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# HIGH-ORDER EXPONENTIAL OPERATOR SPLITTING METHODS FOR TIME-DEPENDENT SCHRÖDINGER EQUATIONS*

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**Abstract.** In this paper, we deduce high-order error bounds for exponential operator splitting methods. The employed techniques are specific to linear differential equations of the form $u'(t) = A\,u(t) + B\,u(t)$, $t \geq 0$, involving an unbounded operator $A$. In particular, evolutionary Schrödinger equations with sufficiently regular initial values are included in the analysis.

**Key words.** exponential operator splitting, Schrödinger equations, high-order methods, convergence, stability

**AMS subject classifications.** 65L05, 65M12, 65J10

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**1. Introduction.** In this paper, we study exponential operator splitting methods for initial value problems of the form

$$u'(t) = A\,u(t) + B\,u(t), \quad t \geq 0, \qquad u(0) \text{ given.} \tag{1.1}$$

We are primarily interested in evolution equations that are related to time-dependent linear Schrödinger equations or spatial discretizations thereof. That is, we allow the operator norm of $A$ to be of arbitrary size and suppose $B$ to be a bounded linear operator.

For the time integration of (1.1), we consider exponential operator splitting methods composed by several exponentials

$$u_n = \prod_{j=1}^{s} \mathrm{e}^{\,b_j hB}\, \mathrm{e}^{a_j hA}\, u_{n-1}, \quad n \geq 1, \qquad u_0 \text{ given,} \tag{1.2}$$

with coefficients $a_j, b_j \in \mathbb{R}$ for $1 \leq j \leq s$. In particular, the symmetric second-order splitting scheme

$$u_n = \mathrm{e}^{\frac{1}{2}hB}\, \mathrm{e}^{hA}\, \mathrm{e}^{\frac{1}{2}hB}\, u_{n-1}, \quad n \geq 1, \qquad u_0 \text{ given,} \tag{1.3}$$

referred to as *Strang* [20] or *symmetric Trotter* [21] splitting, is contained in the method class (1.2).

In Jahnke and Lubich [11] error bounds for (1.3) when applied to pseudospectral discretizations of time-dependent linear Schrödinger equations are given. In the present paper, we extend this approach to splitting methods of the general form (1.2).

So far, despite the fact that exponential operator splitting methods are widely used in the time integration of partial differential equations, it remains open to provide a convergence analysis for the numerical method class (1.2) when applied to stiff problems. In this work, we deduce a theoretical result on the convergence and stability behavior of exponential operator splitting methods that contributes to filling the blank

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for evolutionary linear Schrödinger equations and to justifying the practical use of example methods proposed in the literature for this type of problem; for instance, our error bound is applicable to symmetric symplectic fourth- and sixth-order methods, given in Blanes and Moan [3], and it shows that the schemes retain their convergence orders for time-dependent linear Schrödinger equations with sufficiently regular data.

This paper is organized as follows. In section 2, we introduce the precise assumptions on the linear evolution equation (1.1). Our abstract framework is based on the theory of $\mathscr{C}_0$-(semi)groups on Banach spaces and includes evolutionary linear Schrödinger equations; a thorough treatment of one-parameter (semi)groups and applications to partial differential equations is found in [7, 10, 17]. In section 3, we derive an expansion for the local error of the exponential operator splitting method (1.2) that remains valid within the analytic framework of section 2; for that purpose, extending Jahnke and Lubich [11, Proof of Thm. 2.1], we associate the order conditions with quadrature order conditions for multiple integrals. In section 4, we then prove a global error bound under reasonable regularity requirements on the initial value. Essential tools for our convergence analysis are estimates for repeated commutators; for instance, such bounds are valid for time-dependent linear Schrödinger equations subject to periodic boundary conditions, provided that the potential is sufficiently regular. The error estimate is finally illustrated by a numerical example.

A variety of works is concerned with exponential splitting methods for differential equations; as a small excerpt from the literature we mention [1, 2, 12, 18, 19] and the recent contributions [4, 5, 6, 15]; see also the references therein. In particular, we refer the reader to Lubich [14], where a rigorous convergence analysis of the Strang splitting for the cubic Schrödinger equation is given; Magnus integrators for linear Schrödinger equations involving a time-dependent potential are analyzed in Hochbruck and Lubich [9]. Basic information on splitting methods is also found in the survey article of McLachlan and Quispel [16] and the monograph of Hairer, Lubich, and Wanner [8].

## 2. Splitting methods for evolutionary Schrödinger equations.

In this section, we give the basic hypotheses on the abstract differential equation (1.1). As illustration, we consider time-dependent linear Schrödinger equations and formulate them as evolution equations; for notational simplicity, we restrict ourselves to one space dimension. Moreover, we restate the exponential operator splitting method (1.2) and introduce several auxiliary abbreviations used throughout.

### 2.1. Evolution equations.

We employ the following assumptions on the abstract initial value problem (1.1); see also Engel and Nagel [7, Thm. II.3.8]. To simplify matters, following Jahnke and Lubich [11], we require $\mathrm{e}^{tA}$ to be bounded by one.

HYPOTHESIS 1. *Let $(X, \|\cdot\|_X)$ denote the underlying Banach space and $\|\cdot\|_{X\leftarrow X}$ the induced operator norm. We assume that the densely defined and closed linear operator $A : D \subset X \to X$ is the infinitesimal generator of a $\mathscr{C}_0$-semigroup $\big(\mathrm{e}^{tA}\big)_{t\geq 0}$ on $X$ satisfying the bound*

$$\big\|\mathrm{e}^{tA}\big\|_{X\leftarrow X} \leq 1, \qquad 0 \leq t \leq T. \tag{2.1}$$

*Further, we suppose $B : X \to X$ to be a bounded linear operator.*

The above assumptions ensure that for $u(0) \in D$ the uniquely determined (classical) solution $u \in \mathscr{C}^1([0,\infty), X)$ of the initial value problem (1.1) is given by

$$u(t) = \mathrm{e}^{t(A+B)}\, u(0), \qquad t \geq 0. \tag{2.2a}$$

Moreover, the following representation by the variation-of-constants formula

$$u(t) = \mathrm{e}^{tA}\, u(0) + \int_0^t \mathrm{e}^{(t-\tau)A}\, B\, u(\tau)\, \mathrm{d}\tau, \qquad t \geq 0, \tag{2.2b}$$

is valid; see [7, Chap. II.6/III.1].

For some $\omega \in \mathbb{R}$ and $\vartheta > 0$ the fractional powers $A_\omega^\vartheta$ of the shifted operator $A_\omega = A - \omega I$ are well defined on a subspace of $X$ (see [7, Chap. II.5c]); we denote by $\big(X_\vartheta, \|\cdot\|_{X_\vartheta}\big)$ the domain of $A_\omega^\vartheta$, endowed with the graph norm

$$\|v\|_{X_\vartheta} = \|v\|_X + \big\|A_\omega^\vartheta\, v\big\|_X, \qquad v \in X_\vartheta;$$

in particular, we set $A^0 = I$ and $X_0 = X$.

Henceforth, we assume that the linear operator $B$ remains bounded on $X_\vartheta$ for some $\vartheta \geq 0$, that is, there exists a constant $C > 0$ such that

$$\big\|B\big\|_{X_\vartheta \leftarrow X_\vartheta} \leq C; \tag{2.3a}$$

consequently, the bound

$$\big\|\mathrm{e}^{tB}\big\|_{X_\vartheta \leftarrow X_\vartheta} \leq C, \qquad 0 \leq t \leq T, \tag{2.3b}$$

holds with some constant $C > 0$. Hypothesis 1 implies that $\mathrm{e}^{tA} : X \to X$ is uniformly bounded on finite time intervals; furthermore, for any $\vartheta \geq 0$ it follows that

$$\big\|\mathrm{e}^{tA}\big\|_{X_\vartheta \leftarrow X_\vartheta} \leq 1, \quad \big\|\mathrm{e}^{t(A+B)}\big\|_{X_\vartheta \leftarrow X_\vartheta} \leq C, \qquad 0 \leq t \leq T, \tag{2.3c}$$

with some constant $C > 0$.

For integers $j \geq 0$, the linear operators $\varphi_j(tB)$ are defined through

$$\varphi_0(z) = \mathrm{e}^z, \qquad \varphi_j(z) = \frac{1}{(j-1)!} \int_0^1 \tau^{j-1}\, \mathrm{e}^{(1-\tau)z}\, \mathrm{d}\tau, \quad j \geq 1, \qquad z \in \mathbb{C}. \tag{2.4a}$$

We conclude from the above relation (2.3b) that the estimate

$$\big\|\varphi_j(tB)\big\|_{X_\vartheta \leftarrow X_\vartheta} \leq \frac{1}{j!}\, C, \qquad 0 \leq t \leq T, \tag{2.4b}$$

is valid for $j \geq 0$.

In the situation of Hypothesis 1, the exponential operator splitting method (1.2) is well defined provided that $a_j \geq 0$ for $1 \leq j \leq s$. For schemes with negative coefficients, we employ a stronger framework; in particular, relation (2.3c) then remains valid for $0 \leq |t| \leq T$.

Hypothesis 2. *The densely defined closed linear operator $A : D \subset X \to X$ generates a $\mathscr{C}_0$-group $\big(\mathrm{e}^{\,tA}\big)_{t\in\mathbb{R}}$ on $X$ such that the bound*

$$\big\|\mathrm{e}^{\,tA}\big\|_{X \leftarrow X} \leq 1, \qquad 0 \leq |t| \leq T, \tag{2.5}$$

*is satisfied.*

In order to obtain high-order error bounds for (1.2), we require the solution of the initial value problem (1.1) to fulfill certain commutator bounds on fractional power spaces of $A$. We henceforth employ the standard notation

$$\mathrm{ad}_A^{\,0}(B) = B, \qquad \mathrm{ad}_A^{\,j}(B) = \big[A, \mathrm{ad}_A^{\,j-1}(B)\big], \quad j \geq 1, \tag{2.6}$$

where $[A, L] = AL - LA$ for some linear operator $L$; e.g., see [8, Chap. III.4.1].

HYPOTHESIS 3. *We suppose that for certain $\vartheta, \widetilde{\vartheta} \geq 0$ the estimate*

$$\big\|\mathrm{ad}_A^j(B)\big\|_{X_\vartheta \leftarrow X_{\widetilde{\vartheta}}} \leq C$$

*is valid with constant $C > 0$.*

As indicated in section 2.2, the above hypothesis is reasonable in connection with evolutionary linear Schrödinger equations that are subject to periodic boundary conditions and involve a smooth potential.

**2.2. Time-dependent Schrödinger equations.** Let $V : \Omega = [-\pi, \pi] \to \mathbb{R}$ be a periodic map that fulfills suitable regularity requirements. We consider the time-dependent linear Schrödinger equation

$$\mathrm{i}\, \partial_t U(x,t) = -\,\Delta\, U(x,t) + V(x)\, U(x,t), \qquad x \in \Omega, \quad t \geq 0, \tag{2.7}$$

subject to periodic boundary conditions on $\Omega$ and an initial condition $U(x,0) = U_0(x)$, $x \in \Omega$.

The above initial-boundary value problem is interpreted as an initial value problem of the form (1.1) by setting $u(t) = U(\cdot, t)$ and

$$\big(A\, v\big)(x) = \mathrm{i}\,\Delta\, v(x), \qquad \big(B\, v\big)(x) = -\,\mathrm{i}\, V(x)\, v(x)$$

for $v : \Omega \to \mathbb{C}$ a sufficiently regular function. Similarly as in Pazy [17, Chap. 7.5], it is shown that the linear operators $A : D \to X$ and $B : X \to X$ satisfy the assumptions of Hypothesis 1 with $X = L^2(\Omega, \mathbb{C})$ and $D = \big\{v \in H^2(\Omega, \mathbb{C}) : v \text{ periodic on } \Omega\big\}$. Furthermore, it holds that $X_{k/2} = \big\{v \in H^k(\Omega, \mathbb{C}) : v \text{ periodic on } \Omega\big\}$ for integers $k \geq 1$.

We note that Hypothesis 3 is fulfilled with $\vartheta = k/2$ and $\widetilde{\vartheta} = \vartheta + j/2$ for integers $j, k \geq 0$, provided that $V$ is sufficiently often differentiable. In fact, the commutator of the one-dimensional Laplace operator $\mathscr{A} = \partial_x^2$ and a $j$th-order differential operator

$$\mathscr{B} = \sum_{\ell=0}^{j} \beta_\ell(x)\, \partial_x^\ell$$

with smooth space-dependent coefficients $\beta_\ell$, $0 \leq \ell \leq j$, yields a differential operator of order $j + 1$. More precisely, it follows that

$$\big[\mathscr{A}, \mathscr{B}\big] = \mathscr{A}\mathscr{B} - \mathscr{B}\mathscr{A} = \sum_{\ell=0}^{j} \big(2\, \beta_\ell'\, \partial_x^{\ell+1} + \beta_\ell''\, \partial_x^\ell\big).$$

Proceeding by induction, we conclude that the iterated commutator $\mathrm{ad}_{\mathscr{A}}^j(V)$ is a differential operator of order $j$ and therefore obtain

$$\big\|\mathrm{ad}_{\mathscr{A}}^j(V)\, v\big\|_{H^k(\Omega)} \leq C \|v\|_{H^{k+j}(\Omega)}, \qquad v \in H^{k+j}(\Omega),$$

for $k, j \geq 0$.

It is straightforward to generalize the above considerations to higher space dimensions.

**2.3. Exponential operator splitting methods.** Throughout, the gridpoints associated with a constant stepsize $h > 0$ are denoted by $t_n = nh$ for $n \geq 0$. For an exponential operator splitting method with real coefficients $a_j, b_j \in \mathbb{R}$, $1 \leq j \leq s$, numerical approximation values $u_n \approx u(t_n)$ to the true solution of (1.1) are given by the recurrence formula

$$u_n = \mathrm{e}^{b_s hB}\, \mathrm{e}^{a_s hA} \cdots \mathrm{e}^{b_2 hB}\, \mathrm{e}^{a_2 hA}\, \mathrm{e}^{b_1 hB}\, \mathrm{e}^{a_1 hA}\, u_{n-1}, \quad n \geq 1, \qquad u_0 \text{ given}; \tag{2.8a}$$

see Hypotheses 1 and 2. We note that the linear operators arising in the above product do not commute in general.

In order to write (2.8a) in short notation, it is useful to employ the following abbreviations. For linear operators $L_j : X \to X$, $\ell \leq j \leq k$, we define

$$\prod_{j=\ell}^{k} L_j = L_k \cdots L_{\ell+1}\, L_\ell, \quad k \geq \ell, \qquad \prod_{j=\ell}^{k} L_j = I, \quad k < \ell.$$

Here, $I : X \to X$ denotes the identity operator on $X$. Furthermore, for $k \leq s$ we set

$$P_k = \prod_{j=1}^{k} \mathrm{e}^{b_j hB}\, \mathrm{e}^{a_j hA}, \tag{2.8b}$$

and thus the exponential operator splitting method (2.8a) takes the compact form

$$u_n = P_s\, u_{n-1}, \quad n \geq 1, \qquad u_0 \text{ given}; \tag{2.8c}$$

see (1.2).

Inserting the exact solution values into the numerical scheme (2.8c) defines the defect at time $t_n$

$$u(t_n) = P_s\, u(t_{n-1}) + d_n, \qquad n \geq 1. \tag{2.9}$$

As a consequence, a recurrence relation for the error of the splitting method

$$e_n = u_n - u(t_n) = P_s\, e_{n-1} - d_n, \qquad n \geq 1,$$

follows. Resolving this recursion, we finally obtain

$$e_n = P_s^n\, e_0 - \sum_{j=0}^{n-1} P_s^{n-j-1}\, d_{j+1}, \qquad n \geq 0. \tag{2.10}$$

Our main result in section 4 is a convergence estimate for (2.8). Its proof is based on the above representation; that is, suitable estimations of the splitting operator and the defects are required; in this context, several auxiliary results provided in section 3.1 are of use.

**3. Local error.** In the present section, our concern is to deduce a suitable expansion of the local error

$$d_n = u(t_n) - P_s\, u(t_{n-1}), \qquad n \geq 1, \tag{3.1}$$

that remains well defined within the analytical framework of section 2; see (2.9). Furthermore, from this representation, the order conditions for the exponential operator splitting method (2.8) follow.

We start with expanding the exact solution and the splitting operator.

**3.1. Auxiliary expansions.** (i) *Exact solution.* An expansion of the exact solution value $u(t_n)$ that is specific to evolutionary Schrödinger equations is obtained by means of a reapplication of the variation-of-constants formula (2.2b). Namely, replacing in

$$u(t_n) = u(t_{n-1}+h) = \mathrm{e}^{hA}\, u(t_{n-1}) + \int_0^h \mathrm{e}^{(h-\tau_1)A}\, B\, u(t_{n-1}+\tau_1)\,\mathrm{d}\tau_1$$

the solution value $u(t_{n-1}+\tau_1)$ by

$$u(t_{n-1}+\tau_j) = \mathrm{e}^{\tau_j A}\, u(t_{n-1}) + \int_0^{\tau_j} \mathrm{e}^{(\tau_j-\tau_{j+1})A}\, B\, u(t_{n-1}+\tau_{j+1})\,\mathrm{d}\tau_{j+1}, \tag{3.2}$$

where $j=1$, yields the following relation:

$$\begin{aligned} u(t_n) &= \mathrm{e}^{hA}\, u(t_{n-1}) + \int_0^h \mathrm{e}^{(h-\tau_1)A}\, B\, \mathrm{e}^{\tau_1 A}\, u(t_{n-1})\,\mathrm{d}\tau_1 \\ &\quad + \int_0^h \int_0^{\tau_1} \mathrm{e}^{(h-\tau_1)A}\, B\, \mathrm{e}^{(\tau_1-\tau_2)A}\, B\, u(t_{n-1}+\tau_2)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1. \end{aligned} \tag{3.3}$$

Henceforth, we employ the compact vector notation $\tau = (\tau_1, \tau_2, \dots, \tau_k) \in \mathbb{R}^k$ and set

$$f_k(\tau) = \prod_{\ell=1}^{k} \Bigl(\mathrm{e}^{(\tau_{k-\ell}-\,\tau_{k-\ell+1})A}\, B\Bigr), \qquad g_k(\tau) = f_k(\tau)\,\mathrm{e}^{\tau_k A}, \tag{3.4a}$$

with $\tau_0 = h$; as before, the product is defined downwards. Applying repeatedly the substitution (3.2) to (3.3), we therefore obtain

$$\begin{aligned} u(t_n) &= \mathrm{e}^{hA}\, u(t_{n-1}) + \sum_{k=1}^{p} I_k\, u(t_{n-1}) + R^{(1)}_{p+1}, \\ I_k &= \int_{\Delta_k} g_k(\tau)\,\mathrm{d}\tau, \qquad R^{(1)}_{p+1} = \int_{\Delta_{p+1}} f_{p+1}(\tau)\, u(t_{n-1}+\tau_{p+1})\,\mathrm{d}\tau, \end{aligned} \tag{3.4b}$$

where $\Delta_k = \bigl\{\tau \in \mathbb{R}^k : 0 \le \tau_\ell \le \tau_{\ell-1}, 1 \le \ell \le k\bigr\}$. We note that the above expansion remains well defined in the situation of Hypothesis 1; see also section 4.

(ii) *Splitting operator.* We next specify a representation for the splitting operator $P_s$ that allows, in an easy manner, a comparison with (3.4b). Our main tool for deducing such an expansion is a recurrence formula for the $\varphi$-functions

$$\varphi_j(z) = \frac{1}{j!} + z\,\varphi_{j+1}(z), \qquad j \ge 0, \quad z \in \mathbb{C}, \tag{3.5a}$$

obtained from (2.4a) by a partial integration. Moreover, we make use of the identity

$$\prod_{j=1}^{k} \bigl(K_j + L_j\bigr) = \prod_{\ell=1}^{k} K_\ell + \sum_{j=1}^{k} \prod_{\ell=j+1}^{k} K_\ell\, L_j \prod_{\ell=1}^{j-1} \bigl(K_\ell + L_\ell\bigr) \tag{3.5b}$$

that is valid for (noncommuting) linear operators $K_j, L_j$, $1 \le j \le k$. By applying the relations (3.5) to $P_s$, we obtain

$$P_s = \prod_{j=1}^{s} \mathrm{e}^{\,b_j hB}\, \mathrm{e}^{a_j hA} = \prod_{j=1}^{s} \Bigl(\mathrm{e}^{a_j hA} + h\, b_j\, B\, \varphi_1\bigl(b_j hB\bigr)\, \mathrm{e}^{a_j hA}\Bigr), \tag{3.6}$$

and further the representation

$$P_s = \mathrm{e}^{c_s hA} + h \sum_{j=1}^{s} b_j \, \mathrm{e}^{(c_s - c_j)\, hA} \, B \, \varphi_1(b_j hB) \, \mathrm{e}^{a_j hA} \, P_{j-1}. \tag{3.7}$$

Here, we employ the abbreviation

$$c_k = \sum_{j=1}^{k} a_j, \qquad 1 \le k \le s. \tag{3.8a}$$

Regarding the $h$-expansions (3.4b) and (3.7), it is seen that in (3.1) the $\mathscr{O}(1)$ term vanishes, provided that

$$c_s = 1; \tag{3.8b}$$

thus, we henceforth suppose the above order condition to be fulfilled. For the following considerations, it is useful to introduce the abbreviations

$$\begin{gathered} \Phi_j(\lambda) = F(\lambda) \, \varphi_j(b_{\lambda_k} hB) \, \mathrm{e}^{a_{\lambda_k} hA} \, P_{\lambda_k - 1}, \\ F(\lambda) = \prod_{\ell=1}^{k} b_{\lambda_\ell} \, f_k(c_\lambda h), \qquad G(\lambda) = F(\lambda) \, \mathrm{e}^{c_{\lambda_k} hA} = \prod_{\ell=1}^{k} b_{\lambda_\ell} \, g_k(c_\lambda h), \end{gathered} \tag{3.9}$$

where we set $c_\lambda = (c_{\lambda_1}, c_{\lambda_2}, \dots, c_{\lambda_k})$ for multi-indices $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_k) \in \mathbb{N}^k$ and $\lambda_0 = s$; see (3.4a). With the help of this notation, relation (3.7) can be written as

$$P_s = \mathrm{e}^{hA} + h \sum_{\lambda_1 = 1}^{s} \Phi_1(\lambda_1). \tag{3.10}$$

In order to expand the splitting operator $P_s$ further, we proceed by induction; that is, we repeatedly apply a recurrence relation for $\Phi_j$ to (3.10) which we derive next. Formula (3.5a) implies

$$\Phi_j(\lambda) = \frac{1}{j!} \, F(\lambda) \, \mathrm{e}^{a_{\lambda_k} hA} \, P_{\lambda_k - 1} + h \, \Phi_{j+1}(\lambda, \lambda_k);$$

moreover, from the analogue of (3.7),

$$\begin{aligned} \mathrm{e}^{a_{\lambda_k} hA} \, P_{\lambda_k - 1} &= \mathrm{e}^{c_{\lambda_k} hA} \\ &\quad + h \sum_{\lambda_{k+1} = 1}^{\lambda_k - 1} b_{\lambda_{k+1}} \, \mathrm{e}^{(c_{\lambda_k} - c_{\lambda_{k+1}})\, hA} \, B \, \varphi_1(b_{\lambda_{k+1}} hB) \, \mathrm{e}^{a_{\lambda_{k+1}} hA} \, P_{\lambda_{k+1} - 1}, \end{aligned}$$

we obtain the recurrence formula

$$\Phi_j(\lambda) = \frac{1}{j!} \, G(\lambda) + h \left( \Phi_{j+1}(\lambda, \lambda_k) + \sum_{\lambda_{k+1} = 1}^{\lambda_k - 1} \frac{1}{j!} \, \Phi_1(\lambda, \lambda_{k+1}) \right). \tag{3.11}$$

As an illustration, we apply the above relation twice to (3.10). In a first step, we get

$$\begin{gathered} P_s = \mathrm{e}^{hA} + Q_1 + r_2^{(2)}, \\ Q_1 = h \sum_{\lambda_1 = 1}^{s} G(\lambda_1), \qquad r_2^{(2)} = h^2 \left( \sum_{\lambda_1 = 1}^{s} \Phi_2(\lambda_1, \lambda_1) + \sum_{\lambda_1 = 1}^{s} \sum_{\lambda_2 = 1}^{\lambda_1 - 1} \Phi_1(\lambda_1, \lambda_2) \right). \end{gathered}$$

A further expansion of $r_2^{(2)}$ by means of (3.11) yields

$$\text{(3.12a)}\qquad \begin{aligned} &P_s = \mathrm{e}^{hA} + \sum_{k=1}^{2} Q_k + r_3^{(2)},\\ &Q_1 = h \sum_{\lambda_1=1}^{s} G(\lambda_1), \qquad Q_2 = h^2 \Bigg( \sum_{\lambda_1=1}^{s} \tfrac{1}{2}\, G(\lambda_1,\lambda_1) + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} G(\lambda_1,\lambda_2) \Bigg), \end{aligned}$$

with remainder $r_3^{(2)}$ given by

$$\text{(3.12b)}\qquad \begin{aligned} r_3^{(2)} = h^3 \Bigg( &\sum_{\lambda_1=1}^{s} \Phi_3(\lambda_1,\lambda_1,\lambda_1) + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \tfrac{1}{2}\, \Phi_1(\lambda_1,\lambda_1,\lambda_2)\\ &+ \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \Phi_2(\lambda_1,\lambda_2,\lambda_2) + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} \Phi_1(\lambda_1,\lambda_2,\lambda_3) \Bigg). \end{aligned}$$

By reason of brevity, we write $Q_2$ as

$$\text{(3.12c)}\qquad Q_2 = h^2 \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1} \alpha_{\lambda_1\lambda_2}\, G(\lambda_1,\lambda_2), \qquad \alpha_{\lambda_1\lambda_2} = \begin{cases} \frac{1}{2} & \text{if } \lambda_2 = \lambda_1,\\ 1 & \text{if } \lambda_2 \le \lambda_1 - 1. \end{cases}$$

Applying (3.11) several times to (3.12), we finally end up with the expansion

$$\text{(3.13a)}\qquad P_s = \mathrm{e}^{hA} + \sum_{k=1}^{p} Q_k + r_{p+1}^{(2)}.$$

Here, the multiple sum $Q_k$ comprises terms of the form $h^k\, \alpha_\lambda\, G(\lambda)$ for certain $\alpha_\lambda \in \mathbb{R}$; more precisely, we have

$$\text{(3.13b)}\qquad Q_k = h^k \sum_{\lambda \in \Lambda_k} \alpha_\lambda\, G(\lambda) = h^k \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1} \cdots \sum_{\lambda_k=1}^{\lambda_{k-1}} \alpha_{\lambda_1\lambda_2\cdots\lambda_k}\, G(\lambda_1,\lambda_2,\ldots,\lambda_k),$$

where we denote $\Lambda_k = \big\{ \lambda \in \mathbb{N}^k : 1 \le \lambda_\ell \le \lambda_{\ell-1}, 1 \le \ell \le k \big\}$ with $\lambda_0 = s$, according to (3.4). The coefficients $\alpha_\lambda$ are displayed in Table A.1 for $1 \le k \le 4$. The remainder $r_{p+1}^{(2)}$ is given by

$$\text{(3.13c)}\qquad r_{p+1}^{(2)} = h^{p+1} \sum_{j=1}^{p+1} \sum_{\lambda \in \Lambda_{p+1}} \widetilde{\alpha}_{j\lambda}\, \Phi_j(\lambda)$$

for certain $\widetilde{\alpha}_{j\lambda} \in \mathbb{R}$; we omit further details and refer the reader to the MATLAB code `recurrence`, available at http://techmath.uibk.ac.at/mecht/research/research.html, that determines the coefficients $\alpha_\lambda$ and $\widetilde{\alpha}_{j\lambda}$.

(iii) *Quadrature formulas.* From the above considerations, we obtain the following expansion of the defect:

$$\text{(3.14)}\qquad d_n = \sum_{k=1}^{p} \big( I_k - Q_k \big)\, u(t_{n-1}) + R_{p+1}^{(1)} - R_{p+1}^{(2)}, \qquad R_{p+1}^{(2)} = r_{p+1}^{(2)}\, u(t_{n-1});$$

see also (3.1), (3.4), (3.8), and (3.13). We next relate the difference $I_k - Q_k$ to the error of quadrature formulas for multiple integrals. Regarding (3.9) and (3.13b), we write $Q_k$ as

$$Q_k = h^k \sum_{\lambda\in\Lambda_k} \beta_\lambda \, g_k(c_\lambda h), \qquad \beta_\lambda = \beta_{\lambda_1\lambda_2\cdots\lambda_k} = \alpha_{\lambda_1\lambda_2\cdots\lambda_k} \prod_{\ell=1}^{k} b_{\lambda_\ell}; \tag{3.15}$$

see (3.4a) for the definition of $g_k$. As usual, in order to determine the defects of the quadrature formula (3.15), we employ a Taylor series expansion of order $M = p - k$:

$$\begin{aligned} g_k(\tau) &= \sum_{m=0}^{p-k} \frac{1}{m!}\, g_k^{(m)}(0)\, \tau^m + \varrho_{k,p-k+1}(\tau), \\ \varrho_{k,M+1}(\tau) &= \frac{1}{M!}\int_0^1 (1-z)^M\, g_k^{(M+1)}(z\,\tau)\,\tau^{M+1}\,\mathrm{d}z. \end{aligned} \tag{3.16a}$$

In view of section 4, we next specify the $m$th derivative of $g_k$. It holds that

$$g_k^{(m)}(\sigma)\,\tau^m = \sum_{\substack{\mu\in\mathbb{N}^k\\ |\mu|=m}} \frac{m!}{\mu!}\,\partial_\tau^\mu g_k(\sigma)\,\tau^\mu; \tag{3.16b}$$

here, for $\mu = (\mu_1, \mu_2, \dots, \mu_k) \in \mathbb{N}^k$ and $\tau = (\tau_1, \tau_2, \dots, \tau_k) \in \mathbb{R}^k$, we let

$$|\mu| = \sum_{\ell=1}^{k} \mu_\ell, \qquad \mu! = \prod_{\ell=1}^{k} \mu_\ell!, \qquad \tau^\mu = \prod_{\ell=1}^{k} \tau_\ell^{\mu_\ell}, \qquad \partial_\tau^\mu = \prod_{\ell=1}^{k} \partial_{\tau_\ell}^{\mu_\ell}. \tag{3.16c}$$

Proceeding by induction, it follows that

$$\partial_\tau^\mu\, g_k(\tau) = (-1)^{|\mu|} \prod_{\ell=1}^{k} \Big( \mathrm{e}^{(\tau_{k-\ell} - \tau_{k-\ell+1})A}\, \mathrm{ad}_A^{\mu_{k-\ell+1}}(B) \Big)\, \mathrm{e}^{\tau_k A}; \tag{3.16d}$$

we recall definition (2.6) of the repeated commutators. In particular, we have

$$\partial_\tau^\mu\, g_k(0) = (-1)^{|\mu|}\, \mathrm{e}^{hA} \prod_{\ell=1}^{k} \mathrm{ad}_A^{\mu_{k-\ell+1}}(B). \tag{3.16e}$$

Inserting the Taylor series expansion (3.16) into

$$I_k - Q_k = \int_{\Delta_k} g_k(\tau)\,\mathrm{d}\tau - h^k \sum_{\lambda\in\Lambda_k} \beta_\lambda\, g_k(c_\lambda h)$$

(see (3.4b) and (3.15)) and making use of the fact that

$$\int_{\Delta_k} \tau^\mu\,\mathrm{d}\tau = h^{k+|\mu|} \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1}, \tag{3.17}$$

we obtain the representation

$$\begin{aligned} I_k - Q_k = {} & \sum_{m=0}^{p-k} h^{k+m} \sum_{\substack{\mu\in\mathbb{N}^k\\ |\mu|=m}} \frac{1}{\mu!} \left( \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1} - \sum_{\lambda\in\Lambda_k} \beta_\lambda\, c_\lambda^\mu \right) \partial_\tau^\mu g_k(0) \\ & + \int_{\Delta_k} \varrho_{k,p-k+1}(\tau)\,\mathrm{d}\tau - h^k \sum_{\lambda\in\Lambda_k} \beta_\lambda\, \varrho_{k,p-k+1}(c_\lambda h). \end{aligned}$$

Altogether, inserting the above relation into (3.14) implies

$$d_n = \sum_{k=1}^{p} \sum_{m=0}^{p-k} h^{k+m} \sum_{\substack{\mu\in\mathbb{N}^k \\ |\mu|=m}} \frac{1}{\mu!} \Bigg( \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1} - \sum_{\lambda\in\Lambda_k} \beta_\lambda\, c_\lambda^\mu \Bigg)$$
$$\times\, \partial_\tau^\mu g_k(0)\, u(t_{n-1}) + R_{p+1}^{(1)} - R_{p+1}^{(2)} + R_{p+1}^{(3)},$$
$$R_{p+1}^{(3)} = \sum_{k=1}^{p} \Bigg( \int_{\Delta_k} \varrho_{k,p-k+1}(\tau)\, \mathrm{d}\tau - h^k \sum_{\lambda\in\Lambda_k} \beta_\lambda\, \varrho_{k,p-k+1}(c_\lambda h) \Bigg) u(t_{n-1});$$

see also (3.4b) and (3.13c) for the definition of $R_{p+1}^{(1)}$ and $R_{p+1}^{(2)}$.

**3.2. Local error expansion and order conditions.** In Lemma 1, we restate the expansion for the defect (3.1) deduced in section 3.1. In view of section 4, we resume the employed abbreviations; see also (2.2a), (2.4a), (2.6), and (3.16c).

LEMMA 1. *We set* $\Lambda_k = \big\{\lambda = (\lambda_1, \lambda_2, \dots, \lambda_k) \in \mathbb{N}^k : 1 \le \lambda_\ell \le \lambda_{\ell-1}, 1 \le \ell \le k\big\}$ *and* $\Delta_k = \big\{\tau = (\tau_1, \tau_2, \dots, \tau_k) \in \mathbb{R}^k : 0 \le \tau_\ell \le \tau_{\ell-1}, 1 \le \ell \le k\big\}$*, where* $\lambda_0 = s$ *and* $\tau_0 = h$*. Further, we denote* $c_k = a_1 + a_2 + \cdots + a_k$ *for* $1 \le k \le s$*. Provided that the condition* $c_s = 1$ *is fulfilled, the defect of the exponential operator splitting method* (2.8) *equals*

(3.18)
$$d_n = \sum_{k=1}^{p} \sum_{\substack{\mu\in\mathbb{N}^k \\ |\mu|\le p-k}} \frac{(-1)^{|\mu|}}{\mu!} h^{k+|\mu|} \Bigg( \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1} - \sum_{\lambda\in\Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell} c_{\lambda_\ell}^{\mu_\ell} \Bigg)$$
$$\times\, \mathrm{e}^{hA} \prod_{\ell=1}^{k} \mathrm{ad}_A^{\mu_{k-\ell+1}}(B)\, \mathrm{e}^{t_{n-1}(A+B)}\, u(0) + R_{p+1}.$$

*The remainder* $R_{p+1} = R_{p+1}^{(1)} - R_{p+1}^{(2)} + R_{p+1}^{(3)}$ *is given by*

$$R_{p+1}^{(1)} = \int_{\Delta_{p+1}} \prod_{j=1}^{p+1} \Big( \mathrm{e}^{(\tau_{p+1-j} - \tau_{p+1-j+1})A}\, B \Big)\, \mathrm{e}^{(t_{n-1}+\tau_{p+1})(A+B)}\, u(0)\, \mathrm{d}\tau,$$
$$R_{p+1}^{(2)} = h^{p+1} \sum_{j=1}^{p+1} \sum_{\lambda\in\Lambda_{p+1}} \widetilde{\alpha}_{j\lambda} \prod_{\ell=1}^{p+1} \Big( b_{\lambda_\ell}\, \mathrm{e}^{(c_{\lambda_{p-\ell+1}} - c_{\lambda_{p-\ell+2}})\, hA}\, B \Big)$$
$$\times\, \varphi_j(b_{\lambda_{p+1}} hB)\, \mathrm{e}^{a_{\lambda_{p+1}} hA}\, P_{\lambda_{p+1}-1}\, \mathrm{e}^{t_{n-1}(A+B)}\, u(0),$$

$$\varrho_{k,p-k+1}(\tau) = (p-k+1) \int_0^1 (1-z)^{p-k} \sum_{\substack{\mu\in\mathbb{N}^k \\ |\mu|=p-k+1}} \frac{(-1)^{|\mu|}}{\mu!}$$
$$\times \prod_{\ell=1}^{k} \Big( \mathrm{e}^{(\tau_{k-\ell} - \tau_{k-\ell+1})\, zA}\, \mathrm{ad}_A^{\mu_{k-\ell+1}}(B) \Big)\, \mathrm{e}^{\tau_k zA}\, \tau^\mu\, \mathrm{d}z,$$

$$R_{p+1}^{(3)} = \sum_{k=1}^{p} \Big( \int_{\Delta_k} \varrho_{k,p-k+1}(\tau)\, \mathrm{d}\tau - h^k \sum_{\lambda\in\Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell}\, \varrho_{k,p-k+1}(c_\lambda h) \Big)\, \mathrm{e}^{t_{n-1}(A+B)}\, u(0).$$

*The coefficients $\alpha_\lambda$ and $\widetilde{\alpha}_{m\lambda}$ are obtained by recurrence.*[1]

Obviously, the first term in the local error expansion (3.18) vanishes whenever (combinations of) the coefficients

$$C_\mu = \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1} - \sum_{\lambda \in \Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell} c_{\lambda_\ell}^{\mu_\ell} \tag{3.19}$$

vanish for all $1 \le k \le p$ and $|\mu| \le p - k$. In order to show that the classical order conditions for a general exponential operator splitting method (2.8) coincide with the stiff order conditions, we meanwhile assume (1.1) to be a *nonstiff* problem; that is, we require the linear operator $A$ to be bounded on $X$. In this situation, the expansion

$$\mathrm{e}^{hA} = \sum_{j=0}^{\infty} \frac{1}{j!}\, h^j A^j$$

is well defined on $X$ and further yields

$$d_\mu = \sum_{\substack{k\ge 1,\, j \ge 0,\, \mu\in\mathbb{N}^k\\ k+j+|\mu|\le p}} \frac{(-1)^{|\mu|}}{j!\,\mu!}\, h^{k+j+|\mu|}\, C_\mu\, E_{j\mu}(A,B)\, \mathrm{e}^{t_{\mu-1}(A+B)}\, \mu(0) + \mathscr{O}(\mu^{p+1}),$$

$$E_{j\mu}(A,B) = A^j \prod_{\ell=1}^{k} \mathrm{ad}_A^{\mu_{k-\ell+1}}(B).$$

The splitting method is consistent of order $p$ iff for any $1 \le q \le p$ the term involving $h^q$ vanishes. Thus, taking into account all combinations of $k \ge 1$, $j \ge 0$, and $\mu \in \mathbb{N}^k$ such that $k + |j| + |\mu| = q$ for some $1 \le q \le p$ fixed, we conclude that

$$\sum_{\substack{k\ge 1,\, j \ge 0,\, \mu\in\mathbb{N}^k\\ k+j+|\mu| = q}} \frac{(-1)^{|\mu|}}{j!\,\mu!}\, C_\mu\, E_{j\mu}(A,B) = 0.$$

For $j > 0$, due to lower order conditions, the corresponding terms vanish; if $j = 0$, the same conditions as in the stiff case arise.

Alternatively, in order to show that for evolutionary Schrödinger equations the stiff and nonstiff order conditions coincide, one could also derive the classical order conditions by means of the Campbell–Baker–Hausdorff formula (see [8]); however, as further tedious calculations are involved, we did not follow this approach here.

The proof of our convergence result for general exponential operator splitting methods (2.8) relies on a suitable estimation of the local error expansion given in Lemma 1. Provided that the conditions

(3.20)

$$\sum_{\ell=1}^{s} a_\ell = 1,$$

$$\sum_{\lambda \in \Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell} c_{\lambda_\ell}^{\mu_\ell} = \prod_{\ell=1}^{k} \frac{1}{\mu_\ell + \cdots + \mu_k + k - \ell + 1}, \qquad 1 \le k \le p, \quad |\mu| \le p - k,$$

[1] A MATLAB code `recurrence` is available at http://techmath.uibk.ac.at/mecht/research/research.html.

are fulfilled (see also (3.19)), the first term in the local error expansion vanishes and it remains to estimate $R_{p+1}$. Clearly, for *nonstiff* problems (1.1), the iterated commutators are bounded; however, whenever the differential equation involves an unbounded linear operator $A$, this is not true in general. For evolutionary Schrödinger equations, reasonable regularity assumptions on the initial value allow us to estimate the decisive term $R_{p+1}^{(3)}$ by means of Hypothesis 3.

**3.3. Example methods.** As an illustration, we next specify various exponential operator splitting methods and verify that the conditions (3.20) are satisfied; see also Appendix A. Our main result in section 4 ensures that the example methods retain their convergence orders for evolutionary Schrödinger equations.

*Order* 1. The conditions for $p = 1$ are given in (A.1a). In particular, for $s = 1$ it follows that $a_1 = 1 = b_1$, and we retain the *Lie–Trotter* splitting

$$u_n = \mathrm{e}^{hB}\,\mathrm{e}^{hA}\,u_{n-1}, \quad n \geq 1, \qquad u_0 \text{ given.}$$

*Order* 2. For $p = 2$ the additional conditions are given in (A.1b). Choosing $s = 2$ and simplifying (A.1a) and (A.1b) yields $a_1 + a_2 = 1$, $b_1 + b_2 = 1$, and $b_1 a_1 + b_2 = \frac{1}{2}$. For the choice $a_1 = 0$ we thus retain the *Strang* splitting (1.3); alternatively, by setting $a_1 = \frac{1}{2}$ it follows that

$$u_n = \mathrm{e}^{\frac{1}{2}hA}\,\mathrm{e}^{hB}\,\mathrm{e}^{\frac{1}{2}hA}\,u_{n-1}, \quad n \geq 1, \qquad u_0 \text{ given.}$$

*Order* 4/6. Symmetric symplectic methods that can be cast in the form (2.8) are proposed in Blanes and Moan [3, Tables 2–3]. The coefficients of a fourth- and sixth-order scheme are collected in Table 3.1; the conditions (3.20) are fulfilled (up to machine precision) for $p = 4$ and $p = 6$, respectively (see also Appendix A).

TABLE 3.1
*Coefficients of a fourth-order method given in Blanes and Moan* [3].

| $j$ | $a_j$ |
|---|---|
| 1,7 | 0.0792036964311957 |
| 2,6 | 0.3531729060497740 |
| 3,5 | $-$ 0.0420650803577195 |
| 4 | $1 - 2\,(a_1 + a_2 + a_3)$ |

| $j$ | $b_j$ |
|---|---|
| 1,6 | 0.209515106613362 |
| 2,5 | $-$ 0.143851773179818 |
| 3,4 | $1/2 - (b_1 + b_2)$ |
| 7 | 0 |

**4. Global error.** In this section, we derive a convergence result for the exponential operator splitting method (2.8) when applied to the abstract initial value problem (1.1) and further illustrate the error bound by a numerical example.

**4.1. Global error bound in terms of the initial value.** In the formulation of Theorem 1, we focus on evolutionary linear Schrödinger equations; that is, the unbounded linear operator $A$ is related to the Laplacian. Provided that the method coefficients $a_j$ are nonnegative for $1 \leq j \leq s$, it suffices to require that $A$ generates a $\mathscr{C}_0$-semigroup; see Hypothesis 1.

THEOREM 1. *Assume that the coefficients of the exponential operator splitting method* (2.8) *fulfill the classical order conditions for some integer* $p \geq 1$. *Suppose further that the linear operators* $A$ *and* $B$ *satisfy the requirements of Hypotheses* 2 *and* 3 *with* $\vartheta = k/2$ *and* $\vartheta = (j+k)/2$ *for integers* $j, k \geq 0$ *such that* $j + k \leq p$. *Then, provided that* $u(0) \in X_{p/2}$, *the error estimate*

$$\big\|u_n - u(t_n)\big\|_X \leq C\,\big\|u(0) - u_0\big\|_X + C\,h^p\,\big\|u(0)\big\|_{X_{p/2}}, \qquad 0 \leq nh \leq T,$$

*is valid with some constant $C > 0$ depending in particular on $T$ but not on $n$ and $h$.*

*Proof.* Our main tools for deriving the above convergence result are a stability bound for the splitting operator and an estimate for the defect of the exponential operator splitting method (2.8). For notational simplicity, we do not distinguish the arising constants.

We first verify the boundedness of $P_s^n$. To that purpose, we employ the relation

$$P_s = \prod_{j=1}^{s} \big(I + h\, b_j\, B\, \varphi_1(b_j hB)\big)\, \mathrm{e}^{a_j hA}$$

obtained by means of (3.5a); see also (3.6). Applying (2.3) and (2.4) and using that $1 + z \le \mathrm{e}^z$ for $z > 0$, it follows that

$$\begin{aligned}\big\|P_s\big\|_{X\leftarrow X} &\le \prod_{j=1}^{s} \big\|I + h\, b_j\, B\, \varphi_1\big(b_j hB\big)\big\|_{X\leftarrow X}\, \big\|\mathrm{e}^{a_j hA}\big\|_{X\leftarrow X}\\ &\le \prod_{j=1}^{s} \big(1 + C\, h\, |b_j|\big) \le \mathrm{e}^{Ch}.\end{aligned}$$

Furthermore, we conclude that for any $h > 0$ the estimate

$$\big\|P_s^n\big\|_{X\leftarrow X} \le C, \qquad 0 \le nh \le T, \tag{4.1}$$

holds true on finite time intervals with constant $C > 0$ depending on $T$ but not on $n$ and $h$.

We next deduce a suitable bound for the defects. Regarding the expansion given in Lemma 1 and using that the order conditions (3.20) are fulfilled, it remains to estimate the remainder. By means of (2.3), we obtain

$$\begin{aligned}\big\|R_{p+1}^{(1)}\big\|_X &\le \int_{\Delta_{p+1}} \prod_{j=1}^{p+1} \Big(\big\|\mathrm{e}^{(\tau_{k-j}-\tau_{k-j+1})A}\big\|_{X\leftarrow X}\, \|B\|_{X\leftarrow X}\Big)\\ &\qquad \times \big\|\mathrm{e}^{(t_{n-1}+\tau_{p+1})(A+B)}\big\|_{X\leftarrow X}\, \big\|u(0)\big\|_X\, \mathrm{d}\tau\\ &\le C\, h^{p+1}\, \big\|u(0)\big\|_X;\end{aligned}$$

set $|\mu| = 0$ in (3.17). In a similar manner, it follows that

$$\big\|R_{p+1}^{(2)}\big\|_X \le C\, h^{p+1} \big\|u(0)\big\|_X.$$

Hypothesis 3, together with (2.3), implies

$$\big\|\varrho_{k,p-k+1}(\tau)\big\|_{X\leftarrow X_{\vartheta_k}} \le C \sum_{|\mu|=p-k+1} \frac{\tau^\mu}{\mu!}, \qquad \vartheta_k = \frac{p-k+1}{2}\,. \tag{4.2}$$

Thus, by means of (3.17), we obtain

$$\begin{aligned}&\Big(\int_{\Delta_k} \big\|\varrho_{k,p-k+1}(\tau)\big\|_{X\leftarrow X_{\vartheta_k}}\, \mathrm{d}\tau + h^k \sum_{\lambda\in\Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} |b_{\lambda_\ell}|\, \big\|\varrho_{k,p-k+1}(c_\lambda h)\big\|_{X\leftarrow X_{\vartheta_k}}\Big)\\ &\qquad \times \big\|\mathrm{e}^{t_{n-1}(A+B)}\big\|_{X_{\vartheta_k}\leftarrow X_{\vartheta_k}}\, \big\|u(0)\big\|_{X_{\vartheta_k}}\\ &\quad \le C\, h^{p+1}\, \big\|u(0)\big\|_{X_{\vartheta_k}}.\end{aligned}$$

Employing the reasonable assumption

$$\|v\|_{X_\vartheta} \leq \|v\|_{X_{\widetilde{\vartheta}}}, \qquad \vartheta \leq \widetilde{\vartheta}, \quad v \in X_{\widetilde{\vartheta}}, \tag{4.3}$$

this finally gives the bound

$$\big\|R_{p+1}^{(3)}\big\|_X \leq C\, h^{p+1}\, \big\|u(0)\big\|_{X_{p/2}}.$$

From the above considerations, we obtain the following estimate for the defect:

$$\big\|d_n\big\|_X = \big\|R_{p+1}\big\|_X \leq C\, h^{p+1} \big\|u(0)\big\|_{X_{p/2}};$$

see also Lemma 1, (3.20), and (4.3). With the help of (4.1), it is now straightforward to estimate the global error; see (2.10). Altogether, we obtain

$$\begin{aligned} \big\|e_n\big\|_X &\leq \big\|P_s^n\big\|_{X\leftarrow X}\, \big\|e_0\big\|_X + \sum_{j=0}^{n-1} \big\|P_s^{n-j-1}\big\|_{X\leftarrow X}\, \big\|d_{j+1}\big\|_X \\ &\leq C\, \big\|e_0\big\|_X + C\, h^p\, \big\|u(0)\big\|_{X_{p/2}}, \qquad 0 \leq nh \leq T, \end{aligned}$$

with constant $C > 0$ depending in particular on $T$. ◻

In the present situation, as seen in the proof of Theorem 1, general exponential splitting methods remain stable for any choice of the time stepsize $0 < h \leq T$; however, for evolutionary Schrödinger equations (1.1) involving a time-dependent or solution-dependent operator $B$, in general, a stepsize restriction is expected; see [9, 14].

The above error bound implies that the example methods given in section 3.2 retain their convergence orders when applied to time-dependent Schrödinger equations subject to a periodic boundary condition, provided that the data are sufficiently differentiable. For less regular initial values, the following convergence result holds true; order reduction phenomena for the Strang splitting are also studied in [11, 13].

Corollary 1. *Under the assumptions of Theorem* 1, *whenever* $u(0) \in X_{k/2}$ *but* $u(0) \notin X_{(k+1)/2}$ *for some* $1 \leq k \leq p-1$, *the error bound*

$$\big\|u_n - u(t_n)\big\|_X \leq C\, \big\|u(0) - u_0\big\|_X + C\, h^k\, \big\|u(0)\big\|_{X_{k/2}}, \qquad 0 \leq nh \leq T,$$

*is valid with constant* $C > 0$ *depending on* $T$ *but not on* $n$ *and* $h$.

We note that the above convergence analysis also applies to equations involving a differential operator of higher order; in this case, the relation between the quantities $\vartheta, \widetilde{\vartheta}$ arising in Hypothesis 3 has to be adapted.

**4.2. Numerical example.** We next illustrate the error bound of Theorem 1 by a numerical example for a time-dependent linear Schrödinger equation. In the present paper, we do not recapitulate how the obtained results for abstract differential equations are applicable to pseudospectral discretizations of time-dependent linear Schrödinger equations; in this respect and for a more detailed description of the realization of the numerical example, we refer the reader to Jahnke and Lubich [11, sect. 3].

As test problem, we consider (2.7) with $V(x) = 1 - \cos x$; in order to study numerically the influence of the initial value on the temporal convergence order of an exponential operator splitting method, we choose various initial data that correspond to $u(0) \in X_{k/2}$ for $2 \leq k \leq 6$. The initial-boundary value problem is discretized in space by the Fourier pseudospectral method with $M = 2^{13}$ gridpoints.

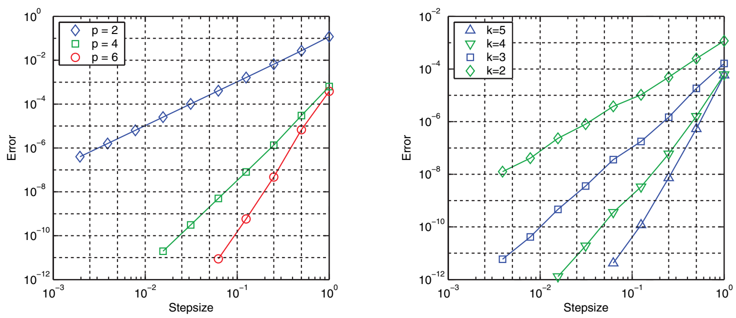


FIG. 4.1. *Numerically observed convergence orders of exponential operator splitting methods. Schemes of various orders (left picture). Initial values of various regularity (right picture).*

For a sufficiently regular initial value, i.e., $k = 6$, we apply the second-order Strang splitting and the fourth- and sixth-order schemes proposed by Blanes and Moan [3] for various time stepsizes (see section 3.3); a reference solution at final time $T = 1$ is computed by the sixth-order splitting method with stepsize $h = 2^{-11}$. The obtained temporal errors, displayed in Figure 4.1 (left picture), confirm the assertion of Theorem 1; the splitting methods retain their convergence orders for time-dependent Schrödinger equations.

For less regular initial values, the order reduction predicted by Corollary 1 is also observed numerically; for the sixth-order scheme the numerical convergence orders are displayed in Figure 4.1 (right picture).

**Appendix A.** In this appendix, we state the coefficients $\alpha_\lambda$, $\lambda \in \Lambda_k$ (see Table A.1), and further specify the conditions (3.20) for $1 \le k \le p = 4$:

$$\text{(A.1a)} \qquad \sum_{\ell=1}^{s} a_\ell = 1, \qquad \sum_{\lambda_1=1}^{s} b_{\lambda_1} = 1,$$

$$\text{(A.1b)} \qquad \sum_{\lambda_1=1}^{s} b_{\lambda_1} c_{\lambda_1} = \frac{1}{2}, \qquad \sum_{\lambda_1=1}^{s} \frac{1}{2} b_{\lambda_1}^2 + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} = \frac{1}{2},$$

TABLE A.1
*Coefficients* $\alpha_{\lambda_\kappa} = \alpha_{\lambda_{\kappa_1}\lambda_{\kappa_2}\cdots\lambda_{\kappa_k}}$ *for* $\kappa = (\kappa_1, \kappa_2, \dots, \kappa_k)$.

| $k$ | $\kappa$ | $\alpha_{\lambda_\kappa}$ |
|---|---|---|
| 1 | 1 | 1 |
| 2 | 11 | 1/2 |
| | 12 | 1 |
| 3 | 111 | 1/6 |
| | 112,122 | 1/2 |
| | 123 | 1 |
| 4 | 1111 | 1/24 |
| | 1112,1222 | 1/6 |
| | 1122 | 1/4 |
| | 1123,1223,1233 | 1/2 |
| | 1234 | 1 |

$$\sum_{\lambda_1=1}^{s} b_{\lambda_1} c_{\lambda_1}^2 = \frac{1}{3},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{2} b_{\lambda_1}^2 c_{\lambda_1} + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} c_{\lambda_1} = \frac{1}{3},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{2} b_{\lambda_1}^2 c_{\lambda_1} + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} c_{\lambda_2} = \frac{1}{6},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{6} b_{\lambda_1}^3 + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \frac{1}{2} b_{\lambda_1} b_{\lambda_2} (b_{\lambda_1} + b_{\lambda_2}) + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} b_{\lambda_1} b_{\lambda_2} b_{\lambda_3} = \frac{1}{6},$$

$$\sum_{\lambda_1=1}^{s} b_{\lambda_1} c_{\lambda_1}^3 = \frac{1}{4},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{2} b_{\lambda_1}^2 c_{\lambda_1}^2 + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} c_{\lambda_1}^2 = \frac{1}{4},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{2} b_{\lambda_1}^2 c_{\lambda_1}^2 + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} c_{\lambda_1} c_{\lambda_2} = \frac{1}{8},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{2} b_{\lambda_1}^2 c_{\lambda_1}^2 + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} c_{\lambda_2}^2 = \frac{1}{12},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{6} b_{\lambda_1}^3 c_{\lambda_1} + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \frac{1}{2} b_{\lambda_1} b_{\lambda_2} c_{\lambda_1} (b_{\lambda_1} + b_{\lambda_2})$$
$$+ \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} b_{\lambda_1} b_{\lambda_2} b_{\lambda_3} c_{\lambda_1} = \frac{1}{8},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{6} b_{\lambda_1}^3 c_{\lambda_1} + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \frac{1}{2} b_{\lambda_1} b_{\lambda_2} (b_{\lambda_1} c_{\lambda_1} + b_{\lambda_2} c_{\lambda_2})$$
$$+ \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} b_{\lambda_1} b_{\lambda_2} b_{\lambda_3} c_{\lambda_2} = \frac{1}{12},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{6} b_{\lambda_1}^3 c_{\lambda_1} + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \frac{1}{2} b_{\lambda_1} b_{\lambda_2} c_{\lambda_2} (b_{\lambda_1} + b_{\lambda_2}) + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} b_{\lambda_1} b_{\lambda_2} b_{\lambda_3} c_{\lambda_3} = \frac{1}{24},$$

$$\sum_{\lambda_1=1}^{s} \frac{1}{24} b_{\lambda_1}^4 + \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} b_{\lambda_1} b_{\lambda_2} \left( \frac{1}{6} b_{\lambda_1}^2 + \frac{1}{4} b_{\lambda_1} b_{\lambda_2} + \frac{1}{6} b_{\lambda_2}^2 \right)$$
$$+ \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} \frac{1}{2} b_{\lambda_1} b_{\lambda_2} b_{\lambda_3} (b_{\lambda_1} + b_{\lambda_2} + b_{\lambda_3})$$
$$+ \sum_{\lambda_1=1}^{s} \sum_{\lambda_2=1}^{\lambda_1-1} \sum_{\lambda_3=1}^{\lambda_2-1} \sum_{\lambda_4=1}^{\lambda_3-1} b_{\lambda_1} b_{\lambda_2} b_{\lambda_3} b_{\lambda_4} = \frac{1}{24}.$$

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