^h (h - \tau)^2 \Big( F''(\varphi_V^\tau(u)) (F(\varphi_V^\tau(u)))^2 + F'(\varphi_V^\tau(u)) F'(\varphi_V^\tau(u)) F(\varphi_V^\tau(u)) \Big) d\tau.$$

We rewrite this relation as

(4.2) 
$$\varphi_V^h(u) = u + \varepsilon h F(u) + \frac{1}{2} \varepsilon^2 h^2 F'(u) F(u) + \varepsilon^3 E_{3,V}(u,\varepsilon,h),$$

where

$$E_{3,V}(u,\varepsilon,h) = \frac{1}{2} \int_0^h (h-\tau)^2 \Big( F''(\varphi_V^\tau(u)) (F(\varphi_V^\tau(u)))^2 + F'(\varphi_V^\tau(u)) F'(\varphi_V^\tau(u)) F(\varphi_V^\tau(u)) \Big) d\tau.$$

Expanding the time-discrete solution associated with the Strang splitting solution, we obtain

(4.3)  

$$\Phi^{h}(u) = e^{ih\Delta/2} \left( e^{ih\Delta/2}u + \varepsilon hF(e^{ih\Delta/2}u) + \frac{1}{2}\varepsilon^{2}h^{2}F'(e^{ih\Delta/2}u)F(e^{ih\Delta/2}u) + \varepsilon^{3}E_{3,V}(e^{ih\Delta/2}u,\varepsilon,h) \right) \\
= e^{ih\Delta} \left( u + \varepsilon hF_{h/2}(u) + \frac{1}{2}\varepsilon^{2}h^{2}F'_{h/2}(u)F_{h/2}(u) \right) \\
+ \varepsilon^{3}e^{ih\Delta/2}E_{3,V}(e^{ih\Delta/2}u,\varepsilon,h).$$

Owing to Lemma 3.1,  $\varphi_V^t(u)$  remains in  $B_R^{\sigma-2}$  for  $0 \le t \le h$ . By Proposition 2.1, we thus get

(4.4) 
$$||E_{3,V}(u,\varepsilon,h)||_{H^{\sigma-2}} \leq \frac{1}{3}M^3h^3.$$

/

**Local error estimate.** Applying the previous expansions, the local truncation error reads

$$(4.5) \qquad \delta^{n}(\varepsilon,h) = \varepsilon e^{ih\Delta} \left( hF_{h/2}(u_{n}^{\varepsilon}) - \int_{0}^{h} F_{\tau}(u_{n}^{\varepsilon})d\tau \right) \\ + \varepsilon^{2} e^{ih\Delta} \left( \frac{1}{2}h^{2}F_{h/2}'(u_{n}^{\varepsilon})F_{h/2}(u_{n}^{\varepsilon}) - \int_{0}^{h} \int_{0}^{\tau} F_{\tau}'(u_{n}^{\varepsilon})F_{\tau_{1}}(u_{n}^{\varepsilon})d\tau_{1}d\tau \right) \\ + \varepsilon^{3} \left( e^{ih\Delta/2}E_{3,V}(e^{ih\Delta/2}u_{n}^{\varepsilon},\varepsilon,h) - e^{ih\Delta}E_{3}(u_{n}^{\varepsilon},\varepsilon,h) \right).$$

Under the assumption  $0 < h < h_0$  we next estimate each term individually.

(i) We use the representation based on the second-order Peano kernel  $\kappa_2$  of the midpoint rule

$$Q_1 = hF_{h/2}(u) - \int_0^h F_{\tau}(u)d\tau = h^3 \int_0^1 \kappa_2(\tau)\partial_{\theta}^2 F_{\theta}(u)\Big|_{\theta=\tau h} d\tau.$$

Owing to (2.2), we obtain

(4.6) 
$$||Q_1||_{H^{\sigma-4}} \le Mh^3 \left(\int_0^1 |\kappa_2(\tau)| d\tau\right).$$

(ii) Inserting the identities

$$F_{\tau_1}(u) = F_{h/2}(u) + \int_{h/2}^{\tau_1} \partial_\theta F_\theta(u) d\theta,$$
  
$$F'_{\tau}(u) = F'_{h/2}(u) + \int_{h/2}^{\tau} \partial_\theta F'_\theta(u) d\theta.$$

into the double integral term, we get

$$\int_0^n \int_0^\tau F'_{\tau}(u) F_{\tau_1}(u) d\tau_1 d\tau = \frac{1}{2} h^2 F'_{h/2}(u) F_{h/2}(u) + r_1,$$

where

$$r_{1} = \int_{0}^{h} \int_{0}^{\tau} F_{h/2}'(u) \left( \int_{h/2}^{\tau_{1}} \partial_{\theta} F_{\theta}(u) d\theta \right) d\tau_{1} d\tau$$
$$+ \int_{0}^{h} \int_{0}^{\tau} \int_{h/2}^{\tau} \partial_{\theta} F_{\theta}'(u) F_{h/2}(u) d\theta d\tau_{1} d\tau$$
$$+ \int_{0}^{h} \int_{0}^{\tau} \left( \int_{h/2}^{\tau} \partial_{\theta} F_{\theta}(u) d\theta \int_{h/2}^{\tau_{1}} \partial_{\theta_{1}} F_{\theta_{1}}(u) d\theta_{1} \right) d\tau_{1} d\tau.$$

This implies the estimate

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

(iii) The third-order term in  $\varepsilon$  is estimated by means of the bounds (4.1) and (4.4).

Altogether, this shows that there exists a constant C > 0 such that the local error estimate

(4.7) 
$$\|\delta^n(\varepsilon,h)\|_{H^{\sigma-4}} \le C\varepsilon h^3$$

holds.

Remark. For later use, we note that the bound

(4.8) 
$$\|\delta^n(\varepsilon,h)\|_{H^{\sigma-2}} \le \widetilde{C}\varepsilon h^2$$

follows, employing instead a representation based on the first-order Peano kernel. Moreover, we observe that the following expansion holds

(4.9) 
$$\delta^n(\varepsilon,h) = \varepsilon e^{ih\Delta} \Lambda_h(u_n^{\varepsilon}) + \varepsilon^2 R_h(u_n^{\varepsilon}),$$

involving the difference

(4.10) 
$$\Lambda_h(u_n^{\varepsilon}) = hF_{h/2}(u_n^{\varepsilon}) - \int_0^h F_{\tau}(u_n^{\varepsilon})d\tau.$$

In accordance with (4.7), we have

$$\|\Lambda_h(u_n^{\varepsilon})\|_{H^{\sigma-4}} \le Ch^3, \qquad \|R_h(u_n^{\varepsilon})\|_{H^{\sigma-2}} \le Ch^3.$$

#### 5. GLOBAL ERROR ESTIMATE

In this section, we deduce a convergence result for the Strang splitting method (1.5) applied to nonlinear Schrödinger equations of the form (1.2). A basic tool for the error analysis is the telescopic identity

$$(\Phi^h)^n(u_0) - u_n^{\varepsilon} = \sum_{\ell=1}^n \left( (\Phi^h)^{n-\ell} \circ \Phi^h(u_{\ell-1}^{\varepsilon}) - (\Phi^h)^{n-\ell}(u_{\ell}^{\varepsilon}) \right),$$

which permits to obtain a global error estimate by means of stability bounds and local error estimates, see Sections 3 and 4. We proceed as follows: In agreement with [4], we start with proving an  $\varepsilon$ -independent global error estimate. Then, we utilise this result in a more refined analysis, first for a time integration over a single period  $T_0 = 1$  and subsequently for the whole time interval  $[0, T/\varepsilon]$ .

**Global error estimate.** The following result generalizes the global error estimate provided in [4] for a cubic nonlinearity.

**Theorem 5.1.** Let  $h_0 = \log(4/3)/(\varepsilon_0 L)$  and  $h_1 = \min\{h_0, RL/(4\widetilde{C}(e^{LT} - 1))\}$ . Then, for any  $0 < h < h_1$ , the Strang splitting method satisfies the second-order error estimate

(5.1) 
$$\|(\Phi^h)^n(u_0) - u^{\varepsilon}(t_n)\|_{H^{\sigma-4}} \le C \frac{e^{LT} - 1}{L} h^2, \quad t_n = nh \le T/\varepsilon,$$

where the positive constants C and L depend on  $\sigma$ , R and f, but are independent of  $\varepsilon$ .

*Proof.* We note that the stability estimates provided by Lemma 3.1 may be employed as long as  $(\Phi^h)^j(u^{\varepsilon}(t_k))$  remains in  $B^{\sigma-2}_{3R/4}$ . The stated telescopic identity implies

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

Furthermore, by means of the local error estimate  $\|\delta^{l-1}(\varepsilon, h)\|_{H^{\sigma-2}} \leq \tilde{C}\varepsilon h^2$ , see (4.8), the geometric series, the relation  $e^x - 1 \geq x$  for  $x \geq 0$ , and due to  $nh \leq T/\varepsilon$ , we get

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

Combining an induction argument and this error estimate thus ensures boundedness of the time-discrete solution in  $H^{\sigma-2}(\mathbb{T}^d)$ , as required by Lemma 3.1, for time stepsizes satisfying the condition  $\widetilde{C}(e^{LT}-1)h/L \leq \frac{R}{4}$ . Using a stability estimate with respect to the  $H^{\sigma-4}$ -norm, again by applying Lemma 3.1, owing to estimate (4.7), the stated second-order error estimate results.

**Refined error estimate over one period.** We now examine more closely the approximation error over a single period  $T_0 = 1$ . A first auxiliary result relates the solutions to (1.2) and the free Schrödinger equation.

**Lemma 5.2.** The following estimate holds for all times  $t \in [0, T_0]$ 

(5.2) 
$$\|u^{\varepsilon}(t) - e^{it\Delta}u_0\|_{H^{\sigma}} \le \varepsilon MT_0$$

*Proof.* For notational simplicity, we set  $u(t) = u^{\varepsilon}(t)$  and  $v(t) = e^{it\Delta}u_0$ . Evidently, we have

$$\begin{cases} u'(t) = i\Delta u(t) + \varepsilon F(u(t)), & t \in [0, T_0], \\ u(0) = u_0, \\ v'(t) = i\Delta v(t), & t \in [0, T_0], \\ v(0) = u_0. \end{cases}$$

The Duhamel formula and Proposition 2.1 imply

$$\|u(t) - v(t)\|_{H^{\sigma}} = \varepsilon \left\| \int_0^t e^{i(t-\tau)\Delta} F(u^{\varepsilon}(\tau)) d\tau \right\|_{H^{\sigma}} \le \varepsilon M T_0,$$

which is the stated result.

The following auxiliary result provides a Lipschitz estimate for the difference between the Strang splitting solution and the solution to the free Schrödinger equation, see (1.7). We note that, according to Theorem 5.1,  $(\Phi^h)^{\ell} \in B^{\sigma-2}_{3R/4}$  for all integers  $0 \leq \ell \leq n$ , where  $nh \leq T/\varepsilon$ , and hence  $(\Phi^h)^{\ell} \in B^s_{3R/4}$  for any exponent  $s \in [0, \sigma - 2]$ . The maximum time stepsize  $h_1$  is defined in Theorem 5.1.

**Lemma 5.3.** Let  $u, v \in H^{\sigma-2}(\mathbb{T}^d)$  be given, and assume that the associated sequences satisfy  $((\Phi^h)^{\ell}(u))_{\ell}, ((\Phi^h)^{\ell}(v))_{\ell} \in B^{\sigma-2}_{3R/4}$  for all integers  $0 \leq \ell \leq n$ with  $nh \leq T_0 = 1$  and time stepsizes  $0 < h < h_1$ . Then, for any exponent  $s \in [0, \sigma - 2]$  and  $0 < h < h_1$  the Lipschitz estimate

$$\|A_{\ell}^{h}(u) - A_{\ell}^{h}(v)\|_{H^{s}} \le \varepsilon LT_{0}e^{\varepsilon LT_{0}}\|u - v\|_{H^{s}}, \qquad 0 \le \ell \le n, \quad nh \le T_{0},$$

holds.

*Proof.* The telescopic identity implies

$$(\Phi^h)^{\ell}(u) - e^{i\ell h\Delta}u = \sum_{k=1}^{\ell} \left( e^{ih(\ell-k)\Delta} \left( \Phi^h - e^{ih\Delta} \right) \circ \left( \Phi^h \right)^{(k-1)} \right) (u)$$

implies the estimate

$$\|A_{\ell}^{h}(u) - A_{\ell}^{h}(v)\|_{H^{s}} \leq \sum_{k=1}^{\ell} \|A_{1}^{h}((\Phi^{h})^{(k-1)}(u)) - A_{1}^{h}((\Phi^{h})^{(k-1)}(v))\|_{H^{s}}.$$

Hence, by Lemma 3.1, we obtain

$$\begin{aligned} \|A_{\ell}^{h}(u) - A_{\ell}^{h}(v)\|_{H^{s}} &\leq \varepsilon Lhe^{L\varepsilon h} \sum_{k=1}^{\ell} \left\| (\Phi^{h})^{(k-1)}(u) - (\Phi^{h})^{(k-1)}(v) \right\|_{H^{s}} \\ &\leq \varepsilon Lh \sum_{k=1}^{\ell} e^{\varepsilon Lkh} \|u - v\|_{H^{s}} \\ &\leq \varepsilon LT_{0} e^{\varepsilon LT_{0}} \|u - v\|_{H^{s}}, \end{aligned}$$

which is the stated result.

By means of the above auxiliary results, the following error estimate is obtained, see Theorem 5.1 for the definition of the maximum time stepsize  $h_1$ .

**Theorem 5.4.** Let  $m = \lfloor \sigma/2 \rfloor$ . For any time stepsize  $0 < h < h_1$ , the Strang splitting method applied to a nonlinear Schrödinger equation of the form (1.2) satisfies the second-order error bound

(5.3) 
$$\|(\Phi^h)^n(u_0) - u^{\varepsilon}(T_0)\|_{H^{\sigma-2m}} \le \widehat{C}(\varepsilon^2 h^2 + \varepsilon h^m), \quad nh = T_0.$$

The arising constant  $\widehat{C}$  depends on  $\sigma$ , R and f, but is independent of  $\varepsilon$ .

*Proof.* The proof proceeds in two steps.

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

$$(\Phi^{h})^{n}(u_{0}) - u^{\varepsilon}(T_{0}) = \sum_{\ell=1}^{n} e^{i(n-\ell)h\Delta} \delta^{\ell-1}(\varepsilon, h) + r,$$
  
$$r = \sum_{\ell=1}^{n} \left( A_{n-\ell}^{h} (\Phi^{h}(u_{\ell-1}^{\varepsilon})) - A_{n-\ell}^{h}(u_{\ell}^{\varepsilon}) \right).$$

By means of Lemma 5.3 and (4.7), we have

$$\begin{aligned} \|r\|_{H^{\sigma-4}} &\leq \varepsilon L T_0 e^{\varepsilon L T_0} \sum_{\ell=1}^n \|\delta^{\ell-1}(\varepsilon,h)\|_{H^{\sigma-4}} \\ &\leq C \varepsilon^2 L T_0^2 e^{\varepsilon L T_0} h^2 \,. \end{aligned}$$

In addition, according to (4.9), we have

$$\sum_{\ell=1}^{n} e^{i(n-\ell)h\Delta} \delta^{\ell-1}(\varepsilon,h) = \varepsilon \sum_{\ell=1}^{n} e^{i(n-\ell+1)h\Delta} \Lambda_h(u_{\ell-1}^{\varepsilon}) + \widetilde{r},$$
$$\widetilde{r} = \varepsilon^2 \sum_{\ell=1}^{n} e^{i(n-\ell)h\Delta} R_h(u_{\ell-1}^{\varepsilon}), \qquad \|\widetilde{r}\|_{H^{\sigma-2}} \le C\varepsilon^2 h^2.$$

Finally, taking into account that

$$\|u_{\ell-1}^{\varepsilon} - e^{i(\ell-1)h\Delta}u_0\|_{H^{\sigma}} \le \varepsilon MT_0,$$

see Lemma 5.2, and that  $\Lambda_h$  satisfies a Lipschitz estimate with a constant of the form  $\tilde{L}_2 h^3$ , see (4.10)-(4.6) and Proposition 2.1, we have

$$\left\| (\Phi^h)^n(u_0) - u^{\varepsilon}(T_0) - \varepsilon \sum_{\ell=1}^n e^{i(n-\ell+1)h\Delta} \Lambda_h(e^{i(\ell-1)h\Delta}u_0) \right\|_{H^{\sigma-4}} \le \text{ Const } \varepsilon^2 h^2.$$

(ii) Estimate of the  $\varepsilon$ -error term. From previous analysis, the main error is concentrated in the term

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

which is of order  $\varepsilon h^2$ . For a refined estimation, we proceed as follows:

$$\sum_{\ell=1}^{n} e^{i(n-\ell+1)h\Delta} \Lambda_h(e^{i(\ell-1)h\Delta} u_0) = h \sum_{\ell=0}^{n-1} F_{(\ell h+h/2)}(u_0) - \int_0^1 F_{\tau}(u_0) d\tau$$
$$= h \sum_{\ell=0}^{n-1} F_{(\ell h+h/2)}(u_0) - \int_0^1 F_{(\tau+h/2)}(u_0) d\tau$$
$$= e^{-ih\Delta/2} E_{Rie}(e^{ih\Delta/2} u_0, h),$$

where  $E_{Rie}$  denotes the error in the approximation by Riemann sums, according to Lemma A.1. Here, we take into account that  $e^{ihn\Delta}$  is the identity operator and that the function  $F_{\tau}(u_0)$  is periodic with respect to  $\tau$  with period  $T_0 = 1$ . From Lemma A.1, we thus have

$$\left\| \sum_{\ell=1}^{n} e^{i(n-\ell+1)h\Delta} \Lambda_{h}(e^{i(\ell-1)h\Delta}u_{0}) \right\|_{H^{\sigma-2m}} \le C_{m}^{Rie} \|\partial_{\tau}^{j}F_{\tau}(u_{0})\|_{H^{\sigma-2m}}h^{m}$$

with constant  $C_m^{Rie} = 2^{1-m} \pi^{-m} \zeta(m)$ . Together with the auxiliary estimate (2.2) of Proposition 2.1, the stated result follows.

Refined global error estimate. In order to deduce a refined global error estimate, we consider the integrator  $\widehat{\Phi}(u) = (\Phi^h)^n(u)$  for  $nh = T_0 = 1$ . Evidently,  $\widehat{\Phi}$  is Lipschitz continuous. The previous result ensures that the approximation error at time  $T_0 = 1$  is of the size  $\widehat{C}\varepsilon(\varepsilon h^2 + h^m)$ . Using a telescopic identity for the representation of  $\widehat{\Phi}^N$ , where  $N = \lfloor T/\varepsilon \rfloor$ , thus implies the desired global error estimate  $\widehat{C}T(\varepsilon h^2 + h^m)$ . We note that the time-discrete solution at any intermediate point within an interval of the form  $[kT_0, (k+1)T_0]$  or  $[N, T/\varepsilon]$  is obtained by a suitable composition of  $\widehat{\Phi}$ and  $\Phi^h$ .

**Theorem 5.5.** Let  $m = \lfloor \sigma/2 \rfloor$ . For any time stepsize h > 0 such that  $T_0/h \in \mathbb{N}$ , the Strang splitting method applied to a nonlinear Schrödinger equation of the form (1.2) satisfies the global error estimate

(5.4) 
$$\|(\Phi^h)^n(u_0) - u^{\varepsilon}(t_n)\|_{H^{\sigma-2m}} \le \widehat{C}T(\varepsilon h^2 + h^m), \quad t_n = nh \le T/\varepsilon.$$

The arising constant  $\widehat{C}$  depends on  $\sigma$ , R and f, but is independent of  $\varepsilon$ .

#### 6. Extension to higher-order splitting methods

In the sequel, we extend our error analysis to higher-order splitting methods given by a composition of the form (1.4). Basic consistency conditions are

$$\gamma_r = 1, \quad \gamma_j = \sum_{k=1}^{j} \alpha_k, \qquad \sum_{j=1}^{r} \beta_j = 1.$$

For a splitting method of order p, we make use of the fact that the local error (1.8) can be written as in (4.9)

$$\delta^n(\varepsilon,h) = \Phi^h(u_n^\varepsilon) - u_{n+1}^\varepsilon = \varepsilon e^{ih\Delta} \Lambda_h(u_n^\varepsilon) + \varepsilon^2 R_h(u_n^\varepsilon),$$

with  $\Lambda_h$  and  $R_h$  satisfying the estimates

$$\|\Lambda_h(u_n^{\varepsilon})\|_{H^{\sigma-2p}} \le Ch^{p+1}, \qquad \|R_h(u_n^{\varepsilon})\|_{H^{\sigma-2p+2}} \le Ch^{p+1}.$$

Next, we identify  $\Lambda_h$  through an  $\varepsilon$ -expansion

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

so that we get

$$\sum_{\ell=1}^{n} e^{i(n-\ell+1)h\Delta} \Lambda_h(e^{i(\ell-1)h\Delta}u_0)$$
$$= \sum_{j=1}^{r} \beta_j \left(h \sum_{\ell=0}^{n-1} F_{(\ell h+\gamma_j h)}(u_0) - \int_0^1 F_{\tau}(u_0) d\tau\right)$$
$$= \sum_{j=1}^{r} \beta_j e^{-i\gamma_j h\Delta} E_{Rie}(e^{i\gamma_j h\Delta}u_0, h).$$

Due to the validity of the order conditions, the relation

$$\Lambda_h(u) = h^{p+1} \int_0^1 \kappa_p(\tau) \partial_\theta^p F_\theta \Big|_{\theta=\tau h}(u) d\tau$$

is obtained, which implies a Lipschitz estimate with a constant of the form  $\tilde{L}_2 h^{p+1}$ . Under the assumption  $\sigma \geq 2p$ , the adaptation of the error analysis for the Strang splitting method shows the following result.

**Theorem 6.1.** Consider a pth-order splitting method applied to a nonlinear Schrödinger equation of the form (1.2), and assume  $\sigma > d/2 + 2$  as well as  $\sigma \geq 2p$ . Then, for any time stepsize h > 0 such that  $T_0/h \in \mathbb{N}$  and  $m = \lfloor \sigma/2 \rfloor$ , the global error estimate

(6.1) 
$$\|(\Phi^h)^n(u_0) - u^{\varepsilon}(t_n)\|_{H^{\sigma-2m}} \le CT(\varepsilon h^p + h^m), \qquad t_n = nh \le T/\varepsilon,$$

holds with constant C that depends on  $\sigma$ , R and f, but is independent of  $\varepsilon$ .

#### 7. Numerical experiments

In this section, we present numerical experiments for the one-dimensional nonlinear Schrödinger equation

(7.1) 
$$\begin{cases} i\partial_t u^{\varepsilon}(x,t) = -\partial_{xx} u^{\varepsilon}(x,t) + 2\varepsilon\cos(2x)|u^{\varepsilon}(x,t)|^2 u^{\varepsilon}(x,t), \\ u^{\varepsilon}(x,0) = u_0(x) = \cos(x) + \sin(x), \quad (x,t) \in [0,2\pi] \times [0,T/\varepsilon], \end{cases}$$

allowing a space-dependent coefficient in the cubic nonlinearity. In the present situation, the time-period is  $T_0 = 2\pi$ . As final time, we choose  $T = \pi/4$ .

**Time discretization.** For the time discretization, we apply the secondorder Strang splitting method (p = 2) and a fourth-order splitting method by Yoshida [7], defined by the composition (1.4) with coefficients

$$p = r = 4: \qquad \beta_4 = 0, \qquad \beta_3 = \frac{1}{2 - \sqrt[3]{2}} = \beta_1, \qquad \beta_2 = -\sqrt[3]{2}\beta_3,$$
$$\alpha_4 = \frac{1}{2}\beta_3 = \alpha_1, \qquad \alpha_3 = \frac{1}{2}(\beta_3 + \beta_2) = \alpha_2.$$

The time stepsize is taken under the form  $T_0/N$  for  $N \in \mathbb{N}^*$ .

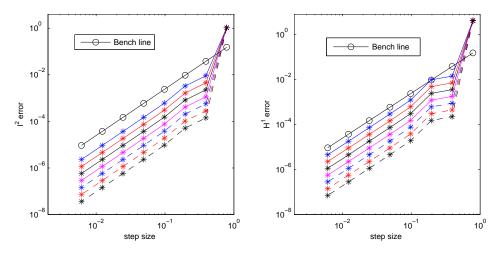


FIGURE 1. Time integration of (7.1) by Strang splitting method for  $\varepsilon = 2^{-6}, 2^{-7}, \ldots, 2^{-12}$  (lines from top to bottom). Global errors with respect to discrete  $L^2$ -norm (left) and discrete  $H^1$ -norm (right) versus time stepsizes. Bench line reflects slope p = 2.

**Space discretization.** For the space discretization, we apply the Fourier spectral method, that is, we employ the approximation

$$u^{\varepsilon}(x,t) \approx \sum_{-N_x/2+1}^{N_x/2} \widehat{u}_k^{\varepsilon}(t) e^{ikx}.$$

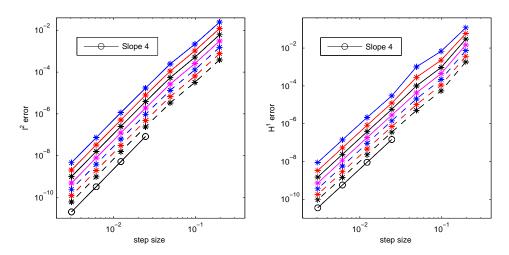


FIGURE 2. Time integration of (7.1) by fourth-order splitting method for  $2^{-3}, 2^{-4}, \ldots, 2^{-9}$  (lines from top to bottom). Global errors with respect to discrete  $L^2$ -norm (left) and discrete  $H^1$ -norm (right) versus time stepsizes. Bench line reflects slope p = 4.

The spectral coefficients are computed numerically by the trapezoidal rule. Setting  $N_x = 256$ , the error originating from the spatial discretization may be considered as negligible.

**Global error.** In view of our convergence result for the Strang splitting method and the extension to high-order splitting methods, see Theorem 6.1, we expect the global errors of the second- and fourth-order splitting methods to depend on the decisive parameter and the time stepsize in the following way

global error = 
$$\mathcal{O}(\varepsilon h^p)$$
.

As the prescribed initial value is highly regular, the exponent  $\sigma$  related to the Sobolev-regularity of the solution is large and the additional contribution  $\mathcal{O}(h^m)$  insignificant. In order to confirm this error behavior, we determine the global error of the discrete solution  $u^{\text{num}}$  with respect to the discrete  $H^s$ -norm

global error = 
$$\|u^{\text{num}}(T/\varepsilon) - u^{\text{ref}}(T/\varepsilon)\|_{H^s}$$
  
=  $\sqrt{\sum_{k=-N_x/2+1}^{N_x/2} (1+|k|^2)^s |\widehat{u_k^{\text{num}}}(T/\varepsilon) - \widehat{u_k^{\text{ref}}}(T/\varepsilon)|^2}.$ 

We in particular consider the discrete  $L^2$ -norm and the  $H^1$ -norm, respectively. The reference solution  $u^{\text{ref}}$  is computed by the fourth-order splitting method, applied with time stepsize  $\Delta t = T_0/10^4$ .

Numerical results (Strang). In Figure 1, we display the results obtained for the Strang splitting method. Each line corresponds to a fixed value of  $\varepsilon$ and shows the global errors with respect to the discrete  $L^2$ -norm and the discrete  $H^1$ -norm, respectively, versus the time stepsizes. The bench line of slope p = 2 reflects the second-order dependence on the time stepsize. Moreover, for a fixed value of the time stepsize, dividing  $\varepsilon$  by a factor two scales the error by this factor. Compared to the stronger discrete  $H^1$ -norm, the error measured with respect to the discrete  $L^2$ -norm is smaller, in accordance with the relation  $\|\cdot\|_{L^2} \leq \|\cdot\|_{H^1}$ . For better visibility, the obtained results illustrating the dependence of the global error on the parameter and the time stepsize are also included in Table 1.

Numerical results (Yoshida). The corresponding results for  $\varepsilon = 2^{-3}, 2^{-4}, \ldots, 2^{-9}$  and the fourth-order splitting method by Yoshida are given in Figure 2 and Table 2. The numerical results confirm the expected global error behavior  $\mathcal{O}(\varepsilon h^4)$ .

#### Acknowledgements

We acknowledge financial support by the Agence nationale de la recherche (ANR) within the Blanc International II Programme under project Modeling and Numerical Simulation of Low Dimensional Quantum Systems (LODI-QUAS), by the Austrian Science Fund (FWF) under SFP Vienna Computational Materials Laboratory (ViCoM) and project P21620-N13, and by the Austrian Ministry of Science and Research via its grant for the WPI.

h	$T_0/2^4$	$T_{0}/2^{5}$	$T_0/2^6$	$T_{0}/2^{7}$	$T_0/2^8$
$\varepsilon = 2^{-6}$	9.037E-3	3.279E-3	6.121E-4	1.489E-4	3.700E-5
$\varepsilon = 2^{-7}$	4.519E-3	1.639E-3	3.060E-4	7.444E-5	1.850E-5
$\varepsilon = 2^{-8}$	2.259E-3	8.196E-4	1.530E-4	3.722E-5	9.249E-6
$\varepsilon = 2^{-9}$	1.130E-3	4.098E-4	7.648E-5	1.861E-5	4.624E-6
$\varepsilon = 2^{-10}$	5.648E-4	2.049E-4	3.824E-5	9.304E-6	2.312E-6
$\varepsilon = 2^{-6}$	1.415E-2	9.691E-3	1.230E-3	2.930E-4	7.244 E-5
$\varepsilon = 2^{-7}$	7.077E-3	4.845E-3	6.142E-4	1.464E-4	$3.621 \text{E}{-5}$
$\varepsilon = 2^{-8}$	3.538E-3	2.423E-3	3.071E-4	7.319E-5	1.810E-5
$\varepsilon = 2^{-9}$	1.769E-3	1.211E-3	1.535E-4	$3.660 \text{E}{-5}$	9.052 E-6
$\varepsilon = 2^{-10}$	8.846E-4	6.056E-4	7.676E-5	1.830E-5	4.526E-6

TABLE 1. Time integration of (7.1) by Strang splitting method for  $\varepsilon = 2^{-6}, 2^{-7}, \ldots, 2^{-12}$ . Global errors with respect to discrete  $L^2$ -norm (up) and discrete  $H^1$ -norm (down) versus time stepsizes.

h	$T_0/2^4$	$T_{0}/2^{5}$	$T_{0}/2^{6}$	$T_{0}/2^{7}$	$T_{0}/2^{8}$	$T_{0}/2^{9}$	$T_0/2^{10}$
$\varepsilon = 2^{-3}$	4.77E-2	2.46E-2	2.19E-3	2.45E-4	1.71E-5	1.14E-6	7.25E-8
$\varepsilon = 2^{-4}$	2.37E-2	1.23E-2	1.04E-3	1.10E-4	7.85E-6	5.11E-7	3.23E-8
$\varepsilon = 2^{-5}$	1.18E-2	6.15E-3	5.18E-4	5.39E-5	3.83E-6	2.48E-7	1.56E-8
$\varepsilon = 2^{-6}$	5.92E-3	3.07E-3	2.58E-4	2.67E-5	1.90E-6	1.23E-7	7.75E-9
$\varepsilon = 2^{-7}$	2.96E-3	1.53E-3	1.29E-4	1.33E-5	9.51E-7	6.14E-8	3.87E-9
$\varepsilon = 2^{-8}$	1.48E-3	7.69E-4	6.44E-5	6.67E-6	4.75E-7	3.07E-8	1.93E-9
$\varepsilon = 2^{-9}$	7.40E-4	3.84E-4	3.22E-5	3.33E-6	2.37E-7	1.53E-8	9.67E-10
$\varepsilon = 2^{-3}$	2.14E-1	1.19E-1	6.80E-3	1.02E-3	2.98E-5	2.13E-6	1.40E-7
$\varepsilon = 2^{-4}$	1.06E-1	5.92E-2	2.28E-3	2.83E-4	1.23E-5	8.23E-7	5.27E-8
$\varepsilon = 2^{-5}$	5.30E-2	2.96E-2	9.49E-4	9.92E-5	5.79E-6	3.77E-7	2.39E-8
$\varepsilon = 2^{-6}$	2.65E-2	1.48E-2	4.47E-4	4.29E-5	2.85E-6	1.84E-7	1.16E-8
$\varepsilon = 2^{-7}$	1.32E-2	7.38E-3	2.20E-4	2.05E-5	1.42E-6	9.15E-8	5.76E-9
$\varepsilon = 2^{-8}$	6.62E-3	3.69E-3	1.10E-4	1.02E-5	7.09E-7	4.57E-8	2.87E-9
$\varepsilon = 2^{-9}$	3.31E-3	1.85E-3	5.48E-5	5.06E-6	3.55E-7	2.28E-8	1.44E-9

TABLE 2. Time integration of (7.1) by fourth-order splitting method for  $2^{-3}, 2^{-4}, \ldots, 2^{-9}$ . Global errors with respect to discrete  $L^2$ -norm (up) and discrete  $H^1$ -norm (down) versus time stepsizes.

The presented numerical results have been achieved by using the Vienna Scientific Cluster.

#### References

- S. ALINHAC, P. GÉRARD, Pseudo-differential Operators and Nash-Moser Theorem. Graduate Studies in Mathematics, Vol. 82, American Mathematical Society, Providence, Rhode Island, 2007.
- F. CASTELLA, P. CHARTIER, F. MÉHATS, A. MURUA, Stroboscopic averaging for the nonlinear Schrödinger equation. Found. Comput. Math 15 (2015) 519–559.
- 3. L. GAUCKLER, Convergence of a split-step Hermite method for the Gross-Pitaevskii equation. IMA J. Numer. Anal. 31 (2011) 396-415.

- CHR. LUBICH, On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations. Math. Comp. 77 (2008) 2141-2153.
- C. MUSCALU, W. SCHLAG, Classical and multilinear harmonic analysis. Vol. II. Cambridge Studies in Advanced Mathematics, 138. Cambridge University Press, Cambridge, 2013.
- J.A.C. WEIDEMAN, B.M. HERBST, Split-step methods for the solution of the nonlinear Schrödinger equation. SIAM J. Numer. Anal. 23 (1986) 485-507.
- H. YOSHIDA, Construction of higher order symplectic integrators. Phys. Lett. A 150 (1990) 262–268.

#### APPENDIX A. AUXILIARY RESULTS

Elementary result for periodic functions. In the sequel, we state an elementary result on the approximation by Riemann sums for periodic functions, see (1.6) for the definition of  $F_{\tau}$ .

**Lemma A.1.** For given h > 0 and  $n \in \mathbb{N}$  such that  $nh = T_0 = 1$ , let

(A.1) 
$$E_{Rie}(u,h) = \frac{1}{n} \sum_{\ell=0}^{n-1} F_{\ell h}(u) - \int_0^1 F_{\tau}(u) d\tau$$

denote the error in the approximation of the integral by its Riemann sum. Then, the following estimate holds with  $m = |\sigma/2|$ 

(A.2) 
$$||E_{Rie}(u,h)||_{H^{\sigma-2m}} \le 2^{1-m}\pi^{-m}\zeta(m)h^m \sup_{\tau\in[0,1]} ||\partial_{\tau}^m F_{\tau}(u)||_{H^{\sigma-2m}}.$$

*Proof.* Our starting point is the Fourier expansion of  $F_{\tau}$ 

$$\sum_{k\in\mathbb{Z}}e^{i2\pi k\tau}\hat{F}_k(u).$$

By the definition of the Fourier coefficients, we have

$$\int_0^1 F_\tau(u)d\theta = \hat{F}_0(u).$$

The numerical counterpart is

$$\frac{1}{n} \sum_{\ell=0}^{n-1} F_{\ell h}(u) = \frac{1}{n} \sum_{\ell=0}^{n-1} \sum_{k \in \mathbb{Z}} e^{i2\pi\ell kh} \hat{F}_k(u)$$
$$= \sum_{k \in \mathbb{Z}} \frac{1}{n} \sum_{\ell=0}^{n-1} e^{i2\pi k\ell h} \hat{F}_k(u)$$
$$= \sum_{q \in \mathbb{Z}} \hat{F}_{nq}(u).$$

Hence, we obtain

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

Owing to the regularity of  $F_{\tau}$ 

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

we have

$$\begin{aligned} \|E_{Rie}(u,h)\|_{H^{\sigma-2m}} &\leq 2 \sup_{\tau \in [0,1]} \|\partial_{\tau}^{m} F_{\tau}(u)\|_{H^{\sigma-2m}} \sum_{q \in \mathbb{N}^{*}} (2\pi nq)^{-m} \\ &= 2(2\pi n)^{-m} \zeta(m) \sup_{\tau \in [0,1]} \|\partial_{\tau}^{m} F_{\tau}(u)\|_{H^{\sigma-2m}}. \end{aligned}$$

This is the stated result.

**Products and functions in Sobolev spaces.** The fractional Leibniz rule for functions defined on a *d*-dimensional torus follows from the standard fractional Leibniz rule for functions defined on  $\mathbb{R}^d$ .

**Lemma A.2** (See [5]). Assume s > 0, and let  $p, q_1, q_2, p_1, p_2 \in (1, \infty)$  be such that  $\frac{1}{p} = \frac{1}{p_1} + \frac{1}{q_1} = \frac{1}{p_2} + \frac{1}{q_2}$ . Then, for all elements  $u \in L^{p_1}(\mathbb{T}^d) \cap W^{s,q_2}(\mathbb{T}^d)$  and  $v \in L^{p_2}(\mathbb{T}^d) \cap W^{s,q_1}(\mathbb{T}^d)$ , the following estimate holds with constant  $\alpha > 0$ 

(A.3) 
$$\|uv\|_{W^{s,p}} \le \alpha \|u\|_{L^{p_1}} \|v\|_{W^{s,q_1}} + \alpha \|u\|_{W^{s,q_2}} \|v\|_{L^{p_2}}$$

The relation remains valid for exponents  $p \in [1, \infty)$  and  $p_1, p_2, q_1, q_2 \in (1, \infty]$ .

The following auxiliary result is used in Section 2.

**Lemma A.3.** Assume  $\sigma > \frac{d}{2}$  and  $s \in [0, \sigma]$ . Then, for all elements  $u \in H^s(\mathbb{T}^d)$  and  $v \in H^{\sigma}(\mathbb{T}^d)$ , the relation

(A.4) 
$$||uv||_{H^s} \le \kappa ||u||_{H^s} ||v||_{H^\sigma}$$

holds. Moreover, for any function  $f \in C^1(\mathbb{R}, \mathbb{R})$  and for all elements  $u, v \in B_R^{\sigma}$  the estimate

(A.5) 
$$||f(u) - f(v)||_{H^s} \le \alpha(f, R) ||u - v||_{H^s}$$

is valid.

*Proof.* We recall that, for any  $\sigma > \frac{d}{2}$ , the continuous Sobolev embedding  $H^{\sigma}(\mathbb{T}^d) \hookrightarrow L^{\infty}(\mathbb{T}^d)$  holds, that is  $\|v\|_{L^{\infty}} \leq c \|v\|_{H^{\sigma}}$ . 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 (A.4). If  $s > \frac{d}{2}$ , the result is well-known, since  $H^s(\mathbb{T}^d)$  is an algebra. If  $0 < s < \frac{d}{2}$ , we apply (A.3) with the admissible set of exponents p = 2,  $p_1 = \frac{2d}{d-2s}$ ,  $q_1 = \frac{d}{s}$ ,  $p_2 = \infty$ ,  $q_2 = 2$ , and use the Sobolev embeddings  $H^{\sigma}(\mathbb{T}^d) \hookrightarrow L^{\infty}(\mathbb{T}^d)$ ,  $H^s(\mathbb{T}^d) \hookrightarrow L^{p_1}(\mathbb{T}^d)$ , and  $H^{\sigma}(\mathbb{T}^d) \hookrightarrow W^{s,q_1}(\mathbb{T}^d)$ . We then have

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

which proves (A.4). If  $s = \frac{d}{2}$ , we obtain the same estimate by applying (A.3) with p = 2,  $p_1 = \frac{1}{\mu}$ ,  $q_1 = \frac{2}{1-2\mu}$ ,  $p_2 = \infty$ ,  $q_2 = 2$ , for  $\mu > 0$  small enough,

such that we also have the embeddings  $H^s(\mathbb{T}^d) \hookrightarrow L^{p_1}(\mathbb{T}^d)$  and  $H^{\sigma}(\mathbb{T}^d) \hookrightarrow W^{s,q_1}(\mathbb{T}^d)$ . Next, to prove (A.5), we employ the identity

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

and apply a tame estimate in  $H^{\sigma}(\mathbb{T}^d)$ , see (2.5). Hence, employing the first estimate, this yields

$$\|f(u) - f(v)\|_{H^s} \le \int_0^1 \|f'(tu + (1-t)v)(u-v)\|_{H^s} dt$$
  
$$\le \int_0^1 \|f'(tu + (1-t)v)\|_{H^\sigma} \|u-v\|_{H^s} dt$$
  
$$\le (\|f'(0)\|_{H^\sigma} + \chi_{f'}(cR)R) \|u-v\|_{H^s}$$

and completes the proof.

INRIA-RENNES, IRMAR, ENS CACHAN BRETAGNE, IPSO PROJECT TEAM, CAMPUS DE BEAULIEU, 35042 RENNES CEDEX, FRANCE.

*E-mail address*: Philippe.Chartier@inria.fr

IRMAR, UNIVERSITE DE RENNES 1, INRIA-RENNES, IPSO PROJECT TEAM, CAM-PUS DE BEAULIEU, 35042 RENNES CEDEX, FRANCE. *E-mail address*: Florian.Mehats@univ-rennes1.fr

LEOPOLD-FRANZENS UNIVERSITÄT INNSBRUCK, INSTITUT FÜR MATHEMATIK, TECH-NIKERSTRASSE 13/VII, 6020 INNSBRUCK, AUSTRIA.

 $E\text{-}mail\ address:\ \texttt{Mechthild.ThalhammerCuibk.ac.at}$ 

WOLFGANG PAULI INSTITUT C/O UNIVERSITÄT WIEN, FAKULTÄT FÜR MATHEMATIK, OSKAR-MORGENSTERN-PLATZ 1, 1090 VIENNA, AUSTRIA. *E-mail address*: Yong.Zhang@univie.ac.at