Convergence analysis of high-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear Schrödinger equations

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This work is devoted to the derivation of a convergence result for high-order commutator-free quasi-Magnus (CFQM) exponential integrators applied to non-autonomous linear Schrödinger equations; a detailed stability and local error analysis is provided for the relevant special case, where the Hamilton operator comprises the Laplacian and a regular space-time-dependent potential. In the context of non-autonomous linear ordinary differential equations, CFQM exponential integrators are composed of exponentials involving linear combinations of certain values of the associated time-dependent matrix; this approach extends to non-autonomous linear evolution equations given by unbounded operators. An inherent advantage of CFQM exponential integrators over other time integration methods such as Runge–Kutta methods or Magnus integrators is that structural properties of the underlying operator family affecting stability are well-preserved; this characteristic is confirmed by a theoretical analysis ensuring unconditional stability in the underlying Hilbert space and the full order of convergence under low regularity requirements on the initial state. Due to the fact that convenient tools for products of matrix exponentials such as the Baker–Campbell–Hausdorff formula involve infinite series and thus cannot be applied in connection with unbounded operators, a certain complexity in the investigation of higher-order CFQM exponential integrators for Schrödinger equations is related to an appropriate treatment of compositions of evolution operators; an effective concept for the derivation of a local error expansion relies on suitable linearisations of the evolution equations for the exact and numerical solutions, representations by the variation-of-constants formula, and Taylor series expansions of parts of the integrands, where the arising iterated commutators determine the regularity requirements on the problem data.

Keywords: Non-autonomous linear evolution equations, Schrödinger equations, Quantum systems, Time integration methods, Exponential integrators, Magnus integrators, Commutator-free quasi-Magnus exponential integrators, Stability, Local error, Convergence

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1. Introduction

Commutator-free quasi-Magnus exponential integrators. Numerical experiments for non-autonomous linear differential equations confirm the favourable stability and error behaviour of exponential methods based on the Magnus expansion in comparison with classical time integration methods, see for instance Blanes, Casas, Oteo, Ros (2009); Blanes, Moan (2006); Hochbruck, Lubich (2003); Iserles, Kropielnicka, Singh (2018) and references given therein; however, in the context of large-scale applications, it is advantageous to avoid the actual computation and storage of commutators. As illustrated in Alvermann, Fehske (2011); Alvermann, Fehske, Littlewood (2012); Bader, Blanes, Kopylov (2018); Blanes, Casas, Thalhammer (2017), the replacement of a single matrix exponential involving iterated commutators by compositions of matrix exponentials leads to numerical approximations that are potentially superior to those obtained by standard Magnus integrators; we refer to this type of time integration methods as commutator-free quasi-Magnus (CFQM) exponential integrators.

In our former works Blanes, Casas, Thalhammer (2017, 2018), the focus is on the study of CFQM exponential integrators applied to dissipative quantum systems or partial differential equations of parabolic type, respectively; during the development of these contributions, we also performed numerical tests for Hamiltonian systems and Schrödinger equations. Our comparisons confirmed the excellent behaviour of CFQM exponential integrators and motivated further theoretical investigations.

Stability and error analysis. In the present work, our objective is the derivation of a convergence result for high-order CFQM exponential integrators in the context of non-autonomous linear Schrödinger equations; we thereby proceed and complete the investigations in Blanes, Casas, Thalhammer (2017, 2018) on the design, numerical comparison, and convergence analysis of CFQM exponential integrators for ordinary and partial differential equations of parabolic type. For the sake of concretion, we provide a detailed stability and local error analysis for the relevant special case, where the Hamilton operator comprises the Laplacian and a regular space-time-dependent potential.

For non-autonomous linear ordinary differential equations, CFQM exponential integrators are composed of exponentials involving linear combinations of certain values of the associated time-dependent matrix; it is straightforward to extend this approach to non-autonomous linear evolution equations that are defined by unbounded operators. Concerning stability, an inherent advantage of CFQM exponential integrators over other classes of time integration methods such as Runge–Kutta methods or standard Magnus integrators is that structural properties of the underlying operator family are well-preserved; this characteristic is confirmed by our theoretical analysis, which implies unconditional stability in the underlying Hilbert space and the full order of convergence under low regularity requirements on the initial state.

Convenient tools for analysing products of matrix exponentials such as the Baker–Campbell–Hausdorff formula involve infinite series and thus cannot be applied in connection with unbounded operators; consequently, a certain complexity in the local error analysis of higher-order CFQM exponential integrators for Schrödinger equations is related to an appropriate treatment of compositions of evolution operators. We explore an effective approach that relies on suitable linearisations of the evolution equations satisfied by the exact and numerical solutions, representations by the variation-of-constants formula, and Taylor series expansions of parts of the integrands; under sufficient regularity requirements on the initial state and the space-time-dependent potential, boundedness of the arising iterated commutators and well-definedness of the resulting local error expansion is ensured.

Outline. The present manuscript has the following structure. In Section 2, we formulate non-
autonomous linear Schrödinger equations as abstract evolution equations on Hilbert spaces and specify fundamental assumptions on the defining Hamilton operators. In Section 3, we introduce CFQM exponential integrators and recapitulate second-order and fourth-order example methods. In Section 4, we provide a detailed stability and local error analysis for the special case, where the Schrödinger equation is given by the Laplacian and a regular space-time-dependent potential. In Section 5, we indicate the extension to the general case.

2. Class of evolution equations

Analytical framework. Our analytical framework for a convergence analysis of CFQM exponential integrators applied to Schrödinger equations relies on the theory of self-adjoint operators on Hilbert spaces; for a comprehensive treatment of basic mathematical means and the principles of quantum theory, we refer to Bangaarts (2015); Engel, Nagel (2000).

Evolution equation. We study the initial value problem for a non-autonomous linear evolution equation of Schrödinger type, cast into the abstract form

\[
\begin{align*}
\begin{cases}
    u'(t) = A(t) u(t) = i H(t) u(t) , & t \in (t_0, T), \\
    u(t_0) \text{ given};
\end{cases}
\end{align*}
\]  

(2.1a)

throughout, we employ the fundamental assumption that the arising time-dependent Hamilton operator is self-adjoint on the underlying Hilbert space

\[
H(t) : \mathcal{D} \subset \mathcal{H} \rightarrow \mathcal{H}, \quad t \in [t_0, T],
\]  

(2.1b)

and that the associated evolution operator is unitary

\[
u(t) = \mathcal{E}(t - t_0, t_0) u(t_0), \quad \| \mathcal{E}(t - t_0, t_0) \|_{\mathcal{H} \rightarrow \mathcal{H}} = 1, \quad t \in [t_0, T].
\]  

(2.1c)

Unitarity. For a regular solution to (2.1a), differentiation with respect to time confirms (2.1c); indeed, with the help of the chain rule and due to the required self-adjointness of the Hamilton operator, the following relations implying the unitarity of the evolution operator are obtained

\[
\begin{align*}
\frac{d}{dt} \| u(t) \|^2_{\mathcal{H}} &= 2 \Re \langle u'(t) | u(t) \rangle_{\mathcal{H}} = 2 \Re \langle i H(t) u(t) | u(t) \rangle_{\mathcal{H}} = 0, \quad t \in (t_0, T), \\
\| u(t) \|^2_{\mathcal{H}} &= \| u(t_0) \|^2_{\mathcal{H}}, \quad t \in [t_0, T].
\end{align*}
\]  

(2.2)

Applications. In view of concrete applications, we primarily study the relevant special case, where the arising Hamilton operator comprises the Laplacian and a space-time-dependent potential, see Section 4; in this situation, it is natural to consider square-integrable complex-valued functions that are defined on the Euclidean space or on a cartesian product of bounded intervals, respectively. That is, the underlying Hilbert space is given by a Lebesgue space

\[
\mathcal{H} = L_2(\Omega, \mathbb{C}), \quad \Omega \subseteq \mathbb{R}^d,
\]

and the common domain of the defining operator family is related to a subspace of a Sobolev space

\[
\mathcal{D} \subseteq H^2(\Omega, \mathbb{C}) = W^2_2(\Omega, \mathbb{C}).
\]

We point out that in the context of Schrödinger equations generally no additional consistency conditions have to be taken into account.
3. Class of time integration methods

**CFQM exponential integrators.** Our main objective is to provide a rigorous convergence analysis for commutator-free quasi-Magnus (CFQM) exponential integrators applied to evolution equations of Schrödinger type (2.1). As standard in a time-stepping approach, we choose time grid points with corresponding time stepsizes and determine approximations to the exact solution values by recurrence

\[ t_0 < \cdots < t_n < \cdots < t_N = T, \quad \tau_n = t_{n+1} - t_n, \]

\[ u_{n+1} = \mathcal{S}(\tau_n, t_n) u_n \approx u(t_{n+1}) = \mathcal{S}(\tau_n, t_n) u(t_n), \quad n \in \{0, 1, \ldots, N-1\}; \tag{3.1a} \]

for a CFQM exponential integrator, the numerical evolution operator is given by the composition of several exponentials that involve linear combinations of certain values of the defining operator

\[ B_j(\tau_n, t_n) = \sum_{k=1}^{K} a_{jk} A(t_n + c_k \tau_n), \quad j \in \{1, \ldots, J\}, \]

\[ \mathcal{S}(\tau_n, t_n) = \prod_{j=1}^{J} e^{\alpha_j B_j(\tau_n, t_n)}, \quad \mathcal{S}(\tau_n, t_n) = e^{\alpha B_1(\tau_n, t_n)}, \quad n \in \{0, 1, \ldots, N-1\}. \tag{3.1b} \]

A proper choice of the underlying quadrature nodes

\[ c_k \in [0, 1], \quad k \in \{1, \ldots, K\}, \tag{3.1c} \]

and of the associated real method coefficients

\[ a_{jk} \in \mathbb{R}, \quad b_j = \sum_{k=1}^{K} a_{jk}, \quad j \in \{1, \ldots, J\}, \quad k \in \{1, \ldots, K\}, \tag{3.1d} \]

permits to attain the desired order of consistency \( p \in \mathbb{N}_{\geq 1} \); that is, in the context of nonstiff nonautonomous linear ordinary differential equations with associated families of regular time-dependent matrices, an expansion of the local error in the first step with respect to the time stepsize leads to a relation of the form

\[ \mathcal{L}(\tau_0, t_0) = \mathcal{S}(\tau_0, t_0) - \mathcal{S}(\tau_0, t_0) = \mathcal{O}\left(\tau_0^{p+1}\right). \]

**Examples.** The simplest instance of a second-order CFQM exponential integrator (3.1) is the exponential midpoint rule

\[ p = 2, \quad J = K = 1, \quad c_1 = \frac{1}{2}, \quad a_{11} = b_1 = 1, \]

\[ \mathcal{S}(\tau_n, t_n) = e^{\alpha A(t_n + \frac{1}{2} \tau_n)}, \quad n \in \{0, 1, \ldots, N-1\}. \tag{3.2} \]

The two-stage Gaussian quadrature rule leads to a canonical fourth-order CFQM exponential integrator

\[ p = 4, \quad J = K = 2, \quad \alpha = \sqrt{\beta}, \quad c_1 = \frac{1}{2} - \alpha, \quad c_2 = \frac{1}{2} + \alpha, \]

\[ a_{11} = a_{22} = \frac{1}{4} + \alpha, \quad a_{12} = a_{21} = \frac{1}{4} - \alpha, \quad b_1 = a_{11} + a_{12} = b_2 = a_{21} + a_{22} = \frac{1}{2}, \]

\[ B_j(\tau_n, t_n) = a_{1j} A(t_n + c_1 \tau_n) + a_{2j} A(t_n + c_2 \tau_n), \quad j \in \{1, 2\}, \]

\[ \mathcal{S}(\tau_n, t_n) = e^{\alpha_j B_2(\tau_n, t_n)} e^{\alpha_j B_1(\tau_n, t_n)}, \quad n \in \{0, 1, \ldots, N-1\}. \tag{3.3} \]

For additional examples and detailed information on order conditions, we refer to Blanes, Casas, Thalhammer (2017, 2018).
Stability. Within the analytical framework introduced in Section 2, Stone’s Theorem implies that any one-parameter group generated by the defining time-dependent linear operator is unitary on the underlying Hilbert space, i.e.

\[
\| e^{\sigma A(t)} \|_{\mathcal{H}^\rightarrow \mathcal{H}} = 1, \quad \sigma \in \mathbb{R}, \quad t \in [t_0, T],
\]

see Engel, Nagel (2000). By means of this fundamental result, we prove that time integration methods of the format (3.1) and in particular the schemes (3.2) and (3.3) are unconditionally stable, in accordance with the characteristics of the exact evolution operator (2.1), see Section 4.2.

Remark. It is natural to compare CFQM exponential integrators of the form (3.1) to Magnus integrators, which are given by a single exponential involving iterated commutators of certain values of the defining operator, see Blanes, Casas, Oteo, Ros (2009); Blanes, Moan (2006); Hochbruck, Lubich (2003); Iserles, Kro{"p}elnicka, Singh (2018) and references given therein. For both classes of methods, it is ensured that the numerical evolution operator is unitary and hence preserves fundamental properties of the exact evolution operator associated with a Schrödinger equation. As indicated before, for CFQM exponential integrators, this result relies on an application of Stone’s Theorem; for a Magnus integrator, it is used that the commutator is hermitian, which in essence follows from the required self-adjointness of the Hamilton operator

\[
\begin{align*}
\left[ [A(s), A(t)] \right] v \big| w \big)_{\mathcal{H}} &= \left( (A(s) A(t) - A(t) A(s)) v \big| w \right)_{\mathcal{H}} = - \left( H(s) H(t) v \big| w \right)_{\mathcal{H}} + \left( H(t) H(s) v \big| w \right)_{\mathcal{H}} \\
&= - \left( H(t) v \big| H(s) w \right)_{\mathcal{H}} + \left( H(s) v \big| H(t) w \right)_{\mathcal{H}} = - \left( v \big| H(t) H(s) w \right)_{\mathcal{H}} + \left( v \big| H(s) H(t) w \right)_{\mathcal{H}} \\
&= \left( v \big| (A(t) A(s) - A(s) A(t)) w \right)_{\mathcal{H}} = - \left( v \big| [A(s), A(t)] w \right)_{\mathcal{H}}.
\end{align*}
\]

However, a basic difference between CFQM exponential integrators and Magnus integrators concerns well-definedness and stability. An inherent advantage of CFQM exponential integrators is that the linear combinations arising in (3.1) preserve the structure of the underlying operator family, and this is reflected in a favourable stability behaviour; contrary, the stability of higher-order Magnus integrators is only ensured in a spatially semi-discrete setting and under major stepsize restrictions, see Hochbruck, Lubich (2003).

Schrödinger versus parabolic equations. In order to ensure the stability of CFQM exponential integrators for non-autonomous linear evolution equations of Schrödinger type, we have to restrict ourselves to schemes involving real coefficients. In the context of dissipative quantum systems and parabolic evolution equations, however, it is of interest to study and design CFQM exponential integrators with complex method coefficients, see Blanes, Casas, Thalhammer (2017, 2018).

4. Special case

Situation. In this section, we focus on non-autonomous linear Schrödinger equations, where the Hamilton operator is given by the Laplacian with respect to the spatial variables and a regular real-valued space-time-dependent potential acting as multiplication operator

\[
H(t) = \Delta + V(t), \quad V(t) = V(\cdot, t) : \Omega \rightarrow \mathbb{R}, \quad t \in [t_0, T];
\]

in view of the abstract formulation (2.1), we again suppress the space dependence. The consideration of this special case is of relevance in applications, see Bader, Blanes, Kopylov (2018); Hochbruck, Lubich (2003); Iserles, Kro{"p}elnicka, Singh (2018) and references given therein.
Assume that the considered non-autonomous linear Schrödinger equation (2.1) is defined
by a Hamilton operator of the special structure (4.1). Provided that the arising real-valued space-time-
dependent potential and the prescribed initial state fulfill suitable regularity requirements such that

\[ L = H^m(\Omega, \mathbb{C}) = W^{2m}_0(\Omega, \mathbb{C}), \quad m \in \mathbb{N}_{\geq 0}, \]

\[ \| G \|_{W^{\ell,m}([t_0,T], \mathbb{K})} = \max_{j \geq 1} \| G^{(j)}(t) \|_{L^\infty([t_0,T], W^{\ell,m}_0(\Omega, \mathbb{K}))}, \quad \ell, m \in \mathbb{N}_{\geq 0}, \]

where \( \mathbb{K} = \mathbb{R} \) or \( \mathbb{K} = \mathbb{C} \), respectively; evidently, \( H^0 \) coincides with the underlying Lebesgue space
\( L = L_2(\Omega, \mathbb{C}) \).

4.1 Convergence result

Theoretical result. In the following, we state a theoretical result, which confirms the favourable
convergence behaviour of CFQM exponential integrators for evolution equations of Schrödinger type;
compared to other classes of time integration methods, stability is ensured without any restriction on the
time stepsizes, and the full order of convergence is obtained under low regularity requirements on the
initial state.

Theorem 1 Assume that the considered non-autonomous linear Schrödinger equation (2.1) is defined
by a Hamilton operator of the special structure (4.1). Provided that the arising real-valued space-time-
dependent potential and the prescribed initial state fulfill suitable regularity requirements such that

\[ C_V = \max_{\ell \in \{1, \ldots, p\}} \| V \|_{W^{\ell/2,p-1}([t_0,T], \mathbb{R})} < \infty, \quad \| u(t_0) \|_{L^p} < \infty, \]

any \( p \)-th order CFQM exponential integrator (3.1) satisfies a global error estimate of the form

\[ \| u_N - u(T) \|_{H^m} \leq \| u_0 - u(t_0) \|_{H^m} + C_C \tau_{\text{max}}^p \| u(t_0) \|_{L^p} \]

\[ \tau_{\text{max}} = \max \{ \tau_n : n \in \{0, 1, \ldots, N-1\} \}; \]

the arising constant depends on an upper bound for the time stepsizes, the length of the considered time
interval \([t_0, T]\), the bound \( C_V \), and the method coefficients, but it is independent of the number of time
steps \( n \) and the actual time stepsizes.

Proof. Our proof relies on stability bounds and local error estimates, which we deduce in the subsequent
Sections 4.2 and 4.3. The constant arising in (4.19) in particular depends on bounds for certain space and
time derivatives of the potential on the interval \([t_0, t_{n+1}]\), where \( n \in \{0, 1, \ldots, N-1\} \); estimation by \( C_V \)
leads to a constant that is independent of \( n \in \{0, 1, \ldots, N-1\} \). Similarly, we estimate the constant
in (4.2) by a constant that depends on the length of the time interval \([t_0, T]\) and the uniform bound \( C_V \).

In order to relate the global error to local errors, we employ the telescopic identity

\[ u_N - u(T) = \prod_{n=0}^{N-1} \mathcal{F}(\tau_n, t_n) \left( u_0 - u(t_0) \right) \]

\[ + \sum_{n=0}^{N-1} \prod_{\nu=n+1}^{N-1} \mathcal{F}(\tau_\nu, t_\nu) \left( \mathcal{F}(\tau_n, t_n) - \mathcal{F}(\tau_\nu, t_\nu) \right) \mathcal{F}(t_\nu - t_0, t_0) u(t_0); \]

due to the fact that the numerical evolution operator associated with a CFQM exponential integrator
involving real coefficients is unitary

\[ \| \mathcal{F}(\tau_n, t_n) \|_{H^m \rightarrow H^m} = 1, \quad n \in \{0, 1, \ldots, N-1\}, \]

\[ \| \mathcal{F} \|_{L_2(\Omega, \mathbb{C})} = 1. \]
see (4.3), straightforward estimation in the underlying Hilbert space yields
\[ \| u_N - u(T) \|_{\mathcal{H}^p} \leq \| u_0 - u(t_0) \|_{\mathcal{H}^p} + \sum_{n=0}^{N-1} \| \mathcal{S}(\tau_n, t_n) - \mathcal{S}(\tau_n, t_n) \|_{\mathcal{H}^p} \mathcal{E}(t_n - t_0, t_0) u(t_0) \|_{\mathcal{H}^p}. \]

In our expansion of the local error operator with respect to the time stepsize, iterated commutators of the Laplacian and the potential up to order \( p - 1 \) arise naturally and lead to an estimate of the form
\[ \| \mathcal{S}(\tau_n, t_n) - \mathcal{S}(\tau_n, t_n) \|_{\mathcal{H}^p} \leq C \tau_n^{p+1}, \quad n \in \{0, 1, \ldots, N-1\}, \]
see (4.19); for this reason, we have to embed the decisive contributions
\[ \{ \mathcal{S}(\tau_n, t_n) - \mathcal{S}(\tau_n, t_n) \} \mathcal{E}(t_n - t_0, t_0) u(t_0), \quad n \in \{0, 1, \ldots, N-1\}, \]
in the Sobolev space \( \mathcal{H}^{p-1} \). Using the stability bound for the exact evolution operator
\[ \| \mathcal{E}(t_n - t_0, t_0) \|_{\mathcal{H}^{p-1}} \leq C, \quad n \in \{0, 1, \ldots, N-1\}, \]
see (4.2) and (4.6), we obtain the relation
\[ \| u_N - u(T) \|_{\mathcal{H}^p} \leq \| u_0 - u(t_0) \|_{\mathcal{H}^p} + C \sum_{n=0}^{N-1} \tau_n^{p+1} \| u(t_0) \|_{\mathcal{H}^{p-1}}, \]
which implies the stated global error estimate. \( \square \)

### 4.2 Stability

**Stability in Sobolev spaces (Exact evolution operator).** The exact solution to the non-autonomous linear Schrödinger equation (2.1) with Hamilton operator given by (4.1) inherits the spatial regularity of the potential and the initial state. As already discussed in Section 2, the evolution operator associated with a self-adjoint Hamilton operator is unitary on the underlying Hilbert space
\[ \| \mathcal{E}(t - t_0, t_0) \|_{\mathcal{H}^m} = 1, \quad t \in [0, T], \]
see (2.1c) and (2.2). Moreover, an estimate of the form
\[ \| \mathcal{E}(t - t_0, t_0) \|_{\mathcal{H}^m} \leq 1 + C_m \left( \mathcal{S}, \| V \|_{\mathcal{H}^m([t_0, T], \Omega, \mathbb{R})} \right)(t - t_0) \leq C, \]
\[ t - t_0 \leq \mathcal{T}, \quad t \in [0, T], \quad m \in \mathbb{N}_{\geq 1}, \]
holds with a constant that depends on an upper bound for the length of the considered time interval and uniform bounds for certain space derivatives of the potential; the form of the bound and in particular the factor \( t - t_0 \) are essential in view of the derivation of an analogous stability bound for compositions of the numerical evolution operator.

In order to exemplify this result, we consider a non-autonomous linear Schrödinger equation in a single space dimension on the unbounded domain
\[ \partial_t \psi(x, t) = i H(x, t) \psi(x, t) = i \left( \partial_x \psi(x, t) + V(x, t) \psi(x, t) \right), \quad (x, t) \in \mathbb{R} \times (t_0, T); \]
the first and second spatial derivatives of the solution
\[ \chi_1 = \partial_x \psi, \quad \chi_2 = \partial_{xx} \psi, \]
satisfy the related evolution equations
\[
R_m(x,t) = \begin{cases} 
\partial_x V(x,t) \psi(x,t) & \text{if } m = 1, \\
2 \partial_x V(x,t) \chi_1(x,t) + \partial_{xx} V(x,t) \psi(x,t) & \text{if } m = 2,
\end{cases} \quad (x,t) \in \mathbb{R} \times (t_0, T).
\]
A representation by means of the variation-of-constants formula together with the application of the unitarity of the evolution operator (2.1c) leads to the estimate
\[
\left\| \chi_1(t) \right\|_{L^2(\Omega,C)} \leq \left\| \chi_1(t_0) \right\|_{L^2(\Omega,C)} + \int_{t_0}^{t} \left\| R_1(s) \right\|_{L^2(\Omega,C)} ds \leq \left\| \chi_1(t_0) \right\|_{L^2(\Omega,C)} + (t - t_0) \left\| \partial_x V \right\|_{L^2(\Omega \times [t_0,t], R)} \sup_{s \in [t_0, t]} \left\| \chi_1(s) \right\|_{L^2(\Omega,C)}
\]
\[
+ (t - t_0) \left( 2 (t - t_0) \left\| \partial_{xx} V \right\|_{L^2(\Omega \times [t_0,t], R)} + \left\| \partial_{xx} V \right\|_{L^2(\Omega \times [t_0,t], R)} \right) \left\| \psi(t_0) \right\|_{L^2(\Omega,C)}, \quad t \in [t_0, T].
\]
Altogether, this yields the following bounds in the associated Sobolev spaces
\[
\left\| \psi(t) \right\|_{H^1(\Omega, C)} \leq \left( 1 + \left\| \partial_x V \right\|_{L^2(\Omega \times [t_0,t], R)} (t - t_0) \right) \left\| \psi(t_0) \right\|_{H^1(\Omega, C)}
\]
\[
\left\| \psi(t) \right\|_{H^2(\Omega, C)} \leq \left( 1 + C_2 \left( \left\| \partial_x V \right\|_{L^2(\Omega \times [t_0,t], R)} \left\| \partial_{xx} V \right\|_{L^2(\Omega \times [t_0,t], R)} (t - t_0) \right) \left\| \psi(t_0) \right\|_{H^2(\Omega, C)}
\]
\[
t - t_0 \leq \tau, \quad t \in [t_0, T],
\]
which are in accordance with (4.2). The extension to higher-order derivatives and higher space dimensions is straightforward.

**Stability in Sobolev spaces (Numerical evolution operator).** Similar considerations permit to deduce a bound for the numerical evolution operator defining a CFQM exponential integrator (3.1); more precisely, provided that the method coefficients are real, the analogous relations
\[
\left\| \mathcal{E} (\tau_n, t_n) \right\|_{\mathcal{W}^m \rightarrow \mathcal{W}^m} = 1,
\]
\[
\left\| \mathcal{E} (\tau_n, t_n) \right\|_{\mathcal{W}^m \rightarrow \mathcal{W}^m} \leq 1 + C_m \left( \left\| \partial_x V \right\|_{L^2(\Omega \times [t_0,t], R)} \left\| \partial_{xx} V \right\|_{L^2(\Omega \times [t_0,t], R)} (t - t_0) \right) \left\| \psi(t_0) \right\|_{H^m(\Omega, C)}, \quad \tau_n \leq \tau, \quad m \in \mathbb{N} \geq 1,
\]
\[n \in \{0,1,\ldots,N-1\}, \quad \text{for } n \geq 1. \]
hold with a constant that depends on an upper bound for the time stepsize, uniform bounds for certain space derivatives of the potential, and the method coefficients. By means of the relation $1 + x \leq e^x$ for $x \geq 0$, we obtain a stability estimate for compositions

$$\left\| \prod_{n=0}^{N-1} \mathcal{J}(\tau_n, t_n) \right\|_{\mathcal{H}^m} \leq \prod_{n=0}^{N-1} e^{C_m(\tau_n, n)} = \left( e^{C_m(\tau_n)} \right)^{n},$$

with constant depending in particular on an upper bound for the time stepsizes, the length of the time space derivatives of the potential, and the method coefficients. By means of the relation $1 + x \leq e^x$ for $x \geq 0$, we obtain a stability estimate for compositions

$$\left\| \prod_{n=0}^{N-1} e^{C_m(\tau_n)} \right\|_{\mathcal{H}^m} \leq e^{C_m(\tau_n)} \leq e^{C_m(\tau_n, n)}(T-t_0) \leq C, \quad \max \{ \tau_n : n \in \{0, 1, \ldots, N-1\} \} \leq T, \quad m \in \mathbb{N} \geq 1,$$

with constant depending in particular on an upper bound for the time stepsizes, the length of the time interval $[t_0, T]$, and uniform bounds for certain space derivatives of the potential.

For a space-time-dependent Hamilton operator of the special structure (4.1), the associated time-independent operators rewrite as

$$B_j(\tau_n, t_n) = \sum_{k=1}^{K} a_{jk} A(t_n + c_k \tau_n) = i \left( b_j + \sum_{k=1}^{K} a_{jk} V(t_n + c_k \tau_n) \right),$$

$$j \in \{1, \ldots, J\}, \quad n \in \{0, \ldots, N-1\}.$$

If $a_{jk} \in \mathbb{R}$ for any $(j, k) \in \{1, \ldots, J\} \times \{1, \ldots, K\}$, Stone’s Theorem ensures unitarity of the arising evolution operators with respect to the norm of the underlying Lebesgue space

$$\left\| e^{\sigma B_j(\tau_n, t_n)} \right\|_{\mathcal{H}^{\sigma+\mathcal{H}}} = 1, \quad \sigma \in \mathbb{R}, \quad j \in \{1, \ldots, J\}, \quad n \in \{0, \ldots, N-1\},$$

and thus unconditional stability of the numerical method follows

$$\left\| \mathcal{J}(\tau_n, t_n) \right\|_{\mathcal{H}^{\sigma+\mathcal{H}}} = 1, \quad n \in \{0, \ldots, N-1\},$$

see also (3.4) and compare with (4.2). Slight modifications of the arguments used in the exemplification of (4.2) imply the validity of the following estimate on bounded time intervals

$$\left\| e^{\sigma B_j(\tau_n, t_n)} \right\|_{\mathcal{H}^{\sigma+\mathcal{H}}} \leq 1 + C_m(\tau_n) \left\| V \right\|_{\mathcal{H}^{\sigma+\mathcal{H}}} \leq e^{C_m(\tau_n, n)} \leq e^{C_m(\tau_n, n)}(T-t_0) \leq C, \quad \max \{ \tau_n : n \in \{0, 1, \ldots, N-1\} \} \leq T, \quad m \in \mathbb{N} \geq 1,$$

and justify the stated result (4.3).

4.3 Local error

**Approach.** In the following, we deduce suitable local error expansions for CFQM exponential integrators (3.1) applied to (2.1), making use of the special structure of the Hamilton operator (4.1). A certain complexity in the treatment of higher-order schemes concerns the correct handling of the arising product of exponentials, since tools that are helpful for matrix exponentials such as the Baker–Campbell–Hausdorff (BCH) formula involve infinite series and thus cannot be applied in the context of unbounded operators. Our approach in the spirit of LUNARDI (1995) relies on linearisations of the evolution equations for the exact and numerical solutions as well as representations by the variation-of-constants formula; together with Taylor series expansions of parts of the integrands and bounds for naturally arising iterated commutators, the stated result is obtained.
Fourth-order scheme. Due to the fact that the treatment of a general high-order CFQM exponential integrator would involve a considerable amount of technicalities, we provide a rigorous derivation of the local error expansion for the fourth-order scheme based on two Gaussian nodes, see (3.1) and (3.3); it suffices to study the error of (3.3) in the first time step

$$\tau = \tau_0 > 0, \quad \mathcal{L}(\tau, t_0) = \mathcal{L}(\tau, t_0) - \mathcal{E}(\tau, t_0), \quad \mathcal{L}(\tau, t_0) = e^{\mathcal{E}B_2(\tau t_0)} e^{\mathcal{E}B_1(\tau t_0)},$$

$$B_j(\tau, t_0) = i \left( b_j A + a_{j1} V(t_0 + c_1 \tau) + a_{j2} V(t_0 + c_2 \tau) \right), \quad j \in \{1, 2\},$$

$$\alpha = \frac{\sqrt{3}}{6}, \quad c_1 = \frac{1}{2} - \alpha, \quad c_2 = \frac{1}{2} + \alpha,$$

$$a_{11} = a_{22} = \frac{1}{4} + \alpha, \quad a_{12} = a_{21} = \frac{1}{4} - \alpha, \quad b_1 = a_{11} + a_{12} = b_2 = a_{21} + a_{22} = \frac{1}{2}.$$

Simplified notation. Henceforth, we specify the arising bounds for space and time derivatives of the potential, but we suppress the dependence of constants on upper bounds for the time stepsize; this slightly simplified notation is also justified by practical implementations, where commonly $\tau \in (0, 1)$. For instance, we use that the relation

$$1 + C_m \left( \frac{1}{\tau} \left| V \right|_{\mathcal{W}^{0, m}([t_0, t_0 + \tau]; \Omega, \mathbb{R})} \right) \tau \leq C_m \left( \left| V \right|_{\mathcal{W}^{0, m}([t_0, t_0 + \tau]; \Omega, \mathbb{R})} \right)$$

is valid with generic constant, see (4.2) and (4.3).

Auxiliary abbreviations and estimates. In view of linearisations of the underlying evolution equations for the exact and numerical solutions about the midpoint of the first subinterval and representations by the variation-of-constants formula, we denote

$$\begin{align*}
A_* &= A(t_0 + \frac{\tau}{2}) = i \left( A + V(t_0 + \frac{\tau}{2}) \right), \quad R(t) = A(t) - A_*, \quad t \in [t_0, t_0 + \tau], \\
S_j(\tau, t_0) &= \frac{1}{b_j} B_j(\tau, t_0) - A_* = 2 \left( a_{j1} R(t_0 + c_1 \tau) + a_{j2} R(t_0 + c_2 \tau) \right), \quad j \in \{1, 2\}.
\end{align*}$$

(4.7a)

We make use of the fact that the remainder is determined by values of the potential such that the following auxiliary estimate holds with generic constant

$$R(t) = i \left( V(t) - V(t_0 + \frac{\tau}{2}) \right),$$

$$\left| R(t) \right|_{\mathcal{W}^m \to \mathcal{W}^{m-1}} + \left| S_j(\tau, t_0) \right|_{\mathcal{W}^m \to \mathcal{W}^{m-1}} \leq C_m \left( \left| V \right|_{\mathcal{W}^{0, m}([t_0, t_0 + \tau]; \Omega, \mathbb{R})} \right),$$

$$t \in [t_0, t_0 + \tau], \quad j \in \{1, 2\}, \quad m \in \mathbb{N}_{\geq 0}.$$  

(4.7b)

in certain places, to prove that a term has the correct order with respect to the time stepsize, we instead use an integral representation involving the first time derivative

$$R(t) = i \int_{t_0 + \frac{\tau}{2}}^{t} V'(\zeta) \, d\zeta,$$

$$\left| R(t) \right|_{\mathcal{W}^m \to \mathcal{W}^{m-1}} + \left| S_j(\tau, t_0) \right|_{\mathcal{W}^m \to \mathcal{W}^{m-1}} \leq C_m \left( \left| V \right|_{\mathcal{W}^{1, m}([t_0, t_0 + \tau]; \Omega, \mathbb{R})} \right) \tau,$$

$$t \in [t_0, t_0 + \tau], \quad j \in \{1, 2\}, \quad m \in \mathbb{N}_{\geq 0}.$$  

(4.7c)

Evolution equations and linearisations. The numerical evolution operator associated with (4.5) is composed by two exponentials

$$\mathcal{J}_j(\tau, t_0) = \mathcal{J}_2(\tau, t_0) \mathcal{J}_1(\tau, t_0),$$

$$\mathcal{J}_j(\tau, t_0) = e^{\sigma B_j(t_0)}, \quad \sigma \in \mathbb{R}, \quad j \in \{1, 2\},$$

(4.8a)
which satisfy autonomous linear evolution equations
\[
\frac{d}{ds} \mathcal{G}(\sigma, \tau, t_0) = B_j(\tau, t_0) \mathcal{G}(\sigma, \tau, t_0) = \frac{1}{2} A_x \mathcal{G}(\sigma, \tau, t_0) + \frac{1}{2} S_j(\tau, t_0) \mathcal{G}(\sigma, \tau, t_0),
\]
\[\sigma \in (0, \tau), \quad j \in \{1, 2\}. \tag{4.8b}\]

For the exact evolution operator, we employ the analogous identity
\[
\mathcal{E}(\tau, t_0) = \mathcal{E}(\frac{\tau}{2}, t_0 + \frac{\tau}{2}) \mathcal{E}(\frac{\tau}{2}, t_0)
\]
and make use of the fact that the associated evolution equation rewrites as
\[
\frac{d}{ds} \mathcal{E}(\sigma, \theta_0) = A(\theta_0 + \sigma) \mathcal{E}(\sigma, \theta_0) = A_x \mathcal{E}(\sigma, \theta_0) + R(\theta_0 + \frac{1}{2} \sigma) \mathcal{E}(\frac{1}{2} \sigma, \theta_0),
\]
\[\sigma \in (0, \tau), \quad \theta_0 \in \{t_0, t_0 + \frac{\tau}{2}\}; \tag{4.9b}\]
evidently, a linear transformation yields the equivalent formulation
\[
\frac{d}{ds} \mathcal{E}(\frac{1}{2} \sigma, \theta_0) = \frac{1}{2} A_x \mathcal{E}(\frac{1}{2} \sigma, \theta_0) + \frac{1}{2} R(\theta_0 + \frac{1}{2} \sigma) \mathcal{E}(\frac{1}{2} \sigma, \theta_0),
\]
\[\sigma \in (0, \tau), \quad \theta_0 \in \{t_0, t_0 + \frac{\tau}{2}\}. \tag{4.9c}\]

**Auxiliary initial value problem.** The evolution equations in (4.8) and (4.9) suggest to study the initial value problem
\[
\begin{aligned}
\mathcal{Y}(\sigma, Z_\sigma, z) &= Z_x \mathcal{Y}(\sigma, Z_\sigma, z) + z(\sigma) \mathcal{Y}(\sigma, Z_\sigma, z), \quad \sigma \in (0, \sigma_0), \\
\mathcal{Y}(0, Z_\sigma, z) &= I,
\end{aligned} \tag{4.10a}
\]
and to distinguish the two cases
\[
\begin{aligned}
Z_x &= \frac{1}{2} A_x, \quad z = \frac{1}{2} S_j(\tau, t_0), \quad j \in \{1, 2\}, \quad \sigma_0 = \tau, \\
Z_x &= A_x, \quad z(\sigma) = R(\theta_0 + \sigma), \quad \theta_0 \in \{t_0, t_0 + \frac{\tau}{2}\}, \quad \sigma \in [0, \sigma_0], \quad \sigma_0 = \frac{\tau}{2}; \tag{4.10b}
\end{aligned}
\]
for the sake of clarity, we indicate the dependence of the solution on the defining linear operator and the defining function. Our previous considerations imply relations of the form
\[
\begin{aligned}
\|z(\sigma)\|_{\mathcal{H}^0(\mathcal{A}, \mathcal{R})} &\leq C_m \left( \|V\|_{\mathcal{H}^m(\mathcal{A}, \mathcal{R})} + \|V\|_{\mathcal{H}^m(\mathcal{A}, \mathcal{R})} \right) \tau, \quad m \in \mathbb{N}_{\geq 0}, \\
\|e^{\sigma Z_x}\|_{\mathcal{H}^0(\mathcal{A}, \mathcal{R})} &\leq 1, \quad \|e^{\sigma Z_x}\|_{\mathcal{H}^m(\mathcal{A}, \mathcal{R})} \leq C_m \left( \|V\|_{\mathcal{H}^m(\mathcal{A}, \mathcal{R})} \right), \\
\|\mathcal{Y}(\sigma, Z_\sigma, z)\|_{\mathcal{H}^0(\mathcal{A}, \mathcal{R})} &\leq 1, \quad \|\mathcal{Y}(\sigma, Z_\sigma, z)\|_{\mathcal{H}^m(\mathcal{A}, \mathcal{R})} \leq C_m \left( \|V\|_{\mathcal{H}^m(\mathcal{A}, \mathcal{R})} \right), \quad \sigma, |\sigma_1| \in [0, \sigma_0], \quad m \in \mathbb{N}_{\geq 1}; \tag{4.11}
\end{aligned}
\]
with generic constants, see Section 4.2, and recall (4.6) as well as (4.7).

**Solution representation and first expansion.** In view of (4.5), we deduce a stepwise expansion of the solution to (4.10). Our starting point is a representation based on the variation-of-constants formula
\[
\mathcal{Y}(\sigma_0, Z_\sigma, z) = e^{\sigma Z_x} + \mathcal{Z}_1(\sigma_0, Z_\sigma, z),
\]
\[
\mathcal{Z}_1(\sigma_0, Z_\sigma, z) = \int_{\sigma_0}^{\sigma} e^{(\sigma_0 - \sigma_1) Z_x} z(\sigma_1) \mathcal{Y}(\sigma_1, Z_\sigma, z) \, d\sigma_1, \tag{4.12}
\]
In view of (4.8) and (4.9), we specify the expansion obtained for a twofold product.

**First expansion for product.** In view of (4.8) and (4.9), we specify the expansion obtained for a twofold product

\[
\mathcal{V}(\sigma_0, z_1) \mathcal{V}(\sigma_0, z_2) = \mathcal{J}_2^{(0)}(\sigma_0, z_1, z_2) + \mathcal{J}_2^{(6)}(\sigma_0, z_1, z_2)
\]
For the convenience of the reader, we recall the Taylor series expansion of order the values of the function and its derivatives read as

$$
\mathcal{F}(0)(\sigma_0, Z, z_1, z_2) = e^{\sigma_0 Z} + e^{\sigma_0 Z} \mathcal{F}(2)(\sigma_0, Z, z_2) + \mathcal{F}(2)(\sigma_0, Z, z_1) e^{\sigma_0 Z} \\
+ e^{\sigma_0 Z} \mathcal{F}(4)(\sigma_0, Z, z_2) + \mathcal{F}(4)(\sigma_0, Z, z_1) e^{\sigma_0 Z} \\
+ \mathcal{F}(2)(\sigma_0, Z, z_1) \mathcal{F}(2)(\sigma_0, Z, z_2),
$$

the remainder comprises several terms

$$
\mathcal{R}(6)(\sigma_0, Z, z_1, z_2) = \mathcal{R}(6)(\sigma_0, Z, z_1) \mathcal{H}(\sigma_0, Z, z_2) + \mathcal{H}(4)(\sigma_0, Z, z_1) \mathcal{R}(2)(\sigma_0, Z, z_2) \\
+ \mathcal{H}(2)(\sigma_0, Z, z_1) \mathcal{H}(4)(\sigma_0, Z, z_2) + e^{\sigma_0 Z} \mathcal{H}(6)(\sigma_0, Z, z_2),
$$

which have the desired order with respect to the time step size

$$
\left\| \mathcal{R}(6)(\sigma_0, Z, z_1, z_2) \right\|_{\mathcal{H}^n \to \mathcal{H}} \leq C_0 \left( \left\| V \right\|_{\mathcal{H}^{1.0}}(t_0, t_0 + \tau, \Omega) \right) \tau^6,
$$

see (4.13) and (4.15).

**Taylor series expansion.** With regard to the integrands in (4.14) and (4.16), we perform a Taylor series expansion of a function of the form

$$
g(\sigma) = e^{-\sigma Z} G e^{\sigma Z}, \quad Z_\sigma = \alpha_1 \left( \Delta + V(t_0 + \frac{\tau}{2}) \right), \quad G = \alpha_2 \left( V(t) - V(t_0 + \frac{\tau}{2}) \right),
$$

by means of the following compact notation for iterated commutators

$$
ad_{Z_\sigma}^0 (G) = G, \quad \text{ad}_{Z_\sigma}^1 (G) = \text{ad}_{Z_\sigma} (G) = [G, Z_\sigma] = GZ_\sigma - Z_\sigma G,
$$

$$
ad_{Z_\sigma}^\ell (G) = [\text{ad}_{Z_\sigma}^\ell-1 (G), Z_\sigma], \quad \ell \in \mathbb{N}_{\geq 2},
$$

the values of the function and its derivatives read as

$$
g^{(\ell)}(\sigma) = e^{-\sigma Z_\sigma} \text{ad}_{Z_\sigma}^\ell (G) e^{\sigma Z_\sigma}, \quad \sigma \in \mathbb{R}, \quad \ell \in \mathbb{N}_{\geq 0}.
$$

For the convenience of the reader, we recall the Taylor series expansion of order $m \in \mathbb{N}_{\geq 0}$ with remainder in integral form

$$
g(\sigma) = \sum_{\ell=0}^m \frac{1}{\ell!} (\sigma - \sigma_\sigma)^\ell g^{(\ell)}(\sigma_\sigma) \\
+ \frac{1}{m!} (\sigma - \sigma_\sigma)^m + 1 \int_0^1 (1 - \theta)^m g^{(m+1)}(\sigma + \theta (\sigma - \sigma_\sigma)) d\theta, \quad \sigma, \sigma_\sigma \in \mathbb{R};
$$

the specification to (4.18) leads to the relation

$$
e^{-\sigma Z_\sigma} G e^{\sigma Z_\sigma} = e^{-\sigma Z_\sigma} \left( \sum_{\ell=0}^m \frac{1}{\ell!} (\sigma - \sigma_\sigma)^\ell \text{ad}_{Z_\sigma}^\ell (G) \\
+ \frac{1}{m!} (\sigma - \sigma_\sigma)^m + 1 \int_0^1 (1 - \theta)^m e^{-\theta (\sigma - \sigma_\sigma)} Z_\sigma \text{ad}_{Z_\sigma}^{m+1} (G) e^{\theta (\sigma - \sigma_\sigma)} Z_\sigma d\theta \right) e^{\sigma Z_\sigma}, \quad \sigma \in \mathbb{R}.
Appropriate choices of the center $\sigma_0 \in \mathbb{R}$ are given below.

**Commutators.** In order to characterise the regularity requirements that apply accordingly to the above expansion, it remains to study the principal terms in the iterated commutators; as the extension to higher space dimensions is straightforward, it suffices to consider a single space dimension. A simple calculation shows that the first commutator of the Laplacian and a multiplication operator is given by a first-order differential operator involving coefficients that depend on the first and second derivatives of the multiplication operator; more precisely, we have

$$
\| [\partial_{xx}, V(t)] \|_{L^2(\Omega, \mathbb{C})} \leq 2 \| \partial_{x} V(t) \|_{L^2(\Omega, \mathbb{R})} \| \partial_{xx} V \|_{L^2(\Omega, \mathbb{C})} + \| \partial_{xx} V(t) \|_{L^2(\Omega, \mathbb{R})} \| V \|_{L^2(\Omega, \mathbb{C})}, \\
v \in H^1(\Omega, \mathbb{C}), \quad t \in [0_1, 0 + \tau];
$$

the second commutator satisfies the relation

$$
\| [\partial_{xx}, [\partial_{xx}, V(t)]] \|_{L^2(\Omega, \mathbb{C})} \leq 2 \| \partial_{xx} V(t) \|_{L^2(\Omega, \mathbb{R})} \| \partial_{xx} V \|_{L^2(\Omega, \mathbb{C})} + 4 \| \partial_{xxx} V(t) \|_{L^2(\Omega, \mathbb{R})} \| \partial_{x} V \|_{L^2(\Omega, \mathbb{C})}, \\
v \in H^2(\Omega, \mathbb{C}), \quad t \in [0_1, 0 + \tau].
$$

By induction, we obtain a bound of the form

$$
\| \text{ad}^m_Z (V(t) - V(t_0 + \frac{\tau}{2})) \|_{H^m \rightarrow H^m} \leq \begin{cases} 
C_m \| V \|_{H^{m_0}(0, 0 + \tau), \Omega, \mathbb{R}} & \text{if } \tau \in [0, 0_1] \text{ and } m \in \mathbb{N}_{\geq 0}, \\
C_m \| V \|_{H^{m_0}(0, 0 + \tau), \Omega, \mathbb{R}} \tau & \text{otherwise},
\end{cases}
$$

involving a generic constant.

**Expansion of principal term.** In order to deduce a suitable representation of the principal term in (4.17), we apply the above stated relations. More precisely, we make use of the following Taylor series expansions

$$
e^{-\sigma Z} z(\sigma) e^{\sigma Z} = e^{-\sigma Z} z(\sigma) e^{\sigma Z} + \mu^{(2)}(\sigma, \sigma, Z, z),
$$

$$
e^{-\sigma Z} z(\sigma) + (\sigma - \sigma) \text{ad}_{Z}(z(\sigma)) + \frac{1}{2} (\sigma - \sigma)^2 \text{ad}_{Z}^2(z(\sigma)) e^{\sigma Z} + \mu^{(4)}(\sigma, \sigma, Z, z), \quad \sigma \in [0, \sigma_0],
$$

with remainders satisfying the bounds

$$
\mu^{(2)}(\sigma, \sigma, Z, z) = (\sigma - \sigma) \int_0^1 e^{-(\sigma + \theta (\sigma - \sigma)) Z} \text{ad}_{Z}(z(\sigma)) e^{(\sigma + \theta (\sigma - \sigma)) Z} d\theta, \\
\| \mu^{(2)}(\sigma, \sigma, Z, z) \|_{H^m \rightarrow H^m} \leq C_1 \| V \|_{H^{m_0}(0, 0 + \tau), \Omega, \mathbb{R}} \tau^2,
$$

$$
\mu^{(4)}(\sigma, \sigma, Z, z) = \frac{1}{2} (\sigma - \sigma)^3 \int_0^1 (1 - \theta)^2 e^{-(\sigma + \theta (\sigma - \sigma)) Z} \text{ad}_{Z}^3(z(\sigma)) e^{(\sigma + \theta (\sigma - \sigma)) Z} d\theta, \\
\| \mu^{(4)}(\sigma, \sigma, Z, z) \|_{H^m \rightarrow H^m} \leq C_1 \| V \|_{H^{m_0}(0, 0 + \tau), \Omega, \mathbb{R}} \tau^4, \quad \sigma \in [0, \sigma_0].
$$

On the one hand, integration implies

$$
\mathcal{J}_{4}^{(2)}(\eta_0, \sigma, Z, z) = \mathcal{J}_{3}^{(2)}(\eta_0, \sigma, Z, z) + \mathcal{J}_{3}^{(3)}(\eta_0, \sigma, Z, z)
$$

$$
= \mathcal{J}_{3}^{(2)}(\eta_0, \sigma, Z, z) + \mathcal{J}_{3}^{(3)}(\eta_0, \sigma, Z, z) + \mathcal{J}_{3}^{(4)}(\eta_0, \sigma, Z, z) + \mathcal{J}_{3}^{(5)}(\eta_0, \sigma, Z, z),
$$
where the principal terms are given by

\[
\mathcal{J}^{(2)}_3(\sigma_0, \sigma_z, Z, z) = e^{(\sigma_0 - \sigma_z)Z} \int_0^{\sigma_0} z(\sigma_1) \, d\sigma_1 \, e^{\sigma_z Z},
\]

\[
\mathcal{J}^{(3)}_3(\sigma_0, \sigma_z, Z, z) = e^{(\sigma_0 - \sigma_z)Z} \int_0^{\sigma_0} (\sigma_1 - \sigma_z) \, \text{ad}_{Z}(z(\sigma_1)) \, d\sigma_1 \, e^{\sigma_z Z},
\]

\[
\mathcal{J}^{(4)}_3(\sigma_0, \sigma_z, Z, z) = e^{(\sigma_0 - \sigma_z)Z} \int_0^{\sigma_0} \frac{1}{2} (\sigma_1 - \sigma_z)^2 \, \text{ad}_{Z}^2(z(\sigma_1)) \, d\sigma_1 \, e^{\sigma_z Z},
\]

and the remainders have the desired orders

\[
\mathcal{J}^{(3)}_3(\sigma_0, \sigma_z, Z, z) = e^{\sigma_0 Z} \int_0^{\sigma_0} r^{(2)}(\sigma_1, \sigma_z, Z, z) \, d\sigma_1,
\]

\[
\|\mathcal{J}^{(3)}_3(\sigma_0, \sigma_z, Z, z)\|_{\mathcal{H} \rightarrow \mathcal{H}^1} \leq C_1 \|V\|_{\mathcal{H}^{1.5}} \tau^3,
\]

\[
\mathcal{J}^{(4)}_4(\sigma_0, \sigma_z, Z, z) = e^{\sigma_0 Z} \int_0^{\sigma_0} \int_0^{\sigma_1} z(\sigma_1) \, z(\sigma_2) \, d\sigma_2 \, d\sigma_1 \, e^{\sigma_z Z},
\]

involving a remainder

\[
\mathcal{J}^{(4)}_4(\sigma_0, \sigma_z, Z, z) = e^{\sigma_0 Z} \int_0^{\sigma_0} \int_0^{\sigma_1} \left( r^{(2)}(\sigma_1, \sigma_z, Z, z) e^{-\sigma_z Z} z(\sigma_2) e^{\sigma_z Z} + e^{-\sigma_z Z} z(\sigma_1) e^{\sigma_z Z} r^{(2)}(\sigma_2, \sigma_z, Z, z) \right) \, d\sigma_2 \, d\sigma_1,
\]

that fulfills an estimate of the form

\[
\|\mathcal{J}^{(4)}_4(\sigma_0, \sigma_z, Z, z)\|_{\mathcal{H} \rightarrow \mathcal{H}^1} \leq C_1 \left( \|V\|_{\mathcal{H}^{1.5}} \right) \tau^5
\]

with generic constant, see (4.11) and (4.16).

**Choices of centers.** As described below, suitable choices of the centers in the Taylor series expansions permit to extract a common exponential factor; accordingly, we rewrite the expansion (4.17) as

\[
\mathcal{J}(\sigma_0, Z, z_1) \mathcal{J}(\sigma_0, Z, z_2) = \mathcal{J}^{(0)}_3(\sigma_0, \zeta, Z, z_1, z_2) + \mathcal{J}^{(5)}_3(\sigma_0, \zeta, Z, z_1, z_2)
\]

with principal term given by

\[
\mathcal{J}^{(0)}_3(\sigma_0, \zeta, Z, z_1, z_2) = e^{2\sigma_0 Z} + e^{\sigma_0 Z} \left( \mathcal{J}^{(2)}_3(\sigma_0, \zeta_1, Z, z_2) + \mathcal{J}^{(3)}_3(\sigma_0, \zeta_1, Z, z_2) + \mathcal{J}^{(4)}_3(\sigma_0, \zeta_1, Z, z_2) \right)
\]

\[
+ \left( \mathcal{J}^{(2)}_3(\sigma_0, \zeta_2, Z, z_1) + \mathcal{J}^{(3)}_3(\sigma_0, \zeta_2, Z, z_1) + \mathcal{J}^{(4)}_3(\sigma_0, \zeta_2, Z, z_1) \right) e^{\sigma_0 Z},
\]

\[
+ e^{\sigma_0 Z} \left( \mathcal{J}^{(4)}_4(\sigma_0, \zeta_3, Z, z_2) + \mathcal{J}^{(4)}_4(\sigma_0, \zeta_4, Z, z_1) \right) e^{\sigma_0 Z},
\]

\[
+ \mathcal{J}^{(2)}_3(\sigma_0, \zeta_5, Z, z_1) \mathcal{J}^{(2)}_3(\sigma_0, \zeta_6, Z, z_2).
\]
the remainder comprises the terms
\[
\mathcal{S}_5^{(5)}(\sigma_0, \xi, Z, z_1, z_2) \\
= \mathcal{S}_2^{(6)}(\sigma_0, Z, z_1, z_2) + e^{\sigma_0 Z} \mathcal{S}_3^{(5)}(\sigma_0, \xi_1, Z, z_2) + \mathcal{S}_3^{(5)}(\sigma_0, \xi_2, Z, z_1) e^{\sigma_0 Z} \\
+ e^{\sigma_0 Z} \mathcal{S}_4^{(5)}(\sigma_0, \xi_3, Z, z_2) + \mathcal{S}_4^{(5)}(\sigma_0, \xi_4, Z, z_1) e^{\sigma_0 Z} \\
+ \mathcal{S}_3^{(5)}(\sigma_0, \xi_5, Z, z_1) \mathcal{S}_4^{(2)}(\sigma_0, Z, z_2) + \mathcal{S}_3^{(2)}(\sigma_0, \xi, Z, z_1) \mathcal{S}_3^{(3)}(\sigma_0, \xi_6, Z, z_2)
\]
and thus satisfies an estimate of the form
\[
\|\mathcal{S}_5^{(5)}(\sigma_0, \xi, Z, z_1, z_2)\| \leq C_3 \left( \|V\|_{\mathcal{H}_{1,0}([0, t_0] \times \Omega, \mathbb{R})} \right) \tau^5,
\]
see again (4.11).

**Local error expansion.** By means of our previous considerations, we obtain a suitable local error expansion for the fourth-order scheme (4.5); more precisely, based on the identity
\[
\mathcal{L}(\tau, t_0) = \mathcal{S}_5^{(2)}(\sigma_0, \xi, A_\tau, V) + \mathcal{S}_6^{(5)}(\sigma_0, \xi, A_\tau, V).
\]
The first summand comprises several terms
\[
\mathcal{S}_6^{(2)}(\tau, t_0, \xi_0, A_\tau, V) = \mathcal{S}_6^{(0)}(\tau, \xi_0, \frac{1}{2} A_\tau, \frac{1}{2} S_2(\tau, t_0), \frac{1}{2} S_1(\tau, t_0)) \\
- \mathcal{S}_5^{(0)}(\tau, \xi_0, \frac{1}{2} A_\tau, \frac{1}{2} R(\tau_0 + \frac{\tau_0}{2} + \frac{1}{2})(\cdot), \frac{1}{2} R(\tau_0 + \frac{1}{2})(\cdot))
\]
which have the desired order four, as we justify in detail below; the remainder
\[
\mathcal{S}_6^{(5)}(\tau, t_0, \xi_0, A_\tau, V) = \mathcal{S}_5^{(5)}(\tau, \xi_0, \frac{1}{2} A_\tau, \frac{1}{2} S_2(\tau, t_0), \frac{1}{2} S_1(\tau, t_0)) \\
- \mathcal{S}_5^{(5)}(\tau, \xi_0, \frac{1}{2} A_\tau, \frac{1}{2} R(\tau_0 + \frac{\tau_0}{2} + \frac{1}{2})(\cdot), \frac{1}{2} R(\tau_0 + \frac{1}{2})(\cdot))
\]
is well-defined when considered as operator from \( \mathcal{H}^3 \) to \( \mathcal{H} \) and satisfies the bound
\[
\|\mathcal{S}_6^{(5)}(\tau, t_0, \xi_0, A_\tau, V)\| \leq C_3 \left( \|V\|_{\mathcal{H}_{1,0}([0, t_0] \times \Omega, \mathbb{R})} \right) \tau^5.
\]
As indicated before, we make use of the fact that the particular choices
\[ \zeta_1 = 0, \quad \zeta_2 = -\tau, \quad \zeta_3 = \tau, \quad \zeta_4 = 0, \quad \zeta_5 = 0, \quad \zeta_6 = \tau, \]
of the centers in the Taylor series expansions employed for the numerical and exact evolution operators permit to extract common exponential factors. On the one hand, we obtain the relations
\[ I_1(t, t_0) = e^{\frac{1}{2} \tau A_0} \left[ I_3(t, t_0) - I_3(t_0) \right] + \left( I_3(t, t_0) - I_3(t_0) \right) e^{\frac{1}{2} \tau A_0} = e^{\frac{1}{2} \tau A_0} I_1(t, t_0), \]
\[ I_2(t, t_0) = \int_0^t \left( S_1(t, t_0) - R(t_0 + \frac{1}{2} \sigma_1) \right) d\sigma_1 + \int_0^t \left( S_2(t, t_0) - R(t_0 + \frac{1}{2} \sigma_1) \right) d\sigma_1, \]
\[ I_3(t, t_0) = \int_0^t \sigma_1 \left( S_1(t, t_0) - R(t_0 + \frac{1}{2} \sigma_1) \right) d\sigma_1 + \int_0^t \left( \sigma_1 + \tau \right) \left( S_2(t, t_0) - R(t_0 + \frac{1}{2} \sigma_1) \right) d\sigma_1, \]
\[ I_4(t, t_0) = \int_0^t \sigma_2 \left( S_1(t, t_0) - R(t_0 + \frac{1}{2} \sigma_1) \right) d\sigma_1 + \int_0^t \left( \sigma_1 + \tau \right)^2 \left( S_2(t, t_0) - R(t_0 + \frac{1}{2} \sigma_1) \right) d\sigma_1. \]
on the other hand, we have
\[ S_4(t, t_0) = e^{\frac{1}{2} \tau A_0} \left[ S_4(t, t_0) + S_4(t_0) \right] + \left( S_4(t, t_0) + S_4(t_0) \right) e^{\frac{1}{2} \tau A_0} = e^{\frac{1}{2} \tau A_0} S_4(t, t_0). \]
special structure. The derivation of the local error expansion based on linearisations of the underlying

For the sake of completeness, we include the extension of Theorem 1 for Hamilton operators without

5. General case

exponential midpoint rule; as the scheme involves a single exponential, the calculations are considerably

exponential midpoint rule.

As a consequence, we arrive at the following result

Straightforward Taylor series expansions of the arising integrands lead to the auxiliary estimates

see also (4.7), and at once imply

As a consequence, we arrive at the following result

Local error estimate. Altogether, this proves that the fourth-order CFQM exponential integrator (3.3) satisfies the local error bound

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Exponential midpoint rule. It is straightforward to apply the above approach in the context of the exponential midpoint rule; as the scheme involves a single exponential, the calculations are considerably simplified.

5. General case

For the sake of completeness, we include the extension of Theorem 1 for Hamilton operators without special structure. The derivation of the local error expansion based on linearisations of the underlying
evolution equations, representations by the variation-of-constants formula, and Taylor series expansions of parts of the integrands in principle applies to the general case as well, see Section 4.3; however, for the specification of regularity assumptions on the problem data, more detailed information on the form of the considered Hamiltonians would be required.

**Theorem 2**  
Assume that the operator family defining the non-autonomous linear Schrödinger equation (2.1) and its exact solution are sufficiently regular such that compositions of the form $A^{(\ell)}(s)u^{(m)}(t)$ with $\ell \in \{0, 1, \ldots, p\}$ and $m \in \{0, 1, \ldots, p - 1\}$ remain bounded. Then, any $p$th-order CFQM exponential integrator (3.1) satisfies a global error estimate of the form

$$\|u_N - u(T)\|_{\mathcal{HF}} \leq \|u_0 - u(t_0)\|_{\mathcal{HF}} + C \tau_{\text{max}}^p;$$

the arising constant depends on the data of the problem, the length of the considered time interval, and the method coefficients, but it is independent of the number of time steps $n$ and the maximal time stepsize.

**Illustrations.**  
Numerical experiments that confirm the global error bound of Theorem 1 and Theorem 2, respectively, are found in BLANES, CASAS, THALHAMMER (2017, 2018), see also BADER, BLANES, KOPYLOV (2018); due to the fact that the exponential midpoint rule is an instance of a Magnus integrator and a CFQM exponential integrator, we also refer to the numerical example given in HOCHBRUCK, LUBICH (2003). For vanishing dissipation parameter $\delta = 0$, the evolution equation considered in BLANES, CASAS, THALHAMMER (2017) is of Schrödinger type; the presented results in particular verify the order of convergence and provide numerical evidence that CFQM exponential integrators are superior in efficiency compared to explicit Runge–Kutta methods and Magnus integrators for differential equations involving a higher degree of freedom.

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**References**


