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CONVERGENCE ANALYSIS OF HIGH-ORDER TIME-SPLITTING PSEUDOSPECTRAL METHODS FOR NONLINEAR SCHRÖDINGER EQUATIONS*

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Abstract. In this work, the issue of favorable numerical methods for the space and time discretization of low-dimensional nonlinear Schrödinger equations is addressed. The objective is to provide a stability and error analysis of high-accuracy discretizations that rely on spectral and splitting methods. As a model problem, the time-dependent Gross–Pitaevskii equation arising in the description of Bose–Einstein condensates is considered. For the space discretization pseudospectral methods collocated at the associated quadrature nodes are analyzed. For the time integration high-order exponential operator splitting methods are studied, where the decomposition of the function defining the partial differential equation is chosen in accordance with the underlying spectral method. The convergence analysis relies on a general framework of abstract nonlinear evolution equations and fractional power spaces defined by the principal linear part. Essential tools in the derivation of a temporal global error estimate are further the formal calculus of Lie-derivatives and bounds for iterated Lie-commutators. Numerical examples for higher-order time-splitting pseudospectral methods applied to time-dependent Gross–Pitaevskii equations illustrate the theoretical result.

Key words. nonlinear Schrödinger equations, time-dependent Gross–Pitaevskii equations, spectral methods, splitting methods, stability, error, convergence

AMS subject classifications. 65L05, 65M12, 65J15

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1. Introduction. *Contents.* In the present work, we address the issue of stable, accurate, and efficient numerical methods for the solution of time-dependent low-dimensional nonlinear Schrödinger equations. Our main objective is to provide a convergence analysis of high-accuracy discretizations that rely on spectral and splitting methods. As a model problem, we consider the time-dependent Gross–Pitaevskii equation, which arises in the description of Bose–Einstein condensates. For the space and time discretization we study pseudospectral methods combined with higher-order exponential operator splitting methods; the decomposition of the right-hand side of the partial differential equation is chosen in accordance with the underlying spectral method, and the solution is collocated at the associated quadrature nodes. We give a detailed derivation of the convergence estimate for the generally most relevant case of the Fourier pseudospectral method and indicate the extension to the Sine and Hermite pseudospectral method. The theoretical result is illustrated by numerical examples for time-splitting pseudospectral methods applied to time-dependent Gross–Pitaevskii equations.

Numerical simulations. The incentive for the present work originates from a variety of contributions devoted to favorable space and time discretizations of low-dimensional Schrödinger equations. We mention the references [4, 6, 7, 10, 25], where numerical comparisons for problems such as time-dependent Gross–Pitaevskii equations with regular analytical solutions provide numerical evidence that time-splitting

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spectral methods are favorable regarding efficiency, accuracy, stability, and the preservation of conserved quantities. In particular, numerical examples given in [10] imply that higher-order splitting methods are superior to other established classes of numerical methods whenever low tolerances are required or long-term computations are carried out. However, so far it remains open to give a complete convergence analysis explaining (certain aspects of) the numerical observations and thus justifying (to some extend) the use of higher-order time-splitting pseudospectral methods for certain classes of time-dependent Schrödinger equations.

Error analysis. The present works contributes to a rigorous error analysis of full discretizations for low-dimensional nonlinear Schrödinger equations by higher-order time-splitting pseudospectral methods. For this purpose, unifying and extending techniques exploited in [15, 20, 22, 23, 28, 30], we utilize an analytical framework of nonlinear evolutionary Schrödinger equations, fractional power spaces defined by the principal linear part, the formal calculus of Lie-derivatives, bounds for iterated Lie-commutators, and results on the approximation error of pseudospectral methods; see also [9, 11, 14, 17, 19, 27].

Extensions and future work. In order to incorporate the relevant cases of the Fourier, Sine, and Hermite pseudospectral methods and in view of generalizations such as to a generalized Laguerre–Fourier–Hermite spectral method capturing an additional rotation term (see, for instance, [6]), we employ an approach which accentuates the common aspects of spectral space discretizations. It is straightforward to extend the theoretical analysis to systems of coupled Gross–Pitaevskii equations or to problems involving more general nonlinearities such as a quartic nonlinearity; this also includes nonlinear Schrödinger equations arising in solid state physics; see, for instance, [5]. The error analysis extends to nonlinear Schrödinger equations of a similar form involving, for instance, a time-dependent trapping potential; in this case a special invariance property is no longer valid and thus an additional numerical approximation of the nonlinear subproblem is needed. In the presence of an additional critical parameter, however, the approach exploited in [12, 13] is better suited in order to obtain error estimates for time-splitting methods that are optimal with respect to the critical parameter, and it remains open to provide a convergence analysis of full discretizations for Schrödinger equations in the semiclassical regime. Furthermore, in the context of variational splitting methods applied to the multiconfiguration time-dependent Hartree–Fock equations arising in electron dynamics (see [22] and references given therein), it is of interest to investigate the convergence behavior of a Galerkin approach combined with higher-order exponential operator splitting methods.

Outline. The present manuscript is organized as follows. Basic definitions and auxiliary results are collected in section 1.1; in particular, we introduce the formal calculus of Lie-derivatives utilized in the derivation of a local error expansion for splitting methods. In section 2, we state the model problem under consideration and the employed analytical framework, and in section 3, we specify the considered space and time discretizations by the Fourier pseudospectral method and higher-order exponential operator splitting methods. In section 4, the main result of the present work, a convergence estimate for the fully discrete solution, is derived and illustrated by numerical examples. To account for situations where the Sine or the Hermite pseudospectral method are advantageous, we indicate the extension of the convergence analysis to these two relevant cases in section 4.5.

1.1. Auxiliary notation and results. *Standard notation.* Throughout, we tacitly make use of the following abbreviations; see also [2]. We denote by $\mathbb{N} = \{m \in$

$\mathbb{Z} : m \geq 0\}$ the set of nonnegative integer numbers. We employ the compact multi-index notation $\mu = (\mu_1, \dots, \mu_d) \in \mathbb{Z}^d$ and the vector notation $x = (x_1, \dots, x_d) \in \mathbb{R}^d$. For $\kappa, \mu \in \mathbb{Z}^d$ the Kronecker symbol is defined by $\delta_{\kappa\mu} = 1$ iff $\kappa = \mu$ and $\delta_{\kappa\mu} = 0$ otherwise. Furthermore, for $\kappa, \mu \in \mathbb{Z}^d$ relations such as $\leq$ are defined componentwise, that is, it holds $\kappa \leq \mu$ iff $\kappa_j \leq \mu_j$ for all $1 \leq j \leq d$. We set $|\mu| = \mu_1 + \dots + \mu_d$ for $\mu \in \mathbb{N}^d$ and $c\mu = (c\mu_1, \dots, c\mu_d)$ for $c \in \mathbb{Z}$ and $\mu \in \mathbb{Z}^d$. For $\mu \in \mathbb{N}^d$ and $x \in \mathbb{R}^d$ we write $x^\mu = x_1^{\mu_1} \cdots x_d^{\mu_d}$ as well as $\partial_x^\mu = \partial_{x_1}^{\mu_1} \cdots \partial_{x_d}^{\mu_d}$ for short and further denote by $\Delta = \partial_{x_1}^2 + \dots + \partial_{x_d}^2$ the d-dimensional Laplace operator. As standard, for any integer number $1 \leq p \leq \infty$ we denote by $L^p(\Omega)$ the Lebesgue space of complex-valued functions on a (suitable) domain $\Omega \subset \mathbb{R}^d$, which forms a Banach space with associated norm given by $\|f\|_{L^p(\Omega)}^p = \int_\Omega |f(x)|^p \,\mathrm{d}x$ for $1 \leq p < \infty$ and $\|f\|_{L^\infty(\Omega)} = \operatorname{ess\,sup}\{|f(x)| : x \in \Omega\}$, respectively; the Sobolev space $W^{m,p}(\Omega)$ comprises all functions with partial derivatives up to order $m \geq 1$ contained in $L^p(\Omega)$. In particular, the Hilbert spaces $H^0(\Omega) = L^2(\Omega)$ and $H^m(\Omega) = W^{m,2}(\Omega)$ for $m \geq 1$ are endowed with the inner product $(\cdot|\cdot)_{H^m(\Omega)}$ defined by $(f\,|\,g)_{L^2(\Omega)} = \int_\Omega f(x)\,\overline{g(x)}\,\mathrm{d}x$ and $(f\,|\,g)_{H^m(\Omega)} = (f\,|\,g)_{L^2(\Omega)} + \sum_{|\mu|=m} (\partial_x^\mu f\,|\,\partial_x^\mu g)_{L^2(\Omega)}$ for $m \geq 1$ and further with the corresponding norm $\|\cdot\|_{H^m(\Omega)}$ defined by $\|f\|_{H^m(\Omega)}^2 = (f\,|\,f)_{H^m(\Omega)}$ for $m \geq 0$; we point out that we choose the inner product to be sesquilinear in the second argument. For $m \geq 0$ the space of m-times continuously differentiable functions is denoted by $\mathscr{C}^m(\Omega)$, and $\mathscr{C}_B^m(\Omega)$ comprises all functions in $\mathscr{C}^m(\Omega)$ with bounded derivatives up to order m. Throughout, we let $\frac{d}{2} < \delta \in \mathbb{N}$ be such that by the Sobolev embedding theorem it holds that $H^\delta(\Omega) \hookrightarrow \mathscr{C}_B(\Omega)$, that is, the bound $\|f\|_{L^\infty(\Omega)} \leq C\,\|f\|_{H^\delta(\Omega)}$ for $f \in H^\delta(\Omega)$ is valid; in particular, we set $\delta = 1$ if $d = 1$ and $\delta = 2$ if $d = 2, 3$. For a (sufficiently regular) function $f : \Omega \to \mathbb{C}$ and a finite set $\mathscr{K} \subset \Omega$ we let $\|f\|_{L^\infty(\mathscr{K})} = \sup_{x \in \mathscr{K}} |f(x)|$. Furthermore, for a family of (unbounded nonlinear) operators $(F_\ell)_{j \leq \ell \leq k}$ the product is defined downward (on a suitably chosen domain), that is, we set $\prod_{\ell=j}^k F_\ell = F_k \cdots F_j$ if $j \leq k$ and $\prod_{\ell=j}^k F_\ell = I$ if $j > k$ with I the identity operator. If not stated otherwise, we do not distinguish the arising constants and denote by $C > 0$ a generic constant.

Calculus of Lie-derivatives. A most useful tool in view of a theoretical error analysis of higher-order exponential operator splitting methods applied to nonlinear evolutionary Schrödinger equations is the calculus of Lie-derivatives. This calculus allows us to formally extend arguments for the less involved linear case to nonlinear problems; see also [19, 22, 27] and references given therein. The analytical solution of an initial value problem of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F\big(u(t)\big)\,, \quad 0 \leq t \leq T\,, \qquad u(0) = u_0\,, \tag{1.1a}$$

involving an unbounded nonlinear operator $F : D(F) \subset X \to X$ defined on a nonempty subspace of the underlying Banach space $(X, \|\cdot\|_X)$ is formally given by

$$u(t) = \mathscr{E}_F(t)\,u_0\,, \qquad 0 \leq t \leq T\,; \tag{1.1b}$$

the nonlinear evolution operator $\mathscr{E}_F$ depends on time and acts on the initial value. Furthermore, it is useful to employ the notation

$$u(t) = \mathrm{e}^{tD_F}\,u_0\,, \qquad 0 \leq t \leq T\,. \tag{1.1c}$$

More precisely, for any unbounded nonlinear operator $G : D(G) \subset X \to X$, defined on a suitably chosen domain, the evolution operator and the Lie-derivative associated with F are given through the relations $\mathrm{e}^{tD_F} G\, v = G\big(\mathscr{E}_F(t)\, v\big)$ for $0 \leq t \leq T$ and $D_F\, G\, v = G'(v)\, F(v)$ with G' denoting the Fréchet derivative of G; if $G = I$ is the identity operator, we write $\mathrm{e}^{tD_F} v = \mathscr{E}_F(t)\, v$ and $D_F\, v = F(v)$ for short. The Lie-commutator of two Lie-derivatives D_F, D_G is given by $[D_F, D_G]\, v = D_F D_G\, v - D_G\, D_F\, v = G'(v)\, F(v) - F'(v)\, G(v)$; more generally, the iterated Lie-commutators are defined through $\mathrm{ad}_{D_F}^{j}(D_G) = \big[D_F, \mathrm{ad}_{D_F}^{j-1}(D_G)\big]$ for $j \geq 1$, where $\mathrm{ad}_{D_F}^{0}(D_G) = D_G$. Along the lines of the linear variation-of-constants formula

$$\frac{\mathrm{d}}{\mathrm{d}t}\, v(t) = L\, v(t) + r(t)\,, \quad v(t) = \mathrm{e}^{tL}\, v(0) + \int_0^t \mathrm{e}^{(t-\tau)L}\, r(\tau)\, \mathrm{d}\tau\,, \qquad 0 \leq t \leq T\,, \tag{1.2}$$

with linear operator L and time-dependent function r, the following result establishes a relation between the solutions of two nonlinear evolution equations.

THEOREM 1 (Gröbner–Alekseev formula). *The solutions to the initial value problems*

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big)\,, \quad u(0) = u_0\,, \quad u(t) = \mathrm{e}^{tD_F} u_0\,, \qquad 0 \leq t \leq T\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, v(t) = F\big(v(t)\big) + R\big(v(t)\big)\,, \quad v(0) = u_0\,, \quad v(t) = \mathrm{e}^{tD_{F+R}}\, u_0\,, \qquad 0 \leq t \leq T\,,$$

are related through the nonlinear variation-of-constants formula

$$\mathrm{e}^{tD_{F+R}}\, u_0 = \mathrm{e}^{tD_F} u_0 + \int_0^t \mathrm{e}^{\tau D_{F+R}}\, D_R\, \mathrm{e}^{(t-\tau)D_F}\, u_0\, \mathrm{d}\tau\,, \qquad 0 \leq t \leq T\,.$$

2. Nonlinear Schrödinger equations.

In this section, we state the considered model equation and formulate it as an abstract evolution equation; see, for example, [11, 14]. Further, we introduce the employed analytical framework and, in particular, the fractional power spaces defined by the principal linear part; the hypotheses on the linear part are in accordance with [31].

2.1. Model problem and abstract formulation.

Model problem. As a model problem, we study the following normalized formulation of the d-dimensional time-dependent Gross–Pitaevskii [18, 26] equation

$$\begin{cases} \mathrm{i}\, \partial_t \psi(x,t) = -\,\Delta\, \psi(x,t) + U(x)\, \psi(x,t) + \vartheta\, \big|\psi(x,t)\big|^2 \psi(x,t)\,, \\ \psi(x,0) \text{ given}\,, \qquad (x,t) \in \Omega \times [0,T]\,, \end{cases} \tag{2.1a}$$

subject to a certain initial condition and asymptotic boundary conditions on the unbounded spatial domain $\Omega = \mathbb{R}^d$. The above problem arises in the description of the complex-valued macroscopic wave function $\psi : \Omega \times [0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$ of a Bose–Einstein condensate at temperatures significantly below the critical condensation temperature. The external real-valued confining potential $U : \Omega \to \mathbb{R}$ comprises a scaled harmonic potential V_γ with positive weights $\gamma_j > 0$ for $1 \leq j \leq d$ and, in addition, a sufficiently regular and bounded potential $W : \Omega \to \mathbb{R}$

$$U = V_\gamma + W\,, \qquad V_\gamma\,(x) = \sum_{j=1}^{d} {\gamma_j}^4 x_j^{\,2}\,, \quad x \in \Omega\,. \tag{2.1b}$$

The interaction strength among the atomic species is described by $\vartheta \in \mathbb{R}$. Concerning existence and uniqueness results for time-dependent nonlinear Schrödinger equations, we refer to the monographs [11, 29].

Abstract formulation as evolution equation. For our convergence analysis, it is useful to employ a compact formulation of the initial boundary value problem (2.1) as an abstract initial value problem for a function $u : [0, T] \to X_0 : t \mapsto u(t) = \psi(\cdot, t)$

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = \mathrm{i}\,F\big(u(t)\big) = A\,u(t) + B\big(u(t)\big)\,u(t)\,, \quad 0 \le t \le T\,, \qquad u(0) \text{ given}\,, \tag{2.2}$$

with unbounded linear differential operator A related to the Laplacian and unbounded nonlinear multiplication operator B comprising the remaining part; see section 2.3. More generally and in view of possible extensions, we assume that both operators $A : D(A) \to X_0$ and $B : D(B) \to X_0$ are defined on suitably chosen dense subspaces of the underlying Hilbert space $(X_0, (\cdot\,|\,\cdot)_{X_0}, \|\cdot\|_{X_0})$ and employ the hypotheses on the linear part A introduced in section 2.2. Formally, the solution to (2.2) is given through $u(t) = \mathrm{e}^{tD_F}u(0) = \mathscr{E}_F(t)\,u(0)$ for $0 \le t \le T$; see (1.1).

2.2. Analytical framework. *Hypotheses on the principal linear part.* We suppose that the densely defined linear operator $A : X_1 = D(A) \subset X_0 \to X_0$ is self-adjoint and positive semidefinite with a pure point spectrum. Thus, the eigenvalue relation

$$A\,\mathscr{B}_\mu = \lambda_\mu\,\mathscr{B}_\mu\,, \qquad \mu \in \mathscr{M}\,, \tag{2.3}$$

holds with countably many eigenfunctions $(\mathscr{B}_\mu)_{\mu\in\mathscr{M}}$ and corresponding nonnegative eigenvalues $(\lambda_\mu)_{\mu\in\mathscr{M}}$; the family $(\mathscr{B}_\mu)_{\mu\in\mathscr{M}}$ forms a complete orthonormal system in X_0,

$$\big(\mathscr{B}_\kappa\,\big|\,\mathscr{B}_\mu\big)_{X_0} = \delta_{\kappa\mu}\,, \qquad \kappa, \mu \in \mathscr{M}\,. \tag{2.4a}$$

Furthermore, for any $v \in X_0$ the spectral representation

$$v = \sum_{\mu\in\mathscr{M}} c_\mu(v)\,\mathscr{B}_\mu\,, \qquad c_\mu(v) = \big(v\,\big|\,\mathscr{B}_\mu\big)_{X_0}\,, \quad \mu \in \mathscr{M}\,, \tag{2.4b}$$

is valid. By Parseval's identity it follows that

$$\|v\|_{X_0}^2 = \sum_{\mu\in\mathscr{M}} \big|c_\mu(v)\big|^2\,, \qquad v \in X_0\,. \tag{2.4c}$$

Fractional power spaces. For $\alpha \in \mathbb{R}$ the linear operator $A^\alpha : X_\alpha \subset X_0 \to X_0$ is given by

$$A^\alpha\,v = \sum_{\mu\in\mathscr{M}} c_\mu(v)\,\lambda_\mu^\alpha\,\mathscr{B}_\mu\,, \qquad X_\alpha = \left\{ v = \sum_{\mu\in\mathscr{M}} c_\mu(v)\,\mathscr{B}_\mu \in X_0 : \|A^\alpha\,v\|_{X_0}^2 < \infty \right\}.$$

The domain X_α forms a Hilbert space with inner product $(v\,|\,w)_{X_\alpha} = (v\,|\,w)_{X_0} + (A^\alpha\,v\,|\,A^\alpha\,w)_{X_0}$ for $v, w \in X_\alpha$; whenever the linear operator A is positive definite (and as well for the case $\alpha = 0$), it suffices to consider instead the equivalent norm $\|\cdot\|_{X_\alpha} = \|A^\alpha(\cdot)\|_{X_0}$.

2.3. Definition of A and B. In the abstract formulation (2.2) we define the linear part A and the remaining nonlinear part B in accordance with the considered spectral method for the space discretization of the time-dependent nonlinear Schrödinger equation (2.1). In connection with the Fourier spectral method, tacitly assuming the analytical solution of (2.1) to be localized due to the confining potential, the unbounded spatial domain is restricted to a sufficiently large bounded domain $\Omega \subset \mathbb{R}^d$; without loss of generality, we suppose $\Omega = (-a_1, a_1) \times \cdots \times (-a_d, a_d) \subset \mathbb{R}^d$ to be the Cartesian product of symmetric intervals with $a_\ell > 0$ sufficiently large for $1 \leq \ell \leq d$. Furthermore, we set $A = -\Delta$, imposing periodic boundary conditions on Ω, as well as $V = U$ and $B(v) = V + \vartheta\,|v|^2$. The hypotheses of section 2.2 are satisfied for with $X_0 = L^2(\Omega)$ chosen as the underlying Hilbert space; see, for instance, [31]. We note that the nonlinearity is well-defined for continuous functions and thus for functions in X_α with exponent $\alpha \geq \frac{\delta}{2} > 0$; see Lemma 1 below.

3. Higher-order time-splitting pseudospectral methods. For the discretization of the time-dependent nonlinear Schrödinger equation (2.1) we study the Fourier pseudospectral method and higher-order exponential operator splitting methods; detailed information on spectral and splitting methods is found, for instance, in [9, 19, 24]. A variety of contributions by Bao and coauthors provide numerical evidence that pseudospectral splitting methods are favorable, with the Fourier pseudospectral method being in general the space discretization of choice [4, 5, 6, 7]; see also [10] for comparisons of the Fourier versus the Hermite pseudospectral method and of various second-, fourth-, and sixth-order time-splitting methods proposed in the literature. We recall auxiliary notations introduced in sections 1.1 and 2.

3.1. Pseudospectral methods. In regard to the spatial discretization of (2.1)–(2.2), we next introduce the interpolant for the approximation of the spectral representation (2.4b). Moreover, we collect the needed basics for the Fourier pseudospectral methods, which also justifies the general approach given in section 3.1.1; for further details, we refer to the monographs [9, 16, 31]. In view of section 4.5 we distinguish the spectral basis functions, denoting the Fourier basis functions by $(\mathscr{F}_\mu)_{\mu\in\mathscr{M}}$; the efficient implementation of the Fourier pseudospectral method relies on fast Fourier transform techniques. We recall the definition of the operator A and the choice $X_0 = L^2(\Omega)$ for the underlying Hilbert space; see section 2.

3.1.1. Interpolant. *Quadrature formula approximation.* Let $\omega : \Omega \subset \mathbb{R}^d \to \mathbb{R}_{>0}$ and $(\eta_\kappa, \xi_\kappa)_{\kappa\in\mathscr{K}_M}$ denote the weight function as well as the quadrature weights and nodes associated with the considered spectral method. For a sufficiently regular function $f : \overline{\Omega} \to \mathbb{C}$ the quadrature formula approximation is then given by

$$\sum_{\kappa\in\mathscr{K}_M} \eta_\kappa\,\omega(\xi_\kappa)\,f(\xi_\kappa) \approx \int_\Omega f(x)\,\mathrm{d}x\,. \tag{3.1}$$

Spectral interpolant. For a sufficiently regular function $v : \overline{\Omega} \to \mathbb{C}$ the associated spectral interpolant $\mathscr{Q}_M\,v \approx v$ for the numerical approximation of the spectral representation (2.4b) results from a truncation of the infinite series and an application of the quadrature formula approximation (3.1)

$$\mathscr{Q}_M\,v = \sum_{\mu\in\mathscr{M}_M} \widetilde{c}_\mu(v)\,\mathscr{B}_\mu\,, \qquad \widetilde{c}_\mu(v) = \sum_{\kappa\in\mathscr{K}_M} \eta_\kappa\,\omega(\xi_\kappa)\,v(\xi_\kappa)\,\overline{\mathscr{B}_\mu(\xi_\kappa)}\,, \quad \mu \in \mathscr{M}_M\,. \tag{3.2}$$

We note that the spectral interpolant is well-defined for continuous functions and thus for functions in X_α with exponent $\alpha \geq \frac{\delta}{2} > 0$ (see also Lemma 1 below); evidently, the mapping $\mathscr{Q}_M$ is linear.

3.1.2. Fourier pseudospectral method. *Fourier spectral method.* For all $1 \leq \ell \leq d$ we choose $a_\ell > 0$ sufficiently large and set $\Omega = (-a_1, a_1) \times \cdots \times (-a_d, a_d) \subset \mathbb{R}^d$ as well as $\mathscr{M} = \mathbb{Z}^d$; see also section 2.3. The complex-valued Fourier basis functions $(\mathscr{F}_\mu)_{\mu \in \mathscr{M}}$ are given by $\mathscr{F}_\mu(x) = \prod_{j=1}^{d} \mathscr{F}_{\mu_j}(x_j) = \prod_{j=1}^{d} \mathrm{e}^{\mathrm{i}\,\mu_j\,\pi\,(x_j/a_j+1)} / \sqrt{(2\,a_j)}$ for $x \in \Omega$ and $\mu \in \mathscr{M}$; clearly, the Fourier basis functions are periodic on the closure $\overline{\Omega}$. Moreover, the eigenvalue relation (2.3) is satisfied with $A = -\Delta$ and $\lambda_\mu = \sum_{j=1}^{d} \lambda_{\mu_j} = \sum_{j=1}^{d} \mu_j^2\,\pi^2/a_j^2$ for $\mu \in \mathscr{M}$. In the present situation, the analytical framework introduced in section 2.2 applies; in particular, the Fourier spectral basis functions fulfill the relations in (2.4) with $X_0 = L^2(\Omega)$.

Fourier pseudospectral method. For a multi-index $0 < M \in \mathbb{N}^d$ comprising even integers, we set $\mathscr{M}_M = \big\{\mu \in \mathscr{M} : -\frac{1}{2}M \leq \mu \leq \frac{1}{2}M - 1\big\}$ and $\mathscr{K}_M = \big\{\kappa \in \mathbb{N}^d : 0 \leq \kappa \leq M - 1\big\}$. Due to $0 \leq \mu_j^2 \leq M_j^2/4$ if $\mu \in \mathscr{M}_M$ or $M_j^2/4 \leq \mu_j^2$ if $\mu \in \mathscr{M} \setminus \mathscr{M}_M$, respectively, it follows that $\lambda_\mu \leq \lambda_{\max}$ for $\mu \in \mathscr{M}_M$ and $\lambda_{\max} \leq \lambda_\mu$ for $\mu \in \mathscr{M} \setminus \mathscr{M}_M$ with $\lambda_{\max} = \sum_{j=1}^{d} M_j^2 \pi^2/(4\,a_j^2)$. For a sufficiently regular and periodic function $f : \overline{\Omega} \to \mathbb{C}$ the multidimensional trapezoidal rule yields a quadrature formula approximation through (3.1), where the weight function and, further, the quadrature nodes and weights are given by $\omega(x) = 1$ for $x \in \mathbb{R}^d$ and $\eta_\kappa = \eta_{\kappa_1} \cdots \eta_{\kappa_d} \in \mathbb{R}_{>0}$ as well as $\xi_\kappa = (\xi_{\kappa_1}, \dots, \xi_{\kappa_d}) \in \mathbb{R}^d$ for $\kappa \in \mathscr{K}_M \subset \mathbb{N}^d$ with $\xi_{\kappa_j} = -a_j + 2\,\kappa_j\,a_j/M_j$ and $\eta_{\kappa_j} = 2\,a_j/M_j$ for $0 \leq \kappa_j \leq M_j - 1$ and $1 \leq j \leq d$.

3.2. Exponential operator splitting methods. *Time-splitting approach.* The class of exponential operator splitting methods applied to a nonlinear evolution equation utilizes the natural decomposition of the function defining the right-hand side of the differential equation into (at least) two parts and the presumption that each of the resulting subproblems is solvable in an efficient and accurate manner. In the context of time-dependent nonlinear Schrödinger equations such as Gross–Pitaevskii systems the decomposition is commonly defined in accordance with the underlying spectral method, and the solutions are collocated at the associated grid points. Compositions of the (numerical) solutions to the subproblems with suitably adjusted time increments in the substeps then yield approximations of a certain order of consistency.

Solutions to subproblems. For our model problem (2.1)–(2.2), the idea suggests itself to consider the subproblem

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,v(t) = A\,v(t)\,, \quad 0 \leq t \leq T\,, \qquad v(0) = v_0\,, \tag{3.3a}$$

with linear differential operator A defined in accordance with the underlying (Fourier) spectral method (see also section 2.3); thus, employing a spectral decomposition of the initial value, the following representation for the analytical solution is obtained:

$$\begin{aligned} &v_0 = \sum_{\mu \in \mathscr{M}} c_\mu(v_0)\,\mathscr{B}_\mu\,, \qquad c_\mu(v_0) = \big(v_0 \,\big|\, \mathscr{B}_\mu\big)_{X_0}\,, \quad \mu \in \mathscr{M}\,, \\ &v(t) = \mathscr{E}_{-\mathrm{i}\,A}(t)\,v_0 = \mathrm{e}^{-\mathrm{i}\,tA}\,v_0 = \sum_{\mu \in \mathscr{M}} c_\mu(v_0)\,\mathrm{e}^{-\mathrm{i}\,t\lambda_\mu}\,\mathscr{B}_\mu\,, \qquad 0 \leq t \leq T\,. \end{aligned} \tag{3.3b}$$

See (2.3) and (2.4b). The remaining terms in (2.1)–(2.2) define the subproblem

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,w(t) = B\big(w(t)\big)\,w(t)\,, \quad 0 \leq t \leq T\,, \qquad w(0) = w_0\,; \tag{3.4a}$$

due to the invariance property $\partial_t\,|\psi(x,t)|^2 = 2\,\Re\big(\overline{\psi(x,t)}\,\partial_t\psi(x,t)\big) = 0$ of the associated analytical solution, which further implies $B(w(t)) = B(w_0)$ for $0 \leq t \leq T$, the initial value problem (3.4a) reduces to the linear problem

$$\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,w(t) = B(w_0)\,w(t)\,, \quad 0 \le t \le T\,, \qquad w(0) = w_0\,, \tag{3.4b}$$

with the solution given through pointwise multiplication

$$w(t) = \mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0 = \mathrm{e}^{-\mathrm{i}\,tB(w_0)}\,w_0\,, \qquad 0 \le t \le T\,. \tag{3.4c}$$

See also section 2.3 for the definition of the nonlinear multiplication operator B in the context of the Fourier spectral method.

General format of splitting methods. As is standard for a time-stepping approach, starting from an initial value $u_0 \approx u(0)$, numerical approximations to the analytical solution values at time grid points $0 = t_0 < t_1 < \cdots < t_N \le T$ with associated time increments $\tau_{n-1} = t_n - t_{n-1}$ for $1 \le n \le N$ are obtained from a recurrence relation of the form

$$\begin{aligned} &u_n = \mathscr{S}_F(\tau_{n-1})\,u_{n-1} \;\approx\; u(t_n) = \mathscr{E}_F(\tau_{n-1})\,u(t_{n-1})\,, \qquad 1 \le n \le N\,,\\ &\mathscr{S}_F(t) = \prod_{j=1}^{s} \mathscr{E}_{-\mathrm{i}\,B}(b_j\,t)\,\mathscr{E}_{-\mathrm{i}\,A}(a_j\,t)\,, \qquad 0 \le t \le T\,. \end{aligned} \tag{3.5}$$

Provided that the (real) method coefficients $(a_j, b_j)_{j=1}^{s}$ fulfill certain order conditions (see [22, 30] and references given therein), the splitting operator is an approximation of order $p \ge 1$ to the analytical evolution operator. Throughout, to avoid possible instabilities due to strongly varying time stepsizes, we employ the standard assumption that the ratios of two subsequent time increments are bounded from below and above.

Numerical realization. For the realization of the splitting approach (3.5) the linear subproblem (3.3) is solved numerically by means of the chosen pseudospectral method; that is, an approximation $\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v_0 \approx v(t) = \mathscr{E}_{-\mathrm{i}\,A}(t)\,v(0)$ is computed by spectral interpolation of the initial value and application of the evolution operator $\mathscr{E}_{-\mathrm{i}\,A}$, which yields

$$\begin{aligned} &\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v_0 = \mathrm{e}^{-\mathrm{i}\,tA}\,\mathscr{Q}_M\,v_0 = \sum_{\mu\in\mathscr{M}_M} \widetilde{c}_\mu(v_0)\,\mathrm{e}^{-\mathrm{i}\,t\lambda_\mu}\,\mathscr{B}_\mu\,, \qquad 0 \le t \le T\,,\\ &\widetilde{c}_\mu(v_0) = \sum_{\kappa\in\mathscr{K}_M} \eta_\kappa\,\omega(\xi_\kappa)\,v_0(\xi_\kappa)\,\overline{\mathscr{B}_\mu(\xi_\kappa)}\,, \quad \mu \in \mathscr{M}_M \end{aligned}$$

(see also (3.2)). We note that in the present situation the analytical solution of the nonlinear subproblem (3.4) is available. Consequently, starting from the initial value $\widetilde{u}_{0M} = u_0 \approx u(0)$, numerical approximations to the analytical solution values are determined through

$$\begin{aligned} &\widetilde{u}_{nM} = \mathscr{T}_F(\tau_{n-1})\,\widetilde{u}_{n-1,M} \;\approx\; u(t_n) = \mathscr{E}_F(\tau_{n-1})\,u(t_{n-1})\,, \qquad 1 \le n \le N\,,\\ &\mathscr{T}_F(t) = \prod_{j=1}^{s} \big(\mathscr{E}_{-\mathrm{i}\,B}(b_j\,t)\,\mathscr{E}_{-\mathrm{i}\,A}(a_j\,t)\,\mathscr{Q}_M\big)\,, \qquad 0 \le t \le T\,; \end{aligned} \tag{3.6}$$

for notational simplicity, we do not indicate the dependence of the nonlinear operator $\mathscr{T}_F$ on the multi-index M.

Examples and illustrations. At certain places, we will illustrate our convergence analysis of exponential operator splitting methods (3.5) on the basis of the least technical example method, the first-order Lie–Trotter splitting method

$$\mathscr{S}_F(t) = \mathscr{E}_{-\mathrm{i}\,B}(t)\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,, \qquad 0 \leq t \leq T\,, \tag{3.7}$$

where $s = 1$ and $a_1 = 1 = b_1$; favorable higher-order splitting methods are proposed, for instance, in [8]. Numerical illustrations for splitting methods of orders $p = 1, 2, 3, 4$ applied to (2.1) are given in section 4.6.

4. Convergence analysis. In the following, we deduce the main result of the present work, a convergence estimate for full discretizations of nonlinear Schrödinger equations (2.1)–(2.2) by high-order time-splitting pseudospectral methods (3.6) (see section 4.4); the theoretical result is illustrated by numerical examples for time-dependent Gross–Pitaevskii equations described in section 4.6. Our approach unifies and extends techniques exploited in [15, 20, 22, 23, 30]. Applying a Lady Windermere's fan argument or, more prosaically, a telescopic identity, the fundamental representation of the global error comprises the numerical evolution operators and defects; thus, the main ingredients for the convergence analysis are stability bounds and estimates for the defect of spectral and splitting methods given in sections 4.2 and 4.3. Various auxiliary results are collected in section 4.1.

4.1. Auxiliary results. In the following, we deduce several auxiliary results that are needed in our convergence analysis; in particular, this includes estimates for the nonlinear part in fractional power spaces and bounds for the spectral interpolant.

4.1.1. Estimates in fractional power spaces. The following result permits to estimate Sobolev norms by the norm of fractional power spaces and further shows that fractional power spaces form a normed algebra for suitably chosen integer exponents. We recall that the constant $\frac{d}{2} < \delta \in \mathbb{N}$ denotes the exponent arising in the Sobolev embedding theorem and that the linear operator A is given by $A = -\Delta$ (see sections 1.1 and 2.3); further, we employ the analytical framework introduced in section 2.2 and the basic relations for the spectral basis functions collected in section 3.1.2. The arising constant depends on the spatial dimension $d \geq 1$.

LEMMA 1. (i) *For any exponent $\alpha \geq 0$ and for any multi-index $\kappa \in \mathbb{N}^d$ the following estimate is valid for the Fourier pseudospectral method:*

$$\big\| A^{\alpha} \partial_x^{\kappa}\, v \big\|_{X_0} \leq \big\| A^{\alpha + |\kappa|/2}\, v \big\|_{X_0}\,, \qquad v \in X_{\alpha + |\kappa|/2}\,.$$

(ii) *For any $\alpha \geq \frac{\delta}{2}$ the bound $\|v\|_{L^\infty(\Omega)} \leq C\,\|v\|_{H^\delta(\Omega)} \leq C\,\|v\|_{X_\alpha}$ holds for $v \in X_\alpha$, and thus the following estimate is valid:*

$$\|v\,w\|_{X_0} \leq C\,\|v\|_{X_0}\,\|w\|_{X_\alpha}\,, \qquad v \in X_0\,, \quad w \in X_\alpha\,.$$

(iii) *For any $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$ the following estimate holds for the Fourier pseudospectral method:*

$$\|v\,w\|_{X_\alpha} \leq C\,\|v\|_{X_\alpha}\,\|w\|_{X_\alpha}\,, \qquad v, w \in X_\alpha\,.$$

Proof. (i) For a function $v \in X_0$ we employ the spectral representation (2.4b). In connection with the Fourier spectral method, due to the relation $\partial_{x_j} \mathscr{F}_\mu = \mathrm{i}\,\lambda_{\mu_j}^{1/2}\,\mathscr{F}_\mu$ for $1 \leq j \leq d$, we obtain $A^\alpha \partial_x^\kappa v = \mathrm{i}^{|\kappa|} \sum_{\mu \in \mathscr{M}} c_\mu(v)\,\lambda_\mu^\alpha \prod_{j=1}^d \lambda_{\mu_j}^{\kappa_j/2}\,\mathscr{F}_\mu$; Parseval's identity yields $\|A^\alpha \partial_x^\kappa v\|_{X_0}^2 = \sum_{\mu \in \mathscr{M}} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} \prod_{j=1}^d \lambda_{\mu_j}^{\kappa_j} \leq \sum_{\mu \in \mathscr{M}} |c_\mu(v)|^2\,\lambda_\mu^{2\,\alpha + |\kappa|} = \|A^{\alpha + |\kappa|/2} v\|_{X_0}^2$, which implies the statement.

(ii) We note that the estimate $\|v\|_{X_\alpha} \leq C\,\|v\|_{X_\beta}$ is valid for exponents $0 \leq \alpha \leq \beta$ and $v \in X_\beta$, since $x^\alpha \leq x^\beta$ for $x \geq 1$, and consequently $\|v\|^2_{X_\alpha} = \|v\|^2_{L^2(\Omega)} + \|A^\alpha v\|^2_{L^2(\Omega)} = \|v\|^2_{L^2(\Omega)} + \sum_{\mu\in\mathscr{M}} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} = \|v\|^2_{L^2(\Omega)} + \sum_{\mu\in\mathscr{M},\,\lambda_\mu<1} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} + \sum_{\mu\in\mathscr{M},\,\lambda_\mu\geq 1} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} \leq C\,\|v\|^2_{L^2(\Omega)} + \sum_{\mu\in\mathscr{M},\,\lambda_\mu\geq 1} |c_\mu(v)|^2\,\lambda_\mu^{2\beta} \leq C\,\|v\|^2_{X_\beta}$. By the Sobolev embedding theorem and statement (i) the estimate $\|v\|^2_{L^\infty(\Omega)} \leq C\,\|v\|^2_{H^\delta(\Omega)} = C\,(\|v\|^2_{L^2(\Omega)} + \sum_{|\kappa|=\delta} \|\partial_x^\kappa v\|^2_{L^2(\Omega)}) \leq C\,(\|v\|^2_{L^2(\Omega)} + \|A^{\delta/2} v\|^2_{L^2(\Omega)}) \leq C\,\|v\|^2_{X_\alpha}$ follows for $\alpha \geq \frac{\delta}{2}$. As an immediate consequence, we obtain the stated bound $\|v\,w\|_{L^2(\Omega)} \leq \|v\|_{L^2(\Omega)}\,\|w\|_{L^\infty(\Omega)} \leq C\,\|v\|_{X_0}\,\|w\|_{X_\alpha}$.

(iii) Let $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$. For the Fourier spectral method, we consider $A^\alpha(v\,w) = (-1)^\alpha\,\Delta^\alpha(v\,w)$; note that by assumption $\alpha \in \mathbb{N}$. For instance, it holds that $\Delta^2 = (\partial^2_{x_1} + \partial^2_{x_2})^2 = \partial^4_{x_1} + \partial^4_{x_2} + 2\,\partial^2_{x_1}\partial^2_{x_2}$ for $d = 2 = \alpha$. Generally, $\Delta^\alpha(v\,w)$ comprises terms of the form $\partial_x^\kappa(v\,w)$ with $\kappa \in \mathbb{N}^d$ such that $|\kappa| = 2\,\alpha$ and thus, by the differentiation rule of Leibnitz, terms of the form $\partial_x^{\kappa-\mu} v\;\partial_x^\mu w$ with $\kappa, \mu \in \mathbb{N}^d$ such that $\mu \leq \kappa$ and $|\kappa| = 2\,\alpha$. Note that all indices are covered by the cases $|\mu| \leq 2\,\alpha - \delta$ or $2\,\alpha - \delta \leq |\mu| \leq 2\,\alpha$, respectively. Without loss of generality, we assume $|\mu| \leq 2\,\alpha - \delta$ or, otherwise, reverse the roles of v and w; in this case, again by the Sobolev embedding theorem and statement (i), we obtain the estimate $\|\partial_x^{\kappa-\mu} v\;\partial_x^\mu w\|_{L^2(\Omega)} \leq \|\partial_x^{\kappa-\mu} v\|_{L^2(\Omega)}\,\|\partial_x^\mu w\|_{L^\infty(\Omega)} \leq C\,\|A^\alpha v\|_{X_0}\,\|w\|_{X_\alpha}$, since $|\kappa-\mu| \leq |\kappa| = 2\,\alpha$ and $|\mu| + \delta \leq 2\,\alpha$. This yields $\|A^\alpha(v\,w)\|_{X_0} \leq C\,\|A^\alpha v\|_{X_0}\,\|w\|_{X_\alpha}$. Altogether, by statement (ii) the bound $\|v\,w\|^2_{X_\alpha} = \|v\,w\|^2_{X_0} + \|A^\alpha(v\,w)\|^2_{X_0} \leq C\,(\|v\|^2_{X_0}\,\|w\|^2_{X_\alpha} + \|A^\alpha v\|^2_{X_0}\,\|w\|^2_{X_\alpha}) \leq C\,\|v\|^2_{X_\alpha}\,\|w\|^2_{X_\alpha}$ follows, which yields the stated result. $\square$

Remark. In the above lemma, for the case of two and three space dimensions the admissable choice $\alpha = \frac{\delta}{2} = 1 \in \mathbb{N}$ yields $\|v\,w\|_{X_0} \leq C\,\|v\|_{X_0}\,\|w\|_{X_1}$ and $\|v\,w\|_{X_1} \leq C\,\|v\|_{X_1}\,\|w\|_{X_1}$, to be compared with the well-known relations $\|v\,w\|_{L^2(\Omega)} \leq C\,\|v\|_{L^2(\Omega)}\,\|w\|_{H^2(\Omega)}$ and $\|v\,w\|_{H^2(\Omega)} \leq C\,\|v\|_{H^2(\Omega)}\,\|w\|_{H^2(\Omega)}$.

4.1.2. Estimates for the nonlinear part in fractional power spaces. As a preliminary step toward a stability bound for the nonlinear part, we next deduce estimates for the unbounded nonlinear operator $B(v) = V + \vartheta\,|v|^2$ in certain fractional power spaces (see section 2.3 for the definition of B); we recall that by Lemma 1 the nonlinearity is well-defined for functions in X_α with exponent $\alpha \geq \frac{\delta}{2} > 0$. We point out that it is not sufficient to derive a bound of the form $\|\mathrm{e}^{-\mathrm{i}\,tB(v_0)} w_0\|_{X_\zeta} \leq C\,\mathrm{e}^{C\,t}\|w_0\|_{X_\zeta}$ for $0 \leq t \leq T$ and $\zeta = 0, \alpha$, where $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$, obtained, for instance, by Lemma 1 together with a straightforward estimation of the power series for the exponential. In order to ensure the stability of exponential operator splitting methods, we instead need to show that a bound of the form $\|\mathrm{e}^{-\mathrm{i}\,tB(v_0)} w_0\|_{X_\zeta} \leq \mathrm{e}^{C\,t}\|w_0\|_{X_\zeta}$ is valid for $0 \leq t \leq T$ and $\zeta = 0, \alpha$. It is straightforward to extend the arguments to more general nonlinearities involving a quartic term such as $B(v) = V + \vartheta_1\,|v|^2 + \vartheta_2\,|v|^4$. The arising constant depends on the spatial dimension $d \geq 1$.

LEMMA 2. *Let $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$. Then the following bounds hold for $\zeta = 0, \alpha$:*

$$\begin{aligned}
\big\|B(v_0)\,w_0\big\|_{X_\zeta} &\leq C\,\big(\|V\|_{X_\alpha} + |\vartheta|\,\|v_0\|^2_{X_\alpha}\big)\,\|w_0\|_{X_\zeta}\,,\\
\big\|\big(B(v_0) - B(\widetilde{v}_0)\big)\,w_0\big\|_{X_\zeta} &\leq C\,|\vartheta|\,\big(\|v_0\|_{X_\alpha} + \|\widetilde{v}_0\|_{X_\alpha}\big)\,\|w_0\|_{X_\alpha}\,\|v_0 - \widetilde{v}_0\|_{X_\zeta}\,,\\
\big\|\mathrm{e}^{-\mathrm{i}\,tB(v_0)} w_0\big\|_{X_\zeta} &\leq \mathrm{e}^{C\,(\|V\|_{X_\alpha} + |\vartheta|\,\|v_0\|^2_{X_\alpha})\,t}\|w_0\|_{X_\zeta}\,, \qquad 0 \leq t \leq T\,.
\end{aligned}$$

Proof. An application of Lemma 1, statements (ii) and (iii), yields the first bound $\|B(v_0)\,w_0\|_{X_\zeta} \leq C\,\|B(v_0)\|_{X_\alpha}\|w_0\|_{X_\zeta} \leq C\,(\|V\|_{X_\alpha} + |\vartheta|\,\|v_0\|^2_{X_\alpha})\,\|w_0\|_{X_\zeta}$ for any $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$ and $\zeta = 0, \alpha$. By means of the identity $(B(v_0) - B(\widetilde{v}_0))\,w_0 =$

$\vartheta\,(v_0\,\overline{v_0} - \widetilde{v}_0\,\overline{\widetilde{v}_0})\,w_0 = \vartheta\,((v_0 - \widetilde{v}_0)\,\overline{v_0} + \overline{(v_0 - \widetilde{v}_0)}\,\widetilde{v}_0)\,w_0$, the second statement follows. In order to deduce the bound for $w(t) = \mathrm{e}^{-\mathrm{i}\,tB(v_0)}w_0$, we consider the initial value problem $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,w(t) = B(v_0)\,w(t)$, $0 \le t \le T$, $w(0) = w_0$. Integration, an application of Lemma 1, and a Gronwall-type inequality yield

$$
\begin{aligned}
w(t) &= w_0 - \mathrm{i}\int_0^t B(v_0)\,w(\tau)\,\mathrm{d}\tau\,,\\
\|w(t)\|_{X_\zeta} &\le \|w_0\|_{X_\zeta} + C\left(\|V\|_{X_\alpha} + |\vartheta|\,\|v_0\|_{X_\alpha}^2\right)\int_0^t \big\|w(\tau)\big\|_{X_\zeta}\,\mathrm{d}\tau\,,\\
\big\|w(t)\big\|_{X_\zeta} &\le \mathrm{e}^{C\,(\|V\|_{X_\alpha} + |\vartheta|\,\|v_0\|_{X_\alpha}^2)\,t}\|w_0\|_{X_\zeta}\,, \qquad 0 \le t \le T\,,
\end{aligned}
$$

which implies the stated result. ∎

4.1.3. Basic relations for orthogonal projection and spectral interpolation. The following auxiliary result summarizes useful relations for the spectral interpolant (3.2) introduced in section 3.1.1. We recall the spectral representation (2.4b) for any function in $X_0 = L^2(\Omega)$. A truncation of the infinite sum defines the orthogonal projection $\mathscr{P}_M\,v \approx v$,

$$
\mathscr{P}_M\,v = \sum_{\mu\in\mathscr{M}_M} c_\mu(v)\,\mathscr{B}_\mu\,, \qquad c_\mu(v) = \big(v\,\big|\,\mathscr{B}_\mu\big)_{X_0}\,, \quad \mu \in \mathscr{M}_M\,, \qquad v \in X_0\,. \tag{4.1}
$$

An orthogonal projection together with an application of the associated quadrature formula approximation yields the spectral interpolant (3.2), which is well-defined for functions $v \in X_\alpha$ with exponent $\alpha \ge \frac{\delta}{2}$; see Lemma 1.

LEMMA 3. (i) *The spectral basis functions fulfill the following discrete orthogonality relations at the associated quadrature nodes:*

$$
\begin{aligned}
&\sum_{\kappa\in\mathscr{K}_M} \eta_\kappa\,\omega(\xi_\kappa)\,\mathscr{B}_\mu(\xi_\kappa)\,\overline{\mathscr{B}_{\widetilde{\mu}}(\xi_\kappa)} = \delta_{\mu\widetilde{\mu}}\,, \qquad \mu,\widetilde{\mu} \in \mathscr{M}_M\,,\\
&\sum_{\mu\in\mathscr{M}_M} \mathscr{B}_\mu(\xi_\kappa)\,\overline{\mathscr{B}_\mu(\xi_{\widetilde{\kappa}})} = \frac{1}{\eta_\kappa\,\omega(\xi_\kappa)}\,\delta_{\kappa\widetilde{\kappa}}\,, \qquad \kappa,\widetilde{\kappa} \in \mathscr{K}_M\,.
\end{aligned}
$$

(ii) *For any $v \in X_0$ the relation $\mathscr{Q}_M\,\mathscr{P}_M\,v = \mathscr{P}_M\,v$ is valid.*

(iii) *For $v \in X_\alpha$ with $\alpha \ge \frac{\delta}{2}$ the interpolation property $(\mathscr{Q}_M\,v)(\xi_\kappa) = v(\xi_\kappa)$ holds for $\kappa \in \mathscr{K}_M$.*

(iv) *Let $v, w \in X_\alpha$ with $\alpha \ge \frac{\delta}{2}$. Then the inner product of the two corresponding interpolants and the norm are given by*

$$
\begin{aligned}
\big(\mathscr{Q}_M\,v\,\big|\,\mathscr{Q}_M\,w\big)_{X_0} &= \sum_{\kappa\in\mathscr{K}_M} \eta_\kappa\,\omega(\xi_\kappa)\,v(\xi_\kappa)\,\overline{w(\xi_\kappa)}\,,\\
\big\|\mathscr{Q}_M\,v\big\|_{X_0}^2 &= \sum_{\kappa\in\mathscr{K}_M} \eta_\kappa\,\omega(\xi_\kappa)\,\big|v(\xi_\kappa)\big|^2\,.
\end{aligned}
$$

Proof. (i) It suffices to deduce the results for a single space dimension only; due to the tensor structure of the spectral basis functions and the approximation by iterated quadrature formulas, the extension to the multidimensional case is then straightforward. We recall the basic relations for the Fourier pseudospectral method collected in section 3.1.2. The stated result is obtained easily by means of the geometric series.

(ii) In order to show that for a function of the form $v = \sum_{\mu\in\mathscr{M}_M} c_\mu(v)\,\mathscr{B}_\mu$ with coefficients $c_\mu(v) = (v\,|\,\mathscr{B}_\mu)_{X_0}$, $\mu \in \mathscr{M}_M$, the quadrature formula approximation of the spectral coefficients is exact, due to linearity, it suffices to consider $v = \mathscr{B}_{\widetilde{\mu}}$ for $\widetilde{\mu} \in \mathscr{M}_M$. Employing the first discrete orthogonality relation as well as the orthogonality of the spectral basis functions, the desired result follows from $\widetilde{c}_\mu(\mathscr{B}_{\widetilde{\mu}}) = \sum_{\kappa \in \mathscr{K}_M} \eta_\kappa \, \omega(\xi_\kappa) \, \mathscr{B}_{\widetilde{\mu}}(\xi_\kappa) \, \overline{\mathscr{B}_\mu(\xi_\kappa)} = \delta_{\mu\widetilde{\mu}} = (\mathscr{B}_{\widetilde{\mu}} \,|\, \mathscr{B}_\mu)_{X_0} = c_\mu(\mathscr{B}_{\widetilde{\mu}})$, $\mu, \widetilde{\mu} \in \mathscr{M}_M$.

(iii) The stated result is an immediate consequence of the definition of the interpolant and the second discrete orthogonality relation $(\mathscr{Q}_M v)(\xi_\kappa) = \sum_{\mu \in \mathscr{M}_M} \widetilde{c}_\mu(v) \mathscr{B}_\mu(\xi_\kappa)$ $= \sum_{\widetilde{\kappa} \in \mathscr{K}_M} \eta_{\widetilde{\kappa}} \omega(\xi_{\widetilde{\kappa}}) v(\xi_{\widetilde{\kappa}}) \sum_{\mu \in \mathscr{M}_M} \overline{\mathscr{B}_\mu(\xi_{\widetilde{\kappa}})} \mathscr{B}_\mu(\xi_\kappa) = \sum_{\widetilde{\kappa} \in \mathscr{K}_M} \eta_{\widetilde{\kappa}} \omega(\xi_{\widetilde{\kappa}}) v(\xi_{\widetilde{\kappa}}) \frac{1}{\eta_\kappa \omega(\xi_\kappa)} \delta_{\kappa\widetilde{\kappa}} = v(\xi_\kappa)$, $\kappa \in \mathscr{K}_M$.

(iv) The defining relation for the spectral interpolant, the orthogonality of the basis functions, and the second discrete orthogonality relation yield the stated result for the inner product $(\mathscr{Q}_M v \,|\, \mathscr{Q}_M w)_{X_0} = \sum_{\mu, \widetilde{\mu} \in \mathscr{M}_M} \widetilde{c}_\mu(v) \, \overline{\widetilde{c}_{\widetilde{\mu}}(w)} \, (\mathscr{B}_\mu \,|\, \mathscr{B}_{\widetilde{\mu}})_{X_0} = \sum_{\mu \in \mathscr{M}_M} \widetilde{c}_\mu(v) \, \overline{\widetilde{c}_\mu(w)} = \sum_{\kappa, \widetilde{\kappa} \in \mathscr{K}_M} \eta_\kappa \, \eta_{\widetilde{\kappa}} \, \omega(\xi_\kappa) \, \omega(\xi_{\widetilde{\kappa}}) \, v(\xi_\kappa) \, \overline{w(\xi_{\widetilde{\kappa}})} \sum_{\mu \in \mathscr{M}_M} \overline{B_\mu(\xi_\kappa)} B_\mu(\xi_{\widetilde{\kappa}})$ $= \sum_{\kappa \in \mathscr{K}_M} \eta_\kappa \, \omega(\xi_\kappa) \, v(\xi_\kappa) \, \overline{w(\xi_\kappa)}$. The given relation for the norm then follows at once. □

4.1.4. Estimates for orthogonal projection and spectral interpolation. Auxiliary estimates for the orthogonal projection (4.1) and the spectral interpolant (3.2) needed in the derivation of our convergence bound are provided by the following result. We recall the values of the quantity $\lambda_{\max} = \lambda_{\max}(\mathscr{M}_M)$ given in section 3.1.2 for the Fourier spectral method. The arising constant depends on the spatial dimension $d \geq 1$.

LEMMA 4. (i) *For $\alpha \geq 0$ the orthogonal projection fulfills the relations*

$$\begin{aligned} \big\| A^\alpha \mathscr{P}_M \, v \big\|_{X_0} &\leq \big\| A^\alpha v \big\|_{X_0} , \qquad v \in X_\alpha \, , \\ \big\| A^\alpha \mathscr{P}_M \, v \big\|_{X_0} &\leq \lambda_{\max}^\alpha \big\| \mathscr{P}_M \, v \big\|_{X_0} \leq \lambda_{\max}^\alpha \, \| v \|_{X_0} \, , \qquad v \in X_0 \, , \end{aligned}$$

and, in particular, for any $\alpha \geq 0$ it follows $\mathscr{P}_M \, v \in X_\alpha$ for $v \in X_0$. For exponents $0 \leq \zeta \leq \alpha$ the truncation error of the orthogonal projection satisfies

$$\big\| A^\zeta (\mathscr{P}_M - I) \, v \big\|_{X_0} \leq \lambda_{\max}^{-(\alpha-\zeta)} \big\| A^\alpha \, v \big\|_{X_0} \, , \qquad v \in X_\alpha \, .$$

(ii) *For $\alpha \geq \frac{\delta}{2}$ the spectral interpolant fulfills the relations*

$$\begin{aligned} \big\| A^\alpha \mathscr{Q}_M \, v \big\|_{X_0} &\leq \lambda_{\max}^\alpha \big\| \mathscr{Q}_M \, v \big\|_{X_0} \, , \qquad v \in X_\alpha \, , \\ \| \mathscr{Q}_M (v \, w) \|_{X_0} \leq \| v \|_{L^\infty(\mathscr{K}_M)} \, \| \mathscr{Q}_M \, w \|_{X_0} &\leq C \, \| v \|_{X_\alpha} \big\| \mathscr{Q}_M \, w \big\|_{X_0} \, , \qquad v, w \in X_\alpha \, . \end{aligned}$$

(iii) *For the Fourier pseudospectral method the estimate*

$$\begin{aligned} \big\| \mathscr{Q}_M \, v \big\|_{X_0}^2 \leq C \Bigg(\| v \|_{X_0}^2 + \sum_{1 \leq \ell_1 \leq d} \frac{1}{M_{\ell_1}^c} \big\| A^{\frac{1}{2}} v \big\|_{X_0}^2 + \sum_{\substack{1 \leq \ell_1, \ell_2 \leq d \\ \ell_1 < \ell_2}} \frac{1}{(M_{\ell_1} M_{\ell_2})^c} \big\| A v \big\|_{X_0}^2 + \cdots \\ + \sum_{\substack{1 \leq \ell_1, \ldots \ell_d \leq d \\ \ell_1 < \cdots < \ell_d}} \frac{1}{(M_{\ell_1} \cdots \, M_{\ell_d})^c} \big\| A^{\frac{d}{2}} v \big\|_{X_0}^2 \Bigg) , \qquad v \in X_\alpha \, , \quad \alpha \geq \frac{d}{2} \, , \end{aligned}$$

is valid with exponent $c = 2$. Furthermore, the following relation holds with quantity $\Lambda(M,\alpha,\zeta)$ involving $\lambda_{\max} = \lambda_{\max}(\mathscr{M}_M)$:

$$\big\|A^{\zeta}\big(\mathscr{Q}_M - I\big)\,v\big\|_{X_0} \leq C\,\Lambda(M,\alpha,\zeta)\,\|v\|_{X_\alpha}\,, \qquad v \in X_\alpha\,, \quad \alpha \geq \frac{\delta}{2}\,, \tag{4.2a}$$

(4.2b)

$$\Lambda(M,\alpha,\zeta) = \lambda_{\max}^{-(\alpha-\zeta)}\left(1 + \lambda_{\max}\sum_{1\leq \ell_1\leq d}\frac{1}{M_{\ell_1}^c} + \cdots + \lambda_{\max}^d \sum_{\substack{1\leq \ell_1,\dots\ell_d\leq d\\ \ell_1<\dots<\ell_d}}\frac{1}{(M_{\ell_1}\cdots\, M_{\ell_d})^c}\right)^{1/2}.$$

Proof. (i) For $v \in X_0$ we employ the spectral representation $v = \sum_{\mu\in\mathscr{M}} c_\mu(v)\,\mathscr{B}_\mu$ with coefficients $c_\mu(v) = (v\,|\,\mathscr{B}_\mu)_{X_0}$, $\mu \in \mathscr{M}$, and the defining relation for the orthogonal projection $\mathscr{P}_M\, v = \sum_{\mu\in\mathscr{M}_M} c_\mu(v)\,\mathscr{B}_\mu$. By means of the relation $A^\alpha\,\mathscr{B}_\mu = \lambda_\mu^\alpha\,\mathscr{B}_\mu$, $\mu \in \mathscr{M}$, Parseval's identity, and the bound $\lambda_\mu \leq \lambda_{\max}$ for $\mu \in \mathscr{M}_M$ the first two relations follow for any $\alpha \geq 0$, namely, $\|A^\alpha\,\mathscr{P}_M\, v\|_{X_0}^2 = \sum_{\mu\in\mathscr{M}_M} |c_\mu(v)|^2\lambda_\mu^{2\alpha} \leq \sum_{\mu\in\mathscr{M}} |c_\mu(v)|^2\lambda_\mu^{2\alpha} = \|A^\alpha v\|_{X_0}^2$ for $v \in X_\alpha$ and $\|A^\alpha\,\mathscr{P}_M\, v\|_{X_0}^2 \leq \lambda_{\max}^{2\alpha}\sum_{\mu\in\mathscr{M}_M} |c_\mu(v)|^2 = \lambda_{\max}^{2\alpha}\,\|\mathscr{P}_M\, v\|_{X_0}^2$ for $v \in X_0$; see also section 3.1.2. Making use of the fact that $\lambda_{\max} \leq \lambda_\mu$ for $\mu \in \mathscr{M}\setminus\mathscr{M}_M$ and that the mapping $\lambda \to \lambda^\beta$ is monotonically increasing for any $\beta \geq 0$, a brief calculation yields the third relation, since $A^\zeta(\mathscr{P}_M - I)\,v = \sum_{\mu\in\mathscr{M}\setminus\mathscr{M}_M} c_\mu(v)\,\lambda_\mu^\zeta\,\mathscr{B}_\mu$ and thus $\|A^\zeta(\mathscr{P}_M - I)\,v\|_{X_0}^2 = \sum_{\mu\in\mathscr{M}\setminus\mathscr{M}_M} |c_\mu(v)|^2\,\lambda_\mu^{2\zeta} \leq \lambda_{\max}^{-2\,(\alpha-\zeta)}\sum_{\mu\in\mathscr{M}\setminus\mathscr{M}_M} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} \leq \lambda_{\max}^{-2\,(\alpha-\zeta)}\sum_{\mu\in\mathscr{M}} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} = \lambda_{\max}^{-2\,(\alpha-\zeta)}\,\|A^\alpha\, v\|_{X_0}^2$ for $v \in X_\alpha$ and $0 \leq \zeta \leq \alpha$; here, we again utilize the spectral representation (2.4b) and Parseval's identity.

(ii) Let $v, w \in X_\alpha$ with $\alpha \geq \frac{\delta}{2}$. A straighforward estimation yields the first relation $\|A^\alpha\mathscr{Q}_M\, v\|_{X_0} = \|\sum_{\mu\in\mathscr{M}_M}\widetilde{c}_\mu(v)\,\lambda_\mu^\alpha\,\mathscr{B}_\mu\|_{X_0} \leq \lambda_{\max}^\alpha\|\mathscr{Q}_M v\|_{X_0}$; the second relation follows from an application of Lemmas 1 and 3, namely, $\|\mathscr{Q}_M\,(vw)\|_{X_0}^2 = \sum_{\kappa\in\mathscr{K}_M}\eta_\kappa\,\omega(\xi_\kappa)\,|v(\xi_\kappa)|^2|w(\xi_\kappa)|^2 \leq \|v\|_{L^\infty(\mathscr{K}_M)}^2\|\mathscr{Q}_M\, w\|_{X_0}^2 \leq C\,\|v\|_{X_\alpha}^2\|\mathscr{Q}_M\, w\|_{X_0}^2$.

(iii) (a) The derivation of the first estimate for the spectral interpolant relies on the following considerations for the one-dimensional case. For the Fourier pseudospectral method we set $\Omega_j = (-\,a_j, a_j)$. In [17, proof of Lemma 3.1] it is shown that the Hermite interpolant of a function $v : \Omega_j \to \mathbb{R} : x_j \mapsto v(x_j)$ such that $v \in H^1(\Omega_j)$ satisfies

$$\sum_{\kappa_j=0}^{M_j-1}\eta_{\kappa_j}\,\omega(\xi_{\kappa_j})\,\big|v(\xi_{\kappa_j})\big|^2 \leq C\left(\int_{\Omega_j}\big|v(x_j)\big|^2\,\mathrm{d}x_j + M_j^{-\frac{1}{3}}\int_{\Omega_j}\big|\partial_x v(x_j)\big|^2\,\mathrm{d}x_j\right); \tag{4.3}$$

the proof uses the following bound for a function $f : [z_0, z_1] \subset \mathbb{R} \to \mathbb{R}$ such that $f \in H^1([z_0, z_1])$:

$$\sup_{z_0\leq z\leq z_1}|f(z)|^2 \leq C\,\frac{1}{z_1 - z_0}\int_{z_0}^{z_1}|f(z)|^2\,\mathrm{d}z + C\,(z_1 - z_0)\int_{z_0}^{z_1}|\partial_z\, f(z)|^2\,\mathrm{d}z\,.$$

For the Fourier pseudospectral method, where $\eta_{\kappa_j} = \frac{2\,a_j}{M_j}$, a straightforward estimation yields the analogous relation to (4.3) with exponent $c = 2$,

$$\begin{aligned}
&\sum_{\kappa_j=0}^{M_j-1} \eta_{\kappa_j}\, \omega(\xi_{\kappa_j})\, \big|v(\xi_{\kappa_j})\big|^2 \\
&\quad \leq C \sum_{\kappa_j=0}^{M_j-1} \bigg(\int_{\xi_{\kappa_j}}^{\xi_{\kappa_j}+\eta_{\kappa_j}} |v(x_j)|^2 \,\mathrm{d}x_j + \eta_{\kappa_j}^2 \int_{\xi_{\kappa_j}}^{\xi_{\kappa_j}+\eta_{\kappa_j}} |\partial_{x_j} v(x_j)|^2 \,\mathrm{d}x_j \bigg) \\
&\quad \leq C \bigg(\int_{\Omega_j} \big|v(x_j)\big|^2 \,\mathrm{d}x_j + M_j^{-c} \int_{\Omega_j} \big|\partial_x v(x_j)\big|^2 \,\mathrm{d}x_j \bigg).
\end{aligned}$$

We next illustrate the extension of the bound to the most relevant case of three space dimensions. A repeated application of the above result yields

$$\begin{aligned}
\big\|\mathscr{Q}_M v\big\|_{X_0}^2 &= \sum_{\kappa_1=0}^{M_1-1} \eta_{\kappa_1}\, \omega(\xi_{\kappa_1}) \sum_{\kappa_2=0}^{M_2-1} \eta_{\kappa_2}\, \omega(\xi_{\kappa_2}) \sum_{\kappa_3=0}^{M_3-1} \eta_{\kappa_3}\, \omega(\xi_{\kappa_3}) \big|v(\xi_{\kappa_1}, \xi_{\kappa_2}, \xi_{\kappa_3})\big|^2 \\
&\leq C \int_\Omega \bigg(\big|v(x)\big|^2 + \frac{1}{M_1^c} \big|\partial_{x_1} v(x)\big|^2 + \frac{1}{M_2^c} \big|\partial_{x_2} v(x)\big|^2 + \frac{1}{M_3^c} \big|\partial_{x_3} v(x)\big|^2 \\
&\qquad + \frac{1}{(M_1 M_2)^c} \big|\partial_{x_1 x_2} v(x)\big|^2 + \frac{1}{(M_1 M_3)^c} \big|\partial_{x_1 x_3} v(x)\big|^2 \\
&\qquad + \frac{1}{(M_2 M_3)^c} \big|\partial_{x_2 x_3} v(x)\big|^2 + \frac{1}{(M_1 M_2 M_3)^c} \big|\partial_{x_1 x_2 x_3} v(x)\big|^2 \bigg) \,\mathrm{d}x;
\end{aligned}$$

see also Lemma 3. Further by Lemma 1,

$$\begin{aligned}
\big\|\mathscr{Q}_M v\big\|_{X_0}^2 \leq C \Bigg(&\|v\|_{X_0}^2 + \sum_{1 \leq \ell_1 \leq 3} \frac{1}{M_{\ell_1}^c} \big\|A^{\frac{1}{2}} v\big\|_{X_0}^2 + \sum_{\substack{1 \leq \ell_1, \ell_2 \leq 3 \\ \ell_1 < \ell_2}} \frac{1}{(M_{\ell_1} M_{\ell_2})^c} \big\|A\, v\big\|_{X_0}^2 \\
&+ \sum_{\substack{1 \leq \ell_1, \ell_2, \ell_3 \leq 3 \\ \ell_1 < \ell_2 < \ell_3}} \frac{1}{(M_{\ell_1}\, M_{\ell_2}\, M_{\ell_3})^c} \big\|A^{\frac{3}{2}} v\big\|_{X_0}^2 \Bigg),
\end{aligned}$$

which yields the first relation for $d = 3$.

(b) Recall that $\mathscr{Q}_M \mathscr{P}_M = \mathscr{P}_M$. We utilize the relation $(\mathscr{Q}_M - I) v = \sum_{\mu \in \mathscr{M}_M} \widetilde{c}_\mu(v) \mathscr{B}_\mu - \sum_{\mu \in \mathscr{M}} c_\mu(v)\, \mathscr{B}_\mu = \sum_{\mu \in \mathscr{M}_M} (\widetilde{c}_\mu(v) - c_\mu(v))\, \mathscr{B}_\mu - \sum_{\mu \in \mathscr{M} \setminus \mathscr{M}_M} c_\mu(v)\, \mathscr{B}_\mu = (\mathscr{Q}_M - \mathscr{P}_M)\, v + (\mathscr{P}_M - I)\, v = \mathscr{Q}_M (I - \mathscr{P}_M)\, v + (\mathscr{P}_M - I)\, v$ and the above considerations to obtain the bound $\|A^\zeta (\mathscr{Q}_M - I)\, v\|_{X_0} \leq \|A^\zeta \mathscr{Q}_M\, (I - \mathscr{P}_M)\, v\|_{X_0} + \|A^\zeta (\mathscr{P}_M - I)\, v\|_{X_0} \leq \lambda_{\max}^\zeta \|\mathscr{Q}_M\, (I - \mathscr{P}_M)\, v\|_{X_0} + \lambda_{\max}^{-(\alpha - \zeta)} \|A^\alpha\, v\|_{X_0}$ and further

$$\begin{aligned}
&\big\|A^\zeta (\mathscr{Q}_M - I)\, v\big\|_{X_0} \\
&\quad \leq C\, \lambda_{\max}^\zeta \Bigg(\big\|(I - \mathscr{P}_M)\, v\big\|_{X_0}^2 + \sum_{1 \leq \ell_1 \leq d} \frac{1}{M_{\ell_1}^c} \big\|A^{\frac{1}{2}} (I - \mathscr{P}_M)\, v\big\|_{X_0}^2 + \cdots \\
&\qquad + \sum_{\substack{1 \leq \ell_1, \ldots, \ell_d \leq d \\ \ell_1 < \cdots < \ell_d}} \frac{1}{(M_{\ell_1} \cdots\, M_{\ell_d})^c} \big\|A^{\frac{d}{2}} (I - \mathscr{P}_M)\, v\big\|_{X_0}^2 \Bigg)^{1/2} + \lambda_{\max}^{-(\alpha - \zeta)} \big\|A^\alpha\, v\big\|_{X_0} \\
&\quad \leq C\, \lambda_{\max}^{-(\alpha - \zeta)} \Bigg(1 + \lambda_{\max} \sum_{1 \leq \ell_1 \leq d} \frac{1}{M_{\ell_1}^c} + \cdots + \lambda_{\max}^d \sum_{\substack{1 \leq \ell_1, \ldots, \ell_d \leq d \\ \ell_1 < \cdots < \ell_d}} \frac{1}{(M_{\ell_1} \cdots\, M_{\ell_d})^c} \Bigg)^{1/2} \|v\|_{X_\alpha},
\end{aligned}$$

which yields the stated result. $\square$

4.2. Stability results for spectral and splitting methods. In this section, we derive stability bounds for the time-discrete evolution operator $\mathscr{S}_F$ and the fully discrete evolution operator $\mathscr{T}_F$; see also (3.5) and (3.6).

4.2.1. Stability results for exponential operator splitting methods. We first study the stability behavior of exponential operator splitting methods for the time integration of the nonlinear evolutionary problem (2.1)–(2.2). We recall that the splitting operator associated with a high-order splitting method is defined by (3.5); that is, starting from some initial value v_0, the arising approximations and intermediate values are given by

$$\begin{cases} v_{\ell 0} = v_\ell \,, \\ v_{\ell k} = \mathscr{E}_{-\mathrm{i}\,B}(b_k\tau_\ell)\,\mathscr{E}_{-\mathrm{i}\,A}(a_k\tau_\ell)\,v_{\ell,k-1}\,, \quad 1\le k\le s\,, \qquad\qquad 0\le \ell\le n-1\,. \\ v_{\ell+1} = v_{\ell s} = \mathscr{S}_F(\tau_\ell)\,v_\ell\,, \end{cases} \tag{4.4}$$

For instance, for the first-order Lie–Trotter splitting method (3.7), the above relations simplify to $v_{\ell+1} = \mathscr{S}_F(\tau_\ell)\,v_\ell = \mathscr{E}_{-\mathrm{i}\,B}(\tau_\ell)\,\mathscr{E}_{-\mathrm{i}\,A}(\tau_\ell)\,v_\ell$ for $0\le\ell\le n-1$. We aim at a stability bound of the form $\big\|\prod_{\ell=j}^{n-1}\mathscr{S}_F(\tau_\ell)\,v_j - \prod_{\ell=j}^{n-1}\mathscr{S}_F(\tau_\ell)\,w_j\big\|_{X_0} \le \mathrm{e}^{C(t_n-t_j)}\,\|v_j - w_j\|_{X_0}$ for $0\le j\le n-1$. However, it turns out that due to the nonlinearity of the problem, the quantity C involves all intermediate values $\|v_{\ell k}\|_{X_\alpha}$, $\|w_{\ell k}\|_{X_\alpha}$ for $1\le k\le s$ and $0\le\ell\le n-1$ (but $\|v_n\|_{X_\alpha}, \|w_n\|_{X_\alpha}$) for some $\frac{\delta}{2}\le\alpha\in\mathbb{N}$; recall that $\delta>\frac{d}{2}$ denotes the exponent arising in the Sobolev embedding theorem (see section 1.1). Thus, provided that the boundedness of the numerical approximation values in X_α for some $\frac{\delta}{2}\le\alpha\in\mathbb{N}$ is ensured, the splitting method remains stable in the underlying function space X_0; this is called *conditional stability* in [23]. For this reason, we also derive an estimate with respect to the X_α-norm for $\frac{\delta}{2}\le\alpha\in\mathbb{N}$ $\big\|\prod_{\ell=j}^{n-1}\mathscr{S}_F(\tau_\ell)\,v_j - \prod_{\ell=j}^{n-1}\mathscr{S}_F(\tau_\ell)\,w_j\big\|_{X_\alpha} \le \mathrm{e}^{C(t_n-t_j)}\,\|v_j-w_j\|_{X_\alpha}$ for $0\le j\le n-1$. Basic auxiliary results for the exact evolution operators $\mathscr{E}_{-\mathrm{i}\,A}$ and $\mathscr{E}_{-\mathrm{i}\,B}$ are provided by Lemma 6. A repeated application yields the following stability result with constant depending on the spatial dimension $d\ge1$ and the method coefficients $(b_j)_{1\le j\le s}$.

LEMMA 5 (stability, $\mathscr{S}_F$). *Let $\frac{\delta}{2}\le\alpha\in\mathbb{N}$ and $0\le j\le n-1$. For starting values v_j, w_j, let $v_{\ell k}$, $w_{\ell k}$ for $1\le k\le s$ and $j\le\ell\le n-1$ denote the corresponding intermediate values arising in the computation of $\mathscr{S}_F(\tau_{n-1})\cdots\mathscr{S}_F(\tau_j)\,v_j$, $\mathscr{S}_F(\tau_{n-1})\cdots\mathscr{S}_F(\tau_j)\,w_j$; see (4.4). Assume that there exist constants $C_V>0$ and $C_\alpha>0$ such that $\|V\|_{X_\alpha}\le C_V$ and $\|v_{\ell k}\|_{X_\alpha}, \|w_{\ell k}\|_{X_\alpha}\le C_\alpha$ for $1\le k\le s$ and $j\le\ell\le n-1$ (but the final approximations v_n, w_n). Then the following estimate is valid for $\zeta=0,\alpha$:*

$$\left\|\prod_{\ell=j}^{n-1}\mathscr{S}_F(\tau_\ell)\,v_j - \prod_{\ell=j}^{n-1}\mathscr{S}_F(\tau_\ell)\,w_j\right\|_{X_\zeta} \le \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,(t_n-t_j)}\,\|v_j-w_j\|_{X_\zeta}\,.$$

Remark. The operators $\mathscr{E}_{-\mathrm{i}\,A}(t)$ and $\mathscr{E}_{-\mathrm{i}\,B}(t)$ are unitary on $X_0=L^2(\Omega)$ for $0\le t\le T$; see Lemma 6 below and note that $\|\mathscr{E}_{-\mathrm{i}\,B}(t)\,v\|_{X_0}^2 = \int_\Omega \big|\mathrm{e}^{-\mathrm{i}\,t(B(v))(x)}\big|^2\,|v(x)|^2\,\mathrm{d}x = \|v\|_{X_0}^2$, since $(B(v))(x) = V(x)+\vartheta\,|v(x)|^2\in\mathbb{R}$. Recall that the nonlinearity is well-defined for continuous functions and thus for functions in X_α with exponent $\alpha\ge\frac{\delta}{2}>0$. For linear Schrödinger equations, that is, if $\vartheta=0$, the constant C_α does not arise in the stability bound; see also [30].

The proof of the following auxiliary estimates utilizes the hypotheses on the linear operator A introduced in section 2.2 and estimates in fractional power spaces given in section 4.1; see also section 2.3 for the definitions of the operators A and B. The arising constant depends on the spatial dimension $d \geq 1$.

LEMMA 6 (stability, $\mathscr{E}_{-\mathrm{i}\,A}, \mathscr{E}_{-\mathrm{i}\,B}$). (i) *The linear operator* $-\mathrm{i}\,A : X_1 \to X_0$ *generates a unitary group* $(\mathrm{e}^{-\mathrm{i}\,tA})_{t\in\mathbb{R}}$ *on* X_α *for any* $\alpha \geq 0$*, that is, it holds*

$$\big\|\mathscr{E}_{-\mathrm{i}\,A}(t)\,v\big\|_{X_\alpha} = \|v\|_{X_\alpha}\,, \qquad t \in \mathbb{R}\,, \quad \alpha \geq 0\,, \quad v \in X_\alpha\,.$$

(ii) *Let* $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$ *and* $v, w \in X_\alpha$. *Assume that there exist constants* $C_V > 0$ *and* $C_\alpha > 0$ *such that* $\|V\|_{X_\alpha} \leq C_V$ *and* $\|v\|_{X_\alpha}, \|w\|_{X_\alpha} \leq C_\alpha$. *Then the following estimate is valid for* $\zeta = 0, \alpha$*:*

$$\big\|\mathscr{E}_{-\mathrm{i}\,B}(t)\,v - \mathscr{E}_{-\mathrm{i}\,B}(t)\,w\big\|_{X_\zeta} \leq \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,t}\,\|v-w\|_{X_\zeta}\,, \qquad 0 \leq t \leq T\,.$$

Proof. (i) For $\alpha = 0$ the stated result is a consequence of Stone's theorem [14]. Generally, for $\alpha \geq 0$ we employ the spectral decomposition $v = \sum_{\mu\in\mathscr{M}} c_\mu(v)\,\mathscr{B}_\mu$, $v \in X_\alpha$, and the relations $A^\alpha\,\mathscr{B}_\mu = \lambda_\mu^\alpha \mathscr{B}_\mu$ as well as $\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{B}_\mu = \mathrm{e}^{-\mathrm{i}\,tA}\,\mathscr{B}_\mu = \mathrm{e}^{-\mathrm{i}\,t\lambda_\mu}\,\mathscr{B}_\mu$ for $\mu \in \mathscr{M}$ and $t \in \mathbb{R}$; recall that all eigenvalues of A are nonnegative. By Parseval's identity, it follows that $\|A^\alpha\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,v\|_{X_0}^2 = \|\sum_{\mu\in\mathscr{M}} c_\mu(v)\,\lambda_\mu^\alpha\,\mathrm{e}^{-\mathrm{i}\,t\lambda_\mu}\mathscr{B}_\mu\|_{X_0}^2 = \sum_{\mu\in\mathscr{M}} |c_\mu(v)|^2\,\lambda_\mu^{2\alpha} = \|A^\alpha\,v\|_{X_0}^2$ and $\|\mathscr{E}_{-\mathrm{i}\,A}(t)\,v\|_{X_\alpha}^2 = \|\mathscr{E}_{-\mathrm{i}\,A}(t)v\|_{X_0}^2 + \|A^\alpha\mathscr{E}_{-\mathrm{i}\,A}(t)v\|_{X_0}^2 = \|v\|_{X_0}^2 + \|A^\alpha\,v\|_{X_0}^2 = \|v\|_{X_\alpha}^2$, which yields the stated result.

(ii) In order to study the dependence of the nonlinear evolution operator $\mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 = \mathrm{e}^{-\mathrm{i}\,tB(v_0)}v_0$ on v_0, we consider the initial value problems $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,v(t) = B(v_0)\,v(t)$, $0 \leq t \leq T$, $v(0) = v_0$, and $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,w(t) = B(w_0)\,w(t)$, $0 \leq t \leq T$, $w(0) = w_0$. Evidently, the difference $(v-w)(t) = \mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 - \mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0$ fulfills the initial value problem $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,(v-w)(t) = B(v_0)\,v(t) - B(w_0)\,w(t)$, $0 \leq t \leq T$, $(v-w)(0) = v_0 - w_0$. In order to extract a factor $\|v_0 - w_0\|_{X_\zeta}$ or $\|v(t) - w(t)\|_{X_\zeta}$, respectively, we rewrite the right-hand side as $B(v_0)\,(v(t) - w(t)) + (B(v_0) - B(w_0))\,w(t)$ and apply the linear variation-of-constants formula (1.2), which yields $\mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 - \mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0 = \mathrm{e}^{-\mathrm{i}\,tB(v_0)}\,(v_0 - w_0) + \int_0^t \mathrm{e}^{-\mathrm{i}\,(t-\tau)B(v_0)}\,(B(v_0) - B(w_0))\,\mathrm{e}^{-\mathrm{i}\,\tau B(w_0)}\,w_0\,\mathrm{d}\tau$. With the help of Lemma 2 and due to $1 + x \leq \mathrm{e}^x$ for $x \geq 0$ we obtain $\|\mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 - \mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0\|_{X_\zeta} \leq (\mathrm{e}^{C\,(\|V\|_{X_\alpha}+|\vartheta|\,\|v_0\|_{X_\alpha}^2)\,t} + C\,|\vartheta|\,(\|v_0\|_{X_\alpha} + \|w_0\|_{X_\alpha})\,\|w_0\|_{X_\alpha} \int_0^t \mathrm{e}^{C\,(\|V\|_{X_\alpha}+|\vartheta|\,\|v_0\|_{X_\alpha}^2)\,(t-\tau)}\,\mathrm{e}^{C\,(\|V\|_{X_\alpha}+|\vartheta|\,\|w_0\|_{X_\alpha}^2)\,\tau}\,\mathrm{d}\tau)\,\|v_0 - w_0\|_{X_\zeta} \leq \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,t}(1 + 2\,C\,|\vartheta|\,C_\alpha^2\,t)\|v_0 - w_0\|_{X_\zeta} \leq \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,t}\,\|v_0 - w_0\|_{X_\zeta}$, which implies the stated result. ∎

4.2.2. Stability results for time-splitting pseudospectral methods. In the following, we deduce stability bounds for time-splitting pseudospectral methods (3.6) applied to the nonlinear Schrödinger equation (2.1)–(2.2). Starting from an initial value $\widetilde{v}_0$, the arising approximations and intermediate values are given by

$$\text{(4.5)} \quad \begin{cases} \widetilde{v}_{\ell\,0} = \widetilde{v}_\ell\,, \\ \widetilde{v}_{\ell k} = \mathscr{E}_{-\mathrm{i}\,B}(b_k\tau_\ell)\,\mathscr{E}_{-\mathrm{i}\,A}(a_k\tau_\ell)\,\mathscr{Q}_M\,\widetilde{v}_{\ell,k-1}\,, \quad 1 \leq k \leq s\,, \\ \widetilde{v}_{\ell+1} = \widetilde{v}_{\ell s} = \mathscr{T}_F(\tau_\ell)\,\widetilde{v}_\ell\,, \end{cases} \qquad 0 \leq \ell \leq n-1\,.$$

We aim at a bound of the form $\big\|\prod_{\ell=j}^{n-1} \mathscr{T}_F(\tau_\ell)\,\widetilde{v}_j - \prod_{\ell=j}^{n-1} \mathscr{T}_F(\tau_\ell)\,\widetilde{w}_j\big\|_{X_0} \leq \mathrm{e}^{C(t_n-t_j)}$

$\big\|\mathscr{Q}_M(\widetilde{v}_j - \widetilde{w}_j)\big\|_{X_0}$ for $0 \leq j \leq n-1$. For instance, for the first-order Lie–Trotter splitting method (3.7) and the application of two steps only, we aim at a suitable bound for the quantity $\|\mathscr{E}_{-\mathrm{i}\,B}(\tau_1)\,\mathscr{E}_{-\mathrm{i}\,A}(\tau_1)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(\tau_0)\,\mathscr{E}_{-\mathrm{i}\,A}(\tau_0)\,\mathscr{Q}_M\,\widetilde{v}_0 - \mathscr{E}_{-\mathrm{i}\,B}(\tau_1)\,\mathscr{E}_{-\mathrm{i}\,A}(\tau_1)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(\tau_0)\,\mathscr{E}_{-\mathrm{i}\,A}(\tau_0)\,\mathscr{Q}_M\,\widetilde{w}_0\|_{X_0}$; this illustrates that basic auxiliary results are bounds for the evolution operators $\mathscr{E}_{-\mathrm{i}\,A}$ and $\mathscr{E}_{-\mathrm{i}\,B}$ provided by Lemma 6 as well as bounds for $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}$ and $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}$ given in Lemma 8 below. A repeated application yields the following stability result with constant depending on the spatial dimension $d \geq 1$ and the method coefficients $(b_j)_{1\leq j\leq s}$.

LEMMA 7 (stability, $\mathscr{T}_F$). *Let $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$ and $0 \leq j \leq n-1$. For starting values $\widetilde{v}_j$, $\widetilde{w}_j$, let $\widetilde{v}_{\ell k}$, $\widetilde{w}_{\ell k}$ for $1 \leq k \leq s$ and $j \leq \ell \leq n-1$ denote the corresponding intermediate values arising in the computation of $\mathscr{T}_F(\tau_{n-1})\cdots\mathscr{T}_F(\tau_j)\,\widetilde{v}_j$, $\mathscr{T}_F(\tau_{n-1})\cdots\mathscr{T}_F(\tau_j)\,\widetilde{w}_j$; see (4.5). Assume that there exist constants $C_V > 0$ and $C_\alpha > 0$ such that $\|V\|_{X_\alpha} \leq C_V$ and further $\|\mathscr{Q}_M\,\widetilde{v}_{\ell k}\|_{X_\alpha}, \|\mathscr{Q}_M\,\widetilde{w}_{\ell k}\|_{X_\alpha} \leq C_\alpha$ for $1 \leq k \leq s$ and $j \leq \ell \leq n-1$ (but the final approximations $\widetilde{v}_n, \widetilde{w}_n$). Then the following estimate is valid:*

$$\bigg\|\prod_{\ell=j}^{n-1}\mathscr{T}_F(\tau_\ell)\,\widetilde{v}_j - \prod_{\ell=j}^{n-1}\mathscr{T}_F(\tau_\ell)\,\widetilde{w}_j\bigg\|_{X_0} \leq \mathrm{e}^{C\,(C_V + |\vartheta|\,C_\alpha^2)\,(t_n - t_j)}\,\big\|\mathscr{Q}_M(\widetilde{v}_j - \widetilde{w}_j)\big\|_{X_0}\,.$$

The proof of the following auxiliary estimates in particular utilizes bounds for the spectral interpolant (3.2) provided by Lemma 4; the arising constant depends on the spatial dimension.

LEMMA 8 (stability, $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{Q}_M, \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}$). (i) *For $v \in X_\alpha$ with $\alpha \geq \frac{\delta}{2}$ it holds that*

$$\big\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v\big\|_{X_0} = \big\|\mathscr{Q}_M\,v\big\|_{X_0}\,, \qquad 0 \leq t \leq T\,.$$

(ii) *Let $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$ and $v, w \in X_\alpha$. Assume that there exist constants $C_V > 0$ and $C_\alpha > 0$ such that $\|V\|_{X_\alpha} \leq C_V$ and $\|v\|_{X_\alpha}, \|w\|_{X_\alpha} \leq C_\alpha$. Then the following estimate is valid for $0 \leq t \leq T$:*

$$\big\|\mathscr{Q}_M\left(\mathscr{E}_{-\mathrm{i}\,B}(t)\,v - \mathscr{E}_{-\mathrm{i}\,B}(t)\,w\right)\big\|_{X_0} \leq \mathrm{e}^{C\,(C_V + |\vartheta|\,C_\alpha^2)\,t}\big\|\mathscr{Q}_M(v-w)\big\|_{X_0}\,, \qquad 0 \leq t \leq T\,.$$

Proof. (i) By Lemma 3 it holds that $\mathscr{Q}_M\,\mathscr{P}_M\,v = \mathscr{P}_M\,v$; thus, the stated result follows from the relations $\mathscr{Q}_M\,v = \sum_{\mu\in\mathscr{M}_M} c_\mu(\mathscr{Q}_M\,v)\,\mathscr{B}_\mu$ and $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v = \mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v = \sum_{\mu\in\mathscr{M}_M} c_\mu(\mathscr{Q}_M\,v)\,\mathrm{e}^{-\mathrm{i}\lambda_\mu t}\mathscr{B}_\mu$, which yield $\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v\|_{X_0}^2 = \|\mathscr{E}_{-\mathrm{i}\,A}(t)\,\mathscr{Q}_M\,v\|_{X_0}^2 = \sum_{\mu\in\mathscr{M}_M}|c_\mu(\mathscr{Q}_M\,v)|^2 = \|\mathscr{Q}_M\,v\|_{X_0}^2$.

(ii) In order to derive the stated bound, we consider the initial value problems $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,v(t) = B(v_0)\,v(t)$, $0 \leq t \leq T$, $v(0) = v_0$, and $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,w(t) = B(w_0)\,w(t)$, $0 \leq t \leq T$, $w(0) = w_0$. The interpolant of the difference $\mathscr{Q}_M(v-w)(t) = \mathscr{Q}_M(\mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 - \mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0)$ fulfills the initial value problem $\mathrm{i}\,\mathscr{Q}_M\,\frac{\mathrm{d}}{\mathrm{d}t}\,(v-w)(t) = \mathscr{Q}_M(B(v_0)\,v(t) - B(w_0)\,w(t))$, $0 \leq t \leq T$, $\mathscr{Q}_M(v-w)(0) = \mathscr{Q}_M(v_0 - w_0)$. Integration and estimation in X_0 thus yields $\|\mathscr{Q}_M(v-w)(t)\|_{X_0} \leq \|\mathscr{Q}_M(v_0-w_0)\|_{X_0} + \int_0^t \|\mathscr{Q}_M(B(v_0)\,v - B(w_0)\,w)(\tau)\|_{X_0}\,\mathrm{d}\tau$. To extract a factor $\|\mathscr{Q}_M(v_0-w_0)\|_{X_0}$ or $\|\mathscr{Q}_M(v-w)(\tau)\|_{X_0}$, respectively, we rewrite the integrand as $\mathscr{Q}_M(B(v_0)\,v - B(w_0)\,w) = \mathscr{Q}_M\,(V(v-w)) + \vartheta\,\mathscr{Q}_M(|v_0|^2(v-w) + v_0\,w\,\overline{(v_0-w_0)} + (v_0-w_0)\,\overline{w_0}\,w)$ and apply Lemma 4 as well as

Lemma 2 to obtain $\|\mathscr{Q}_M(v-w)(t)\|_{X_0} \leq (\|V\|_{L^\infty(\mathscr{K}_M)} + |\vartheta|\,\|v_0\|^2_{L^\infty(\mathscr{K}_M)}) \int_0^t \|\mathscr{Q}_M(v-w)(\tau)\|_{X_0}\,\mathrm{d}\tau + (1+|\vartheta|\,(\|v_0\|_{L^\infty(\mathscr{K}_M)} + \|w_0\|_{L^\infty(\mathscr{K}_M)}) \int_0^t \|\mathrm{e}^{-\mathrm{i}\,\tau\,B(w_0)}\,w_0\|_{L^\infty(\mathscr{K}_M)}\,\mathrm{d}\tau)\,\|\mathscr{Q}_M(v_0-w_0)\|_{X_0} \leq (1 + C\,|\vartheta|\,C_\alpha^2 \int_0^t \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,\tau}\,\mathrm{d}\tau)\,\|\mathscr{Q}_M(v_0-w_0)\|_{X_0} + C\,(C_V + |\vartheta|\,C_\alpha^2) \int_0^t \|\mathscr{Q}_M(v-w)(\tau)\|_{X_0}\,\mathrm{d}\tau$ and furthermore $\|\mathscr{Q}_M(v-w)(t)\|_{X_0} \leq \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,t}\,\|\mathscr{Q}_M(v_0-w_0)\|_{X_0} + C\,(C_V+|\vartheta|\,C_\alpha^2)\int_0^t \|\mathscr{Q}_M(v-w)(\tau)\|_{X_0}\,\mathrm{d}\tau$. A Gronwall-type inequality yields the stated result. $\square$

4.3. Estimates for the defect of spectral and splitting methods. In this section, we deduce suitable estimates for the defects $\mathscr{S}_F(\tau)\,v - \mathscr{E}_F(\tau)\,v$ as well as $\mathscr{T}_F(\tau)\,v - \mathscr{Q}_M\mathscr{S}_F(\tau)\,v$; in particular, we specify the regularity assumptions on the argument v to retain the full order of consistency for high-order exponential splitting methods.

4.3.1. Estimates for the defect of exponential operator splitting methods. We first state a local error expansion for high-order exponential operator splitting methods (3.5) applied to nonlinear evolution equations of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F\big(u(t)\big) = F_1\big(u(t)\big) + F_2\big(u(t)\big)\,, \qquad 0 \leq t \leq T\,; \tag{4.6}$$

the representation remains suitable in the presence of unbounded nonlinear operators and applies to other problem classes such as parabolic problems. For the linear case the local error representation is deduced in [30]. By the formal calculus of Lie-derivatives the result then carries over to nonlinear evolution equations by exchanging the (linear) operators F_1, F_2 with their Lie-derivatives D_{F_1}, D_{F_2} and reversing the sequence of the operators. Essential tools in the derivation of the local error representation are a repeated application of the (non)linear variation-of-constants formula (see Theorem 1), a stepwise expansion of the splitting operator, and quadrature formulae for multiple integrals, where iterated Lie-commutators naturally arise from a Taylor series expansion of the integrands; see [22] for further details. In the context of the nonlinear Schrödinger equation (2.1)–(2.2), we define F_1, F_2 through $F_1(v) = -\,\mathrm{i}\,Av$ with $A = -\,\Delta$ and $F_2(v) = -\,\mathrm{i}\,B(v)\,v$ with $B(v) = V + \vartheta\,|v|^2$; see also section 2. We denote by $p \geq 1$ the (nonstiff) order of consistency of the splitting method; a MATLAB code to determine the coefficients $\alpha_\lambda, \widetilde{\alpha}_{j\lambda}$ is available at http://techmath.uibk.ac.at/mecht/research/research.html.

THEOREM 2 (local error expansion). *Let* $c_k = a_1 + a_2 + \cdots + a_k$ *for* $1 \leq k \leq s$, *and set* $\Lambda_k = \{\lambda \in \mathbb{N}^k : 1 \leq \lambda_k \leq \cdots \leq \lambda_1 \leq \lambda_0 = s\}$ *as well as* $\Sigma_k = \{\sigma \in \mathbb{R}^k : 0 \leq \sigma_k \leq \cdots \leq \sigma_1 \leq \sigma_0 = \tau\}$. *Provided that the condition* $c_s = 1$ *is satisfied, the local error of the exponential operator splitting method* (3.5) *applied to the nonlinear evolutionary problem* (4.6) *admits the following expansion for* $0 \leq q \leq p$:

$$\mathscr{S}_F(\tau)\,v - \mathscr{E}_F(\tau)\,v = \sum_{k=1}^{q} \sum_{\substack{\mu\in\mathbb{N}^k\\ |\mu|\leq q-k}} \frac{1}{\mu!}\,\tau^{k+|\mu|}\,C_{k\mu} \prod_{\ell=1}^{k} \mathrm{ad}_{D_{F_1}}^{\mu_\ell}(D_{F_2})\,\mathrm{e}^{\tau D_{F_1}}\,v + \mathscr{R}_{q+1}(\tau)\,v\,,$$

$$C_{k\mu} = \sum_{\lambda\in\Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell}\,c_{\lambda_\ell}^{\mu_\ell} - \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1}\,.$$

The remainder $\mathscr{R}_{q+1} = \mathscr{R}_{q+1}^{(1)} - \mathscr{R}_{q+1}^{(2)} - \mathscr{R}_{q+1}^{(3)}$ *comprises the following terms:*

$$\mathscr{R}_{q+1}^{(1)}(\tau)\, v = \int_{\Sigma_{q+1}} \mathrm{e}^{\sigma_{q+1} D_F} \prod_{j=1}^{q+1} \Big(D_{F_2}\, \mathrm{e}^{(\sigma_{j-1}-\sigma_j) D_{F_1}} \Big)\, v \,\mathrm{d}\sigma\,,$$

$$\mathscr{R}_{q+1}^{(2)}(\tau)\, v = \tau^{q+1} \sum_{j=1}^{q+1} \sum_{\lambda \in \Lambda_{q+1}} \widetilde{\alpha}_{j\lambda} \prod_{\ell=1}^{\lambda_{q+1}-1} \Big(\mathrm{e}^{a_{\lambda_{q+1-\ell}} \tau D_{F_1}}\, \mathrm{e}^{b_{\lambda_{q+1-\ell}} \tau D_{F_2}} \Big)$$

$$\times\, \mathrm{e}^{a_{\lambda_{q+1}} \tau D_{F_1}}\, \varphi_j(b_{\lambda_{q+1}} \tau D_{F_2}) \prod_{\ell=1}^{q+1} \Big(b_{\lambda_\ell}\, D_{F_2}\, \mathrm{e}^{(c_{\lambda_{\ell-1}} - c_{\lambda_\ell})\, \tau D_{F_1}} \Big)\, v\,,$$

$$\mathscr{R}_{q+1}^{(3)}(\tau)\, v = \sum_{k=1}^{q} \bigg(\int_{\Sigma_k} \varrho_{k,q-k+1}(\sigma)\, v \,\mathrm{d}\sigma - \tau^k \sum_{\lambda \in \Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell}\, \varrho_{k,q-k+1}(c_\lambda \tau)\, v \bigg)\,,$$

$$\varrho_{k,q-k+1}(\sigma)\, v = (q-k+1) \int_0^1 (1-\zeta)^{q-k} \sum_{\substack{\mu \in \mathbb{N}^k \\ |\mu| = q-k+1}} \frac{(-1)^{|\mu|}}{\mu!}\, \sigma^\mu\, \mathrm{e}^{\sigma_k \zeta D_{F_1}}$$

$$\times \prod_{\ell=1}^{k} \big(\mathrm{ad}_{D_{F_1}}^{\mu_\ell}(D_{F_2})\, \mathrm{e}^{(\sigma_{\ell-1}-\sigma_\ell)\, \zeta D_{F_1}} \big) v \,\mathrm{d}\zeta\,.$$

Provided that the coefficients of the splitting method (3.5) fulfill the order conditions $C_{k\mu} = 0$ for $\mu \in \mathbb{N}^k$ with $|\mu| \leq p-k$ and $1 \leq k \leq p$, the local error expansion of Theorem 2 simplifies to $\mathscr{S}_F(\tau)\, v - \mathscr{E}_F(\tau)\, v = \mathscr{R}_{p+1}(\tau)\, v = \mathscr{O}(\tau^{p+1})$. It remains to specify the regularity requirements on v such that the local error representation is well-defined in certain fractional power spaces and that the full order of convergence is retained in X_0. For the Lie–Trotter splitting method, where $p = s = a_1 = b_1 = 1$, it is evident that the dominant local error term comprises the first Lie-commutator; in general, the regularity requirements when applying the iterated Lie-commutator $\mathrm{ad}_{D_{F_1}}^p(D_{F_2})$ have to be determined. We obtain the following local error estimates, which also include the case of a possible order reduction. Again, the arising constant depends on the spatial dimension $d \geq 1$ and further involves the bound for the potential, which we indicate by the notation $C(C_V)$.

LEMMA 9 (defect, $\mathscr{S}_F - \mathscr{E}_F$). *Let* $0 \leq q \leq p$ *and assume that the coefficients of the splitting method* (3.5) *satisfy the conditions* $C_{k\mu} = 0$ *for* $\mu \in \mathbb{N}^k$ *with* $|\mu| \leq q-k$ *and* $1 \leq k \leq q$. *Then the defect fulfills the following estimates for* $\frac{\delta}{2} \leq \zeta \in \mathbb{N}$*:*

$$\big\| \mathscr{S}_F(\tau)\, v - \mathscr{E}_F(\tau)\, v \big\|_{X_0} \leq C(C_V)\, \tau^{q+1} \|v\|_{X_\alpha}^3\,, \qquad \alpha \geq \max\left\{ \frac{\delta}{2}, q \right\}\,,$$

$$\big\| \mathscr{S}_F(\tau)\, v - \mathscr{E}_F(\tau)\, v \big\|_{X_\zeta} \leq C(C_V)\, \tau^{q+1} \|v\|_{X_\alpha}^3\,, \qquad \alpha \geq \zeta + q\,,$$

provided that $\|V\|_{X_\alpha} \leq C_V$.

Proof. In the following, we indicate the estimation of the dominant local error term involving the qth iterated Lie-commutator. We recall that the first iterated Lie-commutator equals $\mathrm{ad}_{D_{F_1}}(D_{F_2}) v = [D_{F_1}, D_{F_2}]\, v = D_{F_1} D_{F_2}\, v - D_{F_2} D_{F_1}\, v = F_2'(v)\, F_1(v) - F_1'(v)\, F_2(v)$. For instance, in a single space dimension we have $F_1(v) = \mathrm{i}\, \partial_x^2 v$ and $F_1'(v) = F_1 = \mathrm{i}\, \partial_x^2$ as well as $F_2(v) = \mathrm{i}\,(V v + \vartheta\, |v|^2 v) = \mathrm{i}\,(V v + \vartheta\, \overline{v}\, v^2)$ and $F_2'(v) = \mathrm{i}\,(V + 2\,\vartheta\, \overline{v}\, v + \vartheta\, v^2 \overline{(\cdot)})$; here, for simplicity, we omit an additional sign in F_2, which does not effect our considerations. A brief calculation yields

$[D_{F_1}, D_{F_2}]\, v = 2\,\partial_x V\,\partial_x v + \partial_x^2 V\, v + 2\,\vartheta\,(\overline{\partial_x^2 v}\, v^2 + 2\,|\partial_x v|^2\, v + (\partial_x v)^2\,\overline{v})$. We point out that the first Lie-commutator involves the second spatial derivative $\overline{\partial_x^2 v}$; by induction, due to the fact that $f(v) = v^2\,\overline{\partial_x^{2(j-1)} v}$, $f'(v) = v^2\,\overline{\partial_x^{2(j-1)}(\cdot)} + 2\,\overline{\partial_x^{2(j-1)} v}\, v$, and $f'(v)\,F_1(v) - F_1'(v)\,f(v) = -2\,\mathrm{i}\,\overline{\partial_x^{2j} v}\, v^2$ + remaining terms for $j \geq 1$, it follows that this term contributes to higher-order spatial derivatives in higher iterated Lie-commutators, namely, to $\overline{\partial_x^{2j} v}\, v^2$ in $\mathrm{ad}_{D_{F_1}}^j(D_{F_2})\, v$ for $j \geq 1$. As the extension to arbitrary space dimensions is more technical but otherwise straightforward, it is seen that the dominant term in the iterated Lie-commutator $\mathrm{ad}_{D_{F_1}}^q(D_{F_2})\, v$ is $\overline{\Delta^q v}\, v^2$. By means of Lemma 1 the bounds $\|\overline{\Delta^q v}\, v^2\|_{L^2(\Omega)} \leq \|v\|_{H^{2q}(\Omega)}\,\|v\|_{H^\delta(\Omega)}^2 \leq \|v\|_{X_q}\,\|v\|_{X_{\delta/2}}^2$ and $\|\overline{\Delta^q v}\, v^2\|_{X_\zeta} \leq \|\Delta^q v\|_{X_\zeta}\,\|v\|_{X_\zeta}^2 \leq \|v\|_{X_{\zeta+q}}\,\|v\|_{X_\zeta}^2 \leq \|v\|_{X_{\zeta+q}}^3$ for $\frac{\delta}{2} \leq \zeta \in \mathbb{N}$ are obtained. We note that lower-order terms are estimated by means of Sobolev embeddings (see [2]); for instance, in two and three space dimensions the relation $\|u\, v\|_{L^2(\Omega)} \leq C\,\|u\|_{L^4(\Omega)}\,\|v\|_{L^4(\Omega)} \leq C\,\|u\|_{H^1(\Omega)}\,\|v\|_{H^1(\Omega)}$ and further the bound $\|u\, v\, w\|_{L^2(\Omega)} \leq C\,\|u\|_{L^6(\Omega)}\,\|v\|_{L^6(\Omega)}\,\|w\|_{L^6(\Omega)} \leq C\,\|u\|_{H^1(\Omega)}\,\|v\|_{H^1(\Omega)}\,\|w\|_{H^1(\Omega)}$ are applied. Altogether, this yields $\|\mathrm{ad}_{D_{F_1}}^q(D_{F_2})\, v\|_{X_0} \leq C\,\|v\|_{X_\alpha}^3$ with $\alpha \geq \max\{\frac{\delta}{2}, q\}$ and $\|\mathrm{ad}_{D_{F_1}}^q(D_{F_2})\, v\|_{X_\zeta} \leq C\,\|v\|_{X_\alpha}^3$ with $\alpha \geq \zeta + q$ and $\frac{\delta}{2} \leq \zeta \in \mathbb{N}$, and thus the stated local error estimates. For related results and further details on the derivation we refer to [3, 13, 15, 22, 23]. ◻

Remark. In the case of a linear Schrödinger equation, that is, if $\vartheta = 0$, the iterated Lie-commutator $\mathrm{ad}_{D_{F_1}}^q(D_{F_2})$ is a differential operator of order q with coefficients involving the spatial derivatives of the potential V up to order $2q$; see [30]. Consequently, the defect fulfills the following estimates for $\frac{\delta}{2} \leq \zeta \in \mathbb{N}$:

$$\begin{aligned} &\big\|\mathscr{S}_F(\tau)\, v - \mathscr{E}_F(\tau)\, v\big\|_{X_0} \leq C(C_V)\,\tau^{q+1}\|v\|_{X_\alpha}^3\,, \qquad \alpha \geq \frac{1}{2}\,\max\{\delta, q\}\,,\\ &\big\|\mathscr{S}_F(\tau)\, v - \mathscr{E}_F(\tau)\, v\big\|_{X_\zeta} \leq C(C_V)\,\tau^{q+1}\|v\|_{X_\alpha}^3\,, \qquad \alpha \geq \zeta + \frac{q}{2}\,; \end{aligned}$$

the regularity requirements on the potential V remain the ones given in Lemma 9.

4.3.2. Estimates for the defect of time-splitting pseudospectral methods. Our aim is to derive a suitable bound for the defect $\mathscr{T}_F(\tau)v - \mathscr{Q}_M\,\mathscr{S}_F(\tau)v$ in X_0; more precisely, in view of relation (4.7b) we wish to extract the factor τ and further a term involving the quantity $\mathscr{Q}_M - I$ which quantifies the approximation rate of the pseudospectral method.

We explain the general approach on the basis of a splitting method involving $s = 2$ stages, since it is then straightforward to extend the considerations to an arbitrary number of stages. Let $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$. We consider the defect $\mathscr{T}_F(\tau)\, u - \mathscr{Q}_M\,\mathscr{S}_F(\tau)\, u = \mathscr{E}_{-\mathrm{i}\,B}(b_2\tau)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(a_2\tau)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(b_1\tau)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(a_1\tau)\,\mathscr{Q}_M\, u - \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(b_2\tau)\,\mathscr{E}_{-\mathrm{i}\,A}(a_2\tau)\,\mathscr{E}_{-\mathrm{i}\,B}(b_1\tau)\,\mathscr{E}_{-\mathrm{i}\,A}(a_1\tau)\, u$; note that the identity $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{Q}_M\, v = \mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{Q}_M\, v$ holds, as shown in the proof of Lemma 8. As this does not affect the considerations, for notational simplicity we henceforth omit the method coefficients a_1, a_2, b_1, b_2. We first rewrite the negative of the defect as $\mathscr{Q}_M\,\mathscr{S}_F\, u - \mathscr{T}_F\, u = Z_1 + Z_2 + Z_3 + Z_4$ with $Z_1 = \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}\, z_1 - \mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{Q}_M\, z_1$ and $Z_j = L_j\, z_j - L_j\,\mathscr{Q}_M\, z_j$ for $j = 2, 3, 4$ involving the nonlinear operators $L_2 = \mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}$, $L_3 = L_2\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}$, and $L_4 = L_3\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}$, and further $z_1 = \mathscr{E}_{-\mathrm{i}\,A}\, z_2$, $z_2 = \mathscr{E}_{-\mathrm{i}\,B}\, z_3$, $z_3 = \mathscr{E}_{-\mathrm{i}\,A}\, z_4$, and $z_4 = u$. For the following, we assume that there exist constants $C_V, C_\alpha > 0$ such that $\|V\|_{X_\alpha} \leq C_V$ and that the quantities $\|\mathscr{Q}_M^c\, u\|_{X_\alpha}$, $\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\, u\|_{X_\alpha}$, $\|\mathscr{Q}_M^c\,\mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{E}_{-\mathrm{i}\,A}\, u\|_{X_\alpha}$, $\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{Q}_M\, u\|_{X_\alpha}$, $\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\, u\|_{X_\alpha}$, $\|\mathscr{Q}_M$

$\mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{E}_{-\mathrm{i}\,A}\,u\|_{X_\alpha}$, and $\|\mathscr{Q}_M^c\,\mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{E}_{-\mathrm{i}\,B}\,\mathscr{E}_{-\mathrm{i}\,A}\,u\|_{X_\alpha}$ are bounded by C_α for $c \in \{0,1\}$, uniformly on $[0,\tau]$. Consequently, applications of Lemma 4, 6, and 8 as well as Lemma 11 given below yield the bounds

$$
\begin{aligned}
\big\|\mathscr{T}_F(\tau)\,u - \mathscr{Q}_M\,\mathscr{S}_F(\tau)\,u\big\|_{X_0} &\le \|Z_1(\tau)\|_{X_0} + \|Z_2(\tau)\|_{X_0} + \|Z_4(\tau)\|_{X_0}\,,\\
\|Z_1(\tau)\|_{X_0} &\le \int_0^\tau \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,(\tau-\sigma)}\|r(\sigma)\|_{X_0}\,\mathrm{d}\sigma\,,\\
\|r\|_{X_0} &\le C\Big(|\vartheta|\,\big(\|\mathscr{Q}_M\,z_1\|_{X_\alpha} + \|z_1\|_{X_\alpha}\big)\,\big\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}\,z_1\big\|_{X_\alpha}\\
&\qquad \big\|(\mathscr{Q}_M - I)z_1\big\|_{X_0} + \|B(z_1)\|_{X_\alpha}\big\|(\mathscr{Q}_M - I)\mathscr{E}_{-\mathrm{i}\,B}z_1\big\|_{X_0}\\
&\qquad + \big\|(\mathscr{Q}_M - I)\,B(z_1)\,z_1\big\|_{X_0}\Big)\\
&\le C\,\big(C_V + |\vartheta|\,C_\alpha^2\big)\,\Lambda(M,\alpha,0)\,\Big(\|z_1\|_{X_\alpha} + \big\|\mathscr{E}_{-\mathrm{i}\,B}\,z_1\big\|_{X_\alpha}\Big)\,,\\
\|Z_j(\tau)\|_{X_0} &\le \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,\tau}\int_0^\tau \big\|[A,\mathscr{Q}_M - I]\,\mathscr{E}_{-\mathrm{i}\,A}(\sigma)\,z_j(\sigma)\big\|_{X_0}\,\mathrm{d}\sigma\\
&\le C\,\mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,\tau}\,\Lambda(M,\alpha,1)\int_0^\tau \|z_j(\sigma)\|_{X_0}\,\mathrm{d}\sigma\,,\\
j &= 2,4\,;
\end{aligned}
$$

note that $\|Z_3\|_{X_0} = 0$ and recall (4.2b). Altogether, this implies the bound

$$
\begin{aligned}
\big\|\mathscr{T}_F(\tau)\,u - \mathscr{Q}_M\,\mathscr{S}_F(\tau)\,u\big\|_{X_0} &\le C\,C_\alpha\,\mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,\tau}\,\tau\\
&\qquad \times \big(\Lambda(M,\alpha,1) + (C_V + |\vartheta|\,C_\alpha^2)\,\Lambda(M,\alpha,0)\big)\,.
\end{aligned}
$$

Similar considerations hold for the general case and yield the following result.

LEMMA 10 (defect, $\mathscr{T}_F - \mathscr{Q}_M\,\mathscr{S}_F$). *Let $\frac{\delta}{2} \le \alpha \in \mathbb{N}$ and assume that there exist constants $C_V, C_\alpha > 0$ such that $\|V\|_{X_\alpha} \le C_V$ and that the intermediate and final values arising in the computation of $\mathscr{Q}_M^{c_{2s}}\,\mathscr{E}_{-\mathrm{i}\,B}(b_s\tau)\,\mathscr{Q}_M^{c_{1s}}\,\mathscr{E}_{-\mathrm{i}\,A}(a_s\tau)\,\mathscr{Q}_M^{c_{0s}}\cdots\mathscr{Q}_M^{c_{21}}\,\mathscr{E}_{-\mathrm{i}\,B}(b_1\tau)\,\mathscr{Q}_M^{c_{11}}\,\mathscr{E}_{-\mathrm{i}\,A}(a_1\tau)\,\mathscr{Q}_M^{c_{01}}\,u$, $c_{jk} \in \{0,1\}$, $j = 0,1,2$, $1 \le k \le s$, are bounded in X_α by C_α, uniformly on $[0,\tau_{\max}]$. Then the following estimate is valid:*

$$
\begin{aligned}
\big\|\mathscr{T}_F(\tau)\,u - \mathscr{Q}_M\,\mathscr{S}_F(\tau)\,u\big\|_{X_0} &\le C\,C_\alpha\,\mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,\tau}\,\tau\\
&\qquad \times \big(\Lambda(M,\alpha,1) + (C_V + |\vartheta|\,C_\alpha^2)\,\Lambda(M,\alpha,0)\big)\,.
\end{aligned}
$$

The above considerations utilize the following auxiliary result providing bounds for the quantities $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\,(\mathscr{Q}_M - I)$ and $\mathscr{E}_{-\mathrm{i}\,B} - \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}$.

LEMMA 11 (defect, $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\,(\mathscr{Q}_M - I), \mathscr{E}_{-\mathrm{i}\,B} - \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}$). (i) *It holds*

$$
\big\|\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,(\mathscr{Q}_M - I)\,v\big\|_{X_0} \le \int_0^t \big\|[A,\mathscr{Q}_M]\,\mathscr{E}_{-\mathrm{i}\,A}(\tau)\,v\big\|_{X_0}\,\mathrm{d}\tau\,, \qquad 0 \le t \le T\,.
$$

(ii) *Let $\frac{\delta}{2} \le \alpha \in \mathbb{N}$ and assume that there exist constants $C_V > 0$ and $C_\alpha > 0$ such that $\|V\|_{X_\alpha} \le C_V$ and further $\|v_0\|_{X_\alpha}, \|w_0\|_{X_\alpha}, \|\mathscr{Q}_M\,w_0\|_{X_\alpha} \le C_\alpha$. Then the* *estimate*

$$\begin{aligned}\big\|\mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 - \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0\big\|_{X_0} &\leq \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,t}\,\big\|v_0 - \mathscr{Q}_M\,w_0\big\|_{X_0}\\ &\quad + \int_0^t \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,(t-\tau)}\|r(\tau)\|_{X_0}\,\mathrm{d}\tau\end{aligned}$$

is valid with the remainder given by

$$\begin{aligned}r(t) &= \vartheta\,\big(\overline{(\mathscr{Q}_M - I)\,w_0}\;\mathscr{Q}_M\,w_0 + \overline{w_0}\,(\mathscr{Q}_M - I)\,w_0\big)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0\\ &\quad + B(w_0)\,(\mathscr{Q}_M - I)\,\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0 + (I - \mathscr{Q}_M)\,B(w_0)\,w_0\,, \qquad 0 \leq t \leq T\,.\end{aligned}$$

Proof. (i) We note that the identity $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{Q}_M\,v = \mathscr{E}_{-\mathrm{i}\,A}\,\mathscr{Q}_M\,v$ holds, as shown in the proof of Lemma 8. To deduce a suitable bound for the quantity $\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,(\mathscr{Q}_M - I)\,v_0 = \mathscr{E}_{-\mathrm{i}\,A}(\tau)\,\mathscr{Q}_M\,v_0 - \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,A}(t)\,v_0$, we consider the initial value problem $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,(w - \mathscr{Q}_M\,v)(t) = A\,w(t) - \mathscr{Q}_M\,A\,v(t)$, $0 \leq t \leq T$, $(w - \mathscr{Q}_M\,v)(0) = 0$, where $w(t) = \mathscr{E}_{-\mathrm{i}\,A}(\tau)\,\mathscr{Q}_M\,v_0$ and $v(t) = \mathscr{E}_{-\mathrm{i}\,A}(t)\,v_0$, and rewrite the differential equation as $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,(w - \mathscr{Q}_M\,v) = A\,(w - \mathscr{Q}_M\,v) + [A, \mathscr{Q}_M]\,v$, where $[A, \mathscr{Q}_M]\,v = A\,(\mathscr{Q}_M\,v) - \mathscr{Q}_M\,(A\,v)$. Thus, an application of the linear variation-of-constants formula and Lemma 6 yields the stated bound $\|(w - \mathscr{Q}_M\,v)(t)\|_{X_0} \leq \int_0^t \|\mathscr{E}_{-\mathrm{i}\,A}(t - \tau)\,[A, \mathscr{Q}_M]\,\mathscr{E}_{-\mathrm{i}\,A}(\tau)\,v_0\|_{X_0}\,\mathrm{d}\tau = \int_0^t \|[A, \mathscr{Q}_M]\,\mathscr{E}_{-\mathrm{i}\,A}(\tau)\,v_0\|_{X_0}\,\mathrm{d}\tau$, $0 \leq t \leq T$.

(ii) For the derivation of a suitable bound for $(v - \mathscr{Q}_M\,w)(t) = \mathscr{E}_{-\mathrm{i}\,B}(t)\,v_0 - \mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0$, we consider the initial value problem $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,(v - \mathscr{Q}_M\,w)(t) = B(v_0)\,v(t) - \mathscr{Q}_M\,(B(w_0)\,w(t))$, $0 \leq t \leq T$, $(v - \mathscr{Q}_M\,w)(0) = v_0 - \mathscr{Q}_M\,w_0$. To extract factors $v_0 - \mathscr{Q}_M\,w_0$ and $(v - \mathscr{Q}_M\,w)(t)$ or to achieve terms involving the quantity $\tau\,(\mathscr{Q}_M - I)$, respectively, we rewrite the differential equation as $\mathrm{i}\,\frac{\mathrm{d}}{\mathrm{d}t}\,(v - \mathscr{Q}_M\,w)(t) = B(v_0)\,(v - \mathscr{Q}_M\,w)(t) + \vartheta\,(\overline{(v_0 - \mathscr{Q}_M\,w_0)}\,v_0 + \overline{\mathscr{Q}_M\,w_0}\,(v_0 - \mathscr{Q}_M\,w_0))\,\mathscr{Q}_M\,(\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0) + r(t)$, $0 \leq t \leq T$, with the remainder given by $r(t) = \vartheta\,(\overline{(\mathscr{Q}_M - I)\,w_0}\;\mathscr{Q}_M\,w_0 + \overline{w_0}\,(\mathscr{Q}_M - I)\,w_0)\,\mathscr{Q}_M\,\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0 + B(w_0)\,(\mathscr{Q}_M - I)\,\mathscr{E}_{-\mathrm{i}\,B}(t)\,w_0 + (I - \mathscr{Q}_M)\,B(w_0)\,w_0$, $0 \leq t \leq T$, and apply the linear variation-of-constants formula to obtain $(v - \mathscr{Q}_M\,w)(t) = \mathrm{e}^{-\mathrm{i}\,t\,B(v_0)}\,(v_0 - \mathscr{Q}_M\,w_0) + \vartheta\,\int_0^t \mathrm{e}^{-\mathrm{i}\,(t-\tau)\,B(v_0)}\,(\overline{(v_0 - \mathscr{Q}_M\,w_0)}\,v_0 + \overline{\mathscr{Q}_M\,w_0}\,(v_0 - \mathscr{Q}_M\,w_0))\,\mathscr{Q}_M\,(\mathscr{E}_{-\mathrm{i}\,B}(\tau)\,w_0)\,\mathrm{d}\tau + \int_0^t \mathrm{e}^{-\mathrm{i}\,(t-\tau)\,B(v_0)}\,r(\tau)\,\mathrm{d}\tau$. The estimation by Lemmas 2 and 4 together with the relation $1 + x \leq \mathrm{e}^x$ for $x \geq 0$ yields $\|(v - \mathscr{Q}_M\,w)(t)\|_{X_0} \leq \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,t}\,\|v_0 - \mathscr{Q}_M\,w_0\|_{X_0} + \int_0^t \mathrm{e}^{C\,(C_V+|\vartheta|\,C_\alpha^2)\,(t-\tau)}\|r(\tau)\|_{X_0}\,\mathrm{d}\tau$ and thus the stated result. $\square$

4.4. Convergence result. *Approach.* We first recall the basic relations for the values of the analytical solution to the nonlinear evolution equation (2.1)–(2.2), for the values of the time-discrete solution obtained by an exponential operator splitting method (3.5), and for the values of the fully discrete solution obtained by the splitting method combined with a Fourier pseudospectral method for the approximate solution of the linear subproblem

$$\begin{aligned}u(t_n) &= \prod_{j=0}^{n-1} \mathscr{E}_F(\tau_j)\,u(0)\,, \quad u_n = \prod_{j=0}^{n-1} \mathscr{S}_F(\tau_j)\,u_0\,,\\ \widetilde{u}_{nM} &= \prod_{j=0}^{n-1} \mathscr{T}_F(\tau_j)\,u_0\,, \qquad 0 \leq n \leq N;\end{aligned}$$

see (3.6). In order to estimate the global error of the fully discrete solution in X_0, a standard approach is to interpose the time-discrete solution

$$\big\|\widetilde{u}_{nM} - u(t_n)\big\|_{X_0} \leq \big\|\widetilde{u}_{nM} - u_n\big\|_{X_0} + \big\|u_n - u(t_n)\big\|_{X_0}\,, \qquad 0 \leq n \leq N\,. \tag{4.7a}$$

By means of a Lady Windermere's fan argument, we obtain the representations

(4.7b)

$$\begin{aligned}
u_n - u(t_n) &= \prod_{\ell=0}^{n-1} \mathscr{S}_F(\tau_\ell)\, u_0 - \prod_{\ell=0}^{n-1} \mathscr{S}_F(\tau_\ell)\, u(0) \\
&\quad + \sum_{j=1}^{n} \left(\prod_{\ell=j}^{n-1} \mathscr{S}_F(\tau_\ell)\, \mathscr{S}_F(\tau_{j-1})\, u(t_{j-1}) - \prod_{\ell=j}^{n-1} \mathscr{S}_F(\tau_\ell)\, \mathscr{E}_F(\tau_{j-1})\, u(t_{j-1}) \right), \\
\widetilde{u}_{nM} - u_n &= (\mathscr{Q}_M - I)\, u_n \\
&\quad + \sum_{j=1}^{n} \left(\prod_{\ell=j}^{n-1} \mathscr{T}_F(\tau_\ell)\, \mathscr{T}_F(\tau_{j-1})\, u_{j-1} - \prod_{\ell=j}^{n-1} \mathscr{T}_F(\tau_\ell)\, \mathscr{Q}_M\, \mathscr{S}_F(\tau_{j-1})\, u_{j-1} \right),
\end{aligned}$$

where we make use of the fact that $\mathscr{T}_F = \mathscr{T}_F \mathscr{Q}_M$. Thus, the main tools for the derivation of a global error estimate, given in Theorem 3, are stability bounds for the numerical evolution operators, provided by Lemmas 5 and 7, as well as estimates for the defects, given in Lemmas 4, 9, and 10.

Problems with regular data. We indicate the derivation of a global error estimate for nonlinear Schrödinger equations (2.1)–(2.2) involving data with high regularity, which we consider to be relevant in view of practical applications; in this case, as confirmed by numerical experiments given, for instance, in [1, 4, 10, 15, 25], pseudospectral methods are favorable in accuracy and higher-order exponential splitting methods retain the full order of consistency. To obtain a compact presentation of the global error estimate, we assume $M_\ell = M_0$ for $1 \leq \ell \leq d$ and introduce the maximal time stepsize $\tau_{\max} = \max\{\tau_j : 0 \leq j \leq n-1\}$ as well as the maximal solution value $\sup\{\|u(t)\|_{X_\beta} : 0 \leq t \leq T\}$ for some $\beta \geq 0$; we recall that the ratios of two subsequent time increments are required to be bounded from below and above. For notational simplicity, we do not distinguish the bounds for the potential V in different fractional power spaces; for our purposes it suffices to indicate the dependence of the arising constants on certain quantities. Under the presumption that Lemmas 5 and 9 as well as Lemmas 4, 7, and 10 are applicable, an estimation of (4.7b) yields

$$\begin{aligned}
&\big\|u_n - u(t_n)\big\|_{X_\zeta} \\
&\quad \leq \mathrm{e}^{C\,(C_V + |\vartheta|\, C_\alpha^2)\, t_n}\, \|u_0 - u(0)\|_{X_\zeta} \\
&\qquad + \sum_{j=1}^{n} \mathrm{e}^{C\,(C_V + |\vartheta|\, C_\alpha^2)\,(t_n - t_j)}\, \big\|\mathscr{S}_F(\tau_{j-1})\, u(t_{j-1}) - \mathscr{E}_F(\tau_{j-1})\, u(t_{j-1})\big\|_{X_\zeta} \\
&\quad \leq \mathrm{e}^{C\,(C_V + |\vartheta|\, C_\alpha^2)\, t_n}\, \|u_0 - u(0)\|_{X_\zeta} + C(C_V) \sum_{j=1}^{n} \mathrm{e}^{C\,(C_V + |\vartheta|\, C_\alpha^2)\,(t_n - t_j)}\, \tau_{j-1}^{q+1}\, \big\|u(t_{j-1})\big\|_{X_\beta}^3 \\
&\quad \leq C(C_V, C_\alpha) \Big(\|u_0 - u(0)\|_{X_\zeta} + \tau_{\max}^q \sup_{0 \leq t \leq T} \big\|u(t)\big\|_{X_\beta}^3 \Big),
\end{aligned}$$

and, in connection with the Fourier pseudospectral method

$$
\begin{aligned}
&\big\|\widetilde{u}_{nM} - u_n\big\|_{X_0} \\
&\quad \leq \big\|(\mathscr{Q}_M - I)\, u_n\big\|_{X_0} + \big\|\mathscr{T}_F(\tau_{n-1})\, u_{n-1} - \mathscr{Q}_M\, \mathscr{S}_F(\tau_{n-1})\, u_{n-1}\big\|_{X_0} \\
&\qquad + \sum_{j=1}^{n-1} \mathrm{e}^{C\,(C_V + |\vartheta|\, C_\alpha^2)\,(t_n - t_j)} \big\|\mathscr{Q}_M\big(\mathscr{T}_F(\tau_{j-1})\, u_{j-1} - \mathscr{S}_F(\tau_{j-1})\, u_{j-1}\big)\big\|_{X_0} \\
&\quad \leq C\, \Lambda(M, \alpha, 0)\, \|u_n\|_{X_\alpha} + C(C_V, C_\alpha)\, \Lambda(M, \alpha, 1) \sum_{j=1}^{n} \mathrm{e}^{C\,(C_V + |\vartheta|\, C_\alpha^2)\,(t_n - t_j)}\, \tau_{j-1} \\
&\quad \leq C(C_V, C_\alpha)\, M_0^{-2\,(\alpha-1)}\,,
\end{aligned}
$$

where it is required that $\beta \geq \max\{\frac{\delta}{2}, q\}$ for $\zeta = 0$ and $\beta \geq \alpha + q$ for $\zeta = \alpha$ for some $\frac{\delta}{2} \leq \alpha \in \mathbb{N}$; here, the arising Riemann sums are estimated by the associated integrals. A justification of the presumption that the stability results Lemmas 5 and 7 are applicable is done in a standard way by combining the above relations; we refer to [15, 22, 23], where the arguments are described in detail. The above estimates show that the regularity properties of the analytical solution determine the temporal convergence order as well as the regularity of the time-discrete solution and thus the spatial accuracy. More precisely, in connection with the Fourier pseudospectral method it follows that

$$
\big\|\widetilde{u}_{nM} - u(t_n)\big\|_{X_0} \leq C\, \|u_0 - u(0)\|_{X_0} + C\, \tau_{\max}^p \sup_{0 \leq t \leq T} \big\|u(t)\big\|_{X_\beta}^3 + C\, M_0^{-2\,(\beta-1)}\,,
$$

provided that the analytical solution values and the potential V remain bounded in X_β for some $\beta \geq \max\{\frac{\delta}{2}, p\}$. Numerical examples illustrating the global error estimate and order reductions encountered for less regular analytical solutions are given in section 4.6.

Theorem 3 (Fourier). *Suppose that the coefficients of the exponential operator splitting method* (3.5) *fulfill the order conditions $C_{k\mu} = 0$ for $\mu \in \mathbb{N}^k$ with $|\mu| \leq p - k$ and $1 \leq k \leq p$ for some $p \geq 1$; see Theorem 2. Assume further that the potential V and the values of the analytical solution to the nonlinear Schrödinger equation* (2.1)–(2.2) *remain bounded in X_β for some $\beta \geq \max\{\frac{\delta}{2}, p\}$. Then the global error estimate*

$$
\big\|\widetilde{u}_{nM} - u(t_n)\big\|_{X_0} \leq C\left(\|u_0 - u(0)\|_{X_0} + \tau_{\max}^p + M_0^{-\widetilde{\beta}}\right), \qquad 0 \leq t_n \leq T\,,
$$

is valid with $\widetilde{\beta} = 2\,(\beta - 1)$ for the Fourier pseudospectral method. The constant $C > 0$ depends on the spatial dimension $d \geq 1$, the parameter value $|\vartheta|$, and the bounds for $\|V\|_{X_\beta}$ as well as $\sup\{\|u(t)\|_{X_\beta} : 0 \leq t \leq T\}$.

Remark. For linear Schrödinger equations the boundedness of the analytical solution in a fractional power space X_β with exponent $\beta \geq \frac{1}{2}\max\{\delta, p\}$ is sufficient to retain the full order of convergence.

4.5. Extension to the Sine and Hermite pseudospectral method. Within the employed general framework it is straightforward to extend our convergence analysis to other pseudospectral methods. Under the hypotheses on the linear part A introduced in section 2.2, it remains to extend the auxiliary results Lemma 1 (statements (i) and (iii)), Lemma 3 (statement (i)), Lemma 4 (statement (iii)), and Lemma 9; we note that the special form of the differential operator A enters in the proof of Lemma 1 (statement (iii)) and Lemma 9.

In situations where it is desirable to avoid the influence of artificial periodic boundary conditions, alternative choices to the Fourier pseudospectral method are the Sine and the Hermite pseudospectral methods; see [9, 16, 31]. Numerical examples given in [10] confirm that the Hermite pseudospectral method is favorable for Gross–Pitaevskii equations with small nonlinearities. For the Sine pseudospectral method minor adaptations of the arguments for the Fourier pseudospectral method are needed; in essence this concerns the analogous relations to section 3.1.2 and the derivation of Lemma 3 (statement (i)). In connection with the Hermite pseudospectral method we consider the model problem (2.1) subject to asymptotic boundary conditions on the unbounded domain $\Omega = \mathbb{R}^d$, and we set $A = -\Delta + V_\gamma$ as well as $V = W$. The construction of the Hermite basis functions as eigenfunctions of the harmonic oscillator through ladder operators is found in [31]; basic results on the Gauss–Hermite quadrature formula are given in [16]. For further details we refer to a preliminary version of the present manuscript, available from the author on request.

THEOREM 4 (Sine, Hermite). (i) *For the Sine pseudospectral method the statement of Theorem* 3 *holds.*

(ii) *For the Hermite pseudospectral method the statement of Theorem* 3 *holds with exponent* $\widetilde{\beta} = \beta - 1 - d/3$.

4.6. Numerical illustrations. In this section, we illustrate the global error estimate given in Theorems 3 and 4 by numerical examples for the two-dimensional time-dependent Gross–Pitaevskii equation under asymptotic boundary conditions

$$\mathrm{i}\,\partial_t \psi(x_1, x_2, t) = \Big(-\frac{1}{2}\,\Delta + \frac{1}{2}\left(x_1^2 + x_2^2\right) + \vartheta\left|\psi(x_1, x_2, t)\right|^2 \Big)\, \psi(x_1, x_2, t)\,, \tag{4.8}$$

where $(x_1, x_2) \in \mathbb{R}^2$ and $0 \leq t \leq 1$. For the space discretization we apply the Fourier and Sine pseudospectral method on the domain $[-8, 8] \times [-8, 8]$ and further the Hermite pseudospectral method; as time integration methods we choose the first-order Lie–Trotter splitting method, the second-order Strang splitting method, an embedded third-order scheme [21] involving $s = 7$ compositions, and a favorable fourth-order splitting scheme by Blanes and Moan [8] with real (and negative) coefficients $(a_j, b_j)_{j=1}^7$, appropriate for the time integration of Hamiltonian systems. From the above theoretical investigations we expect to observe a favorable accuracy behavior in space and to obtain the full (nonstiff) convergence order in time for sufficiently smooth analytical solutions; we note that the dominant spatial error term involves the operator A defining the linear part of the problem. Moreover, we expect that an order reduction is encountered for less regular solutions.

Illustration: Exact reference solution. As a first illustration, we consider problem (4.8) with $\vartheta = 0$, since a reliable reference solution to the linear Schrödinger equation under a harmonic potential is given, for instance, by $\psi(x_1, x_2, t) = \mathrm{e}^{-\frac{1}{2}(x_1^2 + x_2^2)}\, \mathrm{e}^{-\mathrm{i}\,t} / \sqrt{\pi}$ for $(x_1, x_2) \in \mathbb{R}^2$ and $0 \leq t \leq 1$; note that the function ψ is sufficiently often differentiable and that higher-order derivatives satisfy asymptotic boundary conditions. In Figure 4.1 the global errors versus the total number of basis functions are displayed, computed with 1000 equidistant time steps. The numerical results confirm the favorable accuracy properties of the Fourier and Sine pseudospectral method and show that for a larger number of basis functions the global error in L^2 is dominated by the temporal error; the Hermite pseudospectral method integrates the problem exactly. Furthermore, the global errors versus the constant time stepsizes are displayed,

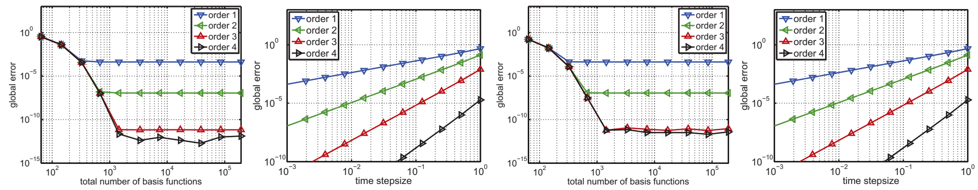

FIG. 4.1. *Space and time discretization of the linear Schrödinger equation by the Fourier (plots $1, 2$, left to right) and Sine (plots $3, 4$) pseudospectral method and splitting methods of orders $1 \leq p \leq 4$. Global errors versus the total numbers of basis functions (plots $1, 3$) and versus the time stepsizes (plots $2, 4$).*

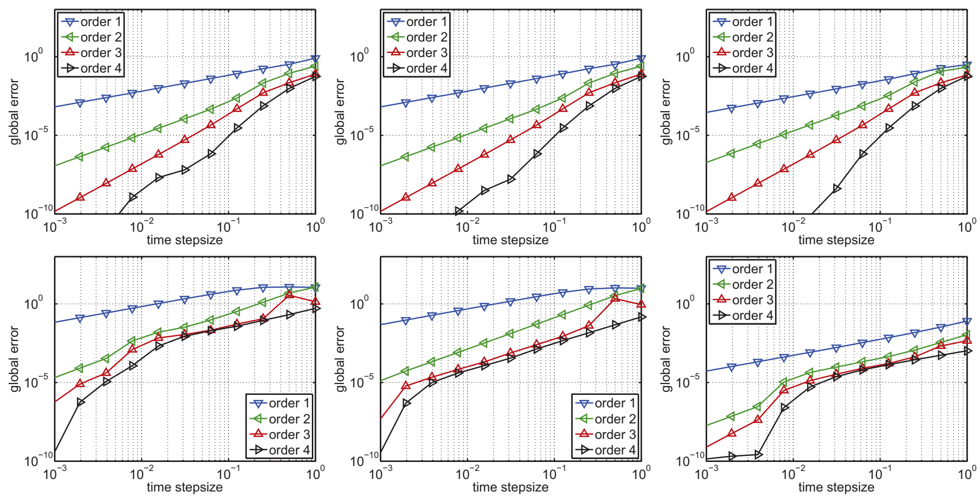

FIG. 4.2. *Space and time discretization of the nonlinear Schrödinger equation by the Fourier (first column), Sine (second column), and Hermite (third column) pseudospectral methods and splitting methods of orders $1 \leq p \leq 4$. Global errors versus the time stepsizes for a regular initial value (first row) and a less regular initial value (second row).*

computed with 256×256 basis functions; the slopes of the lines perfectly reflect the temporal convergence orders of the considered time-splitting methods.

Illustration: Smooth and nonsmooth solutions. To illustrate the error behavior of time-splitting pseudospectral methods for the nonlinear Schrödinger equation (4.8) with $\vartheta = 1$, we distinguish two different situations. On the one hand, we choose the regular initial value $\psi(x_1, x_2, t) = \mathrm{e}^{-(x_1^2+x_2^2)}\ \mathrm{e}^{-\mathrm{i}\ \ln(\exp(x_1+x_2)+\exp(-x_1-x_2))}$ for $(x_1, x_2) \in \mathbb{R}^2$, where we expect that the full (nonstiff) temporal convergence order is retained; on the other hand, to illustrate the order reduction encountered for less regular solutions, we generate a random initial value and apply the operator $(I + A)^{-1}$. The numerical results for 256×256 basis functions are displayed in Figure 4.2; the errors are computed with respect to a reference solution obtained with 2048 equidistant time steps.

Illustration: Numerical approximation of nonlinear subproblem. For the considered class of problems and for nonlinear Schrödinger equations of a similar structure, a special invariance property permits us to reduce (3.4a) to a linear problem with a solution given through exponentials (of scalars) and pointwise multiplications. In view of situations where this invariance property is no longer valid and thus the nu-

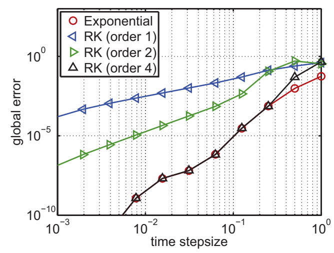

FIG. 4.3. *Space and time discretization of the nonlinear Schrödinger equation with regular initial value by a fourth-order time-splitting Fourier pseudospectral method. Time integration of the nonlinear subproblem by explicit Runge–Kutta methods of orders $p = 1, 2, 4$. Global errors versus the time stepsizes.*

merical solution of (3.4a) is required, we include a further numerical example for (4.8) with $\vartheta = 1$ under a smooth initial condition (as before), applying the Fourier pseudospectral method with 256×256 basis functions for the space discretization and a fourth-order splitting method (as before) in time. To keep the computational effort for the time integration of (3.4a) low, we choose explicit Runge–Kutta methods of orders $p = 1, 2, 4$. As expected, the convergence order of the fourth-order splitting method is retained only when combined with the fourth-order Runge–Kutta method; otherwise the order of the time integrator used for the nonlinear subproblem determines the order of convergence (see Figure 4.3). For smaller time stepsizes there is no significant difference between the results obtained for the solution based on exponentials and its numerical approximation by the fourth-order Runge–Kutta method.

Further numerical experiments on the error behavior of time-splitting pseudospectral methods are found in [1, 4, 10, 15].

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