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The Lie–Trotter splitting for nonlinear evolutionary problems with critical parameters: a compact local error representation and application to nonlinear Schrödinger equations in the semiclassical regime

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In the present work, the error behaviour of the first-order Lie–Trotter splitting method for nonlinear evolutionary problems is analysed. In particular, a local error representation that is suitable in the presence of unbounded nonlinear operators and critical parameters is deduced. Such local error expansions together with stability bounds are the basic ingredients in the derivation of convergence estimates. Essential tools in the theoretical analysis are an abstract formulation of differential equations on function spaces and the formal calculus of Lie derivatives. In order to illustrate the general approach, the application of the Lie–Trotter splitting method to Schrödinger equations in the semiclassical regime is studied. From numerical computations presented in the literature, it is expected that exponential operator splitting methods are favourable for the time integration of nonlinear Schrödinger equations, provided that the time-step size is suitably chosen depending on the magnitude of the critical parameter. For the least technical example method, the first-order Lie–Trotter splitting method, this is substantiated by theoretical considerations for the time-dependent Gross–Pitaevskii equation and confirmed by numerical examples. Numerical illustrations for higher-order exponential operator splitting methods complement the considerations.

Keywords: nonlinear evolutionary problems; time-dependent nonlinear Schrödinger equations; semiclassical regime; exponential operator splitting methods; Lie–Trotter splitting; local error; convergence.

1. Introduction

In this work, our concern is to contribute to the investigation of exponential operator splitting methods for the time integration of abstract nonlinear evolutionary problems

$$\begin{cases} u'(t) = A(u(t)) + B(u(t)), \quad 0 \leqslant t \leqslant T, \\ u(0) \text{ given}; \end{cases} \tag{1.1}$$

for detailed information on abstract evolution equations see Engel & Nagel (2000), Henry (1981), Hille & Phillips (1957), Lunardi (1995); Pazy (1983), and for the investigation and application of splitting

methods see Bao, Jaksch & Markowich (2003), Bao & Shen (2005), Blanes & Moan (2002), Caliari *et al.* (2009), Chin (2007), Descombes *et al.* (2007), Hairer *et al.* (2002), Iserles & Kropielnicka (2011), Jahnke & Lubich (2000), Lubich (2008), McLachlan & Quispel (2002), Pérez-García & Liu (2003); Thalhammer (2008). In particular, our objective is the derivation of a local error representation that is well suited in the presence of unbounded nonlinear operators and critical parameters. A most useful tool for this purpose is the formal calculus of Lie derivatives, which is suggestive of the less involved linear case studied in Descombes & Schatzman (2002) and Descombes & Thalhammer (2010). In order to elucidate the general mechanism, we focus on the least technical example method: the first-order Lie–Trotter splitting method.

In comparison with other local error expansions for splitting methods that are based on the Baker–Campbell–Hausdorff formula (see Iserles & Kropielnicka, 2011) or based on the techniques exploited in Gauckler (2010), Jahnke & Lubich (2000), Lubich (2008) and Thalhammer (2008) in the context of time-dependent Schrödinger equations, the approach presented allows us to capture correctly the error behaviour of time-splitting methods for nonlinear evolutionary problems involving unbounded nonlinear operators and critical parameters. In particular, our theoretical analysis applies to time-dependent nonlinear Schrödinger equations in the semiclassical regime.

As a model problem, we consider the following time-dependent nonlinear Schrödinger equation for $\psi : \mathbb{R}^d \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$:

$$\begin{cases} \mathrm{i}\varepsilon \partial_t \psi(x,t) = -\frac{1}{2}\varepsilon^2 \Delta \psi(x,t) + U(x)\psi(x,t) + \vartheta |\psi(x,t)|^2 \psi(x,t), \\ \psi(x,0) \text{ given}, \quad x \in \mathbb{R}^d, \quad 0 \leqslant t \leqslant T, \end{cases} \tag{1.2}$$

with (small) parameter $\varepsilon > 0$, real-valued external potential $U : \mathbb{R}^d \to \mathbb{R}$ and coupling constant $\vartheta \in \mathbb{R}$, imposing asymptotic boundary conditions on the unbounded domain. The above problem is related to the time-dependent Gross–Pitaevskii equation (see Gross, 1961; Pitaevskii, 1961) which arises in the description of the macroscopic wave function of a Bose–Einstein condensate. Employing an abstract formulation of ordinary differential equations on function spaces, the initial–boundary value problem (1.2) takes the form (1.1) with unbounded linear operator A comprising the Laplacian (and part of the potential) and unbounded nonlinear multiplication operator B involving (part of) the potential and the cubic nonlinearity.

The incentive for this work originates from the question of whether exponential operator splitting methods are favourable for nonlinear evolutionary Schrödinger equations in the semiclassical regime; our interest in this theme is inspired by theoretical and numerical investigations for the first-order Lie–Trotter splitting method and the second-order Strang splitting method provided by Bao *et al.* (2002); Bao, Jin & Markowich (2003) and Faou *et al.* (2009); see also the references given therein.

Numerical comparisons (e.g., given in Bao, Jaksch & Markowich, 2003; Pérez-García & Liu, 2003; Bao & Shen, 2005; Caliari *et al.*, 2009) for nonlinear Schrödinger equations such as (1.2) with $\varepsilon = 1$, show that higher-order splitting schemes are superior to standard integrators when low tolerances are required or long-term integrations are carried out. These numerical observations are also confirmed by theoretical investigations. For instance, for an exponential operator splitting method of (nonstiff) order p, applied to a linear evolutionary Schrödinger equation involving a sufficiently regular bounded potential, the local error expansion exploited in Jahnke & Lubich (2000) and Thalhammer (2008) leads to an error estimate of the form

$$\|u_N - u(t_N)\|_{L^2} \leqslant C(\|u_0 - u(0)\|_{L^2} + h^p \|u(0)\|_{H^p}).$$

Here, as standard, we denote by $(u_n)_{n=0}^N$, the numerical approximation values at the equidistant grid points $t_n = nh$ for $0 \leqslant n \leqslant N$ with time-step size $h = T/N$. As underlying function spaces, we consider the Lebesgue space $L^2(\mathbb{R}^d)$ and the Sobolev space $H^p(\mathbb{R}^d)$; for the definition of the associated norms, see (1.5). In the context of nonlinear Schrödinger equations a seminal contribution is Lubich (2008), where a convergence estimate for the second-order Strang splitting method is derived; main tools in the error analysis are the formal calculus of Lie derivatives and bounds for Lie commutators of the involved nonlinear operators.

However, for small parameter values $0 < \varepsilon \ll 1$, the above-mentioned approach is *not* appropriate to provide optimal local and global error bounds with respect to ε. For instance, in the linear case, the remainder arising in the local error expansion involves $(p+1)$ applications of the operator $B = (1/\varepsilon)U$ implying dependence $\mathcal{O}(1/\varepsilon^{p+1})$ on the critical parameter which is *not* in accordance with numerical experiments. Thus, different techniques are needed for a better theoretical understanding of the error behaviour of exponential operator splitting methods for evolutionary problems and the dependence of the admissible time-step size on the critical parameter.

In our previous work, Descombes & Thalhammer (2010), which is concerned with a local error representation for splitting methods applied to linear equations, we followed an alternative approach based on the derivation of differential equations for splitting operators. In particular, for linear Schrödinger equations and classical Wentzel–Kramers–Brillouin initial values that satisfy the condition $\varepsilon^j \|u(0)\|_{H^j} \leqslant M_j$ with a constant $M_j > 0$ for $0 \leqslant j \leqslant p$, the convergence estimate

$$\|u_N - u(t_N)\|_{L^2} \leqslant \|u_0 - u(0)\|_{L^2} + C\frac{h^p}{\varepsilon}$$

results with constant $C > 0$ depending on M_j, $0 \leqslant j \leqslant p$, L^∞ bounds for the partial derivatives of the potential U (up to order $2p$), and the end time t_N; this dependence $\mathcal{O}(h^p/\varepsilon)$ of the global error on the time-step size h and the critical parameter ε is also confirmed by numerical examples.

In the present paper, we extend the error analysis of Descombes & Thalhammer (2010) for linear equations to nonlinear problems (1.1). In order to illustrate the general mechanism, we focus on the least technical example: the first-order Lie–Trotter splitting method

$$\begin{cases} u_n = e^{hD_A}\, e^{hD_B} u_{n-1}, \quad 1 \leqslant n \leqslant N, \\ u_0 \text{ given.} \end{cases} \tag{1.3}$$

Here, D_F denotes the Lie derivative and e^{tD_F} the nonlinear evolution operator associated with the nonlinear differential equation $u'(t) = F(u(t))$, that is, $u(t) = e^{tD_F}u(0)$ (see below). In the case of the Lie–Trotter splitting method, our approach will lead to a compact local error representation, which is advantageous for further investigation with regard to nonlinear Schrödinger equations such as (1.2). Indeed, the defect operator of the Lie–Trotter splitting method (1.3) possesses the representation

$$\mathscr{L}(t,v) = e^{tD_A}\, e^{tD_B} v - e^{D_{A+B}} v = \int_0^t \int_0^{\tau_1} e^{\tau_1 D_A}\, e^{\tau_2 D_B} [D_A, D_B]\, e^{(\tau_1-\tau_2)D_B}\, e^{(t-\tau_1)D_{A+B}} v \,\mathrm{d}\tau_2\,\mathrm{d}\tau_1. \tag{1.4}$$

In particular, for linear operators A and B the above formula reduces to

$$\mathscr{L}(t,v) = (e^{tB}\, e^{tA} - e^{t(A+B)})v = \int_0^t \int_0^{\tau_1} e^{(t-\tau_1)(A+B)}\, e^{(\tau_1-\tau_2)B}\, [B,A]\, e^{\tau_2 B}\, e^{\tau_1 A} v \,\mathrm{d}\tau_2\,\mathrm{d}\tau_1.$$

Note that in the formal calculus of Lie derivatives, the sequence of the compositions of evolution operators and Lie derivatives is reversed. Local error representations such as (1.4) are an essential ingredient in the derivation of a global error estimate for exponential operator splitting methods applied to nonlinear evolution equations.

The structure of the present work and the main results are as follows: in a first part, we elucidate the general approach, and, in a second part, we discuss the application to nonlinear Schrödinger equations of the form (1.2). In Section 2, we state the abstract nonlinear evolutionary problem and introduce the formal calculus of Lie derivatives. Furthermore, we specify the considered class of exponential operator splitting methods. Section 3 is devoted to the derivation of a local error representation, suitable in the presence of critical parameters; we give a detailed derivation involving marginal technicalities for the first-order Lie–Trotter splitting method and indicate the generalization to high-order methods. We first deduce the statement of Theorem 3.1 by employing standard techniques and notation and then comment on a formal extension of the linear case using the calculus of Lie derivatives. Applications to nonlinear Schrödinger equations in the semiclassical regime are the contents of Section 4. Theoretical considerations, also confirmed by numerical illustrations, imply that the Lie–Trotter splitting method is favourable for the time integration of the Gross–Pitaevskii equation, provided that the time-step sizes are chosen sufficiently small; for a single time step, in the case of a regular initial condition with bounded spatial derivatives, independent of the critical parameter $0 < \varepsilon \ll 1$, time-step sizes of the magnitude of ε are needed, whereas for an initial condition in classical Wentzel–Kramers–Brillouin form, time-step sizes sufficiently smaller than the critical parameter are required. For higher-order exponential operator splitting methods, improved accuracy properties are observed.

Since in the present work, the focus is on the least technical example method (the first-order Lie-Trotter splitting method), we occasionally favour standard notation to the formal calculus of Lie derivatives. In Section 3, the formal calculations are carried out under the tacit requirement that the arising unbounded operators and compositions thereof are well defined on suitably chosen domains and time intervals. The specialization to the time-dependent Gross–Pitaevskii equation is then given in Section 4. Throughout, we denote by $C > 0$ a generic constant, possibly taking different values at different occurrences. As usual, the Lebesgue space $L^2(\Omega) = L^2(\Omega, \mathbb{C})$ of square-integrable complex-valued functions $f : \Omega \subset \mathbb{R}^d \to \mathbb{C}$ is endowed with an inner product $(\cdot|\cdot)_{L^2}$ and the corresponding norm $\|\cdot\|_{L^2}$, given by

$$(f|g)_{L^2} = \int_\Omega f(x)\overline{g(x)}\,\mathrm{d}x, \quad \|f\|_{L^2} = \sqrt{(f|f)_{L^2}}, \ f, g \in L^2(\Omega). \tag{1.5a}$$

The Sobolev space $H^m(\Omega)$ comprises all functions with partial derivatives up to order $m \geqslant 0$ contained in $L^2(\Omega)$, where, in particular, $H^0(\Omega) = L^2(\Omega)$; the associated norm $\|\cdot\|_{H^m}$ is defined through

$$\|f\|_{H^m}^2 = \sum_{\substack{j=(j_1,\dots,j_d)\in\mathbb{N}^d \\ j_1+\cdots+j_d\leqslant m}} \|\partial^j f\|_{L^2}^2, \quad f \in H^m(\Omega). \tag{1.5b}$$

Detailed information on Sobolev spaces is found in the monograph of Adams (1978).

2. Splitting methods for nonlinear evolutionary problems

In this section, we state the abstract nonlinear evolutionary problem, and, for the convenience of the reader, recall the defining relations for the Lie derivative; we point out that the evolution operator and the associated Lie derivative are introduced in such a way that the formalism is appropriate in the context of

unbounded operators. Further, we state the general form of the considered exponential operator splitting methods. For detailed information, we refer to the monographs of Engel & Nagel (2000), Hairer *et al.* (2002), Henry (1981) and Sanz-Serna & Calvo (1994).

2.1 *Nonlinear evolutionary problems*

In the present work, we consider an initial value problem of the form

$$\begin{cases} u'(t) = F(u(t)), \quad 0 \leqslant t \leqslant T, \\ u(0) \text{ given}, \end{cases} \tag{2.1a}$$

where the structure of the unbounded nonlinear operator $F : D(F) \subset X \to X$ suggests a decomposition into two parts with unbounded nonlinear operators $A : D(A) \subset X \to X$ and $B : D(B) \subset X \to X$:

$$F(v) = A(v) + B(v), \quad v \in D(A) \cap D(B); \tag{2.1b}$$

throughout, we tacitly require that the domains are suitably chosen subspaces of the underlying Banach space $(X, \|\cdot\|_X)$ such that $D(F) = D(A) \cap D(B) \neq \emptyset$.

The exact solution of the evolutionary problem (2.1) is (formally) given by

$$u(t) = \mathscr{E}_F(t, u(0)), \quad 0 \leqslant t \leqslant T, \tag{2.2a}$$

with evolution operator $\mathscr{E}_F$ depending on the actual time and the initial value; as the differential equation in (2.1a) is supposed to be autonomous, we may neglect the dependence on the initial time. Besides, we employ the formal notation

$$u(t) = e^{tD_F} u(0), \quad 0 \leqslant t \leqslant T, \tag{2.2b}$$

which is suggestive of the (less involved) linear case. Here, the evolution operator e^{tD_F} and the Lie derivative D_F associated with F are given by

$$e^{tD_F} Gv = G(\mathscr{E}_F(t, v)), \quad 0 \leqslant t \leqslant T, \quad D_F Gv = G'(v)F(v), \tag{2.3a}$$

for any unbounded nonlinear operator $G : D(G) \subset X \to X$ with Fréchet derivative G'; whenever G is the identity operator, we write

$$e^{tD_F} v = \mathscr{E}_F(t, v), \quad 0 \leqslant t \leqslant T, \quad D_F v = F(v) \tag{2.3b}$$

for short. It is notable that the relation $D_F = (\mathrm{d}/\mathrm{d}t)|_{t=0}\, e^{tD_F}$ holds since $(\mathrm{d}/\mathrm{d}t)\mathscr{E}_F(t, v) = F(\mathscr{E}_F(t, v))$ and $\mathscr{E}_F(0, v) = v$ and thus by the chain rule,

$$\left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} e^{tD_F} Gv = \left.\frac{\mathrm{d}}{\mathrm{d}t}\right|_{t=0} G(\mathscr{E}_F(t, v)) = G'(\mathscr{E}_F(t, v))F(\mathscr{E}_F(t, v))|_{t=0} = G'(v)F(v) = D_F Gv.$$

This is in accordance with the identity $Lv = \mathrm{d}/\mathrm{d}t|_{t=0}\, e^{tL} v$, which is valid, for instance, for any bounded linear operator $L : X \to X$ with the exponential function defined by the power series and also extendable to the framework of unbounded linear operators generating a strongly continuous (semi)group.

2.2 *Exponential operator splitting methods*

For the time discretization of the nonlinear evolutionary problem (2.1), we consider the first-order Lie–Trotter splitting method, or, more generally, an exponential operator splitting method of (nonstiff) order $p \geqslant 1$ involving $s \geqslant 1$ compositions (stages). We employ the following general formulation that includes various example methods proposed in the literature.

For some integer $N \in \mathbb{N}$, we let $h = T/N$ denote the time-step size and $t_n = nh$ for $0 \leqslant n \leqslant N$ the associated equidistant time grid points. Starting from an initial value $u_0 \approx u(0)$, numerical approximations u_n to the exact solution values $u(t_n)$ are determined through a recurrence relation of the form

$$\begin{cases} u_n = \mathscr{S}(h, u_{n-1}), \quad 1 \leqslant n \leqslant N, \\ u_0 \text{ given}; \end{cases} \tag{2.4a}$$

here, the splitting operator $\mathscr{S}$ is defined through

$$\mathscr{S}(t, v) = e^{a_1 t D_A}\, e^{b_1 t D_B} \cdots e^{a_s t D_A}\, e^{b_s t D_B} v, \quad 0 \leqslant t \leqslant T, \tag{2.4b}$$

and involves the real method coefficients $(a_j, b_j)_{j=1}^{s}$; see also (2.3).

Low-order example methods that can be cast into the scheme (2.4) are the first-order Lie–Trotter splitting method (1.3), where $p = s = a_1 = b_1 = 1$, and the widely used second-order symmetric Lie–Trotter or Strang splitting method, where

$$p = s = 2, \quad a_1 = a_2 = \tfrac{1}{2}, \quad b_1 = 1, \quad b_2 = 0; \tag{2.5}$$

see Strang (1968) and Trotter (1959). Example methods of higher order that were proposed in the literature are reviewed in Hairer *et al.* (2002) and McLachlan & Quispel (2002); for numerical comparisons of fourth- and sixth-order splitting methods in the context of Schrödinger equations, see also Caliari *et al.* (2009) and the references given therein.

3. Local error of the Lie–Trotter splitting method

In the following, our concern is to deduce an appropriate local error expansion for exponential operator splitting methods (2.4):

$$\mathscr{L}(t, v) = \mathscr{S}(t, v) - \mathscr{E}_F(t, v) = e^{a_1 t D_A}\, e^{b_1 t D_B} \cdots e^{a_s t D_A}\, e^{b_s t D_B} v - e^{t D_F} v, \quad 0 \leqslant t \leqslant T; \tag{3.1}$$

in view of applications to time-dependent nonlinear Schrödinger equations in the semiclassical regime, it is essential that the local error representation remains valid for evolutionary problems (2.1) involving unbounded nonlinear operators and critical parameters. In Section 3.1, we give a detailed depiction of the first-order Lie–Trotter splitting method (1.3) involving marginal technicalities and then indicate the generalization to high-order methods utilizing a formal extension of the linear case studied in Descombes & Thalhammer (2010) by the calculus of Lie derivatives; to keep the presentation tight, several auxiliary results are collected in Section 3.2.

Below, we employ the following notation: recall that the Fréchet derivative of a nonlinear operator $G : D(G) \subset X \to X$ is denoted by G'. The Lie bracket of the nonlinear operators G and H is defined

through

$$[G,H](v) = G'(v)H(v) - H'(v)G(v); \tag{3.2a}$$

clearly, for linear operators G and H, due to $G'(v) = G$ as well as $H'(v) = H$, the above relation reduces to $[G,H](v) = [G,H]v = (GH - HG)v$. In accordance with (3.2a), we further set

$$[D_G, D_H]v = D_G D_H v - D_H D_G v \tag{3.2b}$$

(see (2.3) for the definition of the Lie derivative); note that $[D_G, D_H]v = -[G,H](v)$.

3.1 *A compact local error representation*

For the Lie–Trotter splitting method (1.3), the splitting operator (2.4b) simplifies to

$$\mathscr{S}(t,v) = e^{tD_A}\, e^{tD_B} v = \mathscr{E}_B(t, \mathscr{E}_A(t,v)), \quad 0 \leqslant t \leqslant T. \tag{3.3}$$

With regard to the primal initial value problem

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_F(t,v) = F(\mathscr{E}_F(t,v)), \quad 0 \leqslant t \leqslant T, \\ \mathscr{E}_F(0,v) = v \end{cases} \tag{3.4}$$

(see also (2.1) and (2.2)), we determine the time derivative of (3.3) and rewrite it as

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(t,v) &= B(\mathscr{E}_B(t, \mathscr{E}_A(t,v))) + \partial_2 \mathscr{E}_B(t, \mathscr{E}_A(t,v)) A(\mathscr{E}_A(t,v)) \\ &= F(\mathscr{S}(t,v)) + \partial_2 \mathscr{E}_B(t, \mathscr{E}_A(t,v)) A(\mathscr{E}_A(t,v)) - A(\mathscr{S}(t,v)); \end{aligned}$$

consequently, we obtain the initial value problem

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}(t,v) = F(\mathscr{S}(t,v)) + R(t,v), \quad 0 \leqslant t \leqslant T, \\ \mathscr{S}(0,v) = v, \end{cases} \tag{3.5a}$$

which involves the time-dependent remainder

$$R(t,v) = \partial_2 \mathscr{E}_B(t, \mathscr{E}_A(t,v)) A(\mathscr{E}_A(t,v)) - A(\mathscr{S}(t,v)), \quad 0 \leqslant t \leqslant T. \tag{3.5b}$$

In order to relate the solutions of the initial value problems (3.4) and (3.5), we apply the nonlinear variation-of-constants formula (see Theorem 3.3); this yields the following relation for the defect operator:

$$\mathscr{L}(t,v) = \int_0^t \partial_2 \mathscr{E}_F(t-\tau_1, \mathscr{S}(\tau_1,v)) R(\tau_1,v)\, \mathrm{d}\tau_1, \quad 0 \leqslant t \leqslant T;$$

see (3.1). Furthermore, by Lemma 3.4, we obtain the identity

$$\begin{aligned} R(\tau_1,v) &= \partial_2 \mathscr{E}_B(\tau_1, \mathscr{E}_A(\tau_1,v)) A(\mathscr{E}_A(\tau_1,v)) - A(\mathscr{E}_B(\tau_1, \mathscr{E}_A(\tau_1,v))) \\ &= \int_0^{\tau_1} \partial_2 \mathscr{E}_B(\tau_1 - \tau_2, \mathscr{E}_A(\tau_1,v)) [B,A](\mathscr{E}_B(\tau_2, \mathscr{E}_A(\tau_1,v)))\, \mathrm{d}\tau_2, \quad 0 \leqslant \tau_1 \leqslant t \leqslant T; \end{aligned}$$

see also (3.2) and (3.5b). Altogether, the above considerations imply the following local error representation; for a justification of the compact formal notation, we apply Lemma 3.5 with $G_1 = H_1 = A$, $G_2 = G_3 = H_2 = B$, $G_4 = F$, $t_\ell = \tau_\ell$, $\ell = 1, 2$, $t_3 = \tau_1 - \tau_2$ and $t_4 = t - \tau_1$; see also (2.3).

THEOREM 3.1 (Local error representation, Lie–Trotter splitting) For the nonlinear evolutionary problem (2.1) the defect operator (3.1) of the first-order Lie–Trotter splitting method (1.3) possesses the integral representation

$$\begin{aligned}\mathscr{L}(t,v) &= \int_0^t \int_0^{\tau_1} e^{\tau_1 D_A}\, e^{\tau_2 D_B}[D_A, D_B]\, e^{(\tau_1-\tau_2)D_B}\, e^{(t-\tau_1)D_F} v \,\mathrm{d}\tau_2\,\mathrm{d}\tau_1 \\ &= \int_0^t \int_0^{\tau_1} \partial_2 \mathscr{E}_F(t-\tau_1, \mathscr{S}(\tau_1, v))\partial_2 \mathscr{E}_B(\tau_1-\tau_2, \mathscr{E}_A(\tau_1, v)) \\ &\quad \times [B,A](\mathscr{E}_B(\tau_2, \mathscr{E}_A(\tau_1, v)))\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1, \quad 0 \leqslant t \leqslant T.\end{aligned}$$

REMARK 3.2 (i) In accordance with Descombes & Thalhammer (2010), for initial value problems (2.1) involving unbounded linear operators, the local error representation of Theorem 3.1 reduces to

$$\mathscr{L}(t,v) = \int_0^t \int_0^{\tau_1} e^{(t-\tau_1)(A+B)}\, e^{(\tau_1-\tau_2)B}[B,A] e^{\tau_2 B}\, e^{\tau_1 A} v \,\mathrm{d}\tau_2\,\mathrm{d}\tau_1, \quad 0 \leqslant t \leqslant T.$$

Simplistically, replacing the operators A and B by the associated Lie derivatives D_A and D_B and reversing the order, the result for the nonlinear case is obtained.

(ii) In Section 4.2, we study the local error representation for the Lie–Trotter splitting method when applied to the nonlinear Schrödinger equation (1.2). In particular, we determine the first Lie commutator $[A, B](w)$, which, in general, depends on the argument w and its first- and second-order spatial derivatives as well as on the first- and second-order spatial derivatives of the potential U; on the contrary, in the linear case the Lie commutator $[A, B]$ reduces to a linear differential operator of order one with coefficients involving the first- and second-order spatial derivatives of the potential. In the context of nonlinear Schrödinger equations, it is natural to choose the Lebesgue space $L^2(\Omega)$ as the underlying function space; furthermore, the imposed asymptotic (or periodic) boundary conditions on $\Omega = \mathbb{R}^d$ (or $\Omega \subset \mathbb{R}^d$ a suitably chosen bounded domain) facilitate the considerations.

(iii) A rigorous extension of the local error representation for the first-order Lie–Trotter splitting method to higher-order splitting methods and the investigation for a particular application is left for future work; in this case, it is indispensable to employ the formal calculus of Lie derivatives. However, it is expected that the local error representation for a high-order exponential operator splitting method formally resembles the relation for the linear case, which was deduced in Descombes & Thalhammer (2010), replacing A and B by the associated Lie derivatives and reversing the sequence of the involved operators.

3.2 *Auxiliary results*

In this section, we collect several auxiliary results that are needed for the derivation of our local error representation for exponential operator splitting methods (2.4) applied to nonlinear evolutionary problems (2.1).

In the following, we let $G : D(G) \subset X \to X$ and $H : D(H) \subset X \to X$ denote unbounded nonlinear operators (with suitably chosen domains). With regard to (2.1), we consider the evolutionary problem

$$\begin{cases} v'(t) = G(v(t)), \quad 0 \leqslant t \leqslant T, \\ v(0) = v_0, \end{cases}$$

with exact solution formally given by $v(t) = \mathscr{E}_G(t, v_0)$ for $0 \leqslant t \leqslant T$; see also (2.2). We recall that the evolution operator $\mathscr{E}_G$ and its derivative with respect to the initial value, which we denote by $\partial_2 \mathscr{E}_G$, fulfil the initial value problems

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} \mathscr{E}_G(t, v_0) = G(\mathscr{E}_G(t, v_0)), \quad 0 \leqslant t \leqslant T, \\ \mathscr{E}_G(0, v_0) = v_0, \end{cases}$$
$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t} \partial_2 \mathscr{E}_G(t, v_0) = G'(\mathscr{E}_G(t, v_0)) \partial_2 \mathscr{E}_G(t, v_0), \quad 0 \leqslant t \leqslant T, \\ \partial_2 \mathscr{E}_G(t, v_0)|_{t=0} = I. \end{cases} \tag{3.6}$$

Clearly, the evolution operator $\mathscr{E}_G$ satisfies

$$\mathscr{E}_G(t + s, v_0) = \mathscr{E}_G(s, \mathscr{E}_G(t, v_0)) = \mathscr{E}_G(t, \mathscr{E}_G(s, v_0)), \quad 0 \leqslant t + s \leqslant T;$$

more generally, in the context of parabolic equations, the above relation holds true under the additional restriction $s, t \geqslant 0$. As a consequence, the identity

$$\begin{aligned} \partial_2 \mathscr{E}_G(t, v_0) G(v_0) &= \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} \mathscr{E}_G(t, \mathscr{E}_G(s, v_0)) = \frac{\mathrm{d}}{\mathrm{d}s}\bigg|_{s=0} \mathscr{E}_G(t + s, v_0) \\ &= G(\mathscr{E}_G(t, v_0)), \quad 0 \leqslant t \leqslant T \end{aligned} \tag{3.7}$$

follows.

An essential tool for the derivation of our local error representation is the nonlinear variation-of-constants formula; see, for example, Sanz-Serna & Calvo (1994).

THEOREM 3.3 (Gröbner–Alekseev formula) The analytical solutions of the initial value problems

$$\begin{cases} v'(t) = H(t, v(t)) = G(v(t)) + R(t, v(t)), \quad 0 \leqslant t \leqslant T, \\ v(0) = v_0, \end{cases}$$
$$\begin{cases} v'(t) = G(v(t)), \quad 0 \leqslant t \leqslant T, \\ v(0) = v_0 \end{cases}$$

are related through the nonlinear variation-of-constants formula

$$\mathscr{E}_H(t, v_0) = \mathscr{E}_G(t, v_0) + \int_0^t \partial_2 \mathscr{E}_G(t - \tau, \mathscr{E}_H(\tau, v_0)) R(\tau, \mathscr{E}_H(\tau, v_0)) \, \mathrm{d}\tau, \quad 0 \leqslant t \leqslant T.$$

Proof. With the help of relation (3.7) we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\tau}\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0)) &= -G(\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0)))\\ &\quad + \partial_2\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))H(\tau,\mathscr{E}_H(\tau,v_0))\\ &= -G(\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0)))\\ &\quad + \partial_2\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))G(\mathscr{E}_H(\tau,v_0))\\ &\quad + \partial_2\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))R(\tau,\mathscr{E}_H(\tau,v_0))\\ &= \partial_2\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))R(\tau,\mathscr{E}_H(\tau,v_0)),\quad 0\leqslant\tau\leqslant t\leqslant T;\end{aligned}$$

therefore, the desired result follows at once from

$$\begin{aligned}\mathscr{E}_H(t,v_0)-\mathscr{E}_G(t,v_0) &= \mathscr{E}_G(0,\mathscr{E}_H(t,v_0)) - \mathscr{E}_G(t,\mathscr{E}_H(0,v_0))\\ &= \mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))|_{\tau=0}^{t}\\ &= \int_0^t \frac{\mathrm{d}}{\mathrm{d}\tau}\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))\,\mathrm{d}\tau\\ &= \int_0^t \partial_2\mathscr{E}_G(t-\tau,\mathscr{E}_H(\tau,v_0))R(\tau,\mathscr{E}_H(\tau,v_0))\,\mathrm{d}\tau,\quad 0\leqslant t\leqslant T.\end{aligned}$$

We note that for the nonautonomous problem involving H, the associated evolution operator $\mathscr{E}_H$ depends on the actual time and the initial time, as well as on the initial value; in this case, we write $\mathscr{E}_H(t,v_0) = \mathscr{E}_H(t,0,v_0)$ for short. □

In particular, if G is a time-independent (unbounded) linear operator that generates a semigroup $(e^{tG})_{t\geqslant 0}$, we retain the linear variation-of-constants formula

$$\mathscr{E}_H(t,v_0) = e^{tG}v_0 + \int_0^t e^{(t-\tau)G}R(\tau,\mathscr{E}_H(\tau,v_0))\,\mathrm{d}\tau,\quad 0\leqslant t\leqslant T$$

since $\mathscr{E}_G(t,v_0) = e^{tG}v_0$ and thus $\partial_2\mathscr{E}_G(t,\cdot) = e^{tG}$; see also Engel & Nagel (2000), Henry (1981), Hille & Phillips (1957), Lunardi (1995), Pazy (1983).

In order to further expand terms of the form (3.5b), we apply the following auxiliary result; we refer to (3.2) for the definition of the Lie bracket.

Lemma 3.4 For unbounded nonlinear operators G and H, the identity

$$\partial_2\mathscr{E}_G(t,v)H(v) - H(\mathscr{E}_G(t,v)) = \int_0^t \partial_2\mathscr{E}_G(t-\tau,v)[G,H](\mathscr{E}_G(\tau,v))\,\mathrm{d}\tau,\quad 0\leqslant t\leqslant T$$

holds true.

Proof. In accordance with (3.5b), we set $R(t,v) = \partial_2 \mathscr{E}_G(t,v)H(v) - H(\mathscr{E}_G(t,v))$ for a fixed element v and $0 \leqslant t \leqslant T$. Rewriting the time derivative of R as

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}R(t,v) &= G'(\mathscr{E}_G(t,v))\partial_2\mathscr{E}_G(t,v)H(v) - H'(\mathscr{E}_G(t,v))G(\mathscr{E}_G(t,v)) \\ &= G'(\mathscr{E}_G(t,v))R(t,v) + G'(\mathscr{E}_G(t,v))H(\mathscr{E}_G(t,v)) - H'(\mathscr{E}_G(t,v))G(\mathscr{E}_G(t,v)), \quad 0 \leqslant t \leqslant T\end{aligned}$$

(see (3.6)), and using $R(0,v) = \partial_2\mathscr{E}_G(0,v)H(v) - H(\mathscr{E}_G(0,v)) = 0$ thus yields the linear initial value problem

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}R(t,v) = G'(\mathscr{E}_G(t,v))R(t,v) + [G,H](\mathscr{E}_G(t,v)), \quad 0 \leqslant t \leqslant T, \\ R(0,v) = 0 \end{cases}$$

(see also (3.2) and (3.6)); we note that the evolution operator of the associated homogeneous linear differential equation is given by $\partial_2\mathscr{E}_G(t,v)$ and that $\partial_2\mathscr{E}_G(t-\tau,v)$ is understood as $\partial_2\mathscr{E}_G(t,v)(\partial_2\mathscr{E}_G(\tau,v))^{-1}$. As a consequence, the (linear variant of the) variation-of-constants formula implies the given result; see also Theorem 3.3. □

We next reformulate the composition that arises in the local error representation of the Lie–Trotter splitting by utilizing the formal calculus of Lie derivatives; see (2.3).

LEMMA 3.5 For nonlinear operators G_j, $1 \leqslant j \leqslant 4$ and H_j, $1 \leqslant j \leqslant 2$, the relation

$$\begin{aligned}&e^{t_1 D_{G_1}}\, e^{t_2 D_{G_2}}[D_{H_1}, D_{H_2}]\, e^{t_3 D_{G_3}}\, e^{t_4 D_{G_4}} v_0 \\ &\quad = \partial_2\mathscr{E}_{G_4}(t_4, \mathscr{E}_{G_3}(t_3,v))\partial_2\mathscr{E}_{G_3}(t_3,v)[H_2,H_1](v)|_{v=\mathscr{E}_{G_2}(t_2,\mathscr{E}_{G_1}(t_1,v_0))}\end{aligned}$$

is valid.

Proof. We consider the composition

$$L_1(v) = e^{t_3 D_{G_3}}\, e^{t_4 D_{G_4}} v = \mathscr{E}_{G_4}(t_4, \mathscr{E}_{G_3}(t_3,v))$$

and determine its Fréchet derivative

$$L_1'(v) = \partial_2\mathscr{E}_{G_4}(t_4, \mathscr{E}_{G_3}(t_3,v))\partial_2\mathscr{E}_{G_3}(t_3,v).$$

Moreover, due to the fact that

$$\begin{aligned}L_{1+j}(v) &= D_{H_j}\, e^{t_3 D_{G_3}}\, e^{t_4 D_{G_4}} v = L_1'(v)H_j(v), \quad j = 1,2, \\ L_{1+j}'(v) &= L_1''(v)H_j(v) + L_1'(v)H_j'(v), \quad j = 1,2,\end{aligned}$$

a straightforward calculation yields the relation

$$L_4(v) = [D_{H_1}, D_{H_2}]\, e^{t_3 D_{G_3}}\, e^{t_4 D_{G_4}} v = L_3'(v)H_1(v) - L_2'(v)H_2(v) = L_1'(v)[H_2,H_1](v).$$

Using

$$L_5(v) = e^{t_2 D_{G_2}}[D_{H_1}, D_{H_2}]\, e^{t_3 D_{G_3}}\, e^{t_4 D_{G_4}} v = L_4(\mathscr{E}_{G_2}(t_2,v)),$$

and as a consequence

$$e^{t_1 D_{G_1}}\, e^{t_2 D_{G_2}} [D_{H_1}, D_{H_2}]\, e^{t_3 D_{G_3}}\, e^{t_4 D_{G_4}} v = L_5(\mathscr{E}_{G_1}(t_1, v)),$$

the statement follows. □

4. Nonlinear Schrödinger equations in the semiclassical regime

In this section, we state a convergence estimate for the first-order Lie–Trotter splitting method (1.3) when applied to time-dependent nonlinear Schrödinger equations in the semiclassical regime. In particular, we study the ability of our local error representation given in Theorem 3.1 to provide a local error estimate which correctly captures the dependence on the critical parameter. In Section 4.1, we present numerical examples for the Gross–Pitaevskii equation (1.2) to illustrate and confirm the theoretical considerations of Sections 4.2 and 4.3. Numerical experiments for higher-order exponential operator splitting methods complement our investigations.

In the following, we focus on the local error behaviour of splitting methods. We point out that this is justified by the fact that global error estimates are obtained by a standard approach based on stability bounds and local error estimates; more precisely, by means of a telescopic identity (Lady Windermere's fan argument), the global error is related to compositions of the splitting operator and local errors; see Descombes & Thalhammer (2010), Gauckler (2010), Lubich (2008), and Thalhammer (2008). We believe that in both the numerical example and the theoretical considerations, it gives insight to draw a comparison with the less involved linear case, which was treated in our previous work (Descombes & Thalhammer, 2010). In the following, in order to facilitate the considerations, we suppose the potential to be sufficiently often differentiable with bounded derivatives; techniques exploited in Neuhauser & Thalhammer (2009) allow us to incorporate unbounded potentials such as a scaled harmonic potential, which is relevant in view of physical applications.

For simplicity, we henceforth focus on a model problem in a single space dimension; for our purposes, this restriction is adequate and considerably facilitates the numerical computation as well as the theoretical considerations. We point out that in the numerical example that it is essential to ensure a high spatial resolution in order to observe the expected dependence on the critical parameter; for example, for a one-dimensional problem using an implementation in MATLAB, the computation time of Fig. 1 on a standard notebook[1] amounts to a few seconds (only).

4.1 *Numerical experiments*

In the following, we illustrate the error behaviour of the first-order Lie–Trotter splitting method when applied to the one-dimensional Gross–Pitaevskii equation under an initial condition in classical Wentzel–Kramers–Brillouin form and under a regular initial condition; in particular, we study the dependence of the local error on the time-step size and the critical parameter. Moreover, for comparison, we include the numerical results obtained for exponential operator splitting methods of (nonstiff) orders $p = 2, 3, 4$; for our considerations, the choice of the higher-order splitting methods is not essential. Our model problem conforms to Bao, Jin & Markowich (2003, Example 6).

Model problem (One dimension). We consider the time-dependent nonlinear Schrödinger equation

$$\begin{cases} \mathrm{i}\partial_t \psi(x,t) = \left(-\frac{1}{2}\varepsilon \partial_{xx} + \frac{1}{\varepsilon} U(x) + \frac{1}{\varepsilon}\vartheta |\psi(x,t)|^2 \right) \psi(x,t), \\ \psi(x,0) = \varrho_0(x)\, e^{\mathrm{i}\sigma_0(x)/\varepsilon}, \quad x \in \Omega, \quad 0 \leqslant t \leqslant T, \end{cases} \tag{4.1a}$$

[1] HP Compaq nc8430, Intel(R) Core(TM)2 CPU, T7200 @ 2 GHz, 1.99 GHz, 2 GB RAM.

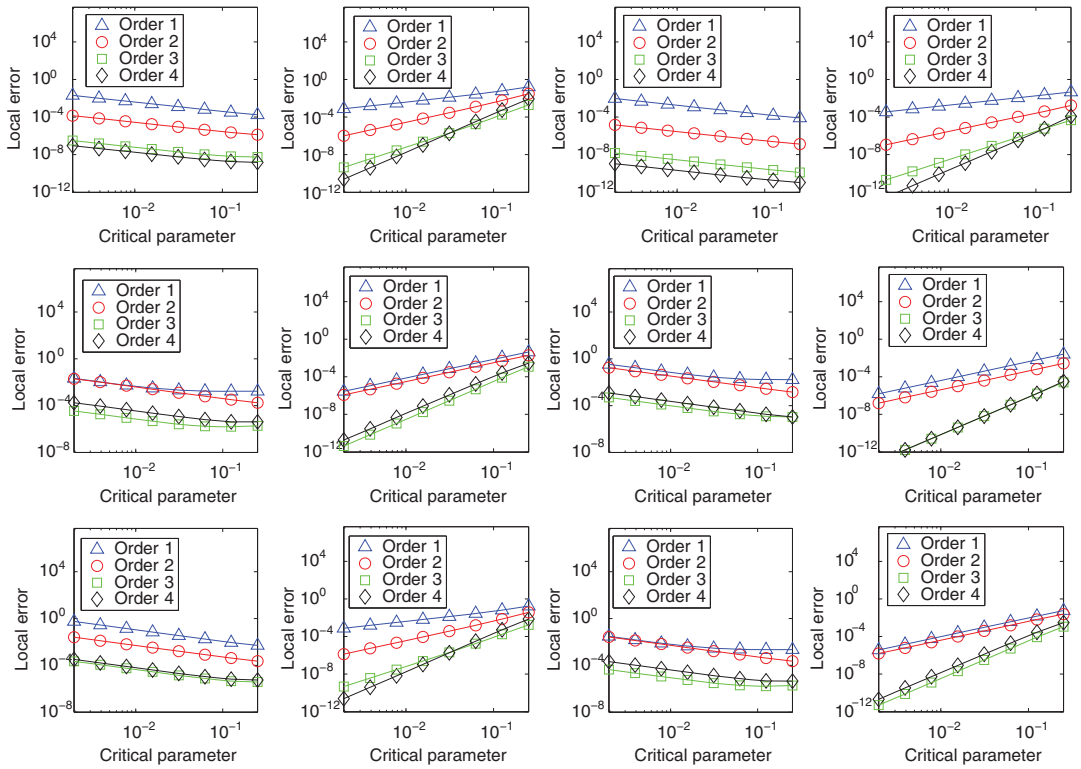

FIG. 1. Dependence of the local error on the critical parameter for different splitting methods applied to problem (4.1) with $M = 4096$ Fourier basis functions. First row: equation under initial condition (4.2) with $\omega = 1$ and $\vartheta = 1$ (columns 1 and 2) or $\vartheta = 0$ (columns 3 and 4). Local error versus critical parameter for time step $h = 10^{-2}$ (columns 1 and 3) and $h = \varepsilon$ (columns 2 and 4). Second row: equation under initial condition (4.3) with $\omega = 1$ and $\vartheta = 1$ (columns 1 and 2) or $\vartheta = 0$ (columns 3 and 4). Local error versus critical parameter for time step $h = 5 \times 10^{-2}$ (column 1) or $h = 2 \times 10^{-1}$ (column 3) and time step $h = \varepsilon$ (columns 2 and 4). Third row: equation under initial condition (4.2) (columns 1 and 2) or (4.3) (columns 3 and 4), with $\omega = 0$ and $\vartheta = 1$. Local error versus critical parameter for time step $h = 5 \times 10^{-2}$ (columns 1 and 3) and $h = \varepsilon$ (columns 2 and 4).

for a function $\psi : \Omega \times [0, T] \to \mathbb{C} : (x, t) \mapsto \psi(x, t)$, where $\Omega \subset \mathbb{R}$ denotes a (suitably chosen) bounded interval. We assume the external real potential $U : \Omega \to \mathbb{R}$ and the functions $\varrho_0, \sigma_0 : \Omega \to \mathbb{R}$ defining the initial condition to be sufficiently often differentiable with bounded derivatives. In particular, we study (4.1a) under the scaled harmonic potential

$$U(x) = \tfrac{1}{2}\omega^2 x^2, \quad x \in \Omega, \tag{4.1b}$$

involving the positive weight $\omega > 0$. In view of Section 4.2, we also consider the special case $\vartheta = 0$ where (4.1a) reduces to a linear Schrödinger equation, and the cubic Schrödinger equation where $\omega = 0$.

Numerical experiments (*Local error*). To study the local error behaviour of splitting methods, the values of the critical parameter $\varepsilon > 0$ are chosen in the range $2^{-9} = 1.953125 \times 10^{-3}$ to $2^{-2} = 2.5 \times 10^{-1}$. Further, we set $\omega = 1$ and $\vartheta = 1$ as well as

$$\varrho_0(x) = e^{-x^2}, \quad \sigma_0(x) = -\ln(e^x + e^{-x}), \quad x \in \Omega. \tag{4.2}$$

With regard to space discretization by the Fourier–spectral method with $M = 4096$ degrees of freedom, we impose periodic boundary conditions on the bounded interval $\Omega = [-a, a]$; in the present situation, $a = 8$ is sufficiently large that the artificial boundary conditions do not cause perturbations of the numerical solution. For the time integration of (4.1), we apply different exponential operator splitting methods: the first-order Lie–Trotter splitting method (1.3), the second-order Strang splitting method (2.5), a fourth-order splitting method by Yoshida, and, in addition, a third-order splitting method.[2] On the one hand, we choose the actual time-step size $h = h_0$ independent of the parameter ε, and, on the other hand, we set $h = \varepsilon$. Numerical reference solutions are computed by a favourable fourth-order Runge–Kutta–Nyström splitting method proposed in Blanes & Moan (2002) with a finer time-step size $h \times 10^{-1}$.

In Fig. 1, the local errors $\mathrm{err}_{\mathrm{local}}(\varepsilon)$ versus the critical parameter values ε are displayed (see also (3.1) for the definition of the local error); for comparison, we include the numerical results for the linear case $\vartheta = 0$ and a regular initial condition independent of ε, namely,

$$\varrho_0(x) = e^{-(x-1/10)^2}, \quad \sigma_0(x) = 0, \quad x \in \Omega, \tag{4.3}$$

as well as for the cubic Schrödinger equation where $\omega = 0$. On a logarithmic scale, the slopes of the lines correspond to the ratios of two subsequent local errors and parameters,

$$\mathrm{ratio}(\varepsilon) = \log\left(\frac{\mathrm{err}_{\mathrm{local}}(\varepsilon)}{\mathrm{err}_{\mathrm{local}}(\varepsilon/2)}\right) \Big/ \log(2). \tag{4.4}$$

For instance, for initial condition (4.2) and a time-step size independent of ε, it is observed that in all cases, within the chosen range of h/ε, the ratios approach the value $\alpha = -1$ which implies dependence $\mathcal{O}(1/\varepsilon)$ of the dominant local error term with respect to the critical parameter. The numerical results are summarized in Table 1 and analysed in Section 4.2; thereby, $\lfloor x \rfloor$ denotes the integer part of $x \in \mathbb{R}$, that is, $\alpha = 2\lfloor (p+1)/2 \rfloor$ yields $\alpha = 2$ if $p = 1, 2$ and $\alpha = 4$ if $p = 3, 4$. We point out that it is crucial to choose the number of Fourier basis functions M sufficiently large to avoid side effects from the spatial approximation and to retain the expected behaviour.

Numerical experiments (*Global error*). The time evolution of the nonlinear Schrödinger equation (4.1) with $\vartheta = 1$ under initial condition (4.2) in classical Wentzel–Kramers–Brillouin form is illustrated in Fig. 2. We display the solution values $|\psi(x,t)|^2$, $(x,t) \in [0, 1.5] \times [0, 3]$ for parameter values $\varepsilon = 1, 10^{-2}$ and the values $\omega = 1, 2$ of the constant in the confining potential; further, the figure mirrors the rapid oscillations that arise for $\varepsilon = 10^{-2}$ in the graph of ψ. We choose the spatial interval $[0, 1.5]$ since the solution is symmetric with respect to the origin and approaches zero outside; the perspective is such that the solution values at time $t = 3$ are visible. For the space integration, we apply the Fourier–spectral method with $M = 8192$ degrees of freedom. The time integration is performed by the above-mentioned fourth-order splitting method by Blanes & Moan (2002) with time-step size $h = \varepsilon/20$. A comparison of the final solution values at time $t = 3$ illustrates that for smaller parameter values it is essential to choose the time-step size sufficiently small; for $\varepsilon = 10^{-2}$ and $h = \varepsilon/20$ the Lie–Trotter splitting method does not capture the correct behaviour, whereas a satisfactory result is obtained for the reduced time-step size $h = \varepsilon/50$.

[2] The coefficients of a four-stage fourth-order splitting method by Yoshida are found in Hairer *et al.* (2002, p. 40, Formula (4.4)). For example, a seven-stage third-order splitting method results from a seven-stage fourth-order Runge–Kutta–Nyström splitting method by Blanes & Moan (2002) when requiring the coefficients $(a_i, b_i)_{i=1}^4$ to coincide and further setting $b_7 = 0$.

TABLE 1 *Problem* (4.1) *with initial condition* (4.2) ($\partial_x \sigma_0 \neq 0$) *or* (4.3) ($\sigma_0 = 0$). *Observed dependence* $\mathcal{O}(\varepsilon^\alpha)$ *of the local error on the critical parameter* ε *for splitting methods of orders* $1 \leqslant p \leqslant 4$

$\omega = 1$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = h_0$	$\alpha \approx -1$
$\omega = 1$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = \varepsilon$	$\alpha \approx p$
$\omega = 1$	$\vartheta = 1$	$\sigma_0 = 0$	$h = h_0$	$\alpha \approx -1$
$\omega = 1$	$\vartheta = 1$	$\sigma_0 = 0$	$h = \varepsilon$	$\alpha \approx 2 \left\lfloor \frac{p+1}{2} \right\rfloor$
$\omega = 1$	$\vartheta = 0$	$\partial_x \sigma_0 \neq 0$	$h = h_0$	$\alpha = -1$
$\omega = 1$	$\vartheta = 0$	$\partial_x \sigma_0 \neq 0$	$h = \varepsilon$	$\alpha = p$
$\omega = 1$	$\vartheta = 0$	$\sigma_0 = 0$	$h = h_0$	$\alpha = -1$
$\omega = 1$	$\vartheta = 0$	$\sigma_0 = 0$	$h = \varepsilon$	$\alpha = 2 \left\lfloor \frac{p+1}{2} \right\rfloor$
$\omega = 0$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = h_0$	$\alpha \approx -1$
$\omega = 0$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$h = \varepsilon$	$\alpha \approx p$
$\omega = 0$	$\vartheta = 1$	$\sigma_0 = 0$	$h = h_0$	$\alpha \approx -1$
$\omega = 0$	$\vartheta = 1$	$\sigma_0 = 0$	$h = \varepsilon$	$\alpha \approx 2 \left\lfloor \frac{p+1}{2} \right\rfloor$

As a further illustration, the global errors $\mathrm{err}_{\mathrm{global}}(h)$ at final time $T = 1$ versus the (constant) time-step sizes $h = 2^{-j}$, $0 \leqslant j \leqslant 10$, are displayed in Fig. 3 for the noncritical parameter value $\varepsilon = 2^{-2}$ and $M = 256$. As expected, the slopes

$$\mathrm{ratio}(h) = \log\left(\frac{\mathrm{err}_{\mathrm{global}}(h)}{\mathrm{err}_{\mathrm{global}}(h/2)}\right) \Big/ \log(2)$$

perfectly reflect the convergence orders of the splitting methods, provided that the time-step sizes are sufficiently small; this implies dependence $\mathcal{O}(h^{p+1})$ of the local error with respect to the time-step size.

4.2 *Local error estimate*

In this section, we study the error behaviour of the Lie–Trotter splitting (1.3) method for the nonlinear Schrödinger equation (4.1) in the semiclassical regime with initial condition chosen in classical Wentzel–Kramers–Brillouin form (4.2) and a regular initial condition (4.3). In particular, we discuss the ability of the local error representation of Theorem 3.1,

$$\begin{aligned}\mathscr{L}(h, u_0) = \int_0^h \int_0^{\tau_1} & \partial_2 \mathscr{E}_F(h - \tau_1, \mathscr{S}(\tau_1, u_0)) \partial_2 \mathscr{E}_B(\tau_1 - \tau_2, \mathscr{E}_A(\tau_1, u_0)) \\ & \times [B, A](\mathscr{E}_B(\tau_2, \mathscr{E}_A(\tau_1, u_0))) \, \mathrm{d}\tau_2 \, \mathrm{d}\tau_1, \end{aligned} \tag{4.5}$$

to explain the dependence of the dominant local error term upon the actual time-step size $h > 0$ and the critical parameter $0 < \varepsilon \ll 1$ observed numerically in Section 4.1. For the theoretical analysis, we first reconsider the linear case (Descombes & Thalhammer, 2010) and further the cubic Schrödinger equation, since then the arguments can be extended to the Gross–Pitaevskii equation (4.1) without

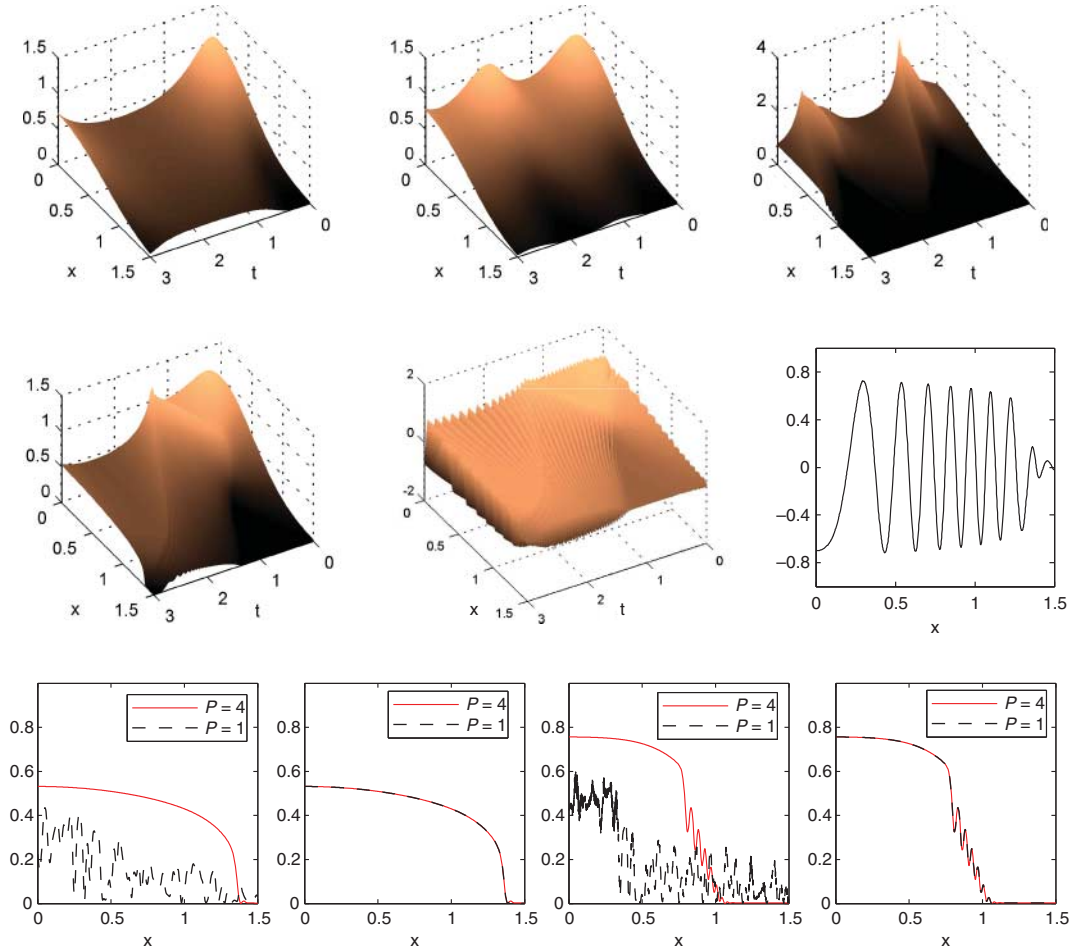

FIG. 2. Time evolution of the time-dependent nonlinear Schrödinger equation (4.1) under initial condition (4.2) with $\vartheta = 1$. First row: equation with $(\varepsilon, \omega) = (1, 1)$ (left), $(\varepsilon, \omega) = (1, 2)$ (middle) and $(\varepsilon, \omega) = (10^{-2}, 2)$ (right). Solution profile $|\psi(x,t)|^2$ for $(x,t) \in [0, 1.5] \times [0, 3]$. Second row: equation with $(\varepsilon, \omega) = (10^{-2}, 1)$. Solution profile $|\psi(x,t)|^2$ (left) and $\Re\psi(x,t)$ (middle) for $(x,t) \in [0, 1.5] \times [0, 3]$ and section at time $t = 3$ (right). Third row: equation with $\varepsilon = 10^{-2}$ and $\omega = 1$ (columns 1 and 2) or $\omega = 2$ (columns 3 and 4). Comparison of the solution profiles $|\psi(x,t)|^2$ for $x \in [0, 1.5]$ at time $t = 3$, computed by the first-order Lie–Trotter ($p = 1$) and a fourth-order splitting method by Blanes & Moan (2002) ($p = 4$). Time-step size $h = \varepsilon/20$ (columns 1 and 3) or $h = \varepsilon/50$ (columns 2 and 4), for $p = 1$. Time-step size $h = \varepsilon/20$ for $p = 4$.

significant difficulty. For suitable choices of the domains of the involved operators, the computation of iterated Lie commutators and a possible extension to unbounded potentials in the context of the Hermite spectral method, we refer to Gauckler (2010), Lubich (2008), Neuhauser & Thalhammer (2009).

Abstract formulation. The nonlinear Schrödinger equation (4.1) may be cast into the form of an abstract initial value problem (2.1) with linear operator $A : D(A) \subset X \to X$ and nonlinear operator $B : D(B) \subset X \to X$ defined by

$$A = \varepsilon \hat{A}, \quad \hat{A} = \frac{1}{2} \mathrm{i} \partial_{xx}, \quad B = \frac{1}{\varepsilon} \hat{B}, \quad \hat{B}(v) = -\mathrm{i}(U + \vartheta |v|^2) v; \tag{4.6}$$

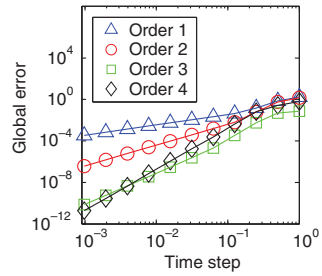

FIG. 3. Numerical convergence orders of different splitting methods applied to problem (4.1) under initial condition (4.2) with $\varepsilon = 2^{-2}$, $\omega = 1$, $\vartheta = 1$, $M = 256$ and final time $T = 1$. Global error versus time-step size.

in accordance with the potential and the imposed boundary conditions on $\Omega \subset \mathbb{R}$, the Sobolev embedding $H^1(\Omega) \subset L^\infty(\Omega)$ suggests suitably chosen subspaces $D(\hat{A}) \subset H^2(\Omega)$ and $D(\hat{B}) \subset H^1(\Omega)$ on the underlying Hilbert space $X = L^2(\Omega)$.

Practical realization. With regard to the practical realization of a splitting method (2.4), it is favourable to rely the numerical solution of the linear subproblem

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_A(t,v) = A\mathscr{E}_A(t,v), \quad 0 \leqslant t \leqslant T, \\ \mathscr{E}_A(0,v) = v, \end{cases}$$

on a spectral decomposition; see Section 4.1 and Caliari *et al.* (2009) for further details. Since $(\mathrm{d}/\mathrm{d}t)|\mathscr{E}_B(t,v)|^2 = 2\Re(\overline{\mathscr{E}_B(t,v)}(\mathrm{d}/\mathrm{d}t)\mathscr{E}_B(t,v)) = 0$, for any $0 \leqslant t \leqslant T$, the invariance property $|\mathscr{E}_B(t,v)|^2 = |v|^2$ follows; therefore, the analytical solution of the nonlinear subproblem

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_B(t,v) = B(\mathscr{E}_B(t,v)), \quad 0 \leqslant t \leqslant T, \\ \mathscr{E}_B(0,v) = v \end{cases}$$

is given in an explicit manner by

$$\mathscr{E}_B(t,v) = e^{-\mathrm{i}t(U+\vartheta|v|^2)/\varepsilon}v, \quad 0 \leqslant t \leqslant T, \tag{4.7}$$

realized numerically by a pointwise multiplication.

Basic properties. The Fréchet derivatives of the operators $\hat{A}$ and $\hat{B}$ equal

$$\hat{A}'(v)w = \hat{A}w = \tfrac{1}{2}\mathrm{i}\partial_{xx}w, \quad \hat{B}'(v)w = -\mathrm{i}(Uw + 2\vartheta|v|^2w + \vartheta v^2\bar{w}), \tag{4.8}$$

and clearly, it holds that $A' = \varepsilon\hat{A}'$ and $B' = (1/\varepsilon)\hat{B}'$; see also (4.6). Stone's theorem (e.g., see Engel & Nagel, 2000) ensures that the linear differential operator $\hat{A}$ and the nonlinear multiplication operator $\hat{B}$ generate unitary evolution operators on $L^2(\Omega)$; moreover, the exact solution operator is unitary on $L^2(\Omega)$. Consequently, for any parameter value $\varepsilon > 0$, it holds that

$$\|\mathscr{E}_A(t,\cdot)\|_{L^2\leftarrow L^2} = 1, \quad \|\mathscr{E}_B(t,\cdot)\|_{L^2\leftarrow L^2} = 1, \quad \|\mathscr{E}_F(t,\cdot)\|_{L^2\leftarrow L^2} = 1, \quad 0 \leqslant t \leqslant T. \tag{4.9}$$

Clearly, it holds that $\partial_2\mathscr{E}_A(t,v) = \mathscr{E}_A(t,\cdot)$ for $0 \leqslant t \leqslant T$, which implies that the derivative of the evolution operator $\mathscr{E}_A$ with respect to the initial value is a unitary operator on $L^2(\Omega)$. For linear Schrödinger

equations, this is also valid for $\partial_2 \mathscr{E}_B(t,u) = \mathscr{E}_B(t,\cdot)$ and $\partial_2 \mathscr{E}_F(t,u) = \mathscr{E}_F(t,\cdot)$, $0 \leqslant t \leqslant T$; more generally, for nonlinear problems the operators $\partial_2 \mathscr{E}_F$ and $\partial_2 \mathscr{E}_B$ satisfy the nonautonomous linear problems

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\partial_2 \mathscr{E}_F(t,v) = (A + B'(\mathscr{E}_F(t,v)))\partial_2 \mathscr{E}_F(t,v), & 0 \leqslant t \leqslant T, \\ \partial_2 \mathscr{E}_F(t,v)|_{t=0} = I, \end{cases}$$

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\partial_2 \mathscr{E}_B(t,v) = B'(\mathscr{E}_B(t,v))\partial_2 \mathscr{E}_B(t,v), & 0 \leqslant t \leqslant T, \\ \partial_2 \mathscr{E}_B(t,v)|_{t=0} = I, \end{cases}$$

with $\partial_2 \mathscr{E}_B$ given explicitly by

$$\partial_2 \mathscr{E}_B(t,v)w = e^{-\mathrm{i}t(U+\vartheta|v|^2)/\varepsilon} w - 2\mathrm{i}\frac{t}{\varepsilon}\vartheta \mathscr{E}_B(t,v)\,\Re(\bar{v}w), \quad 0 \leqslant t \leqslant T; \tag{4.10}$$

see also (3.6) and (4.7).

Lie commutator. In the following, we study the decisive term

$$[A,B](w), \quad w = \mathscr{E}_B(\tau_2, v) = e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon} v, \quad v = \mathscr{E}_A(\tau_1, u_0), \tag{4.11}$$

in the local error representation (4.5). Due to the fact that

$$\begin{aligned} \hat{A}'(w)\hat{B}(w) &= \tfrac{1}{2}\partial_{xx}(Uw + \vartheta|w|^2 w) \\ &= \tfrac{1}{2}(U\partial_{xx}w + 2\partial_x U \partial_x w + \partial_{xx}U w + \vartheta(w^2\partial_{xx}\bar{w} + 4w|\partial_x w|^2 + 2\bar{w}(\partial_x w)^2 + 2|w|^2\partial_{xx}w)), \\ \hat{B}'(w)\hat{A}(w) &= \tfrac{1}{2}(U\partial_{xx}w + 2\vartheta|w|^2\partial_{xx}w - \vartheta w^2\partial_{xx}\bar{w}) \end{aligned}$$

(see (4.6) and (4.8)), the first Lie commutator of A and B is given by

$$\begin{aligned} [A,B](w) &= A'(w)B(w) - B'(w)A(w) = \hat{A}'(w)\hat{B}(w) - \hat{B}'(w)\hat{A}(w) \\ &= \partial_x U \partial_x w + \tfrac{1}{2}\partial_{xx}U w + \vartheta w^2 \partial_{xx}\bar{w} + 2\vartheta w|\partial_x w|^2 + \vartheta\bar{w}(\partial_x w)^2 \end{aligned}$$

(see (3.2)); it is notable that in the nonlinear case the second spatial derivative of w arises, whereas for a linear problem (4.1) with $\vartheta = 0$ the Lie commutator reduces to $[A,B] = \partial_x U \partial_x + \frac{1}{2}\partial_{xx}UI$, a first-order differential operator with coefficients involving the first and second derivative of the potential. A brief calculation yields

$$\begin{aligned} \partial_x w &= \partial_x\, e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon} v + e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon}\partial_x v, \\ \partial_{xx} w &= \partial_{xx}\, e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon} v + 2\partial_x\, e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon}\partial_x v + e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon}\partial_{xx} v, \end{aligned}$$

involving the spatial derivatives

$$\partial_x\, e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon} = -\mathrm{i}\frac{\tau_2}{\varepsilon}\, e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon}(\partial_x U + 2\vartheta\,\Re(\bar{v}\partial_x v)),$$

$$\partial_{xx}\, e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon} = e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon}\left(-\frac{\tau_2^2}{\varepsilon^2}(\partial_x U + 2\vartheta\Re(\bar{v}\partial_x v))^2 - \mathrm{i}\frac{\tau_2}{\varepsilon}(\partial_{xx}U + 4\vartheta|\partial_x v|^2 + 4\vartheta\Re(\bar{v}\partial_{xx}v))\right);$$

inserting the above relations into (4.11) thus gives

$$\begin{aligned}
[A,B](w) &= e^{-\mathrm{i}\tau_2(U+\vartheta|v|^2)/\varepsilon}\left(g_1(v) + \mathrm{i}\frac{\tau_2}{\varepsilon}g_2(v)\right), \quad v = \mathscr{E}_A(\tau_1, u_0),\\
g_1(v) &= \partial_x U\partial_x v + \frac{1}{2}\partial_{xx}Uv + \vartheta\,\partial_{xx}\bar{v}v^2 + 2\vartheta|\partial_x v|^2 v + \vartheta(\partial_x v)^2\bar{v},\\
g_2(v) &= -(\partial_x U)^2 v + \vartheta\,\partial_{xx}U|v|^2 v - 2\vartheta\,\partial_x U\Re(\bar{v}\partial_x v)v\\
&\quad + 2\vartheta^2|\partial_x v|^2|v|^2 v + \vartheta^2\partial_{xx}v|v|^4 + \vartheta^2\partial_{xx}\bar{v}|v|^2 v^2.
\end{aligned} \tag{4.12a}$$

Provided that the linear operator A (with domain $D(A)$ also including the imposed boundary conditions) and the differential operators ∂_x commute (on a suitably chosen subdomain), it follows that

$$\partial_x^j v = \mathscr{E}_A(\tau_1, \partial_x^j u_0), \quad j \geqslant 0, \tag{4.12b}$$

and further that $\|\partial_x^j v\|_{L^2} = \|\partial_x^j u_0\|_{L^2}$ for $j \geqslant 0$; see (4.9). In particular, for initial conditions in classical Wentzel–Kramers–Brillouin form (4.2) with ϱ_0 and σ_0 sufficiently often differentiable, we obtain

$$\begin{aligned}
u_0 &= \varrho_0\, e^{\mathrm{i}\sigma_0/\varepsilon}, \quad \partial_x u_0 = \partial_x\varrho_0\, e^{\mathrm{i}\sigma_0/\varepsilon} + \frac{\mathrm{i}}{\varepsilon}\partial_x\sigma_0 u_0,\\
\partial_{xx}u_0 &= \left(\partial_{xx}\varrho_0 + 2\frac{\mathrm{i}}{\varepsilon}\partial_x\varrho_0\partial_x\sigma_0\right) e^{\mathrm{i}\sigma_0/\varepsilon} + \left(\frac{\mathrm{i}}{\varepsilon}\partial_{xx}\sigma_0 - \frac{1}{\varepsilon^2}(\partial_x\sigma_0)^2\right) u_0.
\end{aligned} \tag{4.12c}$$

In general, for $\partial_x^j\sigma_0 \neq 0$, this implies the estimate $\|\partial_x^j u_0\|_{L^2} \leqslant (1/\varepsilon^j)M_j$ with constant $M_j > 0$ not depending on the critical parameter ε for $j \geqslant 0$; in particular, if $\sigma_0 = 0$ it follows that $\|\partial_x^j u_0\|_{L^2} \leqslant M_j$ for $j \geqslant 0$.

4.2.1 *Linear Schrödinger equation.* For a linear Schrödinger equation, that is, (4.1) with $\vartheta = 0$, the above considerations simplify to

$$[A,B](w) = e^{-\mathrm{i}\tau_2 U/\varepsilon}\left(g_1(v) + \mathrm{i}\frac{\tau_2}{\varepsilon}g_2(v)\right),$$

$$g_1(v) = \partial_x U\partial_x v + \frac{1}{2}\partial_{xx}Uv, \quad g_2(v) = -(\partial_x U)^2 v, \quad v = \mathscr{E}_A(\tau_1, u_0), \quad \partial_x v = \mathscr{E}_A(\tau_1, \partial_x u_0);$$

see (4.12). On the one hand, due to the fact that

$$\|g_1(v)\|_{L^2} \leqslant \|\partial_x U\|_{L^\infty}\|\partial_x v\|_{L^2} + \tfrac{1}{2}\|\partial_{xx}U\|_{L^\infty}\|v\|_{L^2}, \quad \|g_2(v)\|_{L^2} \leqslant \|\partial_x U\|_{L^\infty}^2\|v\|_{L^2},$$

for initial values (4.12c) with $\sigma_0 = 0$ the bound

$$\|[A,B](w)\|_{L^2} \leqslant \|\partial_x U\|_{L^\infty} \|\partial_x u_0\|_{L^2} + \left(\|\partial_{xx} U\|_{L^\infty} + \frac{\tau_2}{\varepsilon} \|\partial_x U\|_{L^\infty}^2 \right) \|u_0\|_{L^2} \tag{4.13}$$

follows, which implies the local error estimate

$$\vartheta = 0, \quad \sigma_0 = 0 : \ \|\mathscr{L}(h,u_0)\|_{L^2} \leqslant \left(C_0 + C_1 \frac{h}{\varepsilon} \right) h^2$$

with constants $C_0, C_1 > 0$ involving $\|\partial_x u_0\|_{L^2}$, $\|u_0\|_{L^2}$, $\|\partial_x U\|_{L^\infty}$ and $\|\partial_{xx} U\|_{L^\infty}$; see also (4.9). Evidently, the Lie–Trotter splitting method has convergence order one; see Fig. 3. Moreover, for a fixed time-step size $h = h_0$ and critical parameter values $0 < \varepsilon < h$ (or, more precisely, $0 < \varepsilon < ch$ for some constant $c > 0$), the dominant local error term is $C_1 h^3/\varepsilon$ and thus the ratio $\alpha = -1$ results, whereas we obtain $\alpha = 2$ for $h = \varepsilon$ (see (4.4)); this is in accordance with the numerical observations summarized in Table 1. On the other hand, for initial values (4.12c) with first spatial derivative involving $1/\varepsilon$ (that is, $\|\partial_x u_0\|_{L^2} \leqslant (1/\varepsilon) M_1$), the bound (4.13) yields

$$\vartheta = 0, \quad \partial_x \sigma_0 \neq 0 : \ \|\mathscr{L}(h,u_0)\|_{L^2} \leqslant \left(C_0 h + C_1 \frac{h}{\varepsilon} \right) h$$

provided that $0 < h < 1$; similarly to before, for ratios h/ε where the local error term $C_1 h^2/\varepsilon$ dominates, we retain $\alpha = -1$ for $h = h_0$, but $\alpha = 1$ for $h = \varepsilon$, both confirming the numerical results given in Table 1.

4.2.2 *Cubic Schrödinger equation.* For the cubic Schrödinger equation it is more involved to deduce a local error estimate.

Regular initial condition. With regard to the regular initial condition (4.3) (see also (4.12c) and let $\sigma_0 = 0$), we first suppose the initial value u_0, and thus $v = \mathscr{E}_A(\tau_1, u_0)$, to be sufficiently regular with derivatives bounded by a constant, independent of ε. We note that the considerations could be made rigorous and that sufficient regularity requirements on u_0 are obtained by means of the Sobolev embedding $H^1(\Omega) \subset L^\infty(\Omega)$; however, as we are primarily concerned with the dependence of the local error on the time-step size and the critical parameter, we do not specify the regularity assumptions on the initial value or the precise form of the constants. Setting $U = 0$ in (4.1), the relations in (4.12) reduce to

$$\begin{aligned} (w) &= e^{-\mathrm{i}\tau_2 \vartheta |v|^2/\varepsilon} \left(g_1(v) + \mathrm{i} \frac{\tau_2}{\varepsilon} g_2(v) \right), \\ g_1(v) &= \vartheta \, \partial_{xx} \bar{v} v^2 + 2\vartheta |\partial_x v|^2 v + \vartheta (\partial_x v)^2 \bar{v}, \\ g_2(v) &= 2\vartheta^2 |\partial_x v|^2 |v|^2 v + \vartheta^2 \partial_{xx} v |v|^4 + \vartheta^2 \partial_{xx} \bar{v} |v|^2 v^2, \\ v = \mathscr{E}_A(\tau_1, u_0), &\quad \partial_x v = \mathscr{E}_A(\tau_1, \partial_x u_0), \quad \partial_{xx} v = \mathscr{E}_A(\tau_1, \partial_{xx} u_0). \end{aligned} \tag{4.14}$$

Therefore, assuming the initial value u_0 to satisfy suitable regularity requirements such that the quantities $g_1(v)$ and $g_2(v)$ remain bounded in $L^2(\Omega)$, the estimate

$$\|[A,B](w)\|_{L^2} \leqslant C_0 + C_1 \frac{h}{\varepsilon}$$

follows. The identity $\partial_2 \mathscr{E}_B(t,v)z = e^{-\mathrm{i}t\vartheta|v|^2/\varepsilon}(z - 2\mathrm{i}(t/\varepsilon)\vartheta\,\Re(\bar{v}z)v)$ (see (4.10)), yields

$$\begin{aligned}
\partial_2 \mathscr{E}_B(\tau_1-\tau_2,v)[A,B](w) &= G_1(v) + \frac{\tau_2}{\varepsilon}G_2(v) + \frac{\tau_1-\tau_2}{\varepsilon}G_3(v) + \frac{(\tau_1-\tau_2)\tau_2}{\varepsilon^2}G_4(v),\\
G_1(v) &= e^{-\mathrm{i}\tau_1\vartheta|v|^2/\varepsilon}g_1(v), \quad G_2(v) = \mathrm{i}\,e^{-\mathrm{i}\tau_1\vartheta|v|^2/\varepsilon}g_2(v),\\
G_3(v) &= -2\mathrm{i}\vartheta\; e^{-\mathrm{i}(\tau_1-\tau_2)\vartheta|v|^2/\varepsilon}\Re(e^{-\mathrm{i}\tau_2\vartheta|v|^2/\varepsilon}g_1(v)\bar{v})v,\\
G_4(v) &= -2\mathrm{i}\vartheta\; e^{-\mathrm{i}(\tau_1-\tau_2)\vartheta|v|^2/\varepsilon}\Re(\mathrm{i}\,e^{-\mathrm{i}\tau_2\vartheta|v|^2/\varepsilon}g_2(v)\bar{v})v,
\end{aligned} \tag{4.15}$$

and further implies the estimate

$$\|\partial_2 \mathscr{E}_B(\tau_1-\tau_2,v)[A,B](w)\|_{L^2} \leqslant C_0 + C_1\frac{h}{\varepsilon} + C_2\frac{h^2}{\varepsilon^2}.$$

With the help of the variation-of-constants formula (see also Theorem 3.3) and a Gronwall inequality, the bound $\|\partial_2 \mathscr{E}_F(t,v)\|_{L^2\leftarrow L^2} \leqslant C(1+h/\varepsilon)$ results and, as a consequence, we finally obtain the local error estimate

$$U=0, \quad \sigma_0 = 0: \ \|\mathscr{L}(h,u_0)\|_{L^2} \leqslant \left(C_0 + C_1\frac{h}{\varepsilon} + C_2\frac{h^2}{\varepsilon^2} + C_3\frac{h^3}{\varepsilon^3}\right)h^2$$

with constants $C_j > 0$ for $0 \leqslant j \leqslant 3$. The above bound shows that for a fixed time-step size $h = h_0$ the size of the ratio h/ε (as well as the size of the involved constants) determines the dominant local error term. Indeed, for ratios h/ε relatively small the term C_0h^2 dominates, whereas for h/ε large the dominant term is C_3h^5/ε^3. Figure 1 and further numerical results given in Table 2 indicate that, in the present example, for h/ε in a certain range the local error of the Lie–Trotter splitting method is dominated by C_1h^3/ε which explains the ratio $\alpha \approx -1$ and that for h/ε exceeding a certain value the local error becomes unsatisfactorily large. On the other hand, for time-step sizes $h = \varepsilon$ the above considerations for the Lie–Trotter splitting method imply $\|\mathscr{L}(\varepsilon,u_0)\|_{L^2} \leqslant C\varepsilon^2$, that is, $\alpha \approx 2$, in accordance with the numerical example; see Table 1.

Wentzel–Kramers–Brillouin (WKB) initial condition. At first glance, the numerical results obtained for classical initial conditions (4.2), that is, for initial values (4.12c) with $\partial_x\sigma_0 \neq 0$, are astonishing. Indeed, with regard to (4.14) one would suppose that the estimate for the first Lie commutator $\|[A,B](w)\|_{L^2} \leqslant C_0(1/\varepsilon^2) + C_1(h/\varepsilon^3)$ and the resulting bound $\|\mathscr{L}(h,u_0)\|_{L^2} \leqslant C_0(h^2/\varepsilon^2) + C_1(h^3/\varepsilon^3) + C_2(h^4/\varepsilon^4) + C_3(h^5/\varepsilon^5)$ capture the dependence on the critical parameter; however, this is not consistent with the numerical experiments. Reconsiderations similar to before lead to the local error bound

$$U=0, \quad \partial_x\sigma_0 \neq 0: \ \|\mathscr{L}(h,u_0)\|_{L^2} \leqslant Q(h/\varepsilon)h, \quad Q(\xi) = \sum_{j=0}^{\infty} C_j\xi^j,$$

in accordance with the numerical results; see also Table 1. In fact, for a fixed time-step size $h = h_0$ the ratio h/ε determines the dominant local error term; in the numerical example, the dominant term is Ch^2/ε. On the other hand, for $h = \varepsilon$ the ratio $\alpha \approx 1$ is observed.

4.2.3 *Gross–Pitaevskii equation.* Altogether, the above considerations for the linear and the cubic Schrödinger equation imply the following local error estimate for the Lie–Trotter splitting method (1.3)

TABLE 2 *Time integration of the cubic Schrödinger equation (4.1) with $\vartheta = 1$ and $\omega = 0$ under initial condition (4.3) by the Lie–Trotter splitting method with $h = 6.25 \times 10^{-2}$. Dependence of the local error on the critical parameter ε*

ε	h/ε	$\mathrm{err}_{\mathrm{local}}(\varepsilon)$	Ratio(ε)
5.000000000000e−1	1.250e−1	3.318314040129623e−3	−1.481542464484375e−002
2.500000000000e−1	2.500e−1	3.352566274062347e−3	−3.987567472693236e−002
1.250000000000e−1	5.000e−1	3.446522721795372e−3	−1.370712693825387e−001
6.250000000000e−2	1.000e + 0	3.790039267831324e−3	−3.789477377625659e−001
3.125000000000e−2	2.000e + 0	4.928540679180661e−3	−6.987314614573381e−001
1.562500000000e−2	4.000e + 0	7.999401116445972e−3	−8.998641518757462e−001
7.812500000000e−3	8.000e + 0	1.492600476861661e−2	−9.725874814930025e−001
3.906250000000e−3	1.600e + 1	2.929014902784553e−2	−9.927998706142481e−001
1.953125000000e−3	3.200e + 1	5.828866680385411e−2	−9.974626176915570e−001
9.765625000000e−4	6.400e + 1	1.163724799946193e−1	−9.964577528699693e−001
4.882812500000e−4	1.280e + 2	2.321742025889134e−1	−9.874763693867023e−001
2.441406250000e−4	2.560e + 2	4.603349719843108e−1	−9.501733704707212e−001
1.220703125000e−4	5.120e + 2	8.894154215722925e−1	−7.779601700474771e−001
6.103515625000e−5	1.024e + 3	1.525084832985217e + 0	4.144601950283195e−001
3.051757812500e−5	2.048e + 3	1.144271421143380e + 0	−4.118896129108623e−001
1.525878906250e−5	4.096e + 3	1.522369868884755e + 0	7.193399857950300e−003
7.629394531250e−6	8.192e + 3	1.514798096013354e + 0	

when applied to the Gross–Pitaevskii equation (4.1) in the semiclassical regime; see also (2.1a). As before, we require that the potential U is twice differentiable with bounded derivatives. For instance, in the case of a regular initial condition (4.3), for time-step sizes $0 < h < 1$ and parameter values $0 < \varepsilon < 1$, the following local error estimate is valid:

$$\sigma_0 = 0 : \ \|\mathscr{L}(h, u_0)\|_{L^2} \leqslant P(h/\varepsilon)h^2, \quad P(\xi) = \sum_{j=0}^{3} C_j \xi^j. \tag{4.16}$$

The local error estimate is in accordance with the numerical experiments given in Section 4.1.

4.3 *Global error estimate*

As standard, a global error estimate for the Lie–Trotter splitting method is obtained by employing a telescopic identity to relate the global error to local errors; see also Descombes & Thalhammer (2010), Lubich (2008), Thalhammer (2008). Thus, essential ingredients are stability bounds such as (4.9) and local error estimates such as (4.16); in particular, similar considerations to before yield bounds for $\|\mathscr{L}(h, u(t_j))\|_{L^2}$. We note that the local error estimates imply that time-step sizes sufficiently small, depending on the critical parameter, are required in order to obtain a reasonable numerical approximation rate. In this noncritical regime, it is then evident that the convergence estimate

$$\|u_N - u(t_N)\|_{L^2} \leqslant C\|u_0 - u(0)\|_{L^2} + Ch^p$$

holds with $p = 1$ for the first-order Lie–Trotter splitting method. This error behaviour is also confirmed by numerical examples not reported here: for time-step sizes relatively large compared with the critical

parameter the approximation is poor, whereas the full order of consistency is only retained for step sizes sufficiently smaller than the critical parameter.

5. Conclusions

The present work is a further attempt to contribute to the study of exponential operator splitting methods for nonlinear evolution equations; our main concern is to expose the derivation of a local error representation that is well suited in the presence of unbounded nonlinear operators as well as critical parameters and its analysis within the context of nonlinear Schrödinger equations in the semiclassical regime. This local error representation is an essential ingredient in the convergence analysis of splitting methods for nonlinear evolution equations. Throughout, as we hoped to thereby enhance clarity, general comprehensibility and readability, we focused on the first-order Lie–Trotter splitting method and considered as a model problem the time-dependent Gross–Pitaevskii equation in a single space dimension (Bao, Jin & Markowich, 2003, Example 6), involving marginal technicalities. Our central theme is to demonstrate that, contrary to other approaches, our local error representation is in agreement with the error behaviour observed in numerical experiments. Our conclusion is that in the case of a regular initial condition with bounded spatial derivatives, independent of the critical parameter $0 < \varepsilon \ll 1$, time-step sizes of the magnitude of ε are needed, whereas for an initial condition in classical Wentzel–Kramers–Brillouin form, time-step sizes sufficiently smaller than the critical parameter are required. For comparison and as an incentive for future work, we further included numerical experiments that confirm the expectation that higher-order exponential operator splitting methods possess improved accuracy properties.

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