Karlsruhe Institute of Technology

Wave phenomena
analysis and numerics

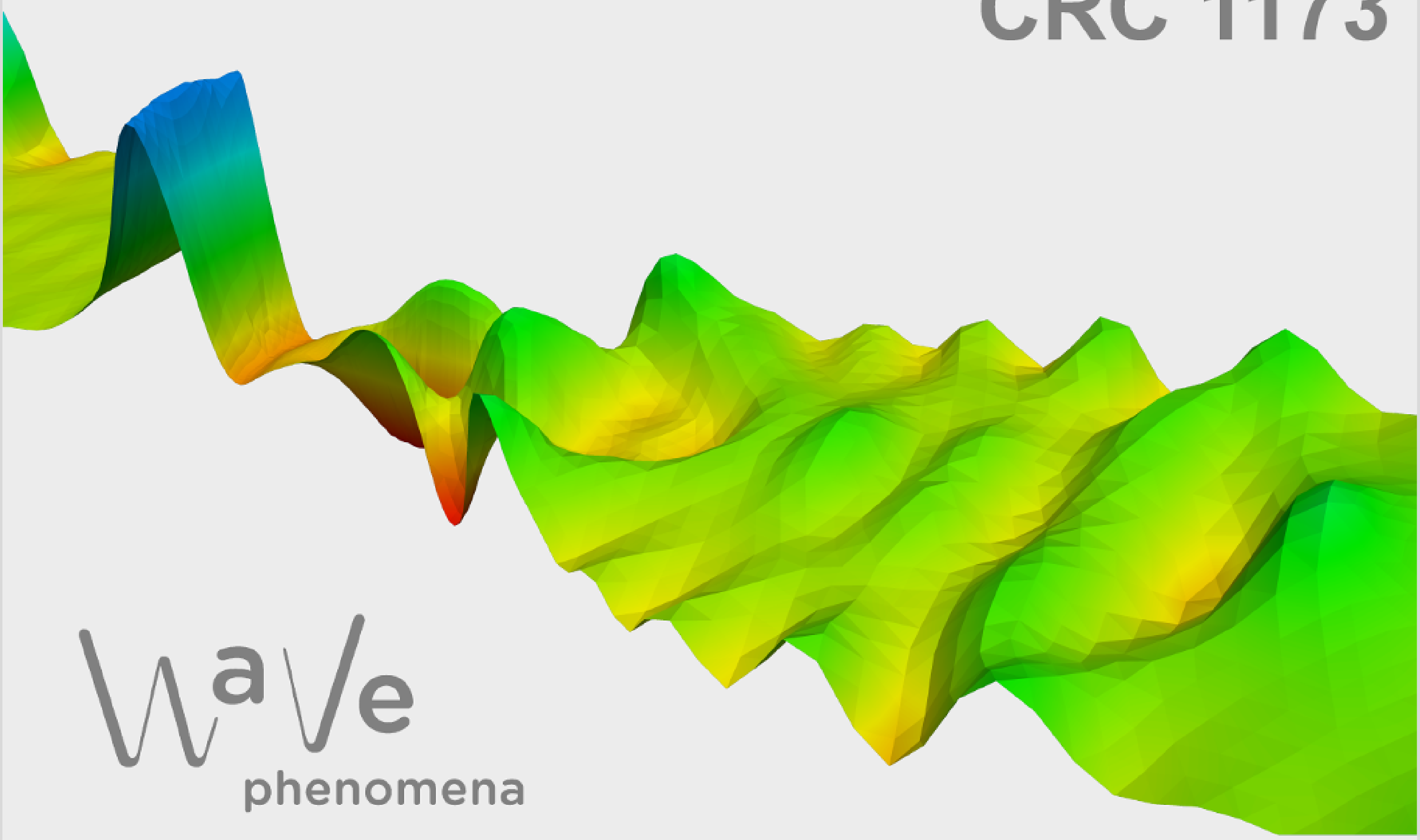
Closing the gap between trigonometric integrators and splitting methods for highly oscillatory differential equations

Simone Buchholz, Ludwig Gauckler, Volker Grimm, Marlis Hochbruck, Tobias Jahnke

CRC Preprint 2016/22, September 2016

KARLSRUHE INSTITUTE OF TECHNOLOGY

CRC 1173



Wave phenomena

Participating universities

Universität Stuttgart

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN

Funded by

DFG

ISSN 2365-662X

Closing the gap between trigonometric integrators and splitting methods for highly oscillatory differential equations

SIMONE BUCHHOLZ†
Karlsruher Institut für Technologie (KIT), Institut für Angewandte und Numerische Mathematik, Kaiserstr. 12, D-76131 Karlsruhe, Germany

LUDWIG GAUCKLER‡
Freie Universität Berlin, Institut für Mathematik, Arnimallee 9, D-14195 Berlin, Germany

VOLKER GRIMM§, MARLIS HOCHBRUCK§ AND TOBIAS JAHNKE§
Karlsruher Institut für Technologie (KIT), Institut für Angewandte und Numerische Mathematik, Kaiserstr. 12, D-76131 Karlsruhe, Germany

[Received on September 23, 2016]

An error analysis of symmetric trigonometric integrators applied to highly oscillatory linear second-order differential equations is given. Second-order convergence is shown uniformly in the high frequencies under a finite-energy condition on the exact solution. The main novelty is the concept to prove these error bounds, which is based on the interpretation of trigonometric integrators as splitting methods for averaged differential equations. This allows one to combine techniques for splitting methods with those for trigonometric integrators. For the bound of the global error, cancellations in the error accumulation have to be studied carefully.

Keywords:

splitting methods; trigonometric integrators; highly oscillatory problems; second-order differential equations; error bounds; summation by parts.

1. Introduction

Many ordinary differential equations in science can be written as

$$u' = F_1(u) + F_2(u) \tag{1.1}$$

with linear or nonlinear vector fields F_1 and F_2, and with the property that solving the two sub-problems

$$v' = F_1(v) \qquad \text{and} \qquad w' = F_2(w)$$

exactly or approximately is numerically much more efficient than solving (1.1) directly. Typical examples include many-body problems and other Hamiltonian systems with a certain structure, but also semi-discretizations of time-dependent partial differential equations such as, e.g., linear or nonlinear Schrödinger equations, linear or nonlinear wave equations, or Maxwell's equations. In such a situation, splitting methods are easy to implement and very efficient, because these integrators compute a

†Corresponding author. Email: simone.buchholz@kit.edu
‡Email: gauckler@math.fu-berlin.de
§Email: {volker.grimm, marlis.hochbruck, tobias.jahnke}@kit.edu

numerical approximation of the full problem by a composition of the flows of the two sub-problems. In many cases the numerical solution inherits certain geometric properties of the exact solution, such as norm conservation or symplecticity of the flow. The order conditions and the accuracy of splitting methods have been analyzed in many papers such as, e.g., Strang (1968), Jahnke & Lubich (2000), Lubich (2008), Hansen & Ostermann (2009), Thalhammer *et al.* (2009), Koch & Lubich (2011), Holden *et al.* (2013), Einkemmer & Ostermann (2014), Einkemmer & Ostermann (2015), Faou *et al.* (2015), Hochbruck *et al.* (2015) and references therein. Overviews have been given, e.g., in McLachlan & Quispel (2002), Hairer *et al.* (2006), Hundsdorfer & Verwer (2007), Holden *et al.* (2010), and Blanes & Casas (2016). The classical procedure is to estimate the local error by proving bounds for certain iterated commutators between the two vector fields. The error bound for the global error then follows by standard arguments like Gronwall inequalities or Lady Windermere's fan.

Unfortunately, the accuracy typically suffers when splitting methods are applied to problems with highly oscillatory solutions. In order to obtain a reasonable approximation, the step-size must be considerably smaller than the inverse of the highest frequency, which reduces the efficiency considerably. We remark, however, that certain invariants of the exact flow are often conserved over long times even in the presence of oscillations, see, e.g., Hairer *et al.* (2006), Faou (2012), Cohen *et al.* (2015).

A particular class of problems with highly oscillatory solutions takes the semilinear form

$$q''(t) = -\Omega^2 q(t) + g(q(t)), \qquad t > 0, \qquad q(0) = q_0, \quad q'(0) = q_0', \tag{1.2}$$

where Ω is a symmetric positive semi-definite matrix of arbitrary large norm, and where g is smooth and bounded. For such problems, trigonometric integrators have been constructed and analyzed in García-Archilla *et al.* (1999), Hochbruck & Lubich (1999), Hairer *et al.* (2006), Grimm & Hochbruck (2006) under a finite-energy condition. These methods involve filter functions which are chosen in such a way that oscillatory parts of the local error do not sum up in the global error. To prove this in the error analysis is a delicate matter and usually excludes to apply the technique of Lady Windermere's fan in a standard way. An exception are semilinear wave equations with polynomial or analytic nonlinearities, see Gauckler (2015).

Hence, it seems that splitting methods and trigonometric integrators are two different approaches, based on different ideas, having different properties, and requiring different techniques for their analysis. Nevertheless, there is a bridge between these two worlds: it is long known that symmetric trigonometric integrators applied to (1.2) can be interpreted as a Strang splitting method applied to an *averaged* version of the first-order formulation of (1.2). This interesting link raises a number of questions: Is it possible to gain a better understanding by considering trigonometric integrators as splitting methods for averaged equations? Does this relation allow to apply the techniques developed for one class of methods to the other one? And, most importantly, is it then possible to construct and analyze efficient numerical integrators for fully nonlinear problems?

These questions are our motivation for the analysis below. In this paper, we will restrict ourselves to the *linear* variant of (1.2), i.e., $g(q) = Gq$ with a matrix G with a moderate norm $\|G\| \ll \|\Omega\|$. Here and in the following, $\|\cdot\|$ denotes the Euclidean vector norm or its induced matrix norm, respectively. The analysis in Lubich (2008) shows that for splitting methods the calculus of Lie derivatives allows, at least to some extent, to carry over techniques developed for linear differential equations to nonlinear ones. After reformulation as a first-order problem, we will derive the corresponding averaged equation and prove a bound for the difference between the solution of both equations; cf. Theorem 4.1. Then, we present an error analysis for the classical Strang splitting applied to the averaged equation, which yields a result very similar but not equivalent to the one obtained in Grimm & Hochbruck (2006).

We stress that the novelty of our analysis is not the error bound itself, but the fact that it is proven by techniques which, to the best of our knowledge, have so far not been considered in the context of trigonometric integrators.

2. Problem setting, assumptions and notation

The situation we have in mind is that the ordinary differential equation

$$q''(t) = -\Omega^2 q(t) + Gq(t), \qquad 0 \leqslant t \leqslant t_{\text{end}}, \qquad q(0) = q_0, \quad q'(0) = q'_0, \tag{2.1}$$

stems from a spatial discretization of a linear wave equation with finite elements, finite differences, or spectral methods on a family of finer and finer meshes. In this situation, the matrix $-\Omega^2$ stems from a spatial discretization of the Laplacian or a more general differential operator, and Ω is a symmetric, positive definite matrix (possibly after shifting $\Omega \to \sqrt{\Omega^2 + I}$ and $G \to G + I$). Then $\|\Omega\|$ becomes arbitrarily large if the spatial mesh width tends to zero, but $\|\Omega^{-1}\|$ remains uniformly bounded independently of the discretization. This motivates the following assumption.

ASSUMPTION 2.1 Let $\Omega \in \mathscr{F}$, where $\mathscr{F}$ is a family of symmetric, positive definite matrices such that there is a constant C_{inv} with

$$\|\Omega^{-1}\| \leqslant C_{\text{inv}} \qquad \text{for all } \Omega \in \mathscr{F}. \tag{2.2}$$

For the matrix G we assume that its norm is bounded independently of Ω.

Our aim is to prove error estimates which are uniform for all matrices in the family $\mathscr{F}$, which means that they are independent of $\|\Omega\|$ (i.e., independent of the spatial discretization). On the other hand, the constant C_{inv} only depends on the coercivity constant of the corresponding differential operator.

For the solution we rely on the following assumption.

ASSUMPTION 2.2 Let the solution $q : [0, t_{\text{end}}] \to \mathbb{R}^d$ of (2.1) fulfill the *finite-energy condition*

$$\|\Omega q(t)\|^2 + \left\|q'(t)\right\|^2 \leqslant K^2, \qquad 0 \leqslant t \leqslant t_{\text{end}}, \tag{2.3}$$

with a constant $K > 0$ on a finite time interval of length t_{end}.

In fact, it can be shown that (2.3) is true on bounded time intervals if the initial data satisfy the bound $\|\Omega q(0)\|^2 + \|q'(0)\|^2 \leqslant K_0^2$ with a sufficiently small $K_0 \leqslant K$; cf. Lemma 4.1 below.

In order to apply a splitting scheme we formulate (2.1) as a first-order problem. We define the new variable

$$u = \begin{bmatrix} q \\ \Omega^{-1} q' \end{bmatrix}, \qquad u_0 = \begin{bmatrix} q_0 \\ \Omega^{-1} q'_0 \end{bmatrix}$$

which solves the differential equation

$$u' = Au + Bu, \qquad u(0) = u_0, \tag{2.4}$$

with matrices

$$A = \begin{bmatrix} 0 & \Omega \\ -\Omega & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 \\ \Omega^{-1} G & 0 \end{bmatrix}.$$

Since A is skew symmetric, the exponential

$$\exp(tA) = \begin{bmatrix} \cos(t\Omega) & \sin(t\Omega) \\ -\sin(t\Omega) & \cos(t\Omega) \end{bmatrix}$$

is unitary, and thus

$$\left\| e^{tA} \right\| = 1, \qquad t \in \mathbb{R}. \tag{2.5}$$

The finite-energy condition (2.3) is equivalent to

$$\|Au(t)\| \leqslant K, \qquad 0 \leqslant t \leqslant t_{\text{end}}. \tag{2.6}$$

The solution of (2.4) could, in principle, be approximated with the classical Strang splitting, but in our setting this method only yields an acceptable accuracy if $\tau \ll \|\Omega\|^{-1}$. Such a severe step-size restriction is not acceptable in practice. We will show that much better approximations are obtained if the Strang splitting is applied to an *averaged* version of (2.4).

The methods considered below involve analytic (mostly trigonometric) matrix functions of $\tau\Omega$. We assume that products of such matrix functions with a given vector can be computed efficiently, e.g., via fast Fourier transforms or (rational) Krylov subspace methods (see, e.g., Grimm & Hochbruck (2008)).

3. Trigonometric integrators as splitting methods

Symmetric one-step trigonometric integrators (Hairer *et al.*, 2006, Section XIII.2.2) and Grimm & Hochbruck (2006) written in terms of the variables $u_n = [q_n, \Omega^{-1}q_n'] \approx u(t_n) = [q(t_n), \Omega^{-1}q'(t_n)]$ at $t_n = n\tau$ are given by

$$u_{n+1} = e^{\tau A}u_n + \frac{\tau}{2}\begin{bmatrix} \sin(\tau\Omega)\Omega^{-1}\widetilde{G}q_n \\ \cos(\tau\Omega)\Omega^{-1}\widetilde{G}q_n + \Omega^{-1}\widetilde{G}q_{n+1} \end{bmatrix}. \tag{3.1}$$

Here, $\tau > 0$ denotes the step-size, and the matrix $\widetilde{G}$ is defined as

$$\widetilde{G} = \Psi_S G \Phi, \qquad \Phi = \phi(\tau\Omega), \qquad \Psi_S = \psi_S(\tau\Omega), \tag{3.2}$$

with appropriate scalar filter functions ϕ and ψ_S. Note that ψ_S was denoted by ψ_1 in Hairer *et al.* (2006) and Grimm & Hochbruck (2006). In these references it was shown that under the assumptions of Section 2 and certain (sufficient) conditions on the filter functions ϕ and ψ_S, these methods yield a global accuracy of $O(\tau^2)$ in the positions q_n and $O(\tau)$ in the velocities q_n'. The constants in the error bounds are independent of $\|\Omega\|$, in spite of the oscillatory nature of the solution.

It is well known that symmetric trigonometric integrators can be interpreted as splitting schemes. With

$$\widetilde{B} = \begin{bmatrix} 0 & 0 \\ \Omega^{-1}\widetilde{G} & 0 \end{bmatrix}, \tag{3.3}$$

the method (3.1) can be written as

$$\left(I - \tfrac{\tau}{2}\widetilde{B}\right)u_{n+1} = e^{\tau A}\left(I + \tfrac{\tau}{2}\widetilde{B}\right)u_n. \tag{3.4}$$

Now we use that

$$e^{\theta\widetilde{B}} = I + \theta\widetilde{B} \qquad \text{for all } \theta \in \mathbb{R} \tag{3.5}$$

due to the particular structure of $\widetilde{B}$. Substituting (3.5) into (3.4) gives

$$u_{n+1} = Su_n, \qquad S = e^{\frac{\tau}{2}\widetilde{B}}e^{\tau A}e^{\frac{\tau}{2}\widetilde{B}}. \tag{3.6}$$

Hence, the trigonometric integrator (3.1) is equivalent to the exponential Strang splitting method applied to the *averaged* equation

$$\widetilde{u}' = A\widetilde{u} + \widetilde{B}\widetilde{u}, \qquad \widetilde{u}(0) = \widetilde{u}_0 = u_0 \tag{3.7}$$

with $\widetilde{B}$ defined in (3.3) and (3.2). This means that applying the Strang splitting to the averaged equation yields very good approximations for step-sizes where the Strang splitting applied to the original problem (2.4) fails if the norm of Ω is large.

We point out that not only the numerical solution u_n depends on the step-size τ, but also the *exact* solution $\widetilde{u}$ of the averaged equation via the filter functions $\Phi = \phi(\tau\Omega)$ and $\Psi_S = \psi_S(\tau\Omega)$. Note that for *semilinear* problems (1.2) the trigonometric integrators can still be interpreted as a Strang splitting applied to a (semilinear) averaged equation.

Our aim is to prove error bounds for the trigonometric integrator (3.1) on the basis of this interpretation as a splitting method (3.6), using a carefully adapted Lady Windermere's fan argument familiar from splitting integrators. In order to analyze the error of the splitting scheme we first study properties of the solution of the averaged problem (3.7). This allows us to bound the error which results from solving the averaged equation instead of (2.4) (Section 4). To analyze the error of the splitting scheme for the averaged problem we first give a new representation of the local error. Unfortunately, this local error still contains a term which is not uniformly of third order in τ and requires a more careful investigation (Section 5).

The error analysis given below relies on the following assumption on the filter functions.

ASSUMPTION 3.1 The filter functions $\chi = \phi$ or $\chi = \psi_S$ are even analytic functions with the properties

$$\chi(0) = 1, \tag{3.8a}$$

$$|\chi(x)| \leqslant M_1, \tag{3.8b}$$

$$|x\chi(x)| \leqslant M_2, \tag{3.8c}$$

$$\left|\cot\left(\frac{x}{2}\right)x\chi(x)\right| \leqslant M_3 \tag{3.8d}$$

for certain constants M_j uniformly for all $x \in \mathbb{R}$.

Even functions χ guarantee that the scheme is symmetric. A popular example used in trigonometric integrators is $\chi(x) = \operatorname{sinc}(x)$. Note that (3.8a) and the condition that χ is even analytic imply

$$\left|x^{-2}(1-\chi(x))\right| \leqslant M_4. \tag{3.8e}$$

In the following C denotes a generic constant which may have different values at different occurrences. Our main result is stated in the following theorem.

THEOREM 3.2 (Main result) Let Assumptions 2.1, 2.2, and 3.1 be fulfilled. Then the global error of (3.6) applied to (2.4) is bounded by

$$\|u_n - u(t_n)\| \leqslant C\tau^2, \qquad 0 \leqslant t_n = n\tau \leqslant t_{\text{end}},$$

with a constant C that only depends on C_{inv}, $\|G\|$, K, M_j, $j = 1, \dots, 4$, and t_{end} but not on $\|\Omega\|$.

Proof. We combine the results from Theorem 4.1 and Theorem 5.1 below to obtain

$$\|u_n - u(t_n)\| \leqslant \|u_n - \widetilde{u}(t_n)\| + \|\widetilde{u}(t_n) - u(t_n)\| \leqslant C\tau^2, \qquad 0 \leqslant t_n = n\tau \leqslant t_{\text{end}},$$

where the constant C only depends on C_{inv}, $\|G\|$, K, M_j, $j = 1, \dots, 4$, and t_{end}. $\square$

4. Properties of the averaged equation

In this section we prove that the solutions of the original problem (2.4) and the averaged equation (3.7) differ only by $O(\tau^2)$.

THEOREM 4.1 Let the assumptions (3.8a) and (3.8b) and the finite-energy condition (2.3) be fulfilled. Let u be the solution of (2.4) and $\widetilde{u}$ be the solution of the averaged system (3.7). Then it holds

$$\|u(t)-\widetilde{u}(t)\| \leqslant C_{\mathrm{av}}\tau^2, \qquad 0 \leqslant t \leqslant t_{\mathrm{end}},$$

where C_{av} only depends on C_{inv}, $\|G\|$, K, M_1, M_4, and t_{end}.

Proof. The variation-of-constants formula yields

$$u(t) = e^{tA}u_0 + \int_0^t e^{(t-s)A}Bu(s)\,ds, \tag{4.1a}$$

$$\widetilde{u}(t) = e^{tA}u_0 + \int_0^t e^{(t-s)A}\widetilde{B}\widetilde{u}(s)\,ds. \tag{4.1b}$$

We define the block diagonal matrices

$$\widehat{\Psi} = \begin{bmatrix} \Psi_S & 0 \\ 0 & \Psi_S \end{bmatrix}, \qquad \widehat{\Phi} = \begin{bmatrix} \Phi & 0 \\ 0 & \Phi \end{bmatrix}. \tag{4.2}$$

Obviously, they satisfy $\left[\widehat{\Psi},A\right] = \left[\widehat{\Phi},A\right] = 0$ and we have $\widetilde{B} = \widehat{\Psi}B\widehat{\Phi}$ so that

$$\begin{aligned} u(t)-\widetilde{u}(t) &= \int_0^t e^{(t-s)A}\Big((I-\widehat{\Psi})Bu(s) + \widehat{\Psi}B(I-\widehat{\Phi})u(s) + \widehat{\Psi}B\widehat{\Phi}\big(u(s)-\widetilde{u}(s)\big)\Big)\,ds \\ &= I_1(t) + I_2(t) + \int_0^t e^{(t-s)A}\widetilde{B}\big(u(s)-\widetilde{u}(s)\big)\,ds \end{aligned}$$

with

$$I_1(t) = \int_0^t e^{(t-s)A}(I-\widehat{\Psi})Bu(s)\,ds, \qquad I_2(t) = \int_0^t e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})u(s)\,ds.$$

For the first term integration by parts yields

$$I_1(t) = -\tau^2 e^{(t-s)A}(\tau A)^{-2}(I-\widehat{\Psi})ABu(s)\Big|_0^t + \tau^2\int_0^t e^{(t-s)A}(\tau A)^{-2}(I-\widehat{\Psi})ABu'(s)\,ds.$$

With (2.2) and (2.6) it follows that

$$\|u\| = \left\|A^{-1}Au\right\| \leqslant C_{\mathrm{inv}}K, \tag{4.3a}$$

$$\left\|u'\right\| \leqslant \|Au\| + \|Bu\| \leqslant K + C_{\mathrm{inv}}^2\,\|G\|\,K. \tag{4.3b}$$

Using in addition (2.5), (3.8e), and

$$\|AB\| = \|G\|, \tag{4.4}$$

this yields the estimate $\|I_1(t)\| \leqslant C\tau^2$ with a constant C depending only on C_{inv}, $\|G\|$, K, M_4, and t_{end}.

For the second term we insert the variation of constants formula once more and obtain

$$\begin{aligned}
I_2(t) &= \int_0^t e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})u(s)\,ds \\
&= \int_0^t e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})e^{sA}u_0\,ds + \int_0^t\int_0^s e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})e^{(s-\sigma)A}Bu(\sigma)\,d\sigma\,ds.
\end{aligned}$$

Integration by parts yields

$$\begin{aligned}
I_2(t) &= e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})A^{-1}e^{sA}u_0\Big|_0^t + \int_0^t e^{(t-s)A}A\widehat{\Psi}B(I-\widehat{\Phi})A^{-1}e^{sA}u_0\,ds \\
&\quad - \int_0^t e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})A^{-1}e^{(s-\sigma)A}Bu(\sigma)\Big|_0^s ds \\
&\quad + \int_0^t\int_0^s e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})A^{-1}e^{(s-\sigma)A}Bu'(\sigma)\,d\sigma\,ds \\
&= \tau^2 e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})(\tau A)^{-2}e^{sA}Au_0\Big|_0^t + \tau^2\int_0^t e^{(t-s)A}\widehat{\Psi}AB(I-\widehat{\Phi})(\tau A)^{-2}e^{sA}Au_0\,ds \\
&\quad - \tau^2\int_0^t e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})(\tau A)^{-2}e^{(s-\sigma)A}ABu(\sigma)\Big|_0^s ds \\
&\quad + \tau^2\int_0^t\int_0^s e^{(t-s)A}\widehat{\Psi}B(I-\widehat{\Phi})(\tau A)^{-2}e^{(s-\sigma)A}ABu'(\sigma)\,d\sigma\,ds.
\end{aligned}$$

By (2.2), (2.5), (3.8), (4.4), and (4.3) we obtain $\|I_2(t)\| \leqslant C\tau^2$, where C depends on C_{inv}, $\|G\|$, K, M_1, M_4, and t_{end}. Hence, we have

$$\|u(t)-\widetilde{u}(t)\| = \left\| I_1(t) + I_2(t) + \int_0^t e^{(t-s)A}\widetilde{B}(u-\widetilde{u})\,ds \right\| \leqslant C\tau^2 + \int_0^t \beta\,\|u(s)-\widetilde{u}(s)\|\,ds$$

with

$$\beta = C_{\text{inv}}\,\|G\|\,M_1^2 \geqslant \left\|\widetilde{B}\right\|. \tag{4.5}$$

An application of Gronwall's Lemma proves the desired result. □

We finally show that the solution of the averaged problem (3.7) inherits the finite-energy condition (2.3) of the original problem.

LEMMA 4.1 Let the assumption (3.8b) and the finite-energy condition (2.3) be fulfilled. Then the solution $\widetilde{u}$ of the averaged system (3.7) satisfies the finite-energy condition

$$\|A\widetilde{u}(t)\| \leqslant \widetilde{K}, \qquad 0 \leqslant t \leqslant t_{\text{end}}, \tag{4.6}$$

where $\widetilde{K}$ depends only on C_{inv}, $\|G\|$, K, M_1, and t_{end}.

Proof. Using (2.5) and the variation of constants formula (4.1b) yields

$$\|A\widetilde{u}(t)\| \leqslant \|Au_0\| + \int_0^t \|A\widetilde{B}\|\,\|A^{-1}\|\,\|A\widetilde{u}(s)\|\,ds.$$

By definition (3.3) and (3.8b) it holds

$$\|A\widetilde{B}\| = \|\widetilde{G}\| \leqslant M_1^2\|G\|, \tag{4.7}$$

and the statement thus follows from (2.2) and Gronwall's Lemma. □

5. Finite-time error analysis of the splitting scheme

In this section we finally study the error of the splitting scheme. We use the notation

$$S = e^{\frac{\tau}{2}\widetilde{B}} e^{\tau A} e^{\frac{\tau}{2}\widetilde{B}}$$

defined in (3.6) for the numerical flow over a time step τ and

$$T = e^{\tau(A+\widetilde{B})}$$

for the exact flow of the averaged equation (3.7). By (3.3) and (3.5) we have

$$\max\left\{\|e^{\theta\widetilde{B}}\|, \|Ae^{\theta\widetilde{B}}A^{-1}\|\right\} \leqslant 1+\theta\beta \leqslant e^{\theta\beta} \tag{5.1}$$

for $\theta \geqslant 0$ with β from (4.5). Together with (2.5), this provides the stability estimate

$$\|S^n\| \leqslant (1+\tfrac{\tau}{2}\beta)^{2n} \leqslant e^{\beta t_{\mathrm{end}}}, \qquad 0 \leqslant t_n \leqslant t_{\mathrm{end}}. \tag{5.2}$$

We next consider the local error.

LEMMA 5.1 (Local error) Assume that the filter functions are bounded as stated in (3.8b) and (3.8c). If the finite-energy condition (4.6) holds true, then the local error at time $t_n = n\tau$, $0 \leqslant t_n \leqslant t_{\mathrm{end}} - \tau$, of the splitting method (3.6) as an approximation to the averaged system (3.7) is given by

$$\delta_n = (S-T)\widetilde{u}(t_n) = \widehat{\delta}_n + D_n,$$

where

$$\widehat{\delta}_n = \frac{1}{2}\int_0^\tau \int_0^\xi \int_0^\theta e^{(\xi-\sigma)A} L e^{(\sigma+\tau-\xi)A}\widetilde{u}(t_n)\, d\sigma\, d\theta\, d\xi, \qquad L = A^2\widetilde{B} + \widetilde{B}A^2, \tag{5.3}$$

and $\|D_n\| \leqslant C\tau^3$. The constant C depends on C_{inv}, $\|G\|$, $\widetilde{K}$, M_1, M_2, and t_{end}.

Proof. We start with the following representation of the local error

$$\begin{aligned}\delta_n &= \int_0^\tau \frac{d}{d\xi}\left(e^{\frac{\xi}{2}\widetilde{B}} e^{\xi A} e^{\frac{\xi}{2}\widetilde{B}} e^{(\tau-\xi)(A+\widetilde{B})}\right)\widetilde{u}(t_n)\, d\xi \\ &= \frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\left(\left[\widetilde{B}, e^{\xi A}\right] e^{\frac{\xi}{2}\widetilde{B}} + 2e^{\xi A}\left[A, e^{\frac{\xi}{2}\widetilde{B}}\right]\right) e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\, d\xi,\end{aligned} \tag{5.4}$$

where $[A_1, A_2] = A_1A_2 - A_2A_1$ denotes the commutator of two matrices A_1 and A_2. The commutators in δ_n are written as integrals

$$\left[\widetilde{B}, e^{\xi A}\right] = \int_0^\xi \frac{d}{d\theta}\left(e^{(\xi-\theta)A}\widetilde{B}e^{\theta A}\right) d\theta = -\int_0^\xi e^{(\xi-\theta)A}\left[A, \widetilde{B}\right] e^{\theta A}\, d\theta$$

and

$$\left[A, e^{\frac{\xi}{2}\widetilde{B}}\right] = \int_0^\xi \frac{d}{d\theta}\left(e^{\frac{\xi-\theta}{2}\widetilde{B}} A e^{\frac{\theta}{2}\widetilde{B}}\right) d\theta = \frac{1}{2}\int_0^\xi e^{\frac{\xi-\theta}{2}\widetilde{B}}\left[A, \widetilde{B}\right] e^{\frac{\theta}{2}\widetilde{B}}\, d\theta.$$

This yields

$$\delta_n = \frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi \Big(-e^{(\xi-\theta)A}\left[A,\widetilde{B}\right]e^{\theta A}e^{\frac{\xi}{2}\widetilde{B}} + e^{\xi A}e^{\frac{\xi-\theta}{2}\widetilde{B}}\left[A,\widetilde{B}\right]e^{\frac{\theta}{2}\widetilde{B}}\Big)e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\theta\,d\xi.$$

We add and subtract the term $e^{\xi A}[A,\widetilde{B}]e^{\frac{\xi}{2}\widetilde{B}}$ inside the brackets, and the local error can be split into $\delta_n = \delta_n^{(1)} + D_n^{(1)}$ where

$$\delta_n^{(1)} = \frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi \Big(e^{\xi A}\left[A,\widetilde{B}\right] - e^{(\xi-\theta)A}\left[A,\widetilde{B}\right]e^{\theta A}\Big)e^{\frac{\xi}{2}\widetilde{B}}e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\theta\,d\xi, \tag{5.5a}$$

$$D_n^{(1)} = \frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi e^{\xi A}\Big(e^{\frac{\xi-\theta}{2}\widetilde{B}}\left[A,\widetilde{B}\right]e^{\frac{\theta}{2}\widetilde{B}} - \left[A,\widetilde{B}\right]e^{\frac{\xi}{2}\widetilde{B}}\Big)e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\theta\,d\xi. \tag{5.5b}$$

The term in brackets in (5.5a) can be written as

$$\begin{aligned} e^{\xi A}\left[A,\widetilde{B}\right] - e^{(\xi-\theta)A}\left[A,\widetilde{B}\right]e^{\theta A} &= -\int_0^\theta \frac{d}{d\sigma}\Big(e^{(\xi-\sigma)A}\left[A,\widetilde{B}\right]e^{\sigma A}\Big)\,d\sigma \\ &= \int_0^\theta e^{(\xi-\sigma)A}\left[A,\left[A,\widetilde{B}\right]\right]e^{\sigma A}\,d\sigma. \end{aligned}$$

For the double commutator we have

$$\left[A,\left[A,\widetilde{B}\right]\right] = L - R, \qquad L = A^2\widetilde{B} + \widetilde{B}A^2, \qquad R = 2A\widetilde{B}A,$$

and we split $\delta_n^{(1)}$ accordingly into $\delta_n^{(1)} = \delta_n^{(2)} + D_n^{(2)}$ with

$$\begin{aligned} \delta_n^{(2)} &= \frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}Le^{\sigma A}e^{\frac{\xi}{2}\widetilde{B}}e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\sigma\;d\theta\,d\xi, \\ D_n^{(2)} &= -\frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}Re^{\sigma A}e^{\frac{\xi}{2}\widetilde{B}}e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\sigma\,d\theta\,d\xi. \end{aligned}$$

To extract the term $\widehat{\delta}_n$ defined in (5.3) from $\delta_n^{(2)}$ we use (3.5) and once more the variation-of-constants formula to obtain

$$\delta_n^{(2)} = \widehat{\delta}_n + D_n^{(3)} + D_n^{(4)} + D_n^{(5)},$$

where

$$\begin{aligned} D_n^{(3)} &= \frac{1}{2}\int_0^\tau\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}Le^{\sigma A}\int_0^{\tau-\xi}e^{(\tau-\xi-\nu)A}\widetilde{B}e^{\nu(A+\widetilde{B})}\,\widetilde{u}(t_n)\,d\nu\,d\sigma\,d\theta\,d\xi, \\ D_n^{(4)} &= \frac{1}{4}\int_0^\tau\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}Le^{\sigma A}\xi\widetilde{B}e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\sigma\,d\theta\,d\xi, \\ D_n^{(5)} &= \frac{1}{4}\int_0^\tau\xi\widetilde{B}\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}Le^{\sigma A}e^{\frac{\xi}{2}\widetilde{B}}e^{(\tau-\xi)(A+\widetilde{B})}\widetilde{u}(t_n)\,d\sigma\,d\theta\,d\xi. \end{aligned}$$

In this way, we end up with the decomposition

$$\delta_n = \widehat{\delta}_n + D_n, \qquad D_n = D_n^{(1)} + D_n^{(2)} + D_n^{(3)} + D_n^{(4)} + D_n^{(5)}$$

of the local error.

To prove the statement of the lemma, we have to estimate the terms $D_n^{(i)}$, $i=1,\ldots,5$. The properties (2.2), (3.8b), (3.8c), (4.4), and (4.7) imply that

$$\|RA^{-1}\| = 2\|A\widetilde{B}\| \leqslant 2M_1^2\|G\|, \tag{5.6a}$$
$$\big\|\tau LA^{-1}\big\| = \Big\|\tau AA\widetilde{B}A^{-1} + \tau\widetilde{B}A\Big\| = \Big\|\big(\tau A\widehat{\Psi}\big)\big(AB\big)\widehat{\Phi}A^{-1} + \widehat{\Psi}B\big(\widehat{\Phi}\tau A\big)\Big\| \leqslant 2C_{\text{inv}}M_1M_2\|G\|, \tag{5.6b}$$

where we use the notation (4.2). Writing

$$D_n^{(2)} = -\frac{1}{2}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}\big(RA^{-1}\big)e^{\sigma A}\big(Ae^{\frac{\xi}{2}\widetilde{B}}A^{-1}\big)A\widetilde{u}(t_n+\tau-\xi)\,d\sigma\,d\theta\,d\xi,$$
$$D_n^{(3)} = \frac{1}{2\tau}\int_0^\tau\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}\big(\tau LA^{-1}\big)e^{\sigma A}\int_0^{\tau-\xi} e^{(\tau-\xi-\nu)A}\big(A\widetilde{B}\big)A^{-1}A\widetilde{u}(t_n+\nu)\,d\nu\,d\sigma\,d\theta\,d\xi,$$
$$D_n^{(4)} = \frac{1}{4\tau}\int_0^\tau \xi\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}\big(\tau LA^{-1}\big)e^{\sigma A}\big(A\widetilde{B}\big)A^{-1}A\widetilde{u}(t_n+\tau-\xi)\,d\sigma\,d\theta\,d\xi,$$
$$D_n^{(5)} = \frac{1}{4\tau}\int_0^\tau \xi\widetilde{B}\int_0^\xi\int_0^\theta e^{(\xi-\sigma)A}\big(\tau LA^{-1}\big)e^{\sigma A}\big(Ae^{\frac{\xi}{2}\widetilde{B}}A^{-1}\big)A\widetilde{u}(t_n+\tau-\xi)\,d\sigma\,d\theta\,d\xi,$$

the above estimates (5.6) and the bounds (2.2), (2.5), (4.5), (4.6), (4.7), and (5.1) yield

$$\big\|D_n^{(2)}\big\| \leqslant \tfrac{1}{6}e^{\tau\beta}\,\|G\|\,M_1^2\widetilde{K}\,\tau^3, \qquad \big\|D_n^{(3)}\big\| \leqslant \tfrac{1}{24}C_{\text{inv}}^2M_1^3M_2\,\|G\|^2\,\widetilde{K}\,\tau^3,$$
$$\big\|D_n^{(4)}\big\| \leqslant \tfrac{1}{16}C_{\text{inv}}^2M_1^3M_2\,\|G\|^2\,\widetilde{K}\,\tau^3, \qquad \big\|D_n^{(5)}\big\| \leqslant \tfrac{1}{16}\beta e^{\tau\beta}C_{\text{inv}}M_1M_2\,\|G\|\,\widetilde{K}\,\tau^3.$$

It remains to bound the integral $D_n^{(1)}$ defined in (5.5b). Using the representation

$$\begin{aligned} e^{\frac{\xi-\theta}{2}\widetilde{B}}\Big[A,\widetilde{B}\Big]e^{\frac{\theta}{2}\widetilde{B}} - \Big[A,\widetilde{B}\Big]e^{\frac{\xi}{2}\widetilde{B}} &= \int_\theta^\xi \frac{d}{d\nu}\Big(e^{\frac{\nu-\theta}{2}\widetilde{B}}\Big[A,\widetilde{B}\Big]e^{\frac{\theta-\nu}{2}\widetilde{B}}\Big)e^{\frac{\xi}{2}\widetilde{B}}\,d\nu \\ &= \frac{1}{2}\int_\theta^\xi e^{\frac{\nu-\theta}{2}\widetilde{B}}\Big[\widetilde{B},\Big[A,\widetilde{B}\Big]\Big]e^{\frac{\xi+\theta-\nu}{2}\widetilde{B}}\,d\nu, \end{aligned}$$

we can write

$$D_n^{(1)} = \frac{1}{4}\int_0^\tau e^{\frac{\xi}{2}\widetilde{B}}\int_0^\xi e^{\xi A}\int_\theta^\xi e^{\frac{\nu-\theta}{2}\widetilde{B}}\Big[\widetilde{B},\Big[A,\widetilde{B}\Big]\Big]A^{-1}\Big(Ae^{\frac{\xi+\theta-\nu}{2}\widetilde{B}}A^{-1}\Big)A\widetilde{u}(t_n+\tau-\xi)\,d\nu\,d\theta\,d\xi.$$

For the double commutator we get from (2.2) and (4.7)

$$\Big\|\Big[\widetilde{B},\Big[A,\widetilde{B}\Big]\Big]A^{-1}\Big\| = \big\|2\widetilde{B}A\widetilde{B}A^{-1} - \widetilde{B}^2 - A\widetilde{B}^2A^{-1}\big\| \leqslant 4C_{\text{inv}}^2M_1^4\|G\|^2,$$

which yields with (2.5) and (5.1)

$$\Big\|D_n^{(1)}\Big\| \leqslant \tfrac{1}{24}e^{\tau\beta}\widetilde{K}\,\Big\|\Big[\widetilde{B},\Big[A,\widetilde{B}\Big]\Big]A^{-1}\Big\|\,\tau^3 \leqslant \tfrac{1}{6}e^{\tau\beta}C_{\text{inv}}^2M_1^4\,\|G\|^2\,\widetilde{K}\tau^3.$$

The assertion now follows from $D_n = D_n^{(1)} + D_n^{(2)} + D_n^{(3)} + D_n^{(4)} + D_n^{(5)}$. □

We now investigate the local error further.

LEMMA 5.2 The dominating part $\widehat{\delta}_n$ of the local error δ_n defined in (5.3) satisfies

$$\widehat{\delta}_n = \widehat{\delta}_n^{(1)} + \widehat{\delta}_n^{(2)}, \qquad \widehat{\delta}_n^{(1)} = A\widehat{\Psi} Z_1 \widetilde{u}(t_n), \qquad \widehat{\delta}_n^{(2)} = Z_2 \widehat{\Phi} A^2 \widetilde{u}(t_n),$$

where

$$\|Z_1\| \leqslant \tfrac{1}{12} M_1 \|G\| \tau^3, \qquad \|Z_2\| \leqslant \tfrac{1}{12} C_{\mathrm{inv}} M_1 \|G\| \tau^3, \qquad \|AZ_2\| \leqslant \tfrac{1}{12} M_1 \|G\| \tau^3.$$

Proof. The matrix L can be written as

$$L = (A\widehat{\Psi})AB\widehat{\Phi} + \widehat{\Psi} B \widehat{\Phi} A^2,$$

since $\widetilde{B} = \widehat{\Psi} B \widehat{\Phi}$ with the notation (4.2). Since the filter functions Ψ_S and Φ are independent of the integration variables, we have by (5.3)

$$\widehat{\delta}_n = A\widehat{\Psi} Z_1 \widetilde{u}(t_n) + Z_2 \widehat{\Phi} A^2 \widetilde{u}(t_n),$$

where

$$Z_1 = \frac{1}{2} \int_0^\tau \int_0^\xi \int_0^\theta e^{(\xi-\sigma)A} AB\widehat{\Phi} e^{(\sigma+\tau-\xi)A}\, d\sigma\, d\theta\, d\xi,$$
$$Z_2 = \frac{1}{2} \int_0^\tau \int_0^\xi \int_0^\theta e^{(\xi-\sigma)A} \widehat{\Psi} B e^{(\sigma+\tau-\xi)A}\, d\sigma\, d\theta\, d\xi.$$

The desired bounds now follow immediately from (2.2), (2.5), (3.8a), and (4.4). □

Although the matrices Z_1, Z_2, and AZ_2 contain a factor of τ^3 this is not sufficient to use a standard Lady Windermere's fan argument to prove that the global error is of second order. The reason are the additional factors of A in $\widehat{\delta}_n^{(1)}$ and $\widehat{\delta}_n^{(2)}$ which would yield a constant depending on $\|\Omega\|$. The proof of the following result treats the two terms defined in Lemma 5.2 separately in an appropriate way by using summation by parts.

THEOREM 5.1 (Global error of the averaged problem) Let the assumptions (3.8) and the finite-energy condition (4.6) be fulfilled. Then the global error of the splitting scheme (3.6) as an approximation to the solution of the averaged system (2.4) is bounded by

$$\|u_n - \widetilde{u}(t_n)\| \leqslant C\tau^2, \qquad 0 \leqslant t_n = n\tau \leqslant t_{\mathrm{end}}, \tag{5.7}$$

where C only depends on C_{inv}, $\|G\|$, $\widetilde{K}$, M_j, $j = 1,2,3$, and t_{end}.

Proof. By a telescopic identity, the global error can be written as

$$\widetilde{e}_n = u_n - \widetilde{u}(t_n) = (S^n - T^n)u_0 = \sum_{j=0}^{n-1} S^{n-j-1}(S-T)T^j u_0 = \sum_{j=0}^{n-1} S^{n-j-1}\delta_j$$

with the local errors δ_j of Lemma 5.1. Lemmas 5.1 and 5.2 motivate to split the error into

$$\widetilde{e}_n = \widetilde{e}_n^{(1)} + \widetilde{e}_n^{(2)} + \widetilde{e}_n^{(3)}, \tag{5.8}$$

where

$$\widetilde{e}_n^{(1)} = \sum_{j=0}^{n-1} S^{n-j-1} \widehat{\delta}_j^{(1)}, \qquad \widetilde{e}_n^{(2)} = \sum_{j=0}^{n-1} S^{n-j-1} \widehat{\delta}_j^{(2)}, \qquad \widetilde{e}_n^{(3)} = \sum_{j=0}^{n-1} S^{n-j-1} D_j.$$

From the stability bound (5.2) and $\|D_j\| \leqslant C\tau^3$ by Lemma 5.1 we thus obtain

$$\left\|\widetilde{e}_n^{(3)}\right\| = \left\|\sum_{j=0}^{n-1} S^{n-j-1} D_j\right\| \leqslant C\tau^2 (n\tau) e^{\beta t_{\mathrm{end}}} \leqslant C\tau^2.$$

To bound $\widetilde{e}_n^{(1)}$ and $\widetilde{e}_n^{(2)}$ we write $\tau A \widehat{\chi}$ for $\widehat{\chi} = \widehat{\Phi}$ and $\widehat{\chi} = \widehat{\Psi}$ (see (4.2)) as

$$\tau A \widehat{\chi} = \tau \widehat{\chi} A = (e^{\tau A} - I)\widehat{\Theta}_\chi = \widehat{\Theta}_\chi (e^{\tau A} - I) \tag{5.9}$$

with

$$\widehat{\Theta}_\chi = \widehat{\theta}_\chi(\tau\Omega), \qquad \widehat{\theta}_\chi(x) = \frac{1}{2}\begin{bmatrix} \cot(\frac{x}{2}) & -1 \\ 1 & \cot(\frac{x}{2}) \end{bmatrix}\begin{bmatrix} x\chi(x) & 0 \\ 0 & x\chi(x) \end{bmatrix}.$$

This representation follows from the identities

$$\sin(x) = \cot(\tfrac{x}{2})\big(1 - \cos(x)\big) \qquad \text{and} \qquad \cos(x) + 1 = \cot(\tfrac{x}{2})\sin(x).$$

Note that by assumptions (3.8c) and (3.8d) on the filter functions χ we have

$$\left\|\widehat{\Theta}_\chi\right\| \leqslant C. \tag{5.10}$$

Next we use summation by parts. With

$$E_j = \sum_{k=0}^{j-1} S^k, \qquad F_j = \sum_{k=0}^{j-1} T^k,$$

it holds

$$\widetilde{e}_n^{(1)} = E_n \widehat{\delta}_0^{(1)} + \sum_{j=0}^{n-2} E_{n-j-1}\big(\widehat{\delta}_{j+1}^{(1)} - \widehat{\delta}_j^{(1)}\big).$$

Using Lemma 5.2 and (5.9) to replace $\widehat{\delta}_j^{(1)}$ by $(e^{\tau A} - I)\widehat{\Theta}_\psi \frac{1}{\tau} Z_1 T^j u_0$, this implies

$$\widetilde{e}_n^{(1)} = E_n (e^{\tau A} - I)\widehat{\Theta}_\psi \tfrac{1}{\tau} Z_1 u_0 + \sum_{j=0}^{n-2} E_{n-j-1}(e^{\tau A} - I)\widehat{\Theta}_\psi Z_1 \tfrac{1}{\tau}(T - I)T^j u_0. \tag{5.11}$$

Now we estimate the matrices in this expression. The matrices $\widehat{\Theta}_\psi$ and Z_1 can be estimated with (5.10) and Lemma 5.2, respectively. To bound $E_{n-j-1}(e^{\tau A} - I)$ in (5.11), we start from

$$E_j(e^{\tau A} - I) = E_j(e^{\tau A} - S) + E_j(S - I) = E_j(e^{\tau A} - S) + S^j - I,$$

and we use the stability bound (5.2) and $\|e^{\tau A} - S\| \leqslant C\tau$ by (2.5), (3.5), and (5.1) to show that

$$\left\|E_j(e^{\tau A} - I)\right\| \leqslant C.$$

To bound $\frac{1}{\tau}(T - I)T^j u_0$ in (5.11), we start from

$$\begin{aligned} \tfrac{1}{\tau}(T - I)T^j u_0 &= \tfrac{1}{\tau}(e^{\tau A} - I)T^j u_0 + \tfrac{1}{\tau}(T - e^{\tau A})T^j u_0 \\ &= (e^{\tau A} - I)(\tau A)^{-1} A\widetilde{u}(t_j) + \frac{1}{\tau}\int_0^\tau e^{(\tau-\xi)A}\widetilde{B}A^{-1}A\widetilde{u}(t_j + \xi)\, d\xi \end{aligned}$$

by the variation-of-constants formula (4.1b), and we use (2.2), the finite-energy condition (4.6) and $\|(e^{\tau A}-I)(\tau A)^{-1}\| = \|\int_0^1 e^{\sigma\tau A} d\sigma\| \leqslant 1$ by (2.5) to show that

$$\left\|\tfrac{1}{\tau}(T-I)T^j u_0\right\| \leqslant C.$$

This yields the estimate $\|\widetilde{e}_n^{(1)}\| \leqslant C\tau^2$ for (5.11) since $\|Z_1\| \leqslant C\tau^3$ by Lemma 5.2.

Analogously, we have by Lemma 5.2 and (5.9)

$$\widetilde{e}_n^{(2)} = \tfrac{1}{\tau} Z_2 \widehat{\Theta}_\phi A(e^{\tau A}-I)F_n u_0 + \sum_{j=0}^{n-2} S^j \tfrac{1}{\tau}(S-I)Z_2\widehat{\Theta}_\phi A(e^{\tau A}-I)F_{n-j-1}u_0.$$

Using the variation-of-constants formula (4.1b) yields

$$\begin{aligned} A(e^{\tau A}-I)F_j u_0 &= A(e^{\tau A}-T)F_j u_0 + A(T^j - I)u_0 \\ &= -\int_0^\tau e^{(\tau-\xi)A} A\widetilde{B} e^{\xi(A+\widetilde{B})} F_j u_0 \, d\xi + A(\widetilde{u}(t_j) - u_0). \end{aligned}$$

The finite-energy condition (4.6) shows

$$\left\|\tau e^{\xi(A+\widetilde{B})} F_j u_0\right\| = \left\|\tau \sum_{k=0}^{j-1} \widetilde{u}(t_k+\xi)\right\| \leqslant t_{\mathrm{end}} C_{\mathrm{inv}} \widetilde{K}.$$

By (4.7) we thus obtain

$$\left\|A(e^{\tau A}-I)F_j u_0\right\| \leqslant C.$$

Moreover, by Lemma 5.2 we have

$$\left\|\tfrac{1}{\tau}(S-I)Z_2\right\| \leqslant \left\|\tfrac{1}{\tau}(S-e^{\tau A})Z_2\right\| + \left\|(e^{\tau A}-I)(\tau A)^{-1} A Z_2\right\| \leqslant C\tau^3$$

since $\|S-e^{\tau A}\| \leqslant C\tau$ and $\|(e^{\tau A}-I)(\tau A)^{-1}\| \leqslant 1$. Together with the stability estimate (5.2) and the bound (5.10), this proves $\|\widetilde{e}_n^{(2)}\| \leqslant C\tau^2$ and thus (5.7) by (5.8). □

REMARK. It is also possible to prove Theorem 5.1 if (5.3) in Lemma 5.1 is replaced by the representation of the local error which has been derived in (Jahnke & Lubich, 2000, Theorem 2.1). While they used quadrature errors to bound the local error, we used the fundamental theorem of calculus as in (5.4). An advantage of the new representation is that $\|G\|$ appears only quadratically in the bounds, while it appears cubically in Jahnke & Lubich (2000). We also believe, that the representation (5.3) is more suitable for a future extension of our approach to nonlinear problems.

6. Discussion and comparison

Error bounds for trigonometric integrators applied to second-order oscillatory differential equations have been previously derived in Grimm & Hochbruck (2006) and, for the case of a single high frequency, in Theorems XIII.4.1 and XIII.4.2 of Hairer *et al.* (2006). They differ from the error bounds of the present paper (Theorem 3.2) in their statement, in the required assumptions on the filter functions and, most notably, in the technique of proof.

The difference in the statement concerns the error bound for the velocities. While the error bounds of Grimm & Hochbruck (2006) and Hairer *et al.* (2006) for the velocities q' are of first order in τ, the error bound of Theorem 3.2 (in the linear case) is of second order in the rescaled velocities $\Omega^{-1}q'$. For small time step-sizes $\tau\|\Omega\| = O(1)$, the latter bound implies the former.

Besides this difference in the statement, there are differences in the assumptions on the filter functions. The splitting method (3.6) with filter functions ϕ and ψ_S coincides with the trigonometric integrator in Grimm & Hochbruck (2006) and Hairer *et al.* (2006) if the filter functions ϕ, ψ, ψ_1, and ψ_0 in Grimm & Hochbruck (2006) and Hairer *et al.* (2006) are chosen in the following way:

$$\phi = \phi, \qquad \psi_1 = \psi_S, \qquad \psi = \operatorname{sinc}(\cdot)\psi_S, \qquad \psi_0 = \cos(\cdot)\psi_S.$$

Now, we can compare the conditions $(11)-(16)$ in Grimm & Hochbruck (2006) and the conditions (XIII.4.1) and (XIII.4.8) in Hairer *et al.* (2006) to our conditions (3.8). Our condition (3.8b) on the boundedness of the filter functions coincides identically with (11) of Grimm & Hochbruck (2006). The conditions $(13)-(16)$ of Grimm & Hochbruck (2006) imply that $\chi = \phi$ and $\chi = \psi_S$ are zero whenever $\sin(\frac{\cdot}{2})$ is zero, meaning for $x = 2k\pi$, $k \in \mathbb{Z}$. This behaviour can also be found in our condition (3.8d). Still, an analogon to our condition (3.8c) is missing in Grimm & Hochbruck (2006) since this condition requires that χ decreases at least like x^{-1} for $x \to \infty$. In comparison to Hairer *et al.* (2006), our conditions (3.8b)–(3.8d) are implied by the conditions (XIII.4.1) and (XIII.4.8) used there, which require in particular that $|\chi(x)|$ and $|x\sin(\frac{1}{2}x)^{-1}\chi(x)|$ are bounded. Note that all sets of conditions are proven to be sufficient but not necessary.

But the main difference in comparison to Grimm & Hochbruck (2006) and Hairer *et al.* (2006) is the technique of proof. It will be interesting to see whether the technique developed in the present paper, namely a Lady Windermere's fan that takes cancellations in the error accumulation into account, can help to gain further insight into the error behaviour of trigonometric integrators and splitting methods, in particular for nonlinear problems.

Acknowledgements

The authors thank Roland Schnaubelt for helpful discussions on the representation of the local error.

We gratefully acknowledge financial support by the Deutsche Forschungsgemeinschaft (DFG) through RTG 1294, CRC 1114, CRC 1173, and project GA 2073/2-1.

REFERENCES

BLANES, S. & CASAS, F. (2016) *A concise introduction to geometric numerical integration*. A Chapman & Hall book: Monographs and research notes in mathematics. Boca Raton: CRC Press.

COHEN, D., GAUCKLER, L., HAIRER, E. & LUBICH, C. (2015) Long-term analysis of numerical integrators for oscillatory Hamiltonian systems under minimal non-resonance conditions. *BIT*, **55**, 705–732.

EINKEMMER, L. & OSTERMANN, A. (2014) Convergence analysis of Strang splitting for Vlasov-type equations. *SIAM J. Numer. Anal.*, **52**, 140–155.

EINKEMMER, L. & OSTERMANN, A. (2015) Overcoming order reduction in diffusion-reaction splitting. Part 1: Dirichlet boundary conditions. *SIAM J. Sci. Comput.*, **37**, A1577–A1592.

FAOU, E. (2012) *Geometric numerical integration and Schrödinger equations*. Zurich Lectures in Advanced Mathematics. Zürich: European Mathematical Society (EMS), pp. xiii+138.

FAOU, E., OSTERMANN, A. & SCHRATZ, K. (2015) Analysis of exponential splitting methods for inhomogeneous parabolic equations. *IMA J. Numer. Anal.*, **35**, 161–178.

GARCÍA-ARCHILLA, B., SANZ-SERNA, J. M. & SKEEL, R. D. (1999) Long-time-step methods for oscillatory differential equations. *SIAM J. Sci. Comput.*, **20**, 930–963.

GAUCKLER, L. (2015) Error analysis of trigonometric integrators for semilinear wave equations. *SIAM J. Numer. Anal.*, **53**, 1082–1106.

GRIMM, V. & HOCHBRUCK, M. (2006) Error analysis of exponential integrators for oscillatory second-order differential equations. *J. Phys. A*, **39**, 5495–5507.

GRIMM, V. & HOCHBRUCK, M. (2008) Rational approximation to trigonometric operators. *BIT*, **48**, 215–229.

HAIRER, E., LUBICH, C. & WANNER, G. (2006) *Geometric numerical integration : structure-preserving algorithms for ordinary differential equations*. Springer series in computational mathematics ; 31, 2. ed. edn. Berlin: Springer.

HANSEN, E. & OSTERMANN, A. (2009) Exponential splitting for unbounded operators. *Math. Comp.*, **78**, 1485–1496.

HOCHBRUCK, M., JAHNKE, T. & SCHNAUBELT, R. (2015) Convergence of an ADI splitting for Maxwell's equations. *Numer. Math.*, **129**, 535–561.

HOCHBRUCK, M. & LUBICH, C. (1999) A Gautschi-type method for oscillatory second-order differential equations. *Numer. Math.*, **83**, 403–426.

HOLDEN, H., KARLSEN, K. H., LIE, K.-A. & RISEBRO, N. H. (2010) *Splitting methods for partial differential equations with rough solutions*. EMS Series of Lectures in Mathematics. Zürich: European Mathematical Society (EMS), pp. viii+226. Analysis and MATLAB programs.

HOLDEN, H., LUBICH, C. & RISEBRO, N. H. (2013) Operator splitting for partial differential equations with Burgers nonlinearity. *Math. Comp.*, **82**, 173–185.

HUNDSDORFER, W. H. & VERWER, J. G. (2007) *Numerical solution of time dependent advection diffusion reaction equations*. Springer series in computational mathematics ; 33, corr. 2. print. edn. Berlin: Springer.

JAHNKE, T. & LUBICH, C. (2000) Error bounds for exponential operator splittings. *BIT*, **40**, 735–744.

KOCH, O. & LUBICH, C. (2011) Variational-splitting time integration of the multi-configuration time-dependent Hartree-Fock equations in electron dynamics. *IMA J. Numer. Anal.*, **31**, 379–395.

LUBICH, C. (2008) On splitting methods for Schrödinger-Poisson and cubic nonlinear Schrödinger equations. *Math. Comp.*, **77**, 2141–2153.

MCLACHLAN, R. I. & QUISPEL, G. R. W. (2002) Splitting methods. *Acta Numerica*, **11**, 341–434.

STRANG, G. (1968) On the construction and comparison of difference schemes. *SIAM Journal on Numerical Analysis*, **5**, 506–517.

THALHAMMER, M., CALIARI, M. & NEUHAUSER, C. (2009) High-order time-splitting Hermite and Fourier spectral methods. *J. Comput. Phys.*, **228**, 822–832.