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Multi-Product Expansion with Suzuki's Method: Generalization

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Abstract. In this paper we discuss the extension to exponential splitting methods with respect to time-dependent operators. We concentrate on the Suzuki's method, which incorporates ideas to the time-ordered exponential of [3, 11, 12, 34]. We formulate the methods with respect to higher order by using kernels for an extrapolation scheme. The advantages include more accurate and less computational intensive schemes to special time-dependent harmonic oscillator problems. The benefits of the higher order kernels are given on different numerical examples.

AMS subject classifications: 65M15, 65L05, 65M71

Key words: Suzuki's method, multiproduct expansion, multiplicate and additive splitting schemes, exponential splitting.

1. Introduction

In this paper we concentrate on approximation to the solution of the linear evolution equation, e.g., time-dependent Schrödinger equation,

$$\partial_t u = L(t)u = (A(t) + B(t))u, \qquad u(0) = u_0, \tag{1.1}$$

where L,A and B are unbounded and time-dependent operators. For such equations, we concentrate on comparing the higher order methods to Suzuki's schemes. Here the Suzuki's methods apply factorized symplectic algorithms with forward derivatives, see, e.g., [11, 12]. Some preliminary comparison are presented in [3, 11], where the benefits of each method are outlined.

In our paper, we like to see the drawback of each method, so for the Magnus integrator, the spiked harmonic oscillator case, see [12] and for the Suzuki's method, geometric properties, which are known to be solved with geometric integrator, e.g. Magnus integrators.

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At least we like to outline an idea to combine the Magnus integrators and the Suzuki's factorization schemes to optimize the methods.

The paper is outlined as follows. In Section 2, we present our Suzuki's rule for decomposing time-ordered integrators. The extrapolation schemes and their generalization are given in Section 3. In Section 4, we present the error analysis of the multi-product splitting based on the extrapolation analysis. The numerical experiments are given in Section 5, here time-dependent problems are discussed. In Section 6, we briefly summarize our results.

2. Exponential splitting method based on Suzuki's time-ordered exponential

Instead of the Magnus expansion, see [10], one can also directly implement the time-ordered exponential as suggested by Suzuki [34]. We deal with a linear evolution equation given as:

$$\frac{dY}{dt} = A(t)Y(t), \tag{2.1}$$

with solution

$$Y(t) = \exp(\Omega(t))Y(0). \tag{2.2}$$

This can be expressed as:

$$Y(t) = \mathscr{T}\left(\exp(\int_0^t A(s)\, ds\right)Y(0)\,, \tag{2.3}$$

where the time-ordering operator $\mathscr{T}$ is given in [15]. Rewriting (2.3) as

$$Y(t+\Delta t) = \mathscr{T}\Big(\exp\int_t^{t+\Delta t} A(s)ds\Big)Y(t). \tag{2.4}$$

Aside from the conventional expansion

$$\begin{aligned}&\mathscr{T}\left(\exp\int_t^{t+\Delta t} A(s)ds\right)\\ =&1+\int_t^{t+\Delta t} A(s_1)ds_1+\int_t^{t+\Delta t} ds_1\int_t^{s_1} ds_2 A(s_1)A(s_2)+\cdots\,,\end{aligned} \tag{2.5}$$

the time-ordered exponential can also be interpreted more intuitively as

$$\begin{aligned}\mathscr{T}\left(\exp\int_t^{t+\Delta t} A(s)ds\right) &= \lim_{n\to\infty}\mathscr{T}\Big(\mathrm{e}^{\frac{\Delta t}{n}\sum_{i=1}^n A\left(t+i\frac{\Delta t}{n}\right)}\Big), &(2.6)\\ &= \lim_{n\to\infty}\mathrm{e}^{\frac{\Delta t}{n}A(t+\Delta t)}\cdots\mathrm{e}^{\frac{\Delta t}{n}A\left(t+\frac{2\Delta t}{n}\right)}\mathrm{e}^{\frac{\Delta t}{n}A\left(t+\frac{\Delta t}{n}\right)}. &(2.7)\end{aligned}$$

The time-ordering is trivially accomplished in going from (2.6) to (2.7). To enforce latter, Suzuki introduces the *forward time derivative* operator

$$D = \frac{\overleftarrow{\partial}}{\partial t} \tag{2.8}$$

such that for any two time-dependent functions $F(t)$ and $G(t)$,

$$F(t)e^{\Delta tD}G(t) = F(t+\Delta t)G(t). \tag{2.9}$$

Trotter's formula then gives

$$\begin{aligned} \exp\left(\Delta t\big(A(t)+D\big)\right) &= \lim_{n\to\infty}\left(e^{\frac{\Delta t}{n}A(t)}e^{\frac{\Delta t}{n}D}\right)^n, \\ &= \lim_{n\to\infty} e^{\frac{\Delta t}{n}A(t+\Delta t)}\cdots e^{\frac{\Delta t}{n}A\left(t+\frac{2\Delta t}{n}\right)}e^{\frac{\Delta t}{n}A\left(t+\frac{\Delta t}{n}\right)}, \end{aligned} \tag{2.10}$$

where property (2.9) has been applied repeatedly and accumulatively. Comparing (2.7) with (2.10) yields Suzuki's decomposition of the time ordered exponential [34]

$$\mathscr{T}\left(\exp\int_t^{t+\Delta t} A(s)ds\right) = \exp\left(\Delta t\big(A(t)+D\big)\right). \tag{2.11}$$

Thus time-ordering can be accomplished by just adding the operator D. For example, we have the following second-order splittings

$$\mathscr{T}_2(\Delta t) = e^{\frac{1}{2}\Delta tD}e^{\Delta tA(t)}e^{\frac{1}{2}\Delta tD} = e^{\Delta tA\left(t+\frac{1}{2}\Delta t\right)}. \tag{2.12}$$

The choice of symmetric products is important, because we archive only odd powers of Δt

$$\mathscr{T}_2(\Delta t) = e^{\Delta t(A(t)+D)} + \Delta t^3E_3 + \Delta t^5E_5 + \cdots. \tag{2.13}$$

Every occurrence of the operator $e^{d_i\Delta tD}$, from right to left, updates the current time t to $t+d_i\Delta t$. If t is the time at the start of the algorithm, then after the first occurrence of $e^{\frac{1}{2}\Delta tD}$, time is $t+\frac{1}{2}\Delta t$. After the second $e^{\frac{1}{2}\Delta tD}$, time is $t+\Delta t$. Thus the leftmost $e^{\frac{1}{2}\Delta tD}$ is not without effect, it correctly updates the time for the next iteration. For example

$$\mathscr{T}_2(\Delta t)\mathscr{T}_2(\Delta t) = e^{\Delta tA\left(t+\frac{3}{2}\Delta t\right)}e^{\Delta tA\left(t+\frac{1}{2}\Delta t\right)}. \tag{2.14}$$

Higher order factorization of (2.11) into a single product form

$$\exp\left(\Delta t\big(A(t)+D\big)\right) = \prod_i e^{a_i\Delta tA(t)}e^{d_i\Delta tD} \tag{2.15}$$

will yield higher order algorithms, but at the cost of exponentially growing number of evaluations of $e^{a_i\Delta tA}$.

To generalize into a Multiproduct expansion, we have:

$$\exp\left(\Delta t\big(A(t)+D\big)\right) = \sum_j \Pi_i c_j e^{a_{ij}\Delta tA(t)}e^{d_{ij}\Delta tD}. \tag{2.16}$$

2.1. Additive and multiplicative higher order splitting methods

A method for the derivation of higher order methods with the multiproduct expansion can be given as following. We have to derive the coefficients:

$$\exp\big((A+B)t\big) - \left(\sum_{i=1}^{m} c_i \prod_{j=1}^{n_i} \exp(a_j A t)\exp(b_j B t)\right) = \mathcal{O}(t^m), \tag{2.17}$$

where $m-1$ is the order of the method and the coefficients have to be derived under the following conditions:

$$\big(1 - f_1(a_1,\cdots,a_{n_m},b_1,\cdots,b_{n_m},c_1,\cdots,c_m)\big) = 0, \tag{2.18}$$
$$\big((A+B) - f_2(a_1,\cdots,a_{n_m},b_1,\cdots,b_{n_m},c_1,\cdots,c_m)\big) = 0. \tag{2.19}$$
$$\vdots$$

Remark 2.1. With respect to efficient schemes, one have to derive with less additive and multiplicative terms. By an effective mixture between exponential splitting methods and extrapolation schemes, higher order methods can be derived.

An Example for a 3rd order is given as:

$$\begin{aligned}\big(\exp((A+B)t) - \big(&a\exp(1/2At)\exp(1/2Bt)\exp(1/2At)\exp(1/2Bt)\\ &+ b\exp(1/2Bt)\exp(1/2At)\exp(1/2Bt)\exp(1/2At)\\ &+ c\exp(At)\exp(Bt) + d\exp(Bt)\exp(At)\big) = \mathcal{O}(t^4).\end{aligned} \tag{2.20}$$

The coefficients are ordered with respect to the operators and derived as:

$$\begin{aligned}&1 - a - c - d - b\\ &\quad + \Big(-dB - dA + A + B - cA - cB - aA - aB - bB - bA\Big)t\\ &\quad + \Big(-1/2cA^2 - cAB - 1/2cB^2 - 1/2dB^2 - dBA - 1/2dA^2 - 1/2bB^2\\ &\quad - 3/4bBA - 1/2bA^2 - 1/4bAB + 1/2(A+B)^2 - 1/2aA^2 - 3/4aAB\\ &\quad - 1/2aB^2 - 1/4aBA\Big)t^2\\ &\quad + \Big(-1/16bA^2B - 5/16aA^2B - 5/16bB^2A + 1/6(A+B)^3\\ &\quad - 1/16aB^2A - 1/2dBA^2 - 1/6cA^3 - 5/16aAB^2 - 1/2cAB^2\\ &\quad - 1/6dA^3 - 1/6cB^3 - 1/2dB^2A - 1/8bBAB - 1/16bAB^2\\ &\quad - 1/6bB^3 - 5/16bBA^2 - 1/6aA^3 - 1/8aBAB - 1/6bA^3 - 1/8bABA\\ &\quad - 1/6aB^3 - 1/6dB^3 - 1/2cA^2B - 1/16aBA^2 - 1/8aABA\Big)t^3\\ =&\mathcal{O}(t^4),\end{aligned} \tag{2.21}$$

which yields

$$\begin{array}{ll}
g1 := 1-a-c-d-b=0; & \\
g21 := 1-a-c-d-b=0; & \text{“}A\text{”} \\
g22 := 1-a-c-d-b=0; & \text{“}B\text{”} \\
g31 := 1-a-c-d-b=0; & \text{“}1/2A^2\text{”} \\
g32 := 1-a-c-d-b=0; & \text{“}1/2B^2\text{”} \\
g33 := -2c-(1/2)b+1-(3/2)a=0; & \text{“}1/2AB\text{”} \\
g34 := -2d-(3/2)b+1-(1/2)a=0; & \text{“}1/2BA\text{”} \\
g41 := 1-a-c-d-b=0; & \text{“}1/6A^3\text{”} \\
g42 := 1-a-c-d-b=0; & \text{“}1/6B^3\text{”} \\
g43 := 1-(15/8)a-(3/8)b-3c=0; & \text{“}1/6A^2B\text{”} \\
g44 := 1-(3/8)a-(15/8)b-3d=0; & \text{“}1/6BA^2\text{”} \\
g45 := 1-(3/8)a-(15/8)b-3d=0; & \text{“}1/6B^2A\text{”} \\
g46 := 1-(15/8)a-(3/8)b-3c=0; & \text{“}1/6AB^2\text{”} \\
g47 := 1-(3/4)a-(3/4)b=0; & \text{“}1/6ABA\text{”} \\
g48 := 1-(3/4)a-(3/4)b=0. & \text{“}1/6BAB\text{”}
\end{array}$$

Solving the linear equation system gives

$$d=d, \quad c=-1/3-d, \quad b=-2d+1/3, \quad a=1+2d,$$

where we have chosen $a=b=4/6$, $c=d=-1/6$.

2.2. Examples of multiproduct expansions

Second Order. For a kernel of second order splitting methods, e.g.,

$$\mathscr{T}_2(\Delta t)=\frac{1}{2}\Big(\exp(A\Delta t)\exp(B\Delta t)+\exp(B\Delta t)\exp(A\Delta t)\Big). \tag{2.22}$$

Fourth Order. For a kernel of fourth order splitting methods, e.g., see [14],

$$\begin{aligned}
&\mathscr{T}_4(\Delta t)=\exp\left(\frac{\tau\tilde{a}}{2}A\right)\exp\left(\frac{\tau}{2}B\right)\exp\left(\frac{\tau}{\sqrt{3}}\tilde{A}\right)\exp\left(\frac{\tau}{2}B\right)\exp\left(\frac{\tau\tilde{a}}{2}A\right),\\
&\tilde{A}=A+\frac{\tau^2}{24}(2\sqrt{3}-3)[B,[B,A]], \qquad \tilde{a}=1-1/\sqrt{3}.
\end{aligned} \tag{2.23}$$

Higher order reconstruction by Taylor expansion, see Subsection 2.1, gives

$$\begin{aligned}
\mathscr{T}_4(\Delta t)=&\frac{2}{3}\exp\left(\frac{1}{2}A\tau\right)\exp\left(\frac{1}{2}B\tau\right)\exp\left(\frac{1}{2}A\tau\right)\exp\left(\frac{1}{2}B\tau\right)\\
&+\frac{2}{3}\exp\left(\frac{1}{2}B\tau\right)\exp\left(\frac{1}{2}A\tau\right)\exp\left(\frac{1}{2}B\tau\right)\exp\left(\frac{1}{2}A\tau\right)\\
&-\frac{1}{6}\exp(A\tau)\exp(B\tau)-\frac{1}{6}\exp(B\tau)\exp(A\tau).
\end{aligned} \tag{2.24}$$

2.3. Symplecticity

The symplecticity and unitarity are important for applications to Hamiltonian problems. Based on the work of [6], we have the following theorem.

Theorem 2.1. ([6]) *If the basic $2n$-th order method $\mathcal{T}_n$ is symmetric and symplectic, then by applying polynomic extrapolation it is possible to construct integration methods of order $2(n+l)$, $l=1,\cdots,n$, which are symplectic up to the order $4n+1$.*

3. Extrapolation scheme

In this section we apply the extrapolation scheme to our higher order splitting kernels.

3.1. Extrapolation to a second-order kernel

Recently, it has been shown that, once one has the second order algorithm (2.12), arbitrary higher order algorithms can be built from the multi-product expansion* of (2.11), with only quadratically growing number of exponentials at high orders. For example,

$$\mathcal{T}_4(\Delta t)=-\frac{1}{3}\mathcal{T}_2(\Delta t)+\frac{4}{3}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right), \tag{3.1}$$

$$\mathcal{T}_6(\Delta t)=\frac{1}{24}\mathcal{T}_2(\Delta t)-\frac{16}{15}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right)+\frac{81}{40}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right), \tag{3.2}$$

$$\mathcal{T}_8(\Delta t)=-\frac{1}{360}\mathcal{T}_2(\Delta t)+\frac{16}{45}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right)-\frac{729}{280}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right)+\frac{1024}{315}\mathcal{T}_2^4\left(\frac{\Delta t}{4}\right), \tag{3.3}$$

$$\begin{aligned}\mathcal{T}_{10}(\Delta t)=&\frac{1}{8640}\mathcal{T}_2(\Delta t)-\frac{64}{945}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right)+\frac{6561}{4480}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right)-\frac{16384}{2835}\mathcal{T}_2^4\left(\frac{\Delta t}{4}\right)\\&+\frac{390625}{72576}\mathcal{T}_2^5\left(\frac{\Delta t}{5}\right).\end{aligned} \tag{3.4}$$

In the case of $A(t)=T+V(t)$, the second-order algorithm is then

$$\mathcal{T}_2(\Delta t)=\mathrm{e}^{\Delta tA\left(t+\frac{1}{2}\Delta t\right)}=\mathrm{e}^{\frac{1}{2}\Delta tT}\mathrm{e}^{\Delta tV\left(t+\frac{\Delta t}{2}\right)}\mathrm{e}^{\frac{1}{2}\Delta tT}+\mathcal{O}(\Delta t^3). \tag{3.5}$$

For the error terms we have the following estimates:

$$\begin{aligned}&\exp\left(\left(\frac{\Delta t}{2}\right)T\right)\exp(\Delta tV)\exp\left(\left(\frac{\Delta t}{2}\right)T\right)\\&=\exp(\Delta t(T+V)+\Delta t3E_3+\Delta t5E_5+\cdots),\end{aligned} \tag{3.6}$$

with

$$E_3=-\left(\frac{1}{24}\right)[TTV]-\left(\frac{1}{12}\right)[VTV], \tag{3.7}$$

$$E_5 = \left(\frac{7}{5760}\right)[TTTTV] + \left(\frac{1}{480}\right)[TTVTV] + \left(\frac{1}{360}\right)[VTTTV] + \left(\frac{1}{120}\right)[VTVTV], \quad (3.8)$$

where $[TTV] = [T,[T,V]]$ and $[TTTTV] = [T,[T,[T,[T,V]]]]$ etc., denotes the nested commutators.

This is for the case we have $[VVTV] = 0$. So an error bound is given as:

$$\begin{aligned} ||E_3|| &= \left\| -\left(\frac{1}{24}\right)[TTV] - \left(\frac{1}{12}\right)[VTV] \right\| \\ &\leq \frac{1}{24}||T^2||||V|| + \frac{1}{12}||T^2||||V^2||, \end{aligned} \quad (3.9)$$

$$\begin{aligned} ||E_5|| &= \left\| \left(\frac{7}{5760}\right)[TTTTV] + \left(\frac{1}{480}\right)[TTVTV] + \left(\frac{1}{360}\right)[VTTTV] + \left(\frac{1}{120}\right)[VTVTV] \right\| \\ &\leq \left(\frac{7}{5760}\right)||T^4||||V|| + \left(\frac{1}{180}\right)||T^3||||V^2|| + \left(\frac{1}{120}\right)||T^2||||V^3||. \end{aligned} \quad (3.10)$$

The Multiproduct expansion can be derived similarly. More generally, for a given set of n distinct whole numbers $k_1, k_2, \cdots, k_n$, one can form a $2n$-order approximation of eh(A+B) via

$$\exp(A+B) = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right) + e_{2n+1}(h_{2n+1}E_{2n+1}). \quad (3.11)$$

3.2. Generalization

The expansion coefficients c_i are determined by a specially simple Vandermonde equation, where the generalization is a shift of the special case of $m = 0$:

3.2.1. Generalization to even kernels

Here we can construct extrapolations with the kernels: $\mathcal{T}_2, \mathcal{T}_4, \mathcal{T}_6$ etc., i.e. $m = 0, 1, 2, \cdots$

Lemma 3.1. *The closed form of the coefficients for the extrapolation is given as with closed form solutions*

$$c_i = \frac{k_i^{2m}}{\sum_{j=1}^n k_j^2} \prod_{j=1(\neq i)}^{n} \frac{k_i^2}{k_i^2 - k_j^2} \quad (3.12)$$

and error coefficient

$$e_{2m+2n+1} = (-1)^{n-1} \frac{k_i^{2m}}{\sum_{j=1}^n k_j^2} \prod_{i=1}^{n} \frac{1}{k_i^2}. \quad (3.13)$$

Here we have closed forms (3.15) *and* (3.16) *and are the keys to the multi-product expansion and its error analysis, see* [6].

Proof. The proof is done with the Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ k_1^{-2m-2} & k_2^{-2m-2} & k_2^{-2m-2} & \cdots & k_n^{-2m-2} \\ k_1^{-2m-4} & k_2^{-2m-4} & k_2^{-2m-4} & \cdots & k_n^{-2m-4} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ k_1^{-2m-2n} & k_2^{-2m-2n} & k_2^{-2m-2n} & \cdots & k_n^{-2m-2n} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \cdots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \cdots \\ 0 \end{pmatrix}. \tag{3.14}$$

The proof is complete by using the induction with the assumption of Eq. (3.11). □

3.2.2. Generalization to odd and prime number kernels

Here we can construct extrapolations with the kernels: $\mathcal{T}_2, \mathcal{T}_3, \mathcal{T}_5$ etc., i.e. $m = 0, 1, 2, \cdots$.

Lemma 3.2. *The closed form of the coefficients for the extrapolation is given as with closed form solutions*

$$c_i = \frac{k_i^{a\,m}}{\sum_{j=1}^n k_j^a} \prod_{j=1(\neq i)}^n \frac{k_i^a}{k_i^a - k_j^a} \tag{3.15}$$

and error coefficient

$$e_{a\,m+a\,n+1} = (-1)^{n-1} \frac{k_i^{a\,m}}{\sum_{j=1}^n k_j^a} \prod_{i=1}^n \frac{1}{k_i^a}. \tag{3.16}$$

Here we have closed forms (3.15) *and* (3.16) *and are the keys to the multi-product expansion and its error analysis, see* [6].

Proof. The proof is also done with the Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 & \cdots & 1 \\ k_1^{-am-a} & k_2^{-am-a} & k_2^{-am-a} & \cdots & k_n^{-am-a} \\ k_1^{-am-2a} & k_2^{-am-2a} & k_2^{-am-2a} & \cdots & k_n^{-am-2a} \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ k_1^{-am-an} & k_2^{-am-an} & k_2^{-am-an} & \cdots & k_n^{-am-an} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \cdots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \cdots \\ 0 \end{pmatrix}. \tag{3.17}$$

Complete induction with the assumption of Eq. (3.15) completes the proof. □

The higher order extrapolation allows to start with more accurate kernels. The higher accuracy starts in a higher order form.

Example 3.1. A 8th order algorithm from an even 4th order kernel function is given as:

$$c_1 = \frac{k_1^6}{(k_1^2 - k_2^2)(k_1^2 - k_3^2)(k_1^2 + k_2^2 + k_3^2)}, \tag{3.18}$$

$$c_2 = \frac{k_2^6}{(k_2^2 - k_1^2)(k_2^2 - k_3^2)(k_1^2 + k_2^2 + k_3^2)}, \tag{3.19}$$

$$c_3 = \frac{k_3^6}{(k_3^2 - k_1^2)(k_3^2 - k_2^2)(k_1^2 + k_2^2 + k_3^2)}. \tag{3.20}$$

Remark 3.1. While Magnus expansion are designed as nice higher order splitting methods, they have also some drawbacks. One of a fundamental weakness of the Magnus approach is that when we apply time integration, we ended up with many terms and all of them are still in the exponential. When we apply to split them, we reach all these terms into individual exponentials. The splitting is then far more laborious than Suzuki's method, while having only two operators to split.

Remark 3.2. We stated, that at higher order, say beyond the sixth order, even direct splitting using Suzuki's method will become inefficient because the number of exponentials will grow exponentially with orders.

Here we can improve the Suzuki's method with multi product expansion. So our multi-product expansion has a niche, while the number of exponential operators now only grows quadratically. We see in experiments that 6th, 8th and 10th order calculations have brilliant accuracy. The 10th order is so accurate that we are running into machine precision problem with using only double precision.

4. Error analysis of the multi-product expansion

While extrapolation methods are well-known to many differential equations, there is a nearly no work done to apply to operators.

While extrapolation methods are known in all details, see [31], we concentrate on applying our results to the operator equations. The multi-product expansion is discussed in [13]. Here our method is based on the Richard-Aitken-Neville extrapolation [20].

We assume that

$$\Gamma_k^l = \sum_{i+0}^{n} |\gamma_{ni}| \leq \Pi_{i=1}^{n} \frac{1+|c_i|}{|1-c_i|},$$

and c_i are the coefficients of the multi-product expansion.

We have the following stability results to our multi-product scheme.

Theorem 4.1. 1.) *The process that generates* $\{\mathcal{T}_2^l(\frac{h}{k})\}_{l=1}^n$ *is stable in that*

$$\sup_j \Gamma_k^l = \sum_i^n |\rho_{ni}| < \infty. \tag{4.1}$$

2.) *Under the condition of monotonicity we have further*

$$\lim_{n\to\infty} \sup_i |\rho_{ni}| \leq \prod_{i=1}^{n} \frac{1+|c_i|}{|1-c_i|} < \infty, \tag{4.2}$$

where the coefficients c_i are given in (3.15). *Here we have consequently a process that* $\sup_k \Gamma_k^l < \infty$.

Proof. 1.) Based on the derivation of the coefficients via the Vandermonde equation the product is bounded. 2.) Some argument as in 1.) can be used. □

The convergence analysis based on a Richardson extrapolation process, see [31] and [13]. Here we have a linear increase of only $n+1$ additional force-evaluation, instead of $2n+2$ for Romberg's extrapolation.

Theorem 4.2. 1.) *The process that generates $\{\mathcal{T}_2^l(\frac{h}{k})\}_{l=1}^n$ is convergent and we have a complete expansion, in that*

$$\begin{aligned}&\left\{\mathcal{T}_2^l\left(\frac{h}{k}\right)\right\}_{l=1}^n - \exp\left(h(A+B)\right)\\ =&e_{2n+1}(h^{2n+1}E_{2n+1}) = \mathcal{O}(h^{2n+1}), \qquad \textit{as } \ n\to\infty.\end{aligned} \tag{4.3}$$

where E_{2n+1} are higher order commutators of A and B.

2.) *The process that generates $\{\mathcal{T}_2^l(\frac{h}{k})\}_{l=1}^n$ is convergent and we have a complete asymptotic expansion, in that*

$$\left\{\mathcal{T}_2^l\left(\frac{h}{k}\right)\right\}_{l=1}^n - \exp\left(h(A+B)\right) \approx O(h^{2n+1}), \qquad \textit{as } \ n\to\infty. \tag{4.4}$$

Proof. 1.) Based on the derivation of the coefficients via the Vandermonde equation the product is bounded and we have:

$$\begin{aligned}\sum_{k=1}^{n} c_k \mathcal{T}_2^k\left(\frac{h}{k}\right) =& \sum_{k=1}^{n} c_k \left(\exp((A+B)h) - (k^{-2}h^3E_3 + k^{-4}h^5E_5 + \cdots)\right)\\ =& \sum_{k=1}^{n} c_k \left(\exp((A+B)h) - \sum_{i}^{n} k^{-2i}h^{2i+1}E_{2i+1}\right)\\ =& \left(\exp((A+B)h) - \sum_{k=1}^{n} c_k \sum_{i}^{n} k^{-2i}h^{2i+1}E_{2i+1}\right)\\ =&\mathcal{O}(h^{2n+1}), \qquad \text{as } \ n\to\infty,\end{aligned} \tag{4.5}$$

where the coefficients are given in (3.15).

2.) Some argument as in 1.) can be applied; see also [31]. □

Lemma 4.1. *We assume $||A(t)||$ to be bounded in the interval $t \in (0,T)$. Then T_2 is nonsingular for sufficiently small $\triangle t$.*

Proof. We use our assumption $|A(t)|$ is to be bounded in the interval $0 < t < T$. So we can find $||A(t)|| < C$ for $0 < t < T$. Therefore T_2 is always non-singular for sufficiently small $\triangle t$. □

Theorem 4.3. *We assume T_2 is non-singular as in Lemma* 4.1. *If T_2 is non-singular, then the entire MPE is non-singular and we have a uniform convergence.*

Proof. Since

$$T_2 = \exp\left(\triangle t A\left(t + \frac{\triangle t}{2}\right)\right) \tag{4.6}$$

for sufficient $\triangle t \ll 1$, we can derive

$$T_2 = 1 + \triangle t\, A(t). \tag{4.7}$$

If we assume the boundedness of $||A(t)||$ in small $\triangle t$, T_2 is nonsingular and bounded and we have uniform convergence, see [33]. □

Remark 4.1. With the uniform convergence of the MPE method, we are more general than for the Magnus series with a convergence radius, see [28].

5. Numerical examples

In the following section, we deal with experiments to verify the benefits of our methods. At the beginning, we propose introductory examples to compare the methods. Then applications to differential equations with stiffness and time-dependent parameters are done.

5.1. An 2×2 ODE system

We deal in the first with an ODE and separate the complex operator in two simpler operators. Consider

$$\partial_t u_1 = -\lambda_1 u_1 + \lambda_2 u_2, \tag{5.1a}$$
$$\partial_t u_2 = \lambda_1 u_1 - \lambda_2 u_2, \tag{5.1b}$$
$$u_1(0) = u_{10}\ ,\ u_2(0) = u_{20}\ \text{ (initial conditions)}, \tag{5.1c}$$

where $\lambda_1, \lambda_2 \in \mathbb{R}^+$ are the decay factors and $u_{10}, u_{20} \in \mathbb{R}^+$. We have the time-interval $t \in [0, T]$.

We rewrite the Eqs. (5.1a)-(5.1b) in operator notation:

$$\partial_t u = A(t)u + B(t)u, \tag{5.2}$$

where $u_1(0) = u_{10} = 1$, $u_2(0) = u_{20} = 1$ are the initial conditions, where we have $\lambda_1(t) = t$ and $\lambda_2(t) = t^2$.

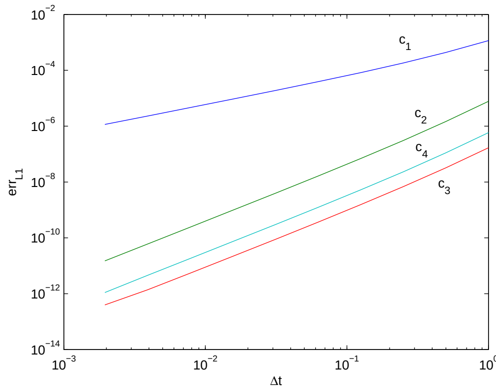

Figure 1: Numerical errors of the methods 1.)-4.), x-axis: time, y-axis: max-error.

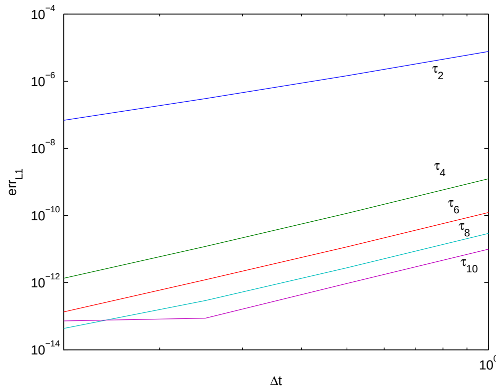

Figure 2: Numerical errors of the methods of a second-order kernel, x-axis: time, y-axis: max-error.

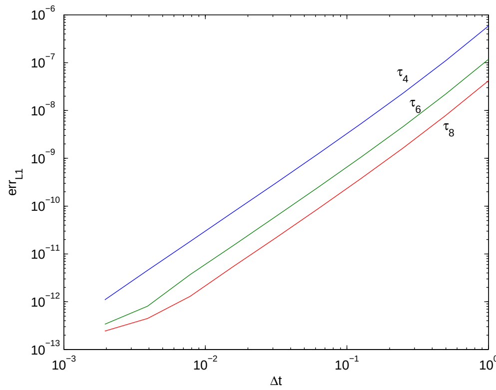

Figure 3: Numerical errors of a fourth-order kernel, x-axis: time, y-axis: max-error.

And our spitted operators are

$$A = \begin{pmatrix} -\lambda_1 & \lambda_2 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ \lambda_1 & -\lambda_2 \end{pmatrix}. \tag{5.3}$$

The concrete parameters for the experiments are given as: $\lambda_1 = 0.05$, $\lambda_2 = 0.01$, $T = 1.0$, $u_0 = (1,1)^t$. The L_1-error is computed as:

$$err_{num,L_1} = \sum_{k=1}^{N} \left| u_{exact}(t_k) - u_{num}(t_k) \right|, \tag{5.4a}$$

where $t_k = k\Delta t$, where $t_0, t_1, \cdots$ and $\triangle t = 0.1$. The L_{max}-error is computed as:

$$err_{num,max} = \max_{k=1}^{N} \left| u_{exact}(t_k) - u_{num}(t_k) \right|, \tag{5.4b}$$

where $t_k = k\Delta t$, where $t_0, t_1, \cdots$ and $\Delta t = 0.1$.

In the first steps we apply the *AB* (method 1.)), Strang (method 2.)) and 3rd-order (method 3.)) and 4th-order-splitting (method 4.)), see Section 2 and compared with the unsplitted solutions. The numerical results for the exponential splitting methods are given in Fig. 1. We see the benefit of the higher order methods with respect to reduce the computational error.

In a next series we apply the extrapolation schemes to our exponential splitting kernels of second and fourth-order.

The numerical results of a second-order kernel are given in Fig. 2. With the second-order kernel, we can improve the numerical error step by step to the machine precision. Strong reductions are obtained between the second and fourth-order method. Here a balance to the amount of computational time and higher order method is at least optimal.

The numerical results of a fourth-order kernel are given in Fig. 3. With the fourth-order kernel, we can really accelerate the convergence rates to machine precision, which is about 10^{-13}. Very fast accelerations are obtained to the fourth and sixth-order method. Here we have an improvement to a fourth-order method done with an extrapolation with a second-order kernel, while we have at least less terms to compute.

Remark 5.1. The numerical experiment present the benefit of the higher order kernel, while large time steps can be chosen to obtain small errors. Additionally extrapolation steps are cheap to obtain and can be embedded to a splitting schemes of 4th order.

5.2. An 10×10 ODE system

We deal in the first with an ODE and separate the complex operator in two simpler operators. Consider

$$\partial_t u_1 = -\lambda_{1,1} u_1 + \lambda_{2,1} u_2 + \cdots + \lambda_{10,1} u_{10}, \tag{5.5a}$$
$$\partial_t u_2 = \lambda_{1,2} u_1 - \lambda_{2,2}(t) u_2 + \cdots + \lambda_{10,2} u_{10}, \tag{5.5b}$$
$$\vdots$$
$$\partial_t u_{10} = \lambda_{1,10} u_1 + \lambda_{2,10}(t) u_2 + \cdots - \lambda_{10,10} u_{10}, \tag{5.5c}$$
$$u_1(0) = u_{1,0}, \quad \cdots, \quad u_{10}(0) = u_{10,0}, \qquad \text{(initial conditions)}, \tag{5.5d}$$

where $\lambda_1(t) \in \mathbb{R}^+$ and $\lambda_2(t) \in \mathbb{R}^+$ are the decay factors and $u_{1,0}, \cdots, u_{10,0} \in \mathbb{R}^+$. We have the time-interval $t \in [0, T]$.

We rewrite Eqs. (5.5a)-(5.5d) in operator notation, we concentrate us to the following equations:

$$\partial_t u = A(t)u + B(t)u, \tag{5.6}$$

where $u_1(0) = u_{10} = 1$, $u_2(0) = u_{20} = 1$ are the initial conditions, where we have $\lambda_1(t) = t$ and $\lambda_2(t) = t^2$.

The spitted operators are

$$A = \begin{pmatrix} -\lambda_{1,1}(t) & \cdots & \lambda_{10,1}(t) \\ \lambda_{1,5}(t) & \cdots & \lambda_{10,5}(t) \\ 0 & \cdots & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & \cdots & 0 \\ \lambda_{1,6}(t) & \cdots & \lambda_{10,6}(t) \\ \lambda_{1,10}(t) & \cdots & -\lambda_{10,10}(t) \end{pmatrix}. \tag{5.7}$$

The parameters are given as:

$$\begin{aligned} &\lambda_{1,1} = 0.09, \quad \lambda_{2,1} = 0.01, \quad \cdots \quad \lambda_{10,1} = 0.01, \\ &\qquad \vdots \\ &\lambda_{1,10} = 0.01, \quad \cdots \quad \lambda_{9,10} = 0.01, \quad \lambda_{10,10} = 0.09. \end{aligned}$$

The higher order schemes with method 1.) − 4.) are presented in Fig. 4. We see the same bahaviour as for lower ODE systems. With higher order schemes, we can really accelerate the convergence rates to machine precision, which is about 10^{-13}. Accelerations are obtained with second-order methods. Here we have an improvement to at least 4th-order method and can balance the computational time to the higher order precision, while we have at least less terms to compute an higher order method.

Remark 5.2. In the numerical experiment we have compared different higher order schemes. With higher order kernels as starting scheme for the extrapolation, we have obtained the best results. Additionally extrapolation steps are cheap to do and increase to higher order schemes.

5.3. A non-singular matrix case

To assess the convergence of the Multi-product expansion with that of the Magnus series, consider the well known example [27] of

$$A(t) = \begin{pmatrix} 2 & t \\ 0 & -1 \end{pmatrix}. \tag{5.8}$$

The exact solution to (2.1) with $Y(0) = I$ is

$$Y(t) = \begin{pmatrix} e^{2t} & f(t) \\ 0 & e^{-t} \end{pmatrix}, \tag{5.9}$$

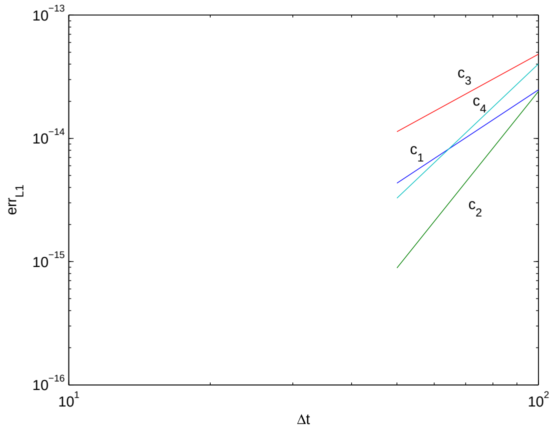

Figure 4: Numerical errors of the methods 1.)-4.), x-axis: time, y-axis: max-error.

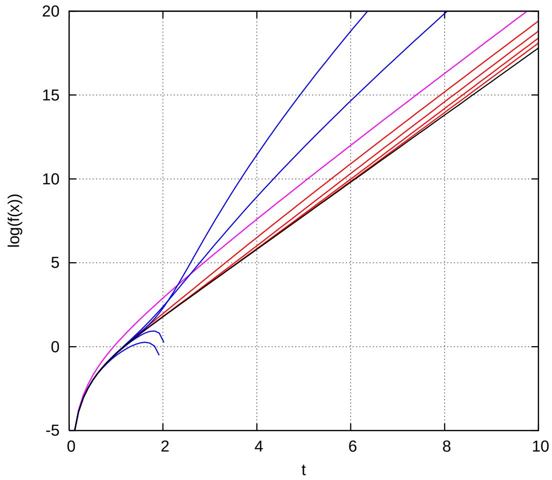

Figure 5: The black line is the exact result (5.10). The blue lines are the Magnus series (5.13a). The red lines are the multi-product expansion. The purple line is their common second-order result.

with

$$f(t) = \frac{1}{9}e^{-t}(e^{3t} - 1 - 3t) \tag{5.10a}$$

$$= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13t^{11}}{178200} + \cdots . \tag{5.10b}$$

For the Magnus expansion, one has the series

$$\Omega(t) = \begin{pmatrix} 2t & g(t) \\ 0 & -t \end{pmatrix}, \tag{5.11}$$

with, up to the 10th-order,

$$g(t) = \frac{1}{2}t^2 - \frac{1}{4}t^3 + \frac{3}{80}t^5 - \frac{9}{1120}t^7 + \frac{81}{44800}t^9 + \cdots \tag{5.12a}$$

$$\to \frac{t(e^{3t} - 1 - 3t)}{3(e^{3t} - 1)}. \tag{5.12b}$$

Exponentiating (5.11) yields (5.9) with

$$f(t) = te^{-t}(e^{3t} - 1)\left(\frac{1}{6} - \frac{1}{12}t + \frac{1}{80}t^3 - \frac{3}{1120}t^5 + \frac{27}{44800}t^7 + \cdots\right) \tag{5.13a}$$

$$\to te^{-t}(e^{3t} - 1)\left(\frac{1}{9t} - \frac{1}{3(e^{3t} - 1)}\right). \tag{5.13b}$$

Whereas the exact solution (5.10) is an entire function of t, the Magnus series (5.12a) and (5.13a) only converge for $|t| < \frac{2}{3}\pi$ due to the pole at $t = \frac{2}{3}\pi i$. The Magnus series (5.13a) is plot in Fig. 5 as blue lines. The pole at $|t| = \frac{2}{3}\pi \approx 2$ is clearly visible. Here we obtain an improvement with the multi-product expansion methods, while we have more precise results. Such precision is obtained by an analytical approach of the function $f(t)$.

From (2.12), by setting $\Delta t = t$ and $t = 0$, we have

$$\mathscr{T}_2(t) = \exp\left[t\begin{pmatrix} 2 & \frac{1}{2}t \\ 0 & -1 \end{pmatrix}\right] = \begin{pmatrix} e^{2t} & f_2(t) \\ 0 & e^{-t} \end{pmatrix} \tag{5.14a}$$

with

$$f_2(t) = \frac{1}{6}te^{-t}(e^{3t} - 1). \tag{5.14b}$$

This is identical to first term of the Magnus series (5.13a) and is an entire function of t. Since higher order MPE uses only powers of $\mathscr{T}_2$, higher order MPE approximations are also entire functions of t. Thus up to the 10th-order, one finds

$$f_4(t) = te^{-t}\left(\frac{e^{3t} - 5}{18} + \frac{2e^{\frac{3t}{2}}}{9}\right), \tag{5.15a}$$

$$f_6(t) = te^{-t}\left(\frac{11e^{3t} - 109}{360} + \frac{9}{40}(e^{2t} + e^t) - \frac{8}{45}e^{\frac{3t}{2}}\right), \tag{5.15b}$$

$$f_8(t) = te^{-t}\left(\frac{151e^{3t} - 2369}{7560} + \frac{256}{945}\left(e^{\frac{9t}{4}} + e^{\frac{3t}{4}}\right) - \frac{81}{280}(e^{2t} + e^t) + \frac{104}{315}e^{\frac{3t}{2}}\right), \tag{5.15c}$$

$$\begin{aligned} f_{10}(t) = te^{-t}\Bigg(&\frac{15619e^{3t} - 347261}{1088640} + \frac{78125}{217728}\left(e^{\frac{12t}{5}} + e^{\frac{9t}{5}} + e^{\frac{6t}{5}} + e^{\frac{3t}{5}}\right) \\ &- \frac{4096}{8505}\left(e^{\frac{9t}{4}} + e^{\frac{3t}{4}}\right) + \frac{729}{4480}(e^{2t} + e^t) - \frac{4192}{8505}e^{\frac{3t}{2}}\Bigg). \end{aligned} \tag{5.15d}$$

These MPE approximations are plotted as red lines in Fig. 5. The convergence seems uniform for all t.

When expanded, the above functions yield

$$f_2(t) = \frac{t^2}{2} + \frac{t^3}{4} + \cdots, \tag{5.16a}$$

$$f_4(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{5t^5}{192} + \cdots, \tag{5.16b}$$

$$f_6(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{384} + \cdots, \tag{5.16c}$$

$$f_8(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{1307t^9}{8601600} + \cdots, \tag{5.16d}$$

$$f_{10}(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13099t^{11}}{232243200}, \tag{5.16e}$$

and agree with the exact solution to the claimed order.

Here we have convergence due to the following theorem.

Theorem 5.1. *We have given the initial value problem* (2.1) *and the exact solution of the initial value problem, see* (5.9)*. Then the approximated* $g(t,\epsilon)$ *done with the MPE method is convergent with the rate:*

$$\left| g_{exact}(t) - g_{MPE,2(i+1)}(t) \right| \le C t^{2(i+1)+1}, \tag{5.17}$$

where C *is independent of* t *and* ϵ *and* $0 \le C \le 0.25$*, for* $i = 0, 1, 2, \cdots$.

Proof. We apply the difference between exact and approximated solution, due to the Taylor expansion of both solutions. We begin with $i = 0$:

$$\begin{aligned} &\left| f_{exact}(t) - f_{MPE,2}(t) \right| \\ =&\left| \frac{\exp(2t)}{9} - \left(\frac{1}{9} + \frac{t}{3}\right)\exp(-t) - \left(\exp(-t)(\exp(3t) - 1)\frac{t}{6}\right) \right| \\ =&\frac{t^3}{4} + \mathcal{O}(t^5) \le C\mathcal{O}(t^5), \end{aligned} \tag{5.18}$$

and $0 \le C \le 0.25$.

For $i \ge 0$: we have the

$$\begin{aligned} &\left| f_{exact}(t) - f_{MPE,2(i+1)}(t) \right| \\ \le&\frac{t^{2(i+1)+1}}{4} \le C\mathcal{O}(t^{2(i+1)+1}), \end{aligned} \tag{5.19}$$

and $0 \le C \le 0.25$. □

Remark 5.3. Here we have uniform convergence because of the non singularities of the MPE products.

5.4. The time-dependent radial Schödinger equation

We consider the radial Schrödinger equation

$$\frac{\partial^2 u}{\partial r^2} = f(r,E)u(r), \tag{5.20a}$$

where

$$f(r,E) = 2V(r) - 2E + \frac{l(l+1)}{r^2}. \tag{5.20b}$$

By relabeling $r \to t$ and $u(r) \to q(t)$, (5.20a) can be viewed as harmonic oscillator with a time dependent spring constant

$$k(t,E) = -f(t,E) \tag{5.21}$$

and Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}k(t,E)q^2. \tag{5.22}$$

Thus any eigenfunction of (5.20a) is an exact time-dependent solution of (5.22). For example, the ground state of the hydrogen atom with $l = 0$, $E = -1/2$ and

$$V(r) = -\frac{1}{r} \tag{5.23}$$

yields the exact solution

$$q(t) = t\exp(-t) \tag{5.24}$$

with initial values $q(0) = 0$ and $p(0) = 1$. Denoting

$$Y(t) = \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}, \tag{5.25}$$

the time-dependent oscillator (5.22) now corresponds to

$$A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} \equiv T + V(t), \tag{5.26}$$

with

$$f(t) = (1 - 2/t). \tag{5.27}$$

In this case, the second-order midpoint algorithm is

$$\begin{aligned} \mathcal{T}_2(h,t) =& \mathrm{e}^{\frac{1}{2}hT}\mathrm{e}^{hV\left(t+\frac{h}{2}\right)}\mathrm{e}^{\frac{1}{2}hT} \\ =& \begin{pmatrix} 1+\frac{1}{2}h^2 f\left(t+\frac{1}{2}h\right) & h+\frac{1}{4}h^3 f\left(t+\frac{1}{2}h\right) \\ hf\left(t+\frac{1}{2}h\right) & 1+\frac{1}{2}h^2 f\left(t+\frac{1}{2}h\right) \end{pmatrix} \end{aligned} \tag{5.28}$$

and for $q(0) = 0$ and $p(0) = 1$, (setting $t = 0$ and $h = t$), correctly gives the second-order result,

$$q_2(t) = t + \frac{1}{4}t^3 f\left(\frac{1}{2}t\right) = t - t^2 + \frac{1}{4}t^3. \tag{5.29}$$

Higher order multi-product expansions using (5.28) yield

$$q_4(t) = t - t^2 + \frac{7t^3}{18} - \frac{t^4}{9} + \frac{t^5}{96}, \tag{5.30a}$$

$$q_6(t) = t - t^2 + \frac{211t^3}{450} - \frac{31t^4}{225} + \frac{17t^5}{600} + \cdots, \tag{5.30b}$$

$$q_8(t) = t - t^2 + \frac{32233t^3}{66150} - \frac{5101t^4}{33075} + \frac{3139t^5}{88200} + \cdots, \tag{5.30c}$$

$$q_{10}(t) = t - t^2 + \frac{88159t^3}{1786050} - \frac{143177t^4}{893025} + \frac{91753t^5}{2381400} + \cdots. \tag{5.30d}$$

Comparing this to the exact solution (5.24):

$$\begin{aligned} q(t) &= t - t^2 + \frac{t^3}{2} - \frac{t^4}{6} + \frac{t^5}{24} - \frac{t^6}{120} + \frac{t^7}{720} - \frac{t^8}{5040} \cdots \\ &= t - t^2 + \frac{t^3}{2} - 0.1667t^4 + 0.0417t^5 - 0.0083t^6 + 0.0014t^7 \cdots, \end{aligned} \tag{5.31}$$

one sees that MPE no longer matches the Taylor expansion beyond second-order. This is due to the singular nature of the Coulomb potential, which makes the problem a challenge to solve. Since $A(t)$ is now singular at $t = 0$, the previous proof of uniform convergence no longer holds. Nevertheless, from the exact solution (5.24), one sees that force (or acceleration)

$$\lim_{t \to 0} f(t)q(t) = -2 \tag{5.32}$$

remains finite. It seems that this is sufficient for uniform convergence as the coefficients of the t^3 and t^4 terms do approach $\frac{1}{2}$ and $\frac{1}{6}$ with increasing order:

$$\begin{aligned} &\frac{7}{18} = 0.3889, \quad \frac{211}{450} = 0.4689, \quad \frac{32233}{66150} = 0.4873, \quad \frac{88159}{1786050} = 0.4936, \\ &\frac{1}{9} = 0.1111, \quad \frac{31}{225} = 0.1378, \quad \frac{5101}{33075} = 0.1542, \quad \frac{143177}{893025} = 0.1603. \end{aligned}$$

Similar results hold for all other coefficients. To see this uniform convergence, Fig. 6 shows how higher order MPE, up to the 100th-order, matches against the exact solution. The calculation is done numerically rather than by evaluating the analytical expressions such as (5.30). For orders 60, 80 and 100, it is necessary to use quadruple precision to circumvent rounding errors. Also shown are some well know fourth-order symplectic algorithm FR (Forest-Ruth [17], 3 force-evaluations), M (McLachlan [26], 4 force-evaluations), BM (Blanes-Moan [5], 6 force-evaluations), Mag4 (Magnus integrator, see below, ≈ 2.5 force-evaluations) and 4B [12] (a *forward* symplectic algorithm with only ≈ 2 evaluations).

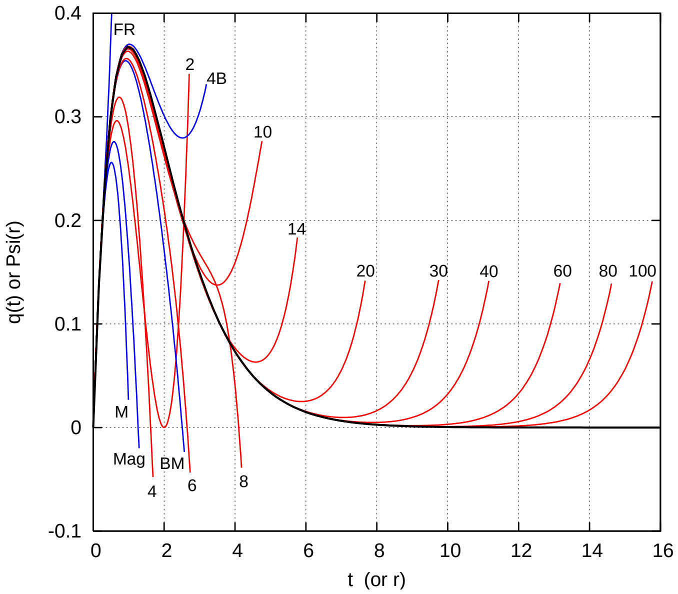

Figure 6: The uniform convergence of the multi-product expansion in solving for the hydrogen ground state wave function. The black line is the exact ground state wave function. The numbers indicates the order of the multi-product expansion. The blue lines denote results of various fourth-order algorithms.

These symplectic integrators steadily improves from FR, to M, to Mag4, to BM to 4B. Forward algorithm 4B is noteworthy in that it is the only fourth-order algorithm that can go around the wave function maximum at $t = 1$, yielding

$$q_{4B}(t) = t - t^2 + \frac{t^3}{2} - 0.1635t^4 + 0.0397t^5 - 0.0070t^6 + 0.0009t^7 \cdots, \tag{5.33}$$

with the correct third-order coefficient and comparable higher order coefficients as the exact solution (5.31). By contrast, the FR algorithm, which is well know to have rather large errors, has the expansion,

$$q_{FR}(t) = t - t^2 - 0.1942t^3 + 3.528t^4 - 2.415t^5 + 0.5742t^6 - 0.0437t^7 \cdots, \tag{5.34}$$

with terms of the wrong signs beyond t^2. The failure of these fourth-order algorithms to converge correctly due to the singular nature of the Coulomb potential is consistent with the findings of Wiebe *et al.* [36]. However, their finding does not explain why the second-order algorithm can converge correctly and only higher order algorithms fail. A deeper understanding of Suzuki's method is necessary to resolve this very interesting, but puzzling issue.

For non-singular potentials such as the radial harmonic oscillator with

$$f(t) = t^2 - 3, \tag{5.35}$$

and exact ground state solution

$$q(t) = te^{-t^2/2} = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{t^{11}}{3840} + \cdots, \tag{5.36}$$

the multi-product expansion now gives,

$$q_2(t) = t - \frac{3t^3}{4} + \frac{t^5}{16}, \tag{5.37a}$$

$$q_4(t) = t - \frac{t^3}{2} + \frac{29t^5}{192} + \cdots, \tag{5.37b}$$

$$q_6(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{13t^7}{576} + \cdots, \tag{5.37c}$$

$$q_8(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{20803t^9}{7741440} + \cdots, \tag{5.37d}$$

$$q_{10}(t) = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{50977t^{11}}{193536000} + \cdots, \tag{5.37e}$$

and matches the Taylor expansion up to the claimed order, as demonstrated in the previous case of (5.16).

The fourth-order Magnus algorithm used is given:

$$\mathcal{T}_4(\Delta t) = \mathrm{e}^{c_3 \Delta t (V_2 - V_1)} \mathrm{e}^{\Delta t \left(T + \frac{1}{2}(V_1 + V_2)\right)} \mathrm{e}^{-c_3 \Delta t (V_2 - V_1)}, \tag{5.38a}$$

where now

$$V_1 = V(t + c_1 \Delta t), \qquad V_2 = V(t + c_2 \Delta t). \tag{5.38b}$$

Normally, one would need to further split the central exponential in (3.38) to fourth-order. In the general case, this would have required three or more force evaluations. However, because the problem is basically a harmonic oscillator, it can be splitted to fourth-order [12] via

$$\mathrm{e}^{\Delta t (T + \frac{1}{2}(V_1 + V_2))} = \mathrm{e}^{c_e \Delta t \frac{1}{2}(V_1 + V_2))} \mathrm{e}^{c_m \Delta t T} \mathrm{e}^{c_e \Delta t \frac{1}{2}(V_1 + V_2)}, \tag{5.39a}$$

where

$$c_e = \frac{1}{2} - f_a \Delta t^2 / 24 \quad \text{and} \quad c_m = 1 + f_a \Delta t^2 / 6. \tag{5.39b}$$

Here $f_a = \frac{1}{2}[f(t + c_1 \Delta t, E) + f(t + c_2 \Delta t, E)]$. Thus the entire algorithm (5.38) needs two evaluations of the potential in $f(t, E)$ but slightly more effort in computing the final force. We assign it as requiring 2.5 force evaluations. Algorithm 4B [12] requires truly two evaluations of the force with an extra multiplication.

5.5. Computing eigenvalues to high precision

In the last study of the hydrogen ground state, the eigenvalue $E = \frac{1}{2}$ was provided initially to test how well each algorithm can integrate the trajectory outward from the origin $t = 0$. All time-dependent algorithms can be used to solve both the wave function and its associated eigenvalue using Killingbeck's method [24]. In this method, one integrate backward from given large time $t = T$ toward $t = 0$ and use Newton's iteration to determine E such that $q(0) = 0$.

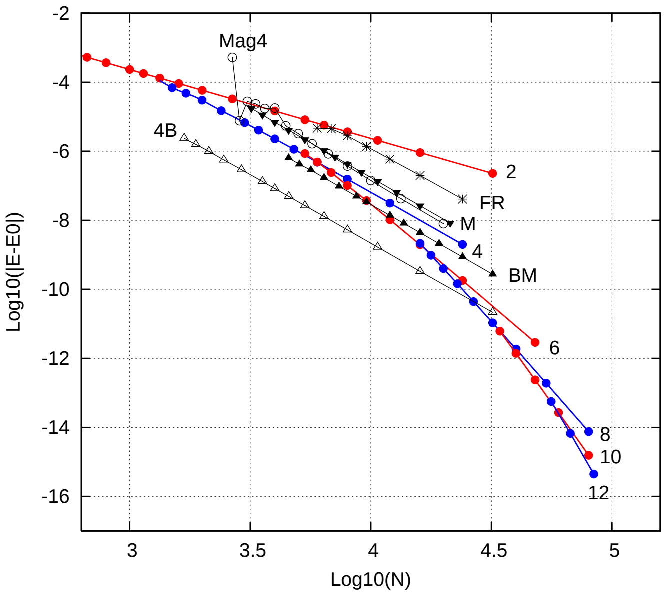

Figure 7: A precision-effort comparison of various fourth-order algorithms with that of MPE for computing the ground state of a spiked harmonic oscillator. N is the number of force-evaluations.

Here, we compare how well MPE can determine the ground state energy and wave function of the spiked harmonic oscillator [1,4,25,30] with potential

$$V(r) = \frac{1}{2}\left(r^2 + \frac{\lambda}{r^M}\right), \tag{5.40}$$

where $M = 6$ and $\lambda = 0.001$. By use of higher-order MPE with quadruple precision, we have first determined that

$$E_0 = 1.6399279129609271073 65. \tag{5.41}$$

We integrate back from $T = 16$, with $q(T) = 0$ and $p(T) = 10^{-10}$. Fig. 7 shows the precision-effort comparison of various fourth-order algorithms as compared to higher-order MPE. If greater precision is desired, it is more efficient to use higher order integrators. The sixth-order MPE out-performs all fourth-order integrators except 4B at the level of 8-digit precision. For about 14 digits, order 10 is near the limit of diminishing return. Among fourth-order algorithms, BM performed the best, except when compared to 4B, which is specially efficient in solving harmonic problems.

Remark 5.4. It is of interest to note that the multi-product expansion, even in singular cases, converges uniformly, and approaches the Taylor expansion asymptotically.

6. Conclusions and discussions

We have presented splitting methods based on Suzuki's ideas and Multi product expansions. Based on the derivation of higher order schemes with the Suzuki's method and Multi product schemes, we can obtain starting splitting schemes of higher order. Extrapolation schemes accelerate the reconstruction to more accurate schemes with less additional computational terms. Numerical examples confirm the applications to differential equations of stiff and time-dependent types. We demonstrate the benefits of our multi-product expansion related to the extrapolation analysis. The benefits are in less force-evaluations, which are necessarily with Magnus expansion or extrapolation schemes based on Romberg. In future we will focus us on the development of improved operator-splitting methods with respect to their application in nonlinear differential equations.

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