Effective highly accurate integrators for linear Klein-Gordon equations from low to high frequency regimes

Karolina Kropielnicka, Karolina Lademann, Katharina Schratz

We introduce an efficient class of numerical schemes for the Klein–Gordon equation which are highly accurate from slowly varying up to highly oscillatory regimes. Their construction is based on Magnus expansions tailored to the structure of the input term which allows us to resolve the oscillations in the system up to second order convergence in time uniformly in all frequencies $\omega_n$. Depending on the nature of the oscillatory term, the proposed methods even show superior convergence, reaching up to fourth order convergence, while maintaining high efficiency and small error constants. Numerically experiments highlight our theoretical findings and underline the efficiency of the new schemes.

---

* Institute of Mathematics, Polish Academy of Sciences, Antoniego Abrahama 18, Sopot, Poland
  kkropielnicka@impan.pl

* Institute of Mathematics, University of Gdańsk, Wita Stwosza 57, Gdańsk, Poland
  karolina.lademann@phdstud.ug.edu.pl

* Laboratoire Jacques-Louis Lions, Sorbonne Université, 4 place Jussieu, Paris, France
  katharina.schratz@sorbonne-universite.fr
I. Introduction

We consider the linear Klein-Gordon equation

$$\partial_t^2 \psi(x, t) = \Delta \psi(x, t) + f(x, t) \psi(x, t)$$

(1)

with initial condition $\psi(x, 0) = \psi_0(x)$ equipped with periodic boundary conditions (that is $x \in \mathbb{T}^d$). Here, $f(x, t)$ is a given periodic function under the form

$$f(x, t) = \alpha(x, t) + \sum_n a_n(x, t)e^{i\omega_n t},$$

(2)

where $\omega_n \in \Omega \subset \mathbb{R}$, $\omega_{\min} = \inf\{|\omega_n|; \; \omega_n \in \Omega\} \geq 1$ and $\omega_{\max} = \sup\{|\omega_n|; \; \omega_n \in \Omega\}$. The input term $f(x, t)$ includes the case of non-oscillatory input terms $\alpha(x, t)$, or purely oscillatory input terms of type

$$\sum_n a_n(x, t)e^{i\omega_n t},$$

as well as the combination of the two. It is enough to assume smoothness of the functions $\alpha$ and $a_n$. For the precise assumptions on system (1) we refer to Section III.

Linear and nonlinear Klein-Gordon equations have recently gained a lot attention in computational mathematics, see for instance [2, 4, 6, 14, 15], and the references therein. The highly oscillatory case $\omega \gg 1$ is thereby particularly challenging as classical methods in general fail to resolve the underlying oscillatory structure of the solution which leads to large errors and huge computational costs. Up to our knowledge there are only two publications devoted to computational approaches in case of space- and time-dependent input terms. Namely, fourth and sixth order splittings proposed in [1] which are based on commutator-free, Magnus type expansions. The latter perform very well in non-oscillatory regimes, however, introduce large error constants in case of high frequencies $\omega \gg 1$. The recent work [5], on the other hand, proposes a method specialized to highly oscillatory input terms, however, drastically fails in non-oscillatory regimes where $\omega \sim 1$.

The aim of this paper lies in closing this gap. We present a new class of highly precise numerical methods which are computationally cheap and allow for small error constants which do not depend on the possibly large parameters $\omega_n$. Our new schemes in particular yield high order approximations for all values of frequencies (i.e., from low $|\omega_n| \sim 1$ up to high frequency regimes $|\omega_n| \gg 1$) uniformly in the time step size $h$ without imposing any CFL type condition. In case of highly oscillatory input terms with $\omega_{\min} \gg 1/h$ as well as slowly oscillatory input terms where $\omega_{\max} \ll 1/h$, our new methods in addition reach superior convergence allowing for 4-th order convergence (see also Figures 1-3). This favorable error behavior together with a rigours error analysis is the main novelty in this work. Note that if the input
term $\sum_n a_n(x, t)e^{i\omega_n t}$ involves several frequencies $\omega_1, \omega_2, \ldots$, reaching low up to extremely high values, the new schemes allow for a much smaller error constant than previously proposed methods. The latter is underlined in our numerical experiments in Section V. Our new schemes are based on a refined approximation of highly oscillatory quadratures which can be treated with any quadrature of choice including Filon methods. Note that classical methods for (1) introduce a time error of type $(h \cdot \omega_{\text{max}})^p$ leading to severe step size restrictions $h < \frac{1}{\omega_{\text{max}}}$, loss of convergence and huge computational costs. In contrast, the time (and spatial) step sizes in our new schemes can be chosen significantly larger than the high frequencies $\omega_{\text{max}}$ of the input term. The interplay between the oscillatory parameter $\omega$ and time step $h$ is illustrated in Figures 1-3. More precisely, depending on the speed of oscillations (see also Theorem 2) the local error scales like $O(h^5 + \min\{h^3, \frac{h^2}{\omega_{\text{min}}}, h^5\omega_{\text{max}}^2\})$ and like $O(\min\{h^3, \frac{h^2}{\omega_{\text{min}}}, h^5\omega_{\text{max}}^2\})$ for $\alpha(x, t) \equiv 0$, respectively.

Figure 1: The local error of the proposed numerical methods strongly depends on the oscillatory nature of input term and the ratio between the oscillations $|\omega_n| > 1$ and time step $h$. The left figure illustrates the accuracy obtained for the monochromatic case ($\omega_{\text{min}} = \omega_{\text{max}}$). The middle figure shows the dependency between the fastest frequency $\omega_{\text{max}}$ and time step $h$, while the right figure illustrates the ratio between the slowest frequency $\omega_{\text{min}}$ and time step $h$. The final accuracy (presented in Figure 3) depends, however on both: $\omega_{\text{min}}$ and $\omega_{\text{max}}$. However, note that in all cases, local third order of convergence is guaranteed. In the above graphs we assume without loss of generality that $\alpha(x, t) \neq 0$.

Figure 2: The left figure illustrates the accuracy in regard of ratio between the fastest frequency $\omega_{\text{max}}$ and time step $h$, while the right figure illustrates the ratio between the slowest frequency $\omega_{\text{min}}$ and time step $h$. In all cases local third order of convergence is guaranteed. Unlikely in Figure 1 we assume here that $\alpha(x, t) = 0$. 

3
Figure 3: The left figure illustrates the accuracy obtained in the monochromatic case ($\omega_{\text{min}} = \omega_{\text{max}}$) and should be understood in the following way: for $\omega_{\text{min}} = h^{-\rho}$ the error of approximation scales like $O(h^{M})$, where $M = \max\{3, 2 + \rho, 5 - 2\rho\}$. The figure on the right hand side covers the case of multifrequencies, where for $\omega_{\text{min}} = h^{-\alpha}$, $\omega_{\text{max}} = h^{-\beta}$ the accuracy of the method is $O(h^{MF})$, and $MF = \max\{3, 2 + \alpha, 5 - 2\beta\}$.

Note that equation (1) is a special case of Klein-Gordon equation with atomic scaling $\hbar = c = 1$

$$(\partial_{t}^{2} - \mathcal{B}) \psi(x, t) = 0, \quad B := \Delta - m^{2},$$

where mass function $m^{2} = m^{2}(x, t)$ is time and space dependent. This type of Klein-Gordon equations with time dependent mass was first proposed by M. Znojil in [17], [18], as a significant contribution to the investigations presented in [13], [12] by Mostafazadeh. Due to Znojil’s improvement, not only non-negativity of probability density is assured but also Lorentz covariance of the interaction is not violated. Moreover, this type of equation can be extended to quantum cosmology, see [13], [16].

To illustrate the idea behind our method we will rewrite the Klein–Gordon equation (1) as follows. Let us set

$$A(x, t) = \begin{bmatrix} 0 & 1 \\ N(x, t) & 0 \end{bmatrix} \quad \text{and} \quad N(x, t) = \Delta + f(x, t).$$

Then, we can easily observe that (1) is equivalent to

$$\partial_{t}z(x, t) = A(x, t)z(x, t), \quad \text{where} \quad z(t, x) = \begin{bmatrix} \psi(x, t) \\ \frac{\partial}{\partial t} \psi(x, t) \end{bmatrix}.$$  

Analytical solutions of (5) can be presented for example as infinite Fer, Magnus or Dyson expansion. In this manuscript we base our analysis on truncation of Magnus series. Magnus expansions have been broadly studied, see, e.g., [3, 9, 10]. We need to be careful, however, because the special structure of our operator $A(x, t)$ defined in (4) causes
that odd components of Magnus expansion form anti-diagonal matrices while even components from diagonal ones and, needless to say, need to be treated separately. Similar structure of the operator $A(x, t)$ was analysed in [8]. The difference, however is in the function $f(x, t)$, which instead of being highly oscillatory like in our case, is growing to infinity along with time (in [8]). So the problem both in [8] and in our case is highly oscillatory, but the oscillations have a different source so require different approaches.

Unlike in [3, 8–10] we deal with Magnus expansion which components do not scale only in terms of time step $h = \Delta t$, but also in terms of the oscillation frequency $\omega$. In this paper we construct schemes which allow us to control these terms efficiently up to high order.

Outline of the paper. In Section II we will present the full derivation of the methods. Section II deals with rigorous estimates of the error terms, which were abandoned in the derivation of the schemes. In Section IV we provide the structure of error committed by the proposed schemes. In Section V we underline our theoretical findings with numerical experiments. In addition, we compare various existing methods with the new approach and highlight the behaviour of the new methods with respect to high frequencies $\omega$. Appendices A and B abound with calculations which may be of interest while reading Section III. In Appendix C we provide detailed derivations of 4-th order compact schemes (15) and (16).

II. Derivation of methods

A. Truncation of Magnus expansion

It is well known that the solution of (5) can be presented via an infinite Magnus series

$$z(x, t + h) = e^{\Theta(x, t + h, t)} z(x, t),$$

where $\Theta(x, t + h, t) = \sum_{k=1}^{\infty} \Theta_k(x, t + h, t)$, and $\Theta_k(x, t + h, t)$ are $k$-th times nested integrals of $(k - 1)$ times nested commutators. Below we write the first few terms of such an expansion,
\[ \Theta_1(x, t + h, t) = \int_0^h A(x, t + t_1)dt_1 \]  
\[ \Theta_2(x, t + h, t) = -\frac{1}{2} \int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] dt_2 dt_1 \]  
\[ \Theta_3(x, t + h, t) = \frac{1}{6} \int_0^h \int_0^{t_1} \int_0^{t_2} [A(x, t + t_1), [A(x, t + t_2), A(x, t + t_1)]] dt_3 dt_2 dt_1 + \frac{1}{6} \int_0^h \int_0^{t_1} \int_0^{t_2} [A(x, t + t_3), [A(x, t + t_2), A(x, t + t_1)]] dt_3 dt_2 dt_1 \]  
\[ \Theta_4(x, t + h, t) = \frac{1}{12} \int_0^h \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} [[[A(x, t + t_1), A(x, t + t_2)], A(x, t + t_3)], A(x, t + t_4)] dt_4 dt_3 dt_2 dt_1 + \frac{1}{12} \int_0^h \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} [A(x, t + t_1), [A(x, t + t_2), A(x, t + t_3)], A(x, t + t_4)] dt_4 dt_3 dt_2 dt_1 + \frac{1}{12} \int_0^h \int_0^{t_1} \int_0^{t_2} \int_0^{t_3} [A(x, t + t_2), [A(x, t + t_3), A(x, t + t_4)], A(x, t + t_1)] dt_4 dt_3 dt_2 dt_1. \]

In our approach we will take the approximation obtained by the two first components only, that is

\[ z(x, t + h) \approx e^{\int_0^h A(x, t + t_1)dt_1} - \frac{1}{2} \int_0^h f_0^h j_{t_1}^h [A(x, t + t_2), A(x, t + t_1)] dt_2 dt_1 z(x, t). \]  

Rigorous estimates of the cut off terms \( \Theta_3(x, t + h, t) \), \( \Theta_4(x, t + h, t) \) and \( \Theta_5(x, t + h, t) \) will be presented in Subsection \[ \text{III.A} \] The terms \( \Theta_r(x, t + h, t), r \geq 6 \) are neglected, because most pessimistic estimates indicate scaling at least like \( h^r \). Indeed, it is enough to observe that the summands \( \Theta_r(x, t + h, t) \) are \( r \) times nested integrals.

### B. Strang splitting

We start with illustrating the Strang splitting. The exponent appearing on the right hand side of \([11]\) is computationally costly. As we will see in Sections \[ \text{IIIC} \] and \[ \text{IID} \] the integrals

\[ \int_0^h A(x, t + t_1)dt_1 \]

and

\[ -\frac{1}{2} \int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] dt_2 dt_1 \]

differ not only because of their structure (the first one is anti-diagonal, while the second is diagonal), but also due to the magnitude of order with which they scale (in terms of \( h \) and \( \omega \)).
For this reason we will exploit the Strang splitting, which for $X = \mathcal{O}(h^a)$ and $Y = \mathcal{O}(h^b)$ reads

$$\exp(X + Y) = \exp(\frac{1}{2}X)\exp(Y)\exp(\frac{1}{2}X) + \mathcal{O}(h^{a+b+1}) .$$

(12)

Applied to (11) this results in the splitting

$$z(x, t + h) \approx e^{\int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] \, dt_2 \, dt_1} e^{\int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] \, dt_2 \, dt_1} e^{\int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] \, dt_2 \, dt_1} z(x, t),$$

(13)

where the outer and inner components require various further kinds of treatment. Note that the terms we are splitting in (13) need much more subtle estimates than the general one in (12). Detailed estimate of the error appearing in splitting (13) is provided in Subsection IIIB.

C. Numerical treatment of the outer term

Although the outer term $e^{\int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] \, dt_2 \, dt_1}$ in the approximation (13) seems to be computationally complicated (because of the double integral of a commutator), we will show that its numerical treatment is unexpectedly straightforward. We start out by computing the commutator in

$$\int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] \, dt_2 \, dt_1$$

$$= \int_0^h \int_0^{t_1} \begin{bmatrix} 0 & 1 \\ N(x, t + t_2) & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ N(x, t + t_1) & 0 \end{bmatrix} \, dt_2 \, dt_1$$

$$= \int_0^h \int_0^{t_1} \begin{bmatrix} N(x, t + t_1) - N(x, t + t_2) & 0 \\ 0 & N(x, t + t_2) - N(x, t + t_1) \end{bmatrix} \, dt_2 \, dt_1$$

$$= \begin{bmatrix} \int_0^h \int_0^{t_1} (f(x, t + t_1) - f(x, t + t_2)) \, dt_2 \, dt_1 & 0 \\ 0 & \int_0^h \int_0^{t_1} (f(x, t + t_2) - f(x, t + t_1)) \, dt_2 \, dt_1 \end{bmatrix}$$

Remark 1 By simple integration by parts we can observe, that the problem of two-dimensional quadratures boils down to the far less computationally costly one-dimensional quadrature:

$$\int_0^h \int_0^{t_1} (f(x, t + t_1) - f(x, t + t_2)) \, dt_2 \, dt_1 = 2 \int_0^h (t + t_1 - \frac{h}{2}) f(x, t + t_1) \, dt_1.$$
Let us notice that after semi-discretization, \( x = (x^1_1, \ldots, x^1_M) \otimes \cdots \otimes (x^d_1, \ldots, x^d_M) \), the considered integral \( \int_0^h \int_0^{t_1} [A(x, t + t_2), A(x, t + t_1)] dt_2 dt_1 \) can be approximated by a diagonal matrix, as a tensor product of diagonal matrices

\[
\begin{bmatrix}
O(x^1_1, t) & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & \cdots & -O(x^1_M, t) \\
\end{bmatrix} \otimes \cdots \otimes
\begin{bmatrix}
O(x^d_1, t) & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & \cdots & 0 \\
\vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & \cdots & 0 & 0 & \cdots & -O(x^d_M, t) \\
\end{bmatrix},
\]

where

\[
O(x^k_i, t) = 2 \int_0^h (t + t_1 - \frac{h}{2}) f(x^k_i, t + t_1) dt_1, \quad k = 1, \ldots, d, i = 1, \ldots, M.
\]

Obviously taking the exponential of a diagonal matrix is computationally straightforward.

### D. Numerical treatment of the inner term

In this subsection we will tackle the inner term

\[
e^{\int_0^h A(x, t + t_1) dt_1} = \exp \begin{bmatrix} 0 & h \\ D + F & 0 \end{bmatrix},
\]

where for sake of clarity we used the notation

\[
D := h\Delta, \quad \text{and} \quad F := \int_0^h f(x, t + t_1) dt_1.
\]

Exponent of the anti-diagonal matrix \([14]\) can be performed by applying hyperbolic functions, more precisely,

\[
\exp \begin{bmatrix} 0 & h \\ D + F & 0 \end{bmatrix} = \begin{bmatrix} \cosh \left( \sqrt{h(D + F)} \right) & \frac{\sqrt{h} \sinh \left( \sqrt{h(D + F)} \right)}{\sqrt{D + F}} \\ \frac{\sqrt{D + F} \sinh \left( \sqrt{h(D + F)} \right)}{\sqrt{h}} & \cosh \left( \sqrt{h(D + F)} \right) \end{bmatrix}.
\]

Needless to say the computation of hyperbolic sine or cosine of \( \sqrt{h(D + F)} \) is very complicated, because it is neither diagonal nor circulant symmetric.

Therefore, we will propose two methods on how to overcome the computational difficulties arising at this stage. In all our approaches we will be willing to split the troublesome matrix \( \begin{bmatrix} 0 & h \\ D + F & 0 \end{bmatrix} \) in such a way, that each components
obtained after the splitting could be easily exponentiated. Let us start with the observations, that each entry of the matrix we have to exponentiate scales like $h$. For this reason Strang decomposition would result in second order splitting only, so it is out of considerations while deriving 4-th order methods. Instead we will resort to the higher order splittings of the following kind:

\[
e^{hX + hY} = e^{\frac{h}{2}X} e^{\frac{h}{2}Y} e^{\frac{h^2}{2} \frac{3}{4} [X, [Y, X]]} e^{\frac{h}{2}Y} e^{\frac{h}{2}X} + \mathcal{O}(h^5) \quad (15)
\]

\[
e^{hX + hY} = e^{\frac{h}{6} - \frac{\sqrt{3}h}{6} X} e^{\frac{\sqrt{3}h}{2} X - \frac{(2 - \sqrt{3})h^3}{24} [X, Y]} e^{\frac{h}{2} Y} e^{\frac{h}{6} - \frac{\sqrt{3}h}{6} X} + \mathcal{O}(h^5), \quad (16)
\]

which can be derived using two times Baker–Campbell–Hausdorff formula and compute order conditions. The derivation of the above splittings is detailed in Appendix C. Despite of the choice of components $X$ and $Y$ (where $X + Y = \begin{bmatrix} 0 & h \\ D & F \end{bmatrix}$) the inner exponent in (16), that is $\exp \left( \frac{\sqrt{3}h}{4} X - \frac{(2 - \sqrt{3})h^3}{24} [X, Y] \right)$ turns out to be computationally costly. Hence, we are left with option (15) only.

1. Inner term - towards scheme $\Gamma_{1}^{[4]}$

In the first presented time splitting we separate the Laplacian part from the potential one and apply (15) concluding with the following splitting of order 4 with respect to time step $h$

\[
\exp \begin{bmatrix} 0 & h \\ D + F & 0 \end{bmatrix} = \exp \left( \begin{bmatrix} 0 & 0 \\ D & 0 \end{bmatrix} + \begin{bmatrix} 0 & h \\ F & 0 \end{bmatrix} \right) = \mathcal{O}(h^5) + \\
\exp \begin{bmatrix} 0 & 0 \\ \frac{h}{6} D & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & \frac{h}{2} \\ \frac{1}{2} F & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & 0 \\ \frac{2}{3} D + \frac{2}{7} h D^2 & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & \frac{h}{2} \\ \frac{1}{2} F & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & 0 \\ \frac{h}{6} D & 0 \end{bmatrix}.
\]

Note that each component is computationally friendly. Indeed, let us observe, that hyperbolic functions of $\sqrt{\frac{hF}{2}}$ appearing in

\[
\exp \begin{bmatrix} 0 & \frac{h}{2} \\ \frac{1}{2} F & 0 \end{bmatrix} = \begin{bmatrix} \cosh \left( \sqrt{\frac{hF}{2}} \right) & \sqrt{\frac{F}{2}} \sinh \left( \sqrt{\frac{hF}{2}} \right) \\ \sqrt{\frac{F}{2}} \sinh \left( \sqrt{\frac{hF}{2}} \right) & \cosh \left( \sqrt{\frac{hF}{2}} \right) \end{bmatrix} = \begin{bmatrix} \cosh \left( \sqrt{\frac{hF}{2}} \right) & \frac{h}{2} \frac{\sinh \left( \sqrt{\frac{hF}{2}} \right)}{\sqrt{F}} \\ \frac{\sqrt{F}}{2} \frac{\sinh \left( \sqrt{\frac{hF}{2}} \right)}{\sqrt{h}} & \cosh \left( \sqrt{\frac{hF}{2}} \right) \end{bmatrix}
\]

can be computed easily because $\sqrt{\frac{hF}{2}}$ becomes a diagonal matrix after semi-discretization. Also the other two matrices
can be exponentiated cheaply, as
\[
\begin{align*}
\exp \begin{bmatrix} 0 & 0 \\ \frac{1}{6}D & 0 \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ \frac{1}{6}D & 1 \end{bmatrix} \text{ and } \\
\exp \begin{bmatrix} 0 & 0 \\ \frac{2}{3}D + \frac{7}{2}hD^2 & 0 \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ \frac{2}{3}D + \frac{7}{2}hD^2 & 1 \end{bmatrix}.
\end{align*}
\]

2. Inner term - towards scheme \( \Gamma_2^{[4]} \)

An alternative splitting may be obtained by keeping the kinetic and potential parts together, for which the sum \( D + F \) is the only nonzero entry of the matrix. After applying the splitting \([15]\) we have to exponentiate matrices with only one nonzero input

\[
\begin{align*}
\exp \begin{bmatrix} 0 & h \\ D + F & 0 \end{bmatrix} &= \exp \begin{bmatrix} 0 & 0 \\ D + F & 0 \end{bmatrix} + \begin{bmatrix} 0 & h \\ 0 & 0 \end{bmatrix} = \mathcal{O}(h^5) + \\
\exp \begin{bmatrix} 0 & 0 \\ \frac{1}{6}(D + F) & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & \frac{1}{2}h \\ 0 & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & 0 \\ \frac{2}{3}(D + F) + \frac{7}{2}h(D + F)^2 & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & \frac{1}{2}h \\ 0 & 0 \end{bmatrix} \exp \begin{bmatrix} 0 & 0 \\ \frac{1}{6}(D + F) & 0 \end{bmatrix},
\end{align*}
\]

which makes the scheme extremely fast computationally.

E. Complete numerical schemes \( \Gamma_1^{[4]} \) and \( \Gamma_2^{[4]} \)

Now, after taking care of numerical treatments of the outer term in Section \( \text{II.C} \) and inner terms in Subsections \( \text{II.D.1} \) and \( \text{II.D.2} \) we are ready to build up upon local approximation presented in \( \text{[13]} \). Adopting simplifications in the notation introduced earlier we define

\[
D := h\Delta, \quad F_k := \int_0^h f(x, t_k + t_1)dt_1 \text{ and } \mathcal{F}_k := \frac{1}{2} \int_0^h (t_k + t_1 - \frac{h}{2})f(x, t_k + t_1)dt_1.
\]

Assuming that the solution \( z(x, t_k) \) is known at \( t_k = kh \), we present the scheme \( \Gamma_1^{[4]} \) as follows:

\[
\begin{align*}
z(x, t_k + h) &\approx \begin{bmatrix} \exp(-\mathcal{F}_k) & 0 \\ 0 & \exp(\mathcal{F}_k) \end{bmatrix} \begin{bmatrix} 1 & 0 \\ \frac{1}{6}D & 1 \end{bmatrix} \begin{bmatrix} \cosh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) & \frac{h}{2} \sinh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) \\ \sqrt{\mathcal{F}_k} \sinh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) & \cosh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) \end{bmatrix} \\
&\cdot \begin{bmatrix} 1 & 0 \\ \frac{2}{3}D + \frac{7}{2}hD^2 & 1 \end{bmatrix} \begin{bmatrix} \cosh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) & \frac{h}{2} \sinh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) \\ \sqrt{\mathcal{F}_k} \sinh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) & \cosh \left( \frac{\sqrt{h}\mathcal{F}_k}{2} \right) \end{bmatrix} \begin{bmatrix} 1 & 0 \\ \frac{1}{6}D & 1 \end{bmatrix} \begin{bmatrix} \exp(-\mathcal{F}_k) & 0 \\ 0 & \exp(\mathcal{F}_k) \end{bmatrix} z(x, t_k).
\end{align*}
\]
The Algorithm for the scheme $\Gamma_1^{[4]}$ is presented in Table 1.

### Table 1: Algorithm $\Gamma_1^{[4]}$

$T$ steps of 4th order algorithm $\Gamma_1^{[4]}

\begin{align*}
\text{do } k &= 0, T - 1 \\
q_0 &= \exp(-F_k)z_1; \quad p_0 = \exp(F_k)z_2 \\
p_1 &= \frac{1}{6}Dq_0 + p_0 \\
q_1 &= \cosh\left(\frac{\sqrt{F_k}}{2}\right)q_0 + \frac{h}{2}\text{sinc}\left(\frac{\sqrt{hF_k}}{2}\right)p_1 \\
p_2 &= \frac{\sqrt{F_k}\sinh\left(\frac{\sqrt{F_k}}{2}\right)}{\sqrt{h}}q_0 + \cosh\left(\frac{h\sqrt{F_k}}{2}\right)p_1 \\
p_3 &= \left(\frac{h}{4}D + \frac{3}{8}hD^2\right)q_1 + p_2 \\
q_2 &= \cosh\left(\frac{h\sqrt{F_k}}{2}\right)q_1 + \frac{h}{2}\text{sinc}\left(\frac{\sqrt{hF_k}}{2}\right)p_3 \\
p_4 &= \frac{\sqrt{F_k}\sinh\left(\frac{\sqrt{F_k}}{2}\right)}{\sqrt{h}}q_1 + \cosh\left(\frac{h\sqrt{F_k}}{2}\right)p_3 \\
p_5 &= \frac{1}{6}Dq_2 + p_4 \\
q_3 &= \exp(-F_k)q_2; \quad p_6 = \exp(F_k)p_5 \\
z_1 \leftarrow q_3; \quad z_2 \leftarrow p_6
\end{align*}

end do

Table 1: Algorithm $\Gamma_1^{[4]}$ for finding the approximate solution on the time interval $[t_0, t_T]$ with $T$ time steps $h = (t_T - t_0)/T$. Note that $z(x, t) = [z_1(x, t), z_2(x, t)]^T$, where the discretisation in space is not yet applied or specified.

In a similar way we present final scheme $\Gamma_2^{[4]}$, and its algorithm is presented in Table 2.

\[
\begin{align*}
\begin{bmatrix}
\exp(-F_k) & 0 \\
0 & \exp(F_k)
\end{bmatrix}
\begin{bmatrix}
1 & 0 \\
\frac{1}{6}(D + F_k) & 1
\end{bmatrix}
\begin{bmatrix}
1 & \frac{1}{2}h \\
\frac{3}{8}(D + F_k) + \frac{3}{8}h(D + F_k)^2 & 1
\end{bmatrix}
\begin{bmatrix}
1 & \frac{1}{2}h \\
0 & 1
\end{bmatrix}
\begin{bmatrix}
\exp(-F_k) & 0 \\
\frac{1}{6}(D + F_k) & 1
\end{bmatrix}
\begin{bmatrix}
z(x, t_k + h)
\end{bmatrix}.
\end{align*}
\]
Table 2: Algorithm $\Gamma_{2}^{[4]}$ for finding the approximate solution on the time interval $[t_0, t_T]$ with $T$ time steps $h = (t_T - t_0)/T$. Note that $z(x, t) = [z_1(x, t), z_2(x, t)]^T$, where the discretisation in space is not yet applied or specified.

III. Estimates of the cut off terms

In this Section we will provide details on estimates of the cut off terms obtained while truncating the Magnus expansion and applying the Strang splitting to gain in computational efficiency. The following theorem will be exploited in these estimates frequently.

**Theorem 1** Let $a \in C^1([0, h])$ be a real function and $h \leq 1$ and $\omega \geq 1$. Then the following estimate holds

$$
\left| \int_0^h \int_0^{t_1} \int_0^{t_2} \ldots \int_0^{t_{m-1}} a(t_k) e^{i\omega t_m} dt_m dt_{m-1} \ldots dt_1 \right| \leq C \mathcal{A} \min \left\{ h^m, \frac{h^{m-1}}{\omega} \right\}, \quad 1 \leq k \leq m, \quad (17)
$$

where $C$ is a constant and $\mathcal{A} = \max_{\xi \in [0, h]} \{|a(\xi)|, |a'(\xi)|\}$.

**a. Proof:** Let us start with an observation that for $r = 0, 1, 2, \ldots$

$$
\left| \int_0^{t_{m-1}} t_m^r a(t_m) e^{i\omega t_m} dt_m \right| \leq (r + 2) C \mathcal{A} \min \left\{ h^{r+1}, \frac{h^r}{\omega} \right\}, \quad 0 \leq t_m < t_{m-1} \leq h. \quad (18)
$$

Indeed, the immediate estimate is

$$
\left| \int_0^{t_{m-1}} t_m^r a(t_m) e^{i\omega t_m} dt_m \right| \leq C \mathcal{A} h^{r+1}, \quad (19)
$$
but by simple integration by parts we observe that for \( r = 0 \)

\[
\int_0^{t_{m-1}} a(t_m) e^{i \omega t_m} dt_m = \frac{1}{i \omega} a(t_{m-1}) e^{i \omega t_{m-1}} - \frac{1}{i \omega} a(0) - \frac{1}{i \omega} \int_0^{t_{m-1}} a'(t_m) e^{i \omega t_m} dt_m,
\]

and that for \( r = 1, 2, \ldots \) we have

\[
\int_0^{t_{m-1}} t_r a(t_m) e^{i \omega t_m} dt_m = \frac{1}{i \omega} t_r a(t_{m-1}) e^{i \omega t_{m-1}} - \frac{1}{i \omega} \int_0^{t_{m-1}} r t_{r-1} a(t_m) e^{i \omega t_m} dt_m - \frac{1}{i \omega} \int_0^{t_{m-1}} t_r a'(t_m) e^{i \omega t_m} dt_m
\]

we can obtain the more subtle result

\[
\left| \int_0^{t_{m-1}} t_r a(t_m) e^{i \omega t_m} dt_m \right| \leq \frac{h}{\omega} C_h + \frac{r}{\omega} C_h + \frac{h^{r+1}}{\omega} C_h, \quad r = 0, 1, 2, \ldots
\]

Combining (19) and (20) we can conclude inequality (18). Inequality (17) is the immediate consequence of (18). □

**Remark 2**

Let \( a_n \in C^1([0,h]) \) be a family of known, real-valued functions. Let us assume, that there exist \( N \geq 0 \) such that for all \( |n| > N \) \( a_n(x,t) \equiv 0 \), and let \( h \leq 1 \) and \( \omega_{\min} \geq 1 \). Then we can show a result similar to the one obtained in Theorem 1, namely, that

\[
\left| \int_0^h \int_0^{t_1} \int_0^{t_2} \ldots \int_0^{t_{m-1}} \sum_n a_n(t_k) e^{i \omega_n t_k} dt_k dt_{m-1} \ldots dt_1 \right| \leq C A \min \left\{ h^m, \frac{h^{m-1}}{\omega_{\min}} \right\}, \quad 1 \leq k \leq m,
\]

where \( C \) is a generic constant and \( A = \max_{\xi \in [0,h]} \{|a_n(\xi)|, |a_n'(\xi)|; |n| < N\} \).

**Remark 3**

For clarity of exposition we will abuse the notation and write

\[
f(t_k) = a(t_k) + \sum_n a_n(t_k) e^{i \omega_n t_k}
\]

instead of

\[
f(x,t + t_k) = a(x,t + t_k) + \sum_n a_n(x,t + t_k) e^{i \omega_n (t + t_k)}.
\]

In further part of the paper we denote by \( \| \cdot \|_s \) the standard \( H^s \) Sobolev norm on the torus \( \mathbb{T}^d \) and assume that that the following Assumption holds

**Assumption 1**

Let us assume that

1. \( \exists N \geq 0 \forall |n| > N a_n(x,t) \equiv 0 \),

2. \( a_n \in C^1([0,T], H^{2+s}(\mathbb{T}^d)) \),

13
3. \( \alpha \in C^2_t([0,T], H^{2+s}(\mathbb{T}^d)) \).

4. \( s \geq 0, \ s + 2 > \frac{d}{2} \).

5. \( \omega_n \in \Omega \subset \mathbb{R} \).

Remark 4 The first assumption on the finite number of nonzero coefficients \( a_n(x,t) \), that is on the finite number of frequencies, is due to practical, computational reasons, namely numerical implementation of the schemes. This assumption is not necessary for delivering the theoretical estimates on error of the methods.

Definition 1 In all calculations of this article we understand that \( C \) is generic constant. Let us define

\[
\omega_{\min} = \inf \{ |\omega_n|; \omega_n \in \Omega \} \geq 1, \quad \omega_{\max} = \sup \{ |\omega_n|; \omega_n \in \Omega \}
\]

and

\[
\mathcal{E}_\omega^h = \min \left\{ h^3, \frac{h^2}{\omega_{\min}}, h^5 \omega_{\max} \right\},
\]

\[
\mathcal{A} = \max_{\xi \in [0,T]} \left\{ \| a_n(\cdot, \xi) \|_{s+2}, \| a_n^2(\cdot, \xi) \|_s, \| \partial_t a_n(\cdot, \xi) \|_{s+2}, \| \partial^2_t a_n(\cdot, \xi) \|_{s+2}; |n| \leq N \right\},
\]

\[
\mathcal{C} = \max_{\xi \in [0,T]} \left\{ \| \alpha(\cdot, \xi) \|_{s+2}, \| \alpha^2(\cdot, \xi) \|_s, \| \partial_t \alpha(\cdot, \xi) \|_{s+2}, \| \partial^2_t \alpha(\cdot, \xi) \|_{s+2}; |n| \leq N \right\},
\]

\[
\mathcal{L}_5 = \max_{\xi \in [0,T]} \left\{ \| \alpha^p(\cdot, \xi) \|_s, \| a_n^q(\cdot, \xi) \|_s; \ p + q = 5, |n| \leq N \right\}.
\]

A. Error committed by the Magnus truncation

The commutators appearing in (9)-(10) are calculated in Appendix A. Let us start with the first truncated term of Magnus expansion:

\[
\Theta_3(x, t + h, t) = \frac{1}{6} \int_0^h \int_0^t \int_0^{t_2} [A(x, t + t_1), [A(x, t + t_2), A(x, t + t_3)]] \ dt_3 \ dt_2 \ dt_1
\]

\[
+ \frac{1}{6} \int_0^h \int_0^{t_1} \int_0^{t_2} [A(x, t + t_3), [A(x, t + t_2), A(x, t + t_1)]] \ dt_3 \ dt_2 \ dt_1
\]

\[
= \frac{1}{6} \int_0^h \int_0^{t_1} \int_0^{t_2} \begin{bmatrix} 0 & H_1 + H_3 \\ H_2 + H_4 & 0 \end{bmatrix} \ dt_3 \ dt_2 \ dt_1,
\]

where

\[
H_1 + H_3 = 2(-f(t_1) + 2f(t_2) - f(t_3));
\]

\[
H_2 + H_4 = \Delta \left( (f(t_3) - 2f(t_2) + f(t_1)) + (f(t_3) - 2f(t_2) + f(t_1)) \Delta
\]

\[
+ 4f(t_1)f(t_3) - 2f(t_1)f(t_2) - 2f(t_3)f(t_2). \]
In the estimates below we separate the non-oscillatory part from the oscillatory and obtain

\[
\left| \int_0^h \int_0^{t_1} \int_0^{t_2} (H_1 + H_3) \, dt_3 \, dt_2 \, dt_1 \right| \leq \left| \int_0^h \int_0^{t_1} \int_0^{t_2} 2 (-\alpha(t_1) + 2\alpha(t_2) - \alpha(t_3)) \, dt_3 \, dt_2 \, dt_1 \right| \\
+ \sum_n \left| \int_0^h \int_0^{t_1} \int_0^{t_2} 2 (-a_n(t_1)e^{i\omega_n t_1} + 2a_n(t_2)e^{i\omega_n t_2} - a_n(t_3)e^{i\omega_n t_3}) \, dt_3 \, dt_2 \, dt_1 \right|
\leq Ch^5 \max_{\mu \in [0,h]} |\alpha''(\mu)| + C\bar{A} \min \left\{ h^3, \frac{h^2}{\omega_{\min}}, h^5\omega_{\max}^2 \right\}
\leq Ch^5 \tilde{L} + C\bar{A}\tilde{E}_h^{\omega}.
\]

The estimate of the first summand may be obtained by expanding \(\alpha(t_i), i = 1, 2, 3\) into a Taylor series at point 0, namely there exist such \(\xi_1, \xi_2, \xi_3 \in [0, h]\) that

\[
\left| \int_0^h \int_0^{t_1} \int_0^{t_2} (\alpha(t_1) - 2\alpha(t_2) + \alpha(t_3)) \, dt_3 \, dt_2 \, dt_1 \right| = \left| \int_0^h \int_0^{t_1} \int_0^{t_2} \alpha'(0)(t_1 - 2t_2 + t_3) \, dt_3 \, dt_2 \, dt_1 \right| \\
+ \left| \int_0^h \int_0^{t_1} \int_0^{t_2} t_1^2\alpha''(\xi_1) - 2t_2^2\alpha''(\xi_2) + t_3^2\alpha''(\xi_3) \, dt_3 \, dt_2 \, dt_1 \right|
\leq 4h^5 \max_{\mu \in [h,T]} |\alpha''(\mu)|,
\]

because the first triple integral vanishes.

More attention should be paid to the case, where Laplace operator \(\Delta\) appears. We need to remember that it is applied not only to the function \(f\), but also to the solution \(\varphi\), and why we raise the norm from \(\| \cdot \|_{s}\) to \(\| \cdot \|_{s+2}\). More precisely, for any \(\varphi\) sufficiently smooth we have in the standard \(H^s\) Sobolev norm that

\[
\left\| \int_0^h \int_0^{t_1} \int_0^{t_2} (H_2 + H_4) \, dt_3 \, dt_2 \, dt_1 \varphi \right\|_s \leq \left\| \int_0^h \int_0^{t_1} \int_0^{t_2} \Delta (f(t_1) - 2f(t_2) + f(t_3)) \, dt_3 \, dt_2 \, dt_1 \varphi \right\|_s \\
+ \left\| \int_0^h \int_0^{t_1} \int_0^{t_2} (f(t_1) - 2f(t_2) + f(t_3)) \Delta dt_3 \, dt_2 \, dt_1 \varphi \right\|_s \\
+ \left\| \int_0^h \int_0^{t_1} \int_0^{t_2} (4f(t_1)f(t_3) - 2f(t_1)f(t_2) - 2f(t_3)f(t_2)) \, dt_3 \, dt_2 \, dt_1 \varphi \right\|_s
\leq C h^5 \tilde{L}\|\varphi\|_{s+2} + C\bar{A} \min \left\{ h^3, \frac{h^2}{\omega_{\min}}, h^5\omega_{\max}^2 \right\}\|\varphi\|_{s+2}
+ C \bar{L} \bar{A} \min \left\{ h^3, \frac{h^2}{\omega_{\min}}, h^5\omega_{\max}^2 \right\}\|\varphi\|_s
\leq C h^5 \tilde{L}\|\varphi\|_{s+2} + C\bar{A}\tilde{E}_h^{\omega}\|\varphi\|_{s+2} + C \bar{L} \bar{A} \bar{E}_h^{\omega}\|\varphi\|_s.
\]
To give a clue on the above inequality we estimate one of the integrands below

$$\| \Delta (f(t_1) - 2f(t_2) + f(t_3)) \varphi \|_{s} \leq C \max_{\mu \in [0,T]} \{ h^2 \| \partial^2_{\alpha} \alpha(\cdot, \mu) \Delta \varphi \|_{s}, h^2 \| \nabla \partial^2_{\alpha} \alpha(\cdot, \mu) \nabla \varphi \|_{s}, h^2 \| \Delta \partial^2_{\alpha} \alpha(\cdot, \mu) \varphi \|_{s} \}$$

$$+ C \min \left\{ h^3 \max_{\mu \in [0,T]} \{ \| a_n(\cdot, \mu) \Delta \varphi \|_{s}, \| \nabla a_n(\cdot, \mu) \nabla \varphi \|_{s}, \| \Delta a_n(\cdot, \mu) \varphi \|_{s} \} , \right\}$$

$$\frac{h^2}{\omega_{\min}} \max_{\mu \in [0,T]} \{ \| \partial_t a_n(\cdot, \mu) \Delta \varphi \|_{s}, \| \nabla \partial_t a_n(\cdot, \mu) \nabla \varphi \|_{s}, \| \Delta \partial_t a_n(\cdot, \mu) \varphi \|_{s} \},$$

$$h^{5} \omega_{\max}^{2} \max_{\mu \in [0,T]} \{ \| \partial^2_{\alpha} a_n(\cdot, \mu) \Delta \varphi \|_{s}, \| \nabla \partial^2_{\alpha} a_n(\cdot, \mu) \nabla \varphi \|_{s}, \| \Delta \partial^2_{\alpha} a_n(\cdot, \mu) \varphi \|_{s} \} \right\}.$$ 

The computations of the commutators appearing in $\Theta_4$ are more complicated (details can be found in Appendix A), but the estimates of obtained formulas are similar to these appearing in $\Theta_3$:

$$\Theta_4(x, t + h, t) = \frac{1}{12} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \left[ [A(x, t + t_1), A(x, t + t_2), A(x, t + t_3), A(x, t + t_4)] dt_4 dt_3 dt_2 dt_1 \right. \left. + \frac{1}{12} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \left[ A(x, t + t_1), [A(x, t + t_2), A(x, t + t_3), A(x, t + t_4)] dt_4 dt_3 dt_2 dt_1 \right. \right.$$ 

$$+ \frac{1}{12} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \left[ A(x, t + t_1), A(x, t + t_2), A(x, t + t_3), A(x, t + t_4)] dt_4 dt_3 dt_2 dt_1 \right. \left. + \frac{1}{12} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \left[ A(x, t + t_2), A(x, t + t_3), A(x, t + t_4), A(x, t + t_1)] dt_4 dt_3 dt_2 dt_1 \right. \right.$$ 

$$\left. = \frac{1}{12} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \left[ \mathcal{H}_1 0 0 \mathcal{H}_2 \right] dt_4 dt_3 dt_2 dt_1, \right.$$ 

where

$$\mathcal{H}_1 = \Delta (2f(t_2) - 2f(t_3)) + 3(2f(t_2) - 2f(t_3)) \Delta + 4f(t_4) (f(t_2) - f(t_3)) + 4f(t_1) (f(t_2) - f(t_3));$$

$$\mathcal{H}_2 = -3 \Delta (2f(t_2) - 2f(t_3)) - (2f(t_2) - 2f(t_3)) \Delta - 4f(t_4) (f(t_2) - f(t_3)) - 4f(t_1) (f(t_2) - f(t_3)).$$

Thanks to Theorem 1 we thus obtain for any $\varphi$ sufficiently smooth

$$\left\| \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \int_{0}^{T} \mathcal{H}_1 dt_4 dt_3 dt_2 dt_1 \varphi \right\|_{s} \leq C h^{5} \tilde{L} \| \varphi \|_{s+2} + C \tilde{A} h \mathcal{E}_0 \| \varphi \|_{s+2} + C \tilde{L} \tilde{A} h \mathcal{E}_0 \| \varphi \|_{s}.$$ 

The estimate of the triple integral in $\mathcal{H}_2$ follows similar calculations as above.

It can be shown that

$$\| \Theta_5(x, t + h, t) \varphi \|_{s} \leq \left( C h^{6} \tilde{L} + \tilde{A} h \mathcal{E}_0 \right) \| \varphi \|_{s+2} + C \tilde{L} \tilde{A} h \mathcal{E}_0 \| \varphi \|_{s},$$

16
but the easiest estimate

\[ \| \Theta_5(\mathbf{x}, t + h, t) \varphi \|_s \leq C h^5 \tilde{\mathcal{L}} \| \varphi \|_{s+2}, \]

can be obtained immediately by the observation, that \( \Theta_5(\mathbf{x}, t + h, t) \) is a five times nested integral of four times nested commutators.

All together, the error committed by truncating the Magnus expansion can be bounded for any \( \varphi \) sufficiently smooth by

\[ \| (\Theta_3(\mathbf{x}, t + h, t) + \Theta_4(\mathbf{x}, t + h, t) + \Theta_5(\mathbf{x}, t + h, t)) \varphi \|_s \]
\[ \leq C h^5 \tilde{\mathcal{L}} \| \varphi \|_{s+2} + C \tilde{\mathcal{L}} \mathcal{E}_h^5 \| \varphi \|_s + C h^5 \tilde{\mathcal{L}} \| \varphi \|_{s+2}. \] (24)

**B. Error committed by the Strang splitting**

To estimate the error of the approximation (13) we exploit Baker-Campbell-Hausdorff formula, which reads

\[ \exp(X + Y) = \exp(\frac{1}{2}X) \exp(Y) \exp(\frac{1}{2}X) + \frac{1}{12} [Y, [Y, X]] - \frac{1}{24} [X, [X, Y]] 
- \frac{1}{720} ([Y, [Y, [Y, X]]] + [X, [X, [X, Y]]]) + \frac{1}{360} ([Y, [Y, [Y, [Y, X]]]] + [Y, [X, [X, [X, Y]]]]) + \cdots \] (25)

where,

\[ Y = \int_0^h \begin{bmatrix} 0 & 1 \\ \Delta + f(\mathbf{x}, t_1) & 0 \end{bmatrix} dt_1, \]

and

\[ X = \int_0^h \int_0^{t_1} [A(\mathbf{x}, t_1), A(\mathbf{x}, t_2)] dt_2 dt_1 = \int_0^h \int_0^{t_1} \begin{bmatrix} f(\mathbf{x}, t_1) - f(\mathbf{x}, t_2) & 0 \\ 0 & f(\mathbf{x}, t_2) - f(\mathbf{x}, t_1) \end{bmatrix} dt_2 dt_1. \]

Obviously, five-times nested commutators scale at least like \( \mathcal{O}(h^5) \), so it is enough to consider \([ [Y, X], X] + [Y, X, Y] \). Denoting

\[ F = \int_0^h f(t + t_1) dt_1, \]
\[ \mathcal{F} = \int_0^h \int_0^{t_1} (f(t + t_2) - f(t + t_1)) dt_2 dt_1 \]
underlying commutators (as is calculated in Appendix B) have the following form

\[
[Y, [Y, X]] = \begin{bmatrix}
-\hbar^2 \Delta F - 3\hbar^2 \Delta - 4\hbar F F & 0 \\
0 & 3\hbar^2 \Delta F + \hbar^2 \Delta + 4\hbar F F
\end{bmatrix};
\]

\[
[X, [X, Y]] = \begin{bmatrix}
0 & 4\hbar F^2 \\
2\hbar F \Delta F + \hbar F^2 \Delta + \hbar \Delta F^2 + 4 F^2 F & 0
\end{bmatrix}.
\]

Using Theorem 1 we obtain the estimates

\[
|F| \leq C h \max_{\mu \in [0, T]} \{\|\alpha(\cdot, \mu)\|_s\} + C \min \left\{h, \frac{1}{\omega_{\min}}\right\} \max_{\mu \in [0, T]} \left\{\|a_n(\cdot, \mu)\|_s, \|\partial_t a_n(\cdot, \mu)\|_s\right\}
\]

\[
\leq C h \tilde{\Lambda} + C \tilde{\Lambda} \min \left\{h, \frac{1}{\omega_{\min}}\right\}
\]

\[
|\mathcal{F}| \leq C h^2 \max_{\mu \in [0, T]} \{h \|\partial_t \alpha(\cdot, \mu)\|_s\} + C \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\} \max_{\mu \in [0, T]} \left\{\|a_n(\cdot, \mu)\|_s, \|\partial_t a_n(\cdot, \mu)\|_s\right\}
\]

\[
\leq C h^3 \tilde{\Lambda} + C \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}
\]

\[
\|\Delta F \varphi\|_s \leq C h^2 \max_{\mu \in [0, T]} \{h \|\partial_t \alpha(\cdot, \mu)\|_s, h \|\nabla \partial_t \alpha(\cdot, \mu)\nabla \varphi\|_s, h \|\Delta \partial_t \alpha(\cdot, \mu)\varphi\|_s\}
\]

\[
+ C \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}
\]

\[
\leq C \left(h^3 \tilde{\Lambda} + \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}\right) \|\varphi\|_{s+2}
\]

\[
\|\mathcal{F} \varphi\|_s \leq C \left(h^3 \tilde{\Lambda} + \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}\right) \|\varphi\|_{s+2}
\]

\[
\|\mathcal{F} \mathcal{F} \varphi\|_s \leq C \left(h^3 \tilde{\Lambda} + \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}\right) \|\varphi\|_{s+2}
\]

\[
\|\Delta \mathcal{F} \varphi\|_s \leq C \left(h^3 \tilde{\Lambda} + \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}\right) \|\varphi\|_{s+2}
\]

\[
\|\mathcal{F} \Delta \mathcal{F} \varphi\|_s \leq C \left(h^3 \tilde{\Lambda} + \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}\right) \|\Delta\| \|\varphi\|_{s+2}
\]

\[
\|\mathcal{F}^2 \varphi\|_s \leq C \left(h^3 \tilde{\Lambda} + \tilde{A} \min \left\{h^2, \frac{h}{\omega_{\min}}, h^3 \omega_{\max}\right\}\right) \|\varphi\|_{s+2}
\]

All together,

\[
\frac{1}{12} |Y, [Y, X]| - \frac{1}{24} |X, [X, Y]| \leq \begin{bmatrix}
G_1 \\
G_2 \\
G_3 \\
G_4
\end{bmatrix}.
\]
where

\[ \|G_1\varphi\|_s \leq C \left( h^5 \tilde{L} + \tilde{A} \min \left\{ h, \frac{h^3}{\omega_{\text{min}}}, h^5 \omega_{\text{max}} \right\} \right) \|\varphi\|_{s+2} + C \left( h^4 \tilde{L} + \tilde{A} \min \left\{ h^3, \frac{h^2}{\omega_{\text{min}}}, h^4 \omega_{\text{max}} \right\} \right) \|\varphi\|_s \]

\[ \|G_2\varphi\|_s \leq C h \left( h^3 \tilde{L} + \tilde{A} \min \left\{ h^2, \frac{h}{\omega_{\text{min}}}, h^3 \omega_{\text{max}} \right\} \right) \|\varphi\|_{s+2} \]

\[ \|G_3\varphi\|_s \leq C h \left( h^3 \tilde{L} + \tilde{A} \min \left\{ h^2, \frac{h}{\omega_{\text{min}}}, h^3 \omega_{\text{max}} \right\} \right) \|\varphi\|_{s+2} \]

\[ \|G_4\varphi\|_s \leq C \left( h^5 \tilde{L} + \tilde{A} \min \left\{ h^4, \frac{h^3}{\omega_{\text{min}}}, h^5 \omega_{\text{max}} \right\} \right) \|\varphi\|_{s+2} \]

### IV. Structure of the error

Taking into account the error committed by Magnus expansion, it is enough to observe that Strang splitting also satisfies

\[ \left\| \frac{1}{12} [Y, [Y, X]] - \frac{1}{24} [X, [X, Y]] \varphi \right\|_s \leq \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} C \left( h^5 \tilde{L} + \tilde{A} \xi_h \right) \|\varphi\|_{s+2} + \tilde{L} \tilde{A} \xi_h \|\varphi\|_{s+2} + h^5 \tilde{A} \xi_5 \|\varphi\|_s \right) \]

#### Theorem 2 (Error scaling)

Let us assume that Assumption \[^7\] holds and let us denote by \( \phi^t \) the exact flow, i.e., \( z(x, t) = \phi^t(z_0) \) and by \( \Phi^h \) the numerical flow, i.e.,

\[ z^{n+1} = \Phi^h(z^n) \]

where \( \Phi^h \) corresponds to Algorithm \( \Gamma_1^{[4]} \) or \( \Gamma_2^{[4]} \). Then, for \( \varphi \in H^{s+2}(\mathbb{T}^d) \) we have that

\[ \|\phi^h(\varphi) - \Phi^h(\varphi)\|_s \leq C \left( h^5 \tilde{L} + \tilde{A} \min \left\{ h, \frac{h^3}{\omega_{\text{min}}}, h^5 \omega_{\text{max}} \right\} \right) \|\varphi\|_{s+2} + C \left( h^5 \tilde{A} \xi_5 + \tilde{L} \tilde{A} \xi_h \right) \|\varphi\|_s \]
\[
\tilde{A} = \max_{\xi \in [0, T]} \left\{ \|a_n(\cdot, \xi)\|_{s+2}, \|a_n^2(\cdot, \xi)\|_s, \|a_n(\cdot, \xi)\|_{s+2}, \|a_n^2(\cdot, \xi)\|_s ; |n| \leq N \right\}, \\
\tilde{L} = \max_{\xi \in [0, T]} \left\{ \|a(\cdot, \xi)\|_{s+2}, \|a^2(\cdot, \xi)\|_s, \|a_t(\cdot, \xi)\|_{s+2}, \|a_{tt}(\cdot, \xi)\|_s ; |n| \leq N \right\}, \\
\tilde{A}_{L5} = \max_{\xi \in [0, T]} \left\{ \|a^p(\cdot, \xi)\|_s \cdot \|a^q(\cdot, \xi)\|_s ; p + q = 5, |n| \leq N \right\}.
\]

V. Numerical experiments

In this section we compare newly constructed numerical approaches with several schemes from the literature. In this respect, the following methods are considered:

• BBCK \([4]\): 4-th order method \(\Sigma^{[4]}_{\text{BBCK}}\) from \([1]\);

• BBCK\([6]\): 6-th order method \(\Sigma^{[6]}_{\text{BBCK}}\) from \([1]\);

• Asympt\([3]\): 3-rd order asymptotic method from \([5]\)

For our experiments, we assume that the solution is confined in a region \([x_0, x_M]\), and periodic boundary conditions are imposed. We divide the spatial region into \(M = 200\) intervals of length \(\Delta x = (x_M - x_0)/M\) and, after spatial discretization, we obtain an equation similar to the first order system \((5)\) where \(z = (z_1, z_2)^T\) and \(z_1(t) \approx z(x, t), z_2(t) \approx z_t(x, t)\).

As a reference solution we take the 6-th order method based on self adjoint basis of Munthe-Kaas & Owren \([3]\) with a step size \(h = 10^{-5}\), and then we carry out the numerical integration with each method using different time steps and measure the \(l_2\) error at the final time. This error is plotted in double-logarithmic scale versus the order of the method and time of calculation expressed in seconds. For Laplacian discretization we use Fourier method, described in detail in \([11]\).

Example 1.

In first example we take a wave equation with time-dependent potential and with frequency \(\omega\), namely

\[
\partial^2_t u = \partial^2_x u - \sigma \left( 1 + \frac{1}{5} \cos(\omega t) \right) x^2 u, \quad x \in [-\pi, \pi], \quad t \in [0, 1];
\]

\[
u(x, 0) = e^{-\frac{1}{2}(x-3)^2} + e^{-\frac{1}{2}(x+3)^2}, \quad u'(x, 0) = 0;
\]

\[
u(-\pi, t) = v(\pi, t), \quad t \in [0, 1].
\]

Figure 4 consists of three graphs. On the first plot we present the initial condition (blue line), solution at final time step for \(\sigma = 1/5, \omega = 50\) (yellow line) and solution at final time step for \(\sigma = 1, \omega = 50\) (red line). Next two graphs show
the evolutions in time of the solutions for $\sigma = 1/5, \omega = 50$ and for $\sigma = 1, \omega = 50$.

Figure 4: Initial condition, solutions at final time step and evolution of the solutions in time of (27) for two pairs of coefficients $\sigma$ and $\omega$.

In Figures 5 and 6 we compare order of methods (first row) and cost in seconds (second row). It can be observed that methods $\Gamma_1[4]$ and $\Gamma_2[4]$ present the same order of convergence, but $\Gamma_2[4]$ is less computationally costly than $\Gamma_1[4]$. It is worth paying attention to the extremely competitive computational time of the $\Gamma_1[4]$ and $\Gamma_2[4]$ methods. As expected, 6-th order method BBCK[6] is delivering smaller errors, but is much more expensive computationally. Indeed, it requires at least 10 times more time then the proposed new methods to achieve the same error of approximation.

Example 2.

Let us consider example featuring large disproportion between the laplacian part and the influx-term part, where the laplacian part is multiplied by the factor $10^{-3}$, and the influx-term is multiplied by its inverse, i.e. $10^3$.

\begin{equation}
\partial_t^2 u = 10^{-3} \partial_x^2 u - 10^3 \left(1 + \frac{1}{5} \cos(\omega t)\right) x^2 u, \quad x \in [-\pi, \pi], \quad t \in [0, 1];
\end{equation}

\begin{align*}
u(x,0) &= e^{-\frac{1}{2}(x-3)^2} + e^{-\frac{1}{2}(x+3)^2}, \quad u'(x,0) = 0; \\
u(-\pi, t) &= u(\pi, t), \quad t \in [0, 1].
\end{align*}

In Figure 7 we compare order of methods (first row) and cost in seconds (second row). It is easy to see, that the disproportion between the laplacian part and the influx-term part, which can be understood as semiclassical-like regime, has a negative effect on all considered methods. For $\omega = 1$ method $\Gamma_1[4]$ is less computationally costly and obtains better accuracy than $\Gamma_2[4]$. Moreover, in this case method $\Gamma_1[4]$ achieves an error only slightly greater than 6-th order method BBCK[6]. However, as the oscillation increases, the $\Gamma_1[4]$ and $\Gamma_2[4]$ methods require much smaller time steps than the BBCK[6] method, but larger than BBCK[4] method. Indeed, for $\omega = 500$ and time step $h = 10^{-4}$ 6-th order method BBCK[6] obtains error scaling like $10^{-11}$, while 4-th order method BBCK[4] achieves error scaling like $10^{-4}$ and new 4-th order methods $\Gamma_1[4]$ and $\Gamma_2[4]$ obtain error scaling like $10^{-8}$. Still, methods $\Gamma_1[4]$ and $\Gamma_2[4]$ are less computationally costly then methods BBCK[4] and BBCK[6].
Figure 5: Comparison of orders (first row) and of costs in seconds (second row) for $\sigma = 1$ and small values of frequency $\omega = 1, 500, 1000$ in example (27). (Similar comparisons for larger values of $\omega$ are displayed in Figure 6.) Method $\Gamma_1^{[4]}$ is more computationally costly than $\Gamma_2^{[4]}$, but both they are cheaper than BBCK$^{[4]}$ and BBCK$^{[6]}$. Moreover, unlike BBCK$^{[4]}$, methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ at some point achieve the same error of approximation that 6-th order method BBCK$^{[6]}$. What is also important, methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ require smaller time step than 6-th order method BBCK$^{[6]}$, but in shorter time can deliver the same small error, which means that are competitive not only to 4-th order method, but also to 6-th order BBCK$^{[6]}$.

Example 3.

Now we consider the equation evolving on wider space interval

$$\partial_t^2 u = \partial_x^2 u - (1 + \varepsilon \cos(\omega t)) x^2 u, \quad x \in [-10, 10], \quad t \in [0, 1],$$

(29)

$$u(x, 0) = e^{-\frac{x^2}{2}}, \quad \partial_t u(x, 0) = 0,$$

$$u(-10, t) = u(10, t), \quad t \in [0, 1].$$

On the first graph in Figure 8 we present the initial condition (blue line), solution at final time step for $\varepsilon = 10, \omega = 10$ (yellow line) and solution at final time step for $\varepsilon = 0.1, \omega = 100$ (red line). Next two graphs show the evolutions in time of the solutions for $\varepsilon = 0.1, \omega = 100$ and for $\varepsilon = 10, \omega = 10$.

Comparisons of costs and accuracy for equation (29) are presented in Figures 9 and 10. First of all let us observe, that asymptotic method Asympt$^{[3]}$ proposed $^{[5]}$ is unbeatable for equation with extremely oscillatory influx terms. Indeed - asymptotic method was designed especially for this type of equations. For small $\omega$ asymptotic method Asympt$^{[3]}$ is ineffective. In the case of smaller oscillations, when $\omega = 10$, methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ preforms predictably - they achieve a worse error than the 6-th order BBCK$^{[6]}$ method, but delivers significantly smaller error than 4-th order method BBCK$^{[4]}$. 

22
On contrary to examples presented in Figure 5 we are concerned here with highly oscillatory regimes where the accurate approximation of integrals is crucial. Here we see clearly that although methods BBCK \(^4\) and BBCK \(^6\) are very effective, they are not designed for high oscillation. The phenomena observed on the first top figure where we witness the change of rate of convergence of methods \(\Gamma^1\) and \(\Gamma^2\) is expected and appears due to the change of ratio between frequency and time step.

and asymptotic method Asympt \(^3\). As the oscillations get larger, \(\omega = 1000\), asymptotic method Asympt \(^3\) starts behaving extraordinary - as it was designed - especially and only for extremely large oscillations. Methods BBCK \(^4\) and BBCK \(^6\) require truly small time steps to handle the oscillations, while our new methods deliver expected errors for all time steps \(h\). Moreover, for \(h > 10^{-2}\) method BBCK \(^6\) coincides with the method BBCK \(^4\). In case of extremely high oscillations, \(\omega = 10^6\), methods BBCK \(^4\) and BBCK \(^6\) present the same order of convergence, close to the second order, while the methods \(\Gamma^4\) and \(\Gamma^4\) achieve the 4-th order of convergence from the first, largest, time step \(h = 1\), what is consistent with the theory. Computational cost of methods \(\Gamma^4\) and \(\Gamma^4\) are impressing in case of all frequencies \(\omega\).

**Example 4.**

In this example we consider a wave equation in two dimensions, namely

\[
\begin{align*}
\partial^2_t u &= \Delta u - \sigma \left(1 + \frac{1}{5} \cos(\omega t)\right) x^2 y^2 u, \quad x, y \in [-\pi, \pi], \quad t \in [0, 1], \\
u(x, y, 0) &= e^{-\frac{1}{2}(x-3)^2} + e^{-\frac{1}{2}(x+3)^2} + e^{-\frac{1}{2}(y-3)^2} + e^{-\frac{1}{2}(y+3)^2}, \quad u'(x, y, 0) = 0; \\
u(-\pi, -\pi, t) &= u(\pi, t) = u(\pi, -\pi, t) = u(\pi, -\pi, t), \quad t \in [0, 1].
\end{align*}
\]

The above example is used to show that methods \(\Gamma^4\) and \(\Gamma^4\) can also be used for problems in higher spatial dimensions. Although we present an example in two spatial dimensions, these methods can be extended to higher dimensions,
Figure 7: Comparison of orders (first row) and of costs in seconds (second row) for equation (28). The semiclassical-like regime shows superiority of $\Gamma_1^{[4]}$ to $\Gamma_2^{[4]}$, especially in the non-oscillatory case where $\omega = 1$. Both new methods are competitive to 4-th order method BBCK$^{[4]}$, but 6-th order method BBCK$^{[6]}$ obtains, as expected, better accuracy.

Figure 8: Initial condition, solutions at final time step and evolution of the solutions in time of (29) for two pairs of coefficients $\varepsilon$ and $\omega$.

but as the number of spatial dimensions $d$ increases, the size of the matrix resulting from semidiscretization grows as $M^d$. Thus, such calculations require computers with very high computing power. Accuracy and efficiency are presented in Figure 11.

Example 5.
Figure 9: Comparison of orders (first row) and of costs in seconds (second row) for equation (29) for $\varepsilon = 0.1$.

Asymptotic method $\text{Asympt}^{[3]}$ fails for small $\omega$, but as the oscillations get higher, the $\text{Asympt}^{[3]}$ method becomes unbeatable - this method was designed especially for case of high oscillations. In case of small $\omega$, 6-th order method $\text{BBCK}^{[6]}$ achieves better error and 4-th order method $\text{BBCK}^{[4]}$ worse error than methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$, as expected. For medium oscillations, $\omega = 10^3$, methods $\text{BBCK}^{[4]}$ and $\text{BBCK}^{[6]}$ require a very small time step to perform theoretical orders of their convergence. In case of extremely high oscillations, methods $\text{BBCK}^{[4]}$ and $\text{BBCK}^{[6]}$ fail, while methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ achieve the 4-th order of convergence for all presented time steps. It is also worth noting that for each oscillation $\omega$ methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ are very cheap computationally.

In this example we consider a wave equation with frequency $\omega$, namely

$$\begin{align*}
\partial_t^2 u &= \partial_x^2 u - \frac{1}{1 + t^2} \left( 1 + \frac{1}{5} \cos(\omega t) \right) x^2 u, \quad x \in [-\pi, \pi], \quad t \in [0, 1]; \\
u(x, 0) &= e^{-\frac{1}{2} (x-3)^2} + e^{-\frac{1}{2} (x+3)^2}, \quad u'(x, 0) = 0; \\
u(-\pi, t) &= u(\pi, t), \quad t \in [0, 1].
\end{align*}$$

(31)

In example (31) we consider the most complicated function, where non-oscillatory part $-\frac{1}{1 + t^2} x^2$ and oscillatory part $\frac{1}{5} \frac{1}{1 + t^2} \cos(\omega t)x^2$ are time and space dependent. Accuracy of the methods are displayed in Figure 12. Methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ present the same accuracy and error constant. Like in Example (27), $\Gamma_1^{[4]}$ is slightly more computationally costly than $\Gamma_2^{[4]}$, but both methods are much more accurate then method $\text{BBCK}^{[4]}$ and much less computationally costly then 6-th order method $\text{BBCK}^{[6]}$.

Example 6.
Asymptotic method Asympt\(^3\) perform good only for high oscillations, as it was designed. 6-th order method BBCK\(^6\) achieves better error than other methods only in case of small oscillations. For medium oscillations, \(\omega = 10^3\), methods BBCK\(^4\) and BBCK\(^6\) require a very small time step to perform theoretical orders of their convergence. Moreover, in case of extremely high oscillations those two methods fail. Methods \(\Gamma_1\)^\(^4\) and \(\Gamma_2\)^\(^4\) achieve the 4-th order of convergence and are very cheap computationally for all presented time steps.

Last but not least we consider an equation where the input term features wide variety of frequencies.

\[
\partial_t^2 u = \partial_x^2 u - \sum_{k=0}^{5} \left(1 + \cos(10^k t)\right) x^2 u, \quad x \in [-10, 10], \quad t \in [0, 1],
\]

\[
u(x, 0) = e^{-\frac{x^2}{2}}, \quad \partial_t u(x, 0) = 0,
\]

\[
u(-10, t) = \nu(10, t), \quad t \in [0, 1].
\]

According to the error estimates (see Figures 1–3 and Theorem 2) the new methods commit an error scaling at least like \(O(h^2)\) globally. In Figure 13 we can observe, that the new methods behave steadily for all time steps. Moreover, as expected, the asymptotic method performs very purely. Indeed, this is due to the slow oscillations \(\omega_1\) which appears in the input term. On the other hand the large oscillations like \(\omega_6\) sabotage other Magnus based methods which fail in approximation of highly oscillatory integrals.

Acknowledgments

The work of Katharina Schratz in this project was financed by the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (grant agreement No. 850941).

The work of Karolina Kropiechnicka and Karolina Lademann in this project was financed by the National Science...
Methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ can be extended to higher dimensions without losing order of convergence. It is worth noting that even in the multidimensional case, methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$ are relatively cheap computationally.

Centre (NCN) project no. 2019/34/E/ST1/00390.

Numerical simulations were carried out by Karolina Lademann at the Academic Computer Center in Gdańsk (CI TASK).

The authors thank the Isaac Newton Institute for Mathematical Sciences for support and hospitality during the programme ”Geometry, compatibility and structure preservation in computational differential equations”, supported by EPSRC grant EP/R014604/1, where this work has been initiated.
Figure 12: Comparison of orders (first row) and of costs in seconds (second row) for equation (31). As in previous examples, increasing the oscillation does not affect the order of the methods $\Gamma_1^{[4]}$ and $\Gamma_2^{[4]}$, it only slightly raises the error constant.

Appendices

A. Commutators erasing in Magnus expansion, in equations (7)-(10)

Let us recall that $f(t) = \alpha(t) + \sum a_n(t)e^{i\omega_nt}$. Then

$$A(t_1) = \begin{bmatrix} 0 & 1 \\ \Delta + f(t_1) & 0 \end{bmatrix}$$

and

$$[A(t_2), A(t_1)] = \begin{bmatrix} f(t_1) - f(t_2) & 0 \\ 0 & f(t_2) - f(t_1) \end{bmatrix}.$$
Figure 13: Here we analyse a very important equation (32) where the input term features very slow oscillations like \( \omega_1 = 1 \) and high like \( \omega_5 = 10^5 \). Asymptotic method fails due to \( \omega_1 \) while BBCK\(^4\) and BBCK\(^6\) fail because of very large oscillations. Note that the new method performs steadily and achieves accuracy at least \( O(h^2) \) globally.

In the following part we are calculating two- and three-times nested commutators.

\[
[A(t_1), [A(t_2), A(t_3)]] = \begin{bmatrix}
0 & 1 & f(t_3) - f(t_2) & 0 \\
\Delta + f(t_1) & 0 & f(t_2) - f(t_3) & 0 \\
0 & f(t_2) - f(t_3) & \Delta + f(t_1) & 0 \\
0 & f(t_2) - f(t_3) & (\Delta + f(t_1))(f(t_3) - f(t_2)) & 0 \\
0 & f(t_3) - f(t_2) & (f(t_2) - f(t_3))(\Delta + f(t_1)) & 0 \\
0 & H_1 & H_2 & 0 \\
\end{bmatrix}
\]
where

\[ H_1 = 2 (f(t_2) - f(t_3)) \]

\[ H_2 = (\Delta + f(t_1)) (f(t_3) - f(t_2)) - (f(t_2) - f(t_3)) (\Delta + f(t_1)) \]

\[ = \Delta f(t_3) + f(t_3) \Delta - f(t_2) \Delta - f(t_2) \Delta + 2 f(t_1) f(t_3) - 2 f(t_1) f(t_2) . \]

Analogously

\[
[A(t_3), [A(t_2), A(t_1)]] = \begin{bmatrix}
0 & H_3 \\
H_4 & 0
\end{bmatrix},
\]

where

\[ H_3 = 2 (f(t_2) - f(t_1)) \]

\[ H_4 = \Delta f(t_1) + f(t_1) \Delta - f(t_2) \Delta + 2 f(t_3) f(t_1) - 2 f(t_3) f(t_2) . \]

For three-time nested commutators we have

\[
[A(t_4), [[A(t_1), A(t_2)], A(t_3)]] = \begin{bmatrix}
0 & 1 \\
\Delta + f(t_4) & 0
\end{bmatrix}
\begin{bmatrix}
0 & H_5 \\
H_6 & 0
\end{bmatrix}
- \begin{bmatrix}
0 & H_5 \\
H_6 & 0
\end{bmatrix}
\begin{bmatrix}
0 & 1 \\
\Delta + f(t_4) & 0
\end{bmatrix}
\]

\[
= \begin{bmatrix}
H_6 & 0 \\
0 & \Delta + f(t_4)
\end{bmatrix}
- \begin{bmatrix}
H_5 (\Delta + f(t_4)) & 0 \\
0 & H_6
\end{bmatrix}
\]

\[
= \begin{bmatrix}
H_6 - H_5 (\Delta + f(t_4)) & 0 \\
0 & \Delta + f(t_4) H_5 - H_6
\end{bmatrix}
\]

where

\[ H_5 = 2 (f(t_2) - f(t_1)) \]

\[ H_6 = \Delta (f(t_1) - f(t_2)) + (f(t_1) - f(t_2)) \Delta + 2 f(t_3) (f(t_1) - f(t_2)) . \]
\[
[A(t_1), [A(t_2), A(t_3)], A(t_4)] = \begin{bmatrix}
0 & 1 & 0 & H_7 \\
\Delta + f(t_1) & 0 & H_7 & 0 \\
H_8 & 0 & H_8 & \Delta + f(t_1) \\
0 & H_7 & 0 & H_7
\end{bmatrix}
\]

\[
= \begin{bmatrix}
H_8 & 0 \\
0 & (\Delta + f(t_1)) H_7 \\
H_8 & 0 \\
0 & (\Delta + f(t_1)) H_7
\end{bmatrix}
\]

\[
= \begin{bmatrix}
H_8 - H_7 (\Delta + f(t_1)) & 0 \\
0 & (\Delta + f(t_1)) H_7 - H_8
\end{bmatrix}
\]

where

\[
H_7 = 2 (f(t_3) - f(t_2))
\]

\[
H_8 = \Delta (f(t_2) - f(t_3)) + (f(t_2) - f(t_3)) \Delta + 2f(t_4) (f(t_2) - f(t_3))
\]

\[
[A(t_1), [A(t_2), [A(t_3), A(t_4)]]] = \begin{bmatrix}
0 & 1 & 0 & H_9 \\
\Delta + f(t_1) & 0 & H_9 & 0 \\
H_{10} & 0 & H_{10} & \Delta + f(t_1) \\
0 & H_9 & 0 & H_9
\end{bmatrix}
\]

\[
= \begin{bmatrix}
H_{10} & 0 \\
0 & (\Delta + f(t_4)) H_9 \\
H_{10} & 0 \\
0 & (\Delta + f(t_4)) H_9
\end{bmatrix}
\]

\[
= \begin{bmatrix}
H_{10} - H_9 (\Delta + f(t_1)) & 0 \\
0 & (\Delta + f(t_1)) H_9 - H_{10}
\end{bmatrix}
\]

where

\[
H_9 = 2 (f(t_3) - f(t_4))
\]

\[
H_{10} = \Delta (f(t_4) - f(t_3)) + (f(t_4) - f(t_3)) \Delta + 2f(t_2) (f(t_4) - f(t_3))
\]
\[
[A(t_2), [A(t_3), [A(t_4), A(t_1)]]] = \begin{bmatrix}
0 & 1 & 0 & H_{11} \\
\Delta + f(t_2) & 0 & H_{12} & 0 \\
0 & \Delta + f(t_2) & 0 & H_{12} \\
0 & 0 & \Delta + f(t_2) & 0
\end{bmatrix}
\]

(33)

where

\[
H_{11} = 2 (f(t_4) - f(t_1))
\]

\[
H_{12} = \Delta (f(t_1) - f(t_4)) + (f(t_1) - f(t_4)) \Delta + 2f(t_3) (f(t_1) - f(t_4))
\]

To estimate term \( \Theta_4 \), we need to sum the matrices resulting from individual commutators. The result is a matrix

\[
\begin{bmatrix}
H_1 & 0 \\
0 & H_2
\end{bmatrix}
\]

where

\[
H_1 = -H_6 + H_5 (\Delta + f(t_4)) + H_8 - H_7 (\Delta + f(t_1)) + H_{10} - H_9 (\Delta + f(t_4)) + H_{12} - H_{11} (\Delta + f(t_2))
\]

\[
= \Delta (f(t_2) - f(t_1)) + (f(t_2) - f(t_1)) \Delta + 2f(t_3) (f(t_2) - f(t_1)) - 2 (f(t_1) - f(t_2)) (\Delta + f(t_4)) + \Delta (f(t_3) - f(t_4)) + (f(t_3) - f(t_4)) \Delta + 2f(t_2) (f(t_3) - f(t_4)) - 2 (f(t_2) - f(t_3)) (\Delta + f(t_1)) + \Delta (f(t_1) - f(t_4)) + (f(t_1) - f(t_4)) \Delta + 2f(t_4) (f(t_1) - f(t_4)) - 2 (f(t_4) - f(t_3)) (\Delta + f(t_2)) + \Delta (2f(t_2) - 2f(t_3)) + 3 (2f(t_2) - 2f(t_3)) \Delta + 4f(t_4) (f(t_2) - f(t_3)) + 4f(t_1) (f(t_2) - f(t_3))
\]

and

\[
H_2 = -3 \Delta (2f(t_2) - 2f(t_3)) - (2f(t_2) - 2f(t_3)) \Delta - 4f(t_4) (f(t_2) - f(t_3)) - 4f(t_1) (f(t_2) - f(t_3)),
\]

where

\[
f(t_k) f(t_l) = \left( \alpha(t_k) + \sum_n a_n(t_k) e^{i\omega_n t_k} \right) \left( \alpha(t_l) + \sum_n a_n(t_l) e^{i\omega_n t_l} \right)
\]

\[
= \alpha(t_k) \alpha(t_l) + \alpha(t_k) \sum_n a_n(t_k) e^{i\omega_n t_k} + \alpha(t_l) \sum_n a_n(t_l) e^{i\omega_n t_l} + \sum_n a_n(t_k) e^{i\omega_n t_k} \sum_m a_m(t_l) e^{i\omega_m t_l}
\]
Taking

\[ X = -\int_{0}^{h} \int_{0}^{t_1} [A(t + t_2), A(t + t_1)] dt_1 dt_2 = \begin{bmatrix} -\mathcal{F} & 0 \\ 0 & \mathcal{F} \end{bmatrix}, \]

\[ Y = \int_{0}^{h} \begin{bmatrix} 0 & 1 \\ \Delta + f(t + t_1) & 0 \end{bmatrix} dt_1 = \begin{bmatrix} 0 & h \\ h\Delta + F & 0 \end{bmatrix}, \]
we have

\[
[Y, X] = \begin{bmatrix}
0 & h \\
-\mathcal{F} & 0 \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
- \begin{bmatrix}
-\mathcal{F} & 0 \\
0 & h \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
= \begin{bmatrix}
0 & h\mathcal{F} \\
-(h\Delta + h\mathcal{F}) & 0 \\
-\mathcal{F}(h\Delta + h\mathcal{F}) & 0
\end{bmatrix}
= \begin{bmatrix}
0 & 2h\mathcal{F} \\
0 & -(h\Delta + h\mathcal{F}) & 0 \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
\]

\[
[Y, [Y, X]] = \begin{bmatrix}
0 & h \\
0 & h\mathcal{F} \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
- \begin{bmatrix}
0 & h\mathcal{F} \\
0 & -(h\Delta + h\mathcal{F}) & 0 \\
-(h\Delta + h\mathcal{F}) & 0
\end{bmatrix}
= \begin{bmatrix}
0 & (h\Delta + h\mathcal{F}) \\
0 & -2h\mathcal{F} \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
- \begin{bmatrix}
0 & (h\Delta + h\mathcal{F}) \\
0 & -2h\mathcal{F} \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
= \begin{bmatrix}
0 & 3h^2\Delta + 2h\mathcal{F} \\
0 & 3h^2\Delta + h^2\mathcal{F} + 2h\mathcal{F}
\end{bmatrix}
\]

\[
[X, Y] = -[Y, X] = \begin{bmatrix}
0 & -2h\mathcal{F} \\
h\Delta + h\mathcal{F} & 0
\end{bmatrix}
- \begin{bmatrix}
-\mathcal{F} & 0 \\
0 & h\Delta + h\mathcal{F} + 2h\mathcal{F}
\end{bmatrix}
= \begin{bmatrix}
-\mathcal{F} & 0 \\
0 & h\Delta + h\mathcal{F} + 2h\mathcal{F}
\end{bmatrix}
- \begin{bmatrix}
-\mathcal{F} & 0 \\
0 & h\Delta + h\mathcal{F} + 2h\mathcal{F}
\end{bmatrix}
= \begin{bmatrix}
0 & 2h\mathcal{F} \\
0 & 4h\mathcal{F}^2
\end{bmatrix}
- \begin{bmatrix}
0 & 2h\mathcal{F} \\
0 & 4h\mathcal{F}^2
\end{bmatrix}
= \begin{bmatrix}
0 & 0 \\
0 & -(h\Delta + h\mathcal{F} + 2h\mathcal{F})(-\mathcal{F})
\end{bmatrix}
= \begin{bmatrix}
0 & 0 \\
0 & -(h\Delta + h\mathcal{F} + 2h\mathcal{F})(-\mathcal{F})
\end{bmatrix}
\]

\[
[X, [X, Y]] = \begin{bmatrix}
-\mathcal{F} & 0 \\
0 & h\Delta + h\mathcal{F} + 2h\mathcal{F}
\end{bmatrix}
- \begin{bmatrix}
0 & 2h\mathcal{F} \\
0 & 4h\mathcal{F}^2
\end{bmatrix}
= \begin{bmatrix}
0 & 0 \\
0 & 0
\end{bmatrix}
- \begin{bmatrix}
0 & 2h\mathcal{F} \\
0 & 4h\mathcal{F}^2
\end{bmatrix}
= \begin{bmatrix}
0 & 0 \\
0 & -(h\Delta + h\mathcal{F} + 2h\mathcal{F})(-\mathcal{F})
\end{bmatrix}
= \begin{bmatrix}
0 & 0 \\
0 & -(h\Delta + h\mathcal{F} + 2h\mathcal{F})(-\mathcal{F})
\end{bmatrix}
\]
Hence

\[
[Y, [Y, X]] = \begin{bmatrix}
-h^2 \Delta F - 3h^2 F \Delta - 4h\mathcal{F}F & 0 \\
0 & 3h^2 \Delta F + h^2 F \Delta + 4h\mathcal{F}F
\end{bmatrix}
\]

\[
[X, [X, Y]] = \begin{bmatrix}
0 & 4h\mathcal{F}^2 \\
2h\mathcal{F} \Delta F + h\mathcal{F}^2 \Delta + h\Delta \mathcal{F}^2 + 4\mathcal{F}^2 F & 0
\end{bmatrix}
\]

C. Fourth order splittings

In section IID we introduced the 4-th order splitting (15) and (16) of the following form

\[e^{X+Y} = e^{c_2 X} e^{c_1 Y} e^{c_0 X + a[[X,Y],X] + b[[X,Y],Y]} e^{c_1 Y} e^{c_2 X} + \mathcal{O}(h^5)\]

where \(a\) or \(b\) vanishes.

In the below calculations we will derive coefficients \(c_0, c_1, c_2\) for both cases: where \(a = 0\) and where \(b = 0\).

Let us recall sBCH formula

\[\exp[Y] \exp[X] \exp[Y] = \exp[sBCH(Y,X)], \text{ where}
\]

\[sBCH(Y,X) = 2Y + X - \frac{1}{6}[[X,Y],Y] - \frac{1}{6}[[X,Y],X] + \mathcal{O}(h^5)\]

1.

\[\frac{e^{c_1 Y} e^{c_0 X} e^{c_1 Y}}{\hat{W}_1} = \exp[sBCH(c_1 Y, c_0 X)]\]

\[sBCH(c_1 Y, c_0 X) = 2c_1 Y + c_0 X - \frac{1}{6} c_0 c_1^2 [[X,Y],Y] - \frac{1}{6} c_0^2 c_1 [[X,Y],X]\]
\[ e^{c_2 X} e^{c_1 Y} e^{c_0 X} e^{c_1 Y} e^{c_2 X} = \exp[s\text{BCH}(c_2 X, W_1)] \]

\[
s\text{BCH}(c_2 X, W_1) = 2c_2 X + W_1 - \frac{1}{6} c_2^2 [[W_1, X], X] - \frac{1}{6} c_2 [[W_1, X], W_1] = 2c_2 X + 2c_1 Y + c_0 X - \frac{1}{6} c_0 c_1^3 [[X, Y], Y] - \frac{1}{6} c_0^2 c_1 [[X, Y], X] - \frac{1}{3} c_1 c_2^2 [[Y, X], X] - \frac{2}{3} c_1 c_2 [[Y, X], Y] - \frac{1}{3} c_0 c_1 c_2 [[Y, X], X] = (c_0 + 2c_2) X + 2c_1 Y + \left(\frac{2}{3} c_1 c_2 - \frac{1}{6} c_0 c_1^2\right) [[X, Y], Y] + \left(\frac{1}{3} c_1 c_2^2 - \frac{1}{6} c_0^2 c_1 + \frac{1}{3} c_0 c_1 c_2\right) [[X, Y], X]
\]

because

\[
-\frac{1}{6} c_2^2 [[W_1, X], X] = -\frac{1}{6} c_2^2 [[2c_1 Y, X], X] - \frac{1}{6} c_2^2 [[c_0 X, X], X] = -\frac{1}{3} c_1 c_2^2 [[Y, X], X]
\]

\[
-\frac{1}{6} c_2 [[W_1, X], W_1] = -\frac{1}{6} c_2 [[2c_1 Y + c_0 X, X], 2c_1 Y + c_0 X] = -\frac{2}{3} c_1 c_2 [[Y, X], Y] - \frac{1}{3} c_0 c_1 c_2 [[Y, X], X],
\]

where we neglected terms with commutators nested more then two times (that is scaling at least like \(O(h^5)\)).

Depending on which of the expressions is more computationally complicated (\([[X, Y], Y]\) or \([[X, Y], X]\)) we will obtain two systems of equations for the coefficients \(c_0, c_1, c_2\):

### Elimination of \([[X, Y], Y]\) - towards (15)

- \(c_0 + 2c_2 = 1\)
- \(2c_1 = 1\)
- \(a = \frac{1}{3} c_1 c_2 - \frac{1}{6} c_0 c_1 + \frac{1}{3} c_0 c_1 c_2\)
- \(b = \frac{2}{3} c_1 c_2 - \frac{1}{6} c_0 c_1^2\)
- \(b = 0\)

### Elimination of \([[X, Y], X]\) towards (16)

- \(c_0 + 2c_2 = 1\)
- \(2c_1 = 1\)
- \(a = \frac{1}{3} c_1 c_2 - \frac{1}{6} c_0 c_1 + \frac{1}{3} c_0 c_1 c_2\)
- \(b = \frac{2}{3} c_1 c_2 - \frac{1}{6} c_0 c_1^2\)
- \(a = 0\)

\[ c_0 = \frac{2}{3}, c_1 = \frac{1}{2}, c_2 = \frac{1}{6} \quad \text{and} \quad a = -\frac{1}{72} \quad c_0 = \frac{1}{\sqrt{3}}, c_1 = \frac{1}{2}, c_2 = \frac{1}{2} - \frac{1}{2\sqrt{3}} \quad \text{and} \quad b = \frac{1}{24} (2 - \sqrt{3}) \]

[1] Bader, P., Blanes, S., Casas, F. and Kopylov, N. [2019], ‘Novel symplectic integrators for the Klein-Gordon equation with space- and time-dependent mass’, *J. Comput. Appl. Math.* **350**, 130–138.

**URL**: [https://doi.org/10.1016/j.cam.2018.10.011](https://doi.org/10.1016/j.cam.2018.10.011)
[2] Bao, W. and Dong, X. [2012], ‘Analysis and comparison of numerical methods for the Klein-Gordon equation in the nonrelativistic limit regime’, *Numer. Math.* **120**(2), 189–229.
URL: https://doi.org/10.1007/s00211-011-0411-2

[3] Blanes, S., Casas, F., Oteo, J. A. and Ros, J. [2009], ‘The Magnus expansion and some of its applications’, *Phys. Rep.* **470**(5-6), 151–238.
URL: https://doi.org/10.1016/j.physrep.2008.11.001

[4] Chen, J.-B. and Liu, H. [2008], ‘Multisymplectic pseudospectral discretizations for (3+1)-dimensional Klein-Gordon equation’, *Commun. Theor. Phys. (Beijing)* **50**(5), 1052–1054.
URL: https://doi.org/10.1088/0253-6102/50/5/07

[5] Condon, M., Kropielnicka, K., Lademann, K. and Perczyński, R. [2021], ‘Asymptotic numerical solver for the linear Klein-Gordon equation with space- and time-dependent mass’, *Applied Mathematics Letters* **115**, 106935.
URL: https://www.sciencedirect.com/science/article/pii/S089396592030481X

[6] Faou, E. and Schratz, K. [2014], ‘Asymptotic preserving schemes for the Klein-Gordon equation in the non-relativistic limit regime’, *Numer. Math.* **126**(3), 441–469.
URL: https://doi.org/10.1007/s00211-013-0567-z

[7] Hairer, E., Lubich, C. and Wanner, G. [2006], *Geometric numerical integration: structure-preserving algorithms for ordinary differential equations*, Vol. 31, Springer Science & Business Media.

[8] Iserles, A. [2002], ‘On the global error of discretization methods for highly-oscillatory ordinary differential equations’, *BIT* **42**(3), 561–599.
URL: https://doi.org/10.1023/A:1022049814688

[9] Iserles, A., Munthe-Kaas, H. Z., Norsett, S. P. and Zanna, A. [2000], Lie-group methods, in ‘Acta numerica, 2000’, Vol. 9 of *Acta Numer.*, Cambridge Univ. Press, Cambridge, pp. 215–365.
URL: https://doi.org/10.1017/S0962492900002154

[10] Iserles, A., Norsett, S. P. and Rasmussen, A. F. [2001], ‘Time symmetry and high-order Magnus methods’, *Appl. Numer. Math.* **39**(3-4), 379–401. Special issue: Themes in geometric integration.
URL: https://doi.org/10.1016/S0168-9274(01)00088-5

[11] Kopriva, D. A. [2009], *Implementing spectral methods for partial differential equations*, Scientific Computation, Springer, Berlin. Algorithms for scientists and engineers.
URL: https://doi.org/10.1007/978-90-481-2261-5

[12] Mostafazadeh, A. [2003], ‘Hilbert space structures on the solution space of klein-gordon-type evolution equations’, *Classical Quantum Gravity* **20**(1), 155–171.
URL: https://iopscience.iop.org/article/10.1088/0264-9381/20/1/312

[13] Mostafazadeh, A. [2004], ‘Quantum mechanics of Klein-Gordon-type fields and quantum cosmology’, *Annals of Physics* **309**(1), 1–48.
URL: https://www.sciencedirect.com/science/article/pii/S0003491603002021

[14] Shakeri, F. and Dehghan, M. [2008], ‘Numerical solution of the Klein-Gordon equation via He’s variational iteration method’, *Nonlinear Dynam.* **51**(1-2), 89–97.
[15] Yusufoğlu, E. [2008], ‘The variational iteration method for studying the Klein-Gordon equation’, *Appl. Math. Lett.* **21**(7), 669–674.

URL: https://doi.org/10.1016/j.aml.2007.07.023

[16] Znojil, M. [2016], ‘Quantization of big bang in crypto-hermitian heisenberg picture’, *Springer Proc. Phys.* **184**, 383–399.

[17] Znojil, M. [2017a], ‘Klein-Gordon equation with the time- and space-dependent mass:Unitary evolution picture’.

URL: arXiv:1702.08493v1

[18] Znojil, M. [2017b], ‘Non-Hermitian interaction representation and its use in relativistic quantum mechanics’, *Ann. Physics* **385**, 162–179.

URL: https://doi.org/10.1016/j.aop.2017.08.009