Multi-product expansion, Suzuki's method and the Magnus integrator for solving time-dependent problems

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Abstract. In this paper we discuss the extention to exponential splitting methods with respect to time-dependent operators. For such extensions, the Magnus integration, see [3], [4] and [5] and the Suzuki's method are incorporating ideas to the time-ordered exponential, see [22], [2], [7] and [8]. We formulate each methods and present their advantages to special time-dependent harmonic oscillator problems. An decisive and comprehensive comparison on the Magnus expansion with Suzuki's method on some problems are given. Here classical and also quantum mechanical can be treated to present the solving in time-dependent problems. We choose a radial Schrodinger equation as a classical time-dependent harmonic oscillation which combine classical and quantum calculations simultaneously. Here we present the different schemes of the integrator based Magnus scheme and the differential based Suzuki's method. Based on the spiked harmonic oscillator case we could analyze the differences.

Keyword Magnus Integrator, Suzuki's method, exponential splitting.

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

1 Introduction

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

$$\partial_t \, u = L(t)u = (A(t) + B(t))u, \; u(0) = u_0, \tag{1}$$

where L, A and B are unbounded operators and time-dependent operators.

For such equations, we concentrate on comparing the higher order methods to Suzuki's and Magnus schemes. Here the Suzuki's methods apply factorized symplectic algorithms with forward derivatives, see [7], [8]. Where on the other hand Magnus schemes apply explicit time integration to obtain higher order methods, see [3].

Such preliminary comparison are presented in [2], [7], where the benefits of each method is outlined.

In our paper, we like to see the drawback of each method, so for the Magnus integrator, the spiked harmonic oscillator case, see [8] and for the Suzuki's method, geometric properties, which are know to be solved with geometric integrator, e.g. Magnus integrators.

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 Magnus expansion and the application to a Hamiltonian system. In Section 3, we present our Suzuki's rule for decomposing time-ordered integrators. 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 Schrödinger equations are discussed and spiked harmonic oscillator. In Section 6, we briefly summarize our results.

2 Exponential Splitting method based on Magnus integrators

The Magnus integrator was introduced as a tool to solve non-autonomous linear differential equations for linear operators of the form

$$\frac{dY}{dt} = A(t)Y(t) \ , \tag{2}$$

with solution

$$Y(t) = \exp(\Omega(t))Y(0) \ . \tag{3}$$

This can be expressed as:

$$Y(t) = \mathcal{T}\left(\exp(\int_0^t A(s)\ ds\right) Y(0) \ , \tag{4}$$

where the time-ordering operator $\mathcal{T}$ is given in [10].

The Magnus expansion is given as:

$$\Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t) \ , \tag{5}$$

where 1.) $\Omega_1' = A$ so that

$$\Omega_1(t) = \int_0^t A(t_1) dt_1 \ , \tag{6}$$

2.) $\Omega_2' = -1/2[\Omega_1, A]$ so that

$$\Omega_2(t) = 1/2 \int_0^t \int_0^{t_1} [A(t_1), A(t_2)] dt_2 dt_1 \ , \tag{7}$$

and so on.

The procedure can be written as Magnus expansion generator:
$\Omega_2' = -1/2[\Omega_1, A]$ so that

$$\Omega_1(t) = \int_0^t A(\tau) d\tau \ , \tag{8}$$

and

$$\Omega_n(t) = \sum_{j=1}^{n-1} \frac{B_j}{j!} \int_0^t S_n^{(j)}(\tau) d\tau \ , \tag{9}$$

for $n \geq 2$, where B_j i the jth Bernoulli number, and

$$S_n^{(j)} = \sum_{m=1}^{n-j} [\Omega_m, S_{n-m}^{(j-1)}] \ , \ 2 \leq j \leq n-1, \tag{10}$$

$$S_n^{(1)} = [\Omega_{n-1}, A], \tag{11}$$

$$S_n^{(n-1)} = ad_{\Omega_1}^{n-1}(A). \tag{12}$$

Remark 1. The Magnus expansion can be generalized in different ways, e.g. Volsamber iterative method, Floquet-Magnus expansion.

Remark 2. Numerical methods based on the Magnus expansion require the evaluation of a matrix exponential which contain nested commutators. Such computing exponential is frequently a most consuming part of the schemes. So it makes sense to have a method which do not involve commutators and still preserving the qualitative properties.

The commutator free Magnus integrators, see [3], is a method, that need not explicit time integration in addition to evaluating higher order commutators.

To apply that this method to the differential equation (1), we can split into two parts.

The commutator free Magnus integrators read:

$$\psi_k^{[q]} = \exp(\tilde{B}_l) \exp(\tilde{A}_l) \cdots \exp(\tilde{B}_1) \exp(\tilde{A}_1), \tag{13}$$

where the matrices are

$$\tilde{A}_i = \Delta t \sum_{j=1}^{k} \rho_{ij} A_j, \ \tilde{B}_i = \Delta t \sum_{j=1}^{k} \sigma_{ij} B_j \exp(\tilde{B}_1) \exp(\tilde{A}_1), \tag{14}$$

and the accuracy is given as

$$\psi_k^{[q]} = \exp(\Omega(t_q + \Delta t)) + O(\Delta t^q). \tag{15}$$

Here the coefficients ρ_{ij}, σ_{ij} depending on coefficients of the chosen quadrature rule.

The fourth order method is given in [5], see also the coefficients in the appendix. The convergence results are given in [17].

In the next we present the algorithms for a Hamiltonian application.

Application to a Hamiltonian

The algorithm is given for a Hamiltonian as:

$$H = T(p,t) + V(q,t) \tag{16}$$

For example :

$$H = p^2/2 + V(q,t), \tag{17}$$

where $T(p,t) = p^2/2$ and $\frac{\partial T(p,t)}{\partial p} = p$ and $\frac{\partial V(q,t)}{\partial q} = -F(q,t)$

Algorithm 21 *Magnus split for the Hamiltonian:*

$q_0 = q(t_n), p_0 = p(t_n)$
do i=1,k
$V_i'(q) = V'(q, t_n + c_i\tau)$;
$T_i'(p) = T'(p, t_n + c_i\tau)$
enddo

do $i = 1, m$
$\tilde{V}_i'(q) = \sigma_{i1} V_1'(q) + \ldots + \sigma_{ik} V_k'(q)$;
$\tilde{T}_i'(p) = \rho_{i1} T_1'(p) + \ldots + \rho_{ik} T_k'(p)$;
$p_i = p_{i-1} - \tau\, \tilde{V}'(q_{i-1})$
$q_i = q_{i-1} + \tau\, \tilde{T}'(p_{i-1})$
enddo

Remark 3. The commutator free Magnus expansion and its application to splitting methods, can expanded their approximation scheme without commutators. The work has to be done to compute the matrix exponentials for some quadrature rules. The process will be simplified by assuming additional constraints to the commutators, e.g. $[B(t_i), [B(t_j), [B(t_k), A(t_l)]]]$.

3 Exponential Splitting method based on Suzuki's time-ordered exponential (Multi-product splitting method)

Instead of the Magnus expansion (5), one can also directly implement the time-ordered exponential as suggested by Suzuki[22]. Rewriting (4) as

$$Y(t + \Delta t) = \mathcal{T}\Big(\exp \int_t^{t+\Delta t} A(s) ds\Big) Y(t), \tag{18}$$

aside from the conventional expansion

$$\mathcal{T}\Big(\exp\int_t^{t+\Delta t} A(s)ds\Big) = 1+\int_t^{t+\Delta t} A(s_1)ds_1+\int_t^{t+\Delta t} ds_1\int_t^{s_1} ds_2 A(s_1)A(s_2)+\cdots\,, \tag{19}$$

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

$$\mathcal{T}\Big(\exp\int_t^{t+\Delta t} A(s)ds\Big) = \lim_{n\to\infty}\mathcal{T}\Big(\mathrm{e}^{\frac{\Delta t}{n}\sum_{i=1}^{n} A(t+i\frac{\Delta t}{n})}\Big), \tag{20}$$

$$= \lim_{n\to\infty}\mathrm{e}^{\frac{\Delta t}{n}A(t+\Delta t)}\cdots\mathrm{e}^{\frac{\Delta t}{n}A(t+\frac{2\Delta t}{n})}\mathrm{e}^{\frac{\Delta t}{n}A(t+\frac{\Delta t}{n})}. \tag{21}$$

The time-ordering is trivially accomplished in going from (20) to (21). To enforce latter, Suzuki introduces the *forward time derivative* operator

$$D = \frac{\overleftarrow{\partial}}{\partial t} \tag{22}$$

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

$$F(t)\mathrm{e}^{\Delta t D}G(t) = F(t+\Delta t)G(t). \tag{23}$$

Trotter's formula then gives

$$\exp[\Delta t(A(t)+D)] = \lim_{n\to\infty}\Big(\mathrm{e}^{\frac{\Delta t}{n}A(t)}\mathrm{e}^{\frac{\Delta t}{n}D}\Big)^n,$$

$$= \lim_{n\to\infty}\mathrm{e}^{\frac{\Delta t}{n}A(t+\Delta t)}\cdots\mathrm{e}^{\frac{\Delta t}{n}A(t+\frac{2\Delta t}{n})}\mathrm{e}^{\frac{\Delta t}{n}A(t+\frac{\Delta t}{n})}, \tag{24}$$

where property (23) has been applied repeatedly and accumulatively. Comparing (21) with (24) yields Suzuki's decomposition of the time-ordered exponential[22]

$$\mathcal{T}\Big(\exp\int_t^{t+\Delta t} A(s)ds\Big) = \exp[\Delta t(A(t)+D)]. \tag{25}$$

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

$$\mathcal{T}_2(\Delta t) = \mathrm{e}^{\frac{1}{2}\Delta t D}\mathrm{e}^{\Delta t A(t)}\mathrm{e}^{\frac{1}{2}\Delta t D} = \mathrm{e}^{\Delta t A(t+\frac{1}{2}\Delta t)}. \tag{26}$$

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

$$\mathcal{T}_2(\Delta t) = \mathrm{e}^{\Delta t(A(t)+D)} + \Delta t^3 E_3 + \Delta t^5 E_5 + \ldots \tag{27}$$

Every occurrence of the operator $\mathrm{e}^{d_i \Delta t D}$, 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 $\mathrm{e}^{\frac{1}{2}\Delta t D}$, time is $t+\frac{1}{2}\Delta t$. After the second $\mathrm{e}^{\frac{1}{2}\Delta t D}$, time is $t+\Delta t$.

Thus the leftmost $e^{\frac{1}{2}\Delta t D}$ is not without effect, it correctly updates the time for the next iteration. For example

$$\mathcal{T}_2(\Delta t)\mathcal{T}_2(\Delta t) = e^{\Delta t A(t+\frac{3}{2}\Delta t)} e^{\Delta t A(t+\frac{1}{2}\Delta t)} \tag{28}$$

Higher order factorization of (25) into a single product form

$$\exp[\Delta t(A(t)+D)] = \Pi_i e^{a_i \Delta t A(t)} e^{d_i \Delta t D} \tag{29}$$

will yield higher order algorithms, but at the cost of exponentially growing number of evaluations of $e^{a_i \Delta t A}$. Recently, it has been shown that, once one has the second order algorithm (26), arbitrary higher order algorithms can be built from the multi-product expansion* of (25), with only quadratically growing number of exponentials at high orders. For example,

$$\mathcal{T}_4(\Delta t) = -\frac{1}{3}\mathcal{T}_2(\Delta t) + \frac{4}{3}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) \tag{30}$$

$$\mathcal{T}_6(\Delta t) = \frac{1}{24}\mathcal{T}_2(\Delta t) - \frac{16}{15}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) + \frac{81}{40}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right) \tag{31}$$

$$\mathcal{T}_8(\Delta t) = -\frac{1}{360}\mathcal{T}_2(\Delta t) + \frac{16}{45}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) - \frac{729}{280}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right) + \frac{1024}{315}\mathcal{T}_2^4\left(\frac{\Delta t}{4}\right) \tag{32}$$

$$\begin{aligned}\mathcal{T}_{10}(\Delta t) = {} & \frac{1}{8640}\mathcal{T}_2(\Delta t) - \frac{64}{945}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) + \frac{6561}{4480}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right) \\ & - \frac{16384}{2835}\mathcal{T}_2^4\left(\frac{\Delta t}{4}\right) + \frac{390625}{72576}\mathcal{T}_2^5\left(\frac{\Delta t}{5}\right)\end{aligned} \tag{33}$$

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

$$\mathcal{T}_2(\Delta t) = e^{\Delta t A(t+\frac{1}{2}\Delta t)} = e^{\frac{1}{2}\Delta t T} e^{\Delta t V(t+\Delta t/2)} e^{\frac{1}{2}\Delta t T} + O(\Delta t^3). \tag{34}$$

For the error terms we have the following estimates:

$$\exp((dt/2)T) exp(dtV) exp((dt/2)T) = \exp(dt(T+V) + dt3E_3 + dt5E_5 + ...), \tag{35}$$

with

$$E_3 = -(1/24)[TTV] - (1/12)[VTV] \tag{36}$$

$$E_5 = (7/5760)[TTTTV] + (1/480)[TTVTV] + (1/360)[VTTTV] + (1/120)[VTVTV] \tag{37}$$

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:

$$
\begin{aligned}
||E_3|| &= || - (1/24)[TTV] - (1/12)[VTV]|| && (38)\\
&\leq \frac{1}{24}||T^2||||V|| + \frac{1}{12}||T^2||||V^2||, \\
||E_5|| &= ||(7/5760)[TTTTV] + (1/480)[TTVTV] && (39)\\
&+(1/360)[VTTTV] + (1/120)[VTVTV]|| \\
&\leq (7/5760)||T^4||||V|| + (1/180)||T^3||||V^2|| + (1/120)||T^2||||V^3||
\end{aligned}
$$

The Multiproduct expansion can be derived as . More generally, for a given set of n distinct whole numbers fk1; k2; :::kng, one can form a 2n-order approximation of eh(A+B) via

$$\exp(A+B) = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i}) + e_{2n+1}(h_{2n+1}E_{2n+1}) \tag{40}$$

The expansion coeffcients c_i are determined by a specially simple Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 \dots & 1 & \\ k_1^{-2} & k_2^{-2} & k_2^{-2} & \dots & k_n^{-2} \\ k_1^{-4} & k_2^{-4} & k_2^{-4} & \dots & k_n^{-4} \\ \dots & \dots & \dots & \dots & \dots \\ k_1^{-2(n-1)} & k_2^{-2(n-1)} & k_2^{-2(n-1)} & \dots & k_n^{-2(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \dots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \dots \\ 0 \end{pmatrix} \tag{41}$$

with closed form solutions

$$c_i = \sum_{j=1(\neq i)}^{n} \frac{k_i^2}{k_i^2 - k_j^2} \tag{42}$$

and error coefficient,

$$e_{2n+1} = (-1)^{n-1} \sum_{i=1}^{n} \frac{1}{k_i^2} \tag{43}$$

Here we have closed forms (42) and (43) and are the keys to the multi-product expansion and its error analysis.

Remark 4. 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 5. 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 wel-known to tremendous differential equations, there is a nearly no work done to apply to operators.

While extrapolation methods are known in all details, see [19], we concentrate on applying our results to the operator equations.

The multi-product expansion is discussed in [9].

Here our method is based on the Richard-Aitken-Neville extrapolation [12].

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

$$\sup_j \Gamma_k^l = \sum_i^n |\rho_{ni}| < \infty, \tag{44}$$

2.) Under the condition of monotonicity we have further

$$\limsup_{n\to\infty} |\rho_{ni}| \leq \Pi_{i=1}^n \frac{1+|c_i|}{|1-c_i|} < \infty, \tag{45}$$

where the coefficients c_i are given in (42). Here we have consequently a process that $\sup_k \Gamma_k^l < \infty$.

Proof. ad 1.) Based on the derivation of the coefficients via the Vandermonde equation the product is bounded.

ad 2.) Some argument as in 1.).

The convergence analysis based on a Richardson extrapolation process, see [19] and [9]. Here we have a linear increase of only $n+1$ additional force-evaluation, instead of $2n+2$ for Romberg's extrapolation.

Theorem 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*

$$\{\mathcal{T}_2^l(\frac{h}{k})\}_{l=1}^n - \exp(h(A+B)) = e_{2n+1}(h^{2n+1}E_{2n+1}), \quad (46)$$
$$= O(h^{2n+1}), \quad (47)$$
$$as\, n \rightarrow \infty. \quad (48)$$

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

$$\{\mathcal{T}_2^l(\frac{h}{k})\}_{l=1}^n - \exp(h(A+B)) \approx O(h^{2n+1}), \quad (49)$$
$$as\, n \rightarrow \infty. \quad (50)$$

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

$$\sum_{k=1}^n c_k \mathcal{T}_2^k(\frac{h}{k}) = \sum_{k=1}^n c_k \left(\exp((A+B)h) - (k^{-2}h^3 E_3 + k^{-4}h^5 E_5 + \ldots)\right), (51)$$
$$= \sum_{k=1}^n c_k \left(\exp((A+B)h) - \sum_i^n k^{-2i} h^{2i+1} E_{2i+1}\right),$$
$$= \left(\exp((A+B)h) - \sum_{k=1}^n c_k \sum_i^n k^{-2i} h^{2i+1} E_{2i+1}\right),$$
$$= O(h^{2n+1}),$$
$$\text{as } n \rightarrow \infty.$$

where the coefficients are given in (42).

ad 2.) Some argument as in 1.), see also [19].

Lemma 1. *We assume $||A(t)||$ to be bounded in the interval $t \in (0,T)$. Then T_2 is non-singular for sufficient small dt.*

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 dt.

Theorem 3. *We assume T_2 is non-singular, see lemma 1. If T_2 is non-singular, then the entire MPE is non-singular and we have a uniform convergence.*

Proof. Since
$$T_2 = \exp(dtlA(t + dt/2)), \quad (52)$$
for sufficient $dt << 1$, we can derive
$$T_2 = 1 + dt\, A(t), \quad (53)$$
If we assume the boundedness of $||A(t)||$ in small dt, T_2 is nonsingular and bounded and we have uniform convergence, see [21].

Remark 6. With the uniform convergence of the MPE method, we are more general than for the Magnus series with a convergence radius, see [17].

5 Numerical Examples

In the following section, we deal with experiments to verify the benefit of our methods. At the beginning, we propose introductory examples to compare the methods. In the next examples, applications to Hamiltonian problems, as Schrödinger equation and harmonic oscillator, are done.

5.1 Simple Examples: First

To assess the convergence of the Multi-product expansion with that of the Magnus series, consider the well known example[16] of

$$A(t) = \begin{pmatrix} 2 & t \\ 0 & -1 \end{pmatrix}, \tag{54}$$

The exact solution to (2) with $Y(0) = I$ is

$$Y(t) = \begin{pmatrix} \mathrm{e}^{2t} & f(t) \\ 0 & \mathrm{e}^{-t} \end{pmatrix}, \tag{55}$$

with

$$\begin{aligned} f(t) &= \frac{1}{9}\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1 - 3t) && (56) \\ &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13t^{11}}{178200} && (57) \end{aligned}$$

For the Magnus expansion, one has the series

$$\Omega(t) = \begin{pmatrix} 2t & g(t) \\ 0 & -t \end{pmatrix}, \tag{58}$$

with, up to the 10th order,

$$\begin{aligned} g(t) &= \frac{1}{2}t^2 - \frac{1}{4}t^3 + \frac{3}{80}t^5 - \frac{9}{1120}t^7 + \frac{81}{44800}t^9 + \cdots && (59) \\ &\to \frac{t(\mathrm{e}^{3t} - 1 - 3t)}{3(\mathrm{e}^{3t} - 1)}. && (60) \end{aligned}$$

Exponentiating (58) yields (55) with

$$\begin{aligned} f(t) &= t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1)\left(\frac{1}{6} - \frac{1}{12}t + \frac{1}{80}t^3 - \frac{3}{1120}t^5 + \frac{27}{44800}t^7 + \cdots\right) && (61) \\ &\to t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1)\left(\frac{1}{9t} - \frac{1}{3(\mathrm{e}^{3t} - 1)}\right) && (62) \end{aligned}$$

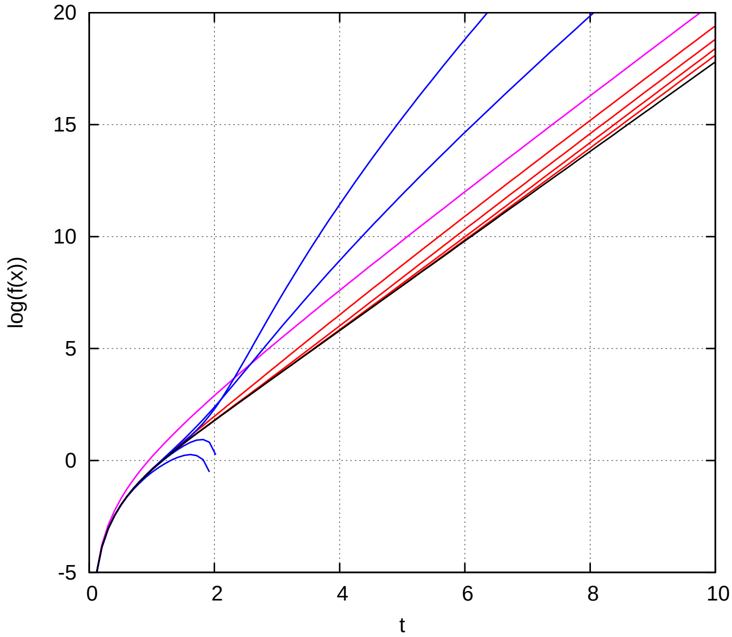

Fig. 1. The black line is the exact result (57). The blue lines are the Magnus series (61). The red lines are the multi-product expansion. The purple line is their common second order result.

Whereas the exact solution (57) is an entire function of t, the Magnus series (59) and (61) only converge for $|t| < \frac{2}{3}\pi$ due to the pole at $t = \frac{2}{3}\pi i$. The Magnus series (61) is plot in Fig.1 as blue lines. The pole at $|t| = \frac{2}{3}\pi \approx 2$ is clearly visible.

By contrast, the multi-product expansion suffers no such drawbacks. ¿From (26), by setting $\Delta t = t$ and $t = 0$, we have

$$\mathcal{T}_2(t) = \exp\left[t\begin{pmatrix} 2 & \frac{1}{2}t \\ 0 & -1 \end{pmatrix}\right] = \begin{pmatrix} \mathrm{e}^{2t} & f_2(t) \\ 0 & \mathrm{e}^{-t} \end{pmatrix} \tag{63}$$

with

$$f_2(t) = \frac{1}{6}t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1). \tag{64}$$

This is identical to first term of the Magnus series (61) and is an entire function of t. Since higher order MPE uses only powers of $\mathcal{T}_2$, higher order MPE approximations are also entire functions of t. Thus up to the 10th order, one finds

$$f_4(t) = t\mathrm{e}^{-t}\left(\frac{\mathrm{e}^{3t} - 5}{18} + \frac{2\mathrm{e}^{3t/2}}{9}\right) \tag{65}$$

$$f_6(t) = t\mathrm{e}^{-t}\left(\frac{11\mathrm{e}^{3t} - 109}{360} + \frac{9}{40}(\mathrm{e}^{2t} + \mathrm{e}^{t}) - \frac{8}{45}\mathrm{e}^{3t/2}\right) \tag{66}$$

$$f_8(t) = t\mathrm{e}^{-t}\left(\frac{151\mathrm{e}^{3t} - 2369}{7560} + \frac{256}{945}(\mathrm{e}^{9t/4} + \mathrm{e}^{3t/4}) - \frac{81}{280}(\mathrm{e}^{2t} + \mathrm{e}^{t}) + \frac{104}{315}\mathrm{e}^{3t/2}\right) \tag{67}$$

$$\begin{aligned} f_{10}(t) = t\mathrm{e}^{-t}\Bigg(&\frac{15619\mathrm{e}^{3t} - 347261}{1088640} + \frac{78125}{217728}(\mathrm{e}^{12t/5} + \mathrm{e}^{9t/5} + \mathrm{e}^{6t/5} + \mathrm{e}^{3t/5}) \\ &- \frac{4096}{8505}(\mathrm{e}^{9t/4} + \mathrm{e}^{3t/4}) + \frac{729}{4480}(\mathrm{e}^{2t} + \mathrm{e}^{t}) - \frac{4192}{8505}\mathrm{e}^{3t/2}\Bigg). \end{aligned} \tag{68}$$

These MPE approximations are plotted as red lines in Fig.1. The convergence seems uniform for all t.

When expanded, the above yields

$$\begin{aligned} f_2(t) &= \frac{t^2}{2} + \frac{t^3}{4} + \cdots \\ f_4(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{5t^5}{192} + \cdots \\ f_6(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{384} + \cdots \\ f_8(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{1307t^9}{8601600} + \cdots \\ f_{10}(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13099t^{11}}{232243200} \end{aligned} \tag{69}$$

and agree with the exact solution to the claimed order.

Here we have convergence due to the following theorem:

Theorem 4. *We have given the initial value problem (2) and the exact solution of the initial value problem, see (55). Then the approximated $g(t, \epsilon)$ done with the MPE method is convergent with the rate:*

$$|g_{exact}(t) - g_{MPE,2(i+1)}(t)| \leq C\mathcal{O}(t^{2(i+1)+1}), \tag{70}$$

where C is independent of t and ϵ and $0 \leq C \leq 0.25$, for $i = 0, 1, 2, \ldots$.

Proof. We apply the difference between exact and approximated solution, due to the Taylor expansion of both solutions:

We begin with $i = 0$:

$$\begin{aligned} &|f_{exact}(t) - f_{MPE,2}(t)| && (71) \\ &= |\frac{\exp(2t)}{9} - (1/9 + t/3)exp(-t) - (\exp(-t)(\exp(3t) - 1)t/6)| && (72) \\ &= \frac{t^3}{4} + \mathcal{O}(t^5) \leq C\mathcal{O}(t^5), && (73) \end{aligned}$$

and $0 \leq C \leq 0.25$.

For $i \geq 0$: We have the

$$|f_{exact}(t) - f_{MPE,2(i+1)}(t)| \leq \frac{t^{2(i+1)+1})}{4} \tag{74}$$

$$\leq C\mathcal{O}(t^{2(i+1)+1}), \tag{75}$$

and $0 \leq C \leq 0.25$.

Remark 7. Here we have uniform convergence because of the non singularities of the MPE products.

5.2 Radial Schödinger equation (highly nonlinear)

We consider the radial Schrödinger equation

$$\frac{\partial^2 u}{\partial r^2} = f(r, E) u(r) \tag{76}$$

where

$$f(r, E) = 2V(r) - 2E + \frac{l(l+1)}{r^2}\ , \tag{77}$$

By relabeling $r \rightarrow t$ and $u(r) \rightarrow q(t)$, (76) can be viewed as harmonic oscillator with a time dependent spring constant

$$k(t, E) = -f(t, E) \tag{78}$$

and Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}k(t, E)q^2. \tag{79}$$

Thus any eigenfunction of (76) is an exact time-dependent solution of (79). For example, the ground state of the hydrogen atom with $l = 0$, $E = -1/2$ and

$$V(r) = -\frac{1}{r} \tag{80}$$

yields the exact solution

$$q(t) = t\exp(-t) \tag{81}$$

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

$$Y(t) = \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}, \tag{82}$$

the time-dependent oscillator (79) now corresponds to

$$A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} \equiv T + V(t), \tag{83}$$

with

$$f(t) = (1 - \frac{2}{t}). \tag{84}$$

In this case, the second-order midpoint algorithm is

$$\begin{aligned} \mathcal{T}_2(h,t) &= \mathrm{e}^{\frac{1}{2}hT}\mathrm{e}^{hV(t+h/2)}\mathrm{e}^{\frac{1}{2}hT} \\ &= \begin{pmatrix} 1+\frac{1}{2}h^2 f(t+\frac{1}{2}h) & h+\frac{1}{4}h^3 f(t+\frac{1}{2}h) \\ hf(t+\frac{1}{2}h) & 1+\frac{1}{2}h^2 f(t+\frac{1}{2}h), \end{pmatrix} \end{aligned} \tag{85}$$

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

$$q_2(t) = t + \frac{1}{4}t^3 f(\frac{1}{2}t) = t - t^2 + \frac{1}{4}t^3. \tag{86}$$

Higher order multi-product expansions, using (85), then yield

$$\begin{aligned} q_4(t) &= t - t^2 + \frac{7t^3}{18} - \frac{t^4}{9} + \frac{t^5}{96} \\ q_6(t) &= t - t^2 + \frac{211t^3}{450} - \frac{31t^4}{225} + \frac{17t^5}{600} + \cdots \\ q_8(t) &= t - t^2 + \frac{32233t^3}{66150} - \frac{5101t^4}{33075} + \frac{3139t^5}{88200} + \cdots \\ q_{10}(t) &= t - t^2 + \frac{88159t^3}{1786050} - \frac{143177t^4}{893025} + \frac{91753t^5}{2381400} + \cdots \end{aligned} \tag{87}$$

Comparing this to the exact solution (81):

$$\begin{aligned} q(t) &= t - t^2 + \frac{t^3}{2} - \frac{t^4}{6} + \frac{t^5}{24} - \frac{t^6}{120} + \frac{t^7}{720} - \frac{t^8}{5040} \cdots, \\ &= t - t^2 + \frac{t^3}{2} - 0.1667t^4 + 0.0417t^5 - 0.0083t^6 + 0.0014t^7 \cdots \end{aligned} \tag{88}$$

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 (81), one sees that force (or acceleration)

$$\lim_{t\to 0} f(t)q(t) = -2 \tag{89}$$

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

$$\frac{7}{18} = 0.3889, \quad \frac{211}{450} = 0.4689, \quad \frac{32233}{66150} = 0.4873, \quad \frac{88159}{1786050} = 0.4936, \tag{90}$$

$$\frac{1}{9} = 0.1111, \quad \frac{31}{225} = 0.1378, \quad \frac{5101}{33075} = 0.1542, \quad \frac{143177}{893025} = 0.1603. \tag{91}$$

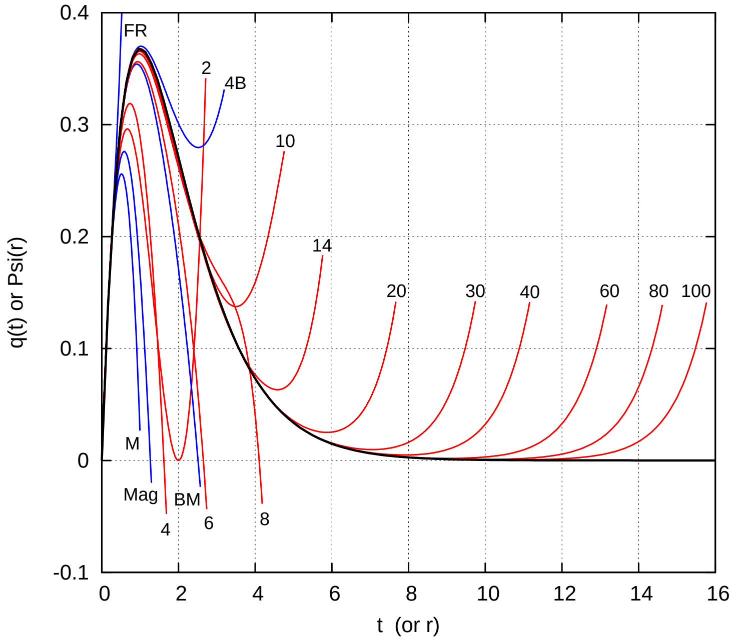

Fig. 2. The uniform convergence of the multi-product expansion in solving for the hydrogen ground state wave function. The black line is the exact ground state wave function. The numbers indicates the order of the multi-product expansion. The blue lines denote results of various fourth-order algorithms.

Similarily with all other coefficients. To see this uniform convergence, we show in Fig.2, 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 (87). 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, 3 force-evaluations), M (MacLachlan, 4 force-evaluations), BM (Blanes-Moan, 6 force-evaluations), Mag (Magnus integrator, see below, ≈ 2.5 force-evaluations) and 4B (a *forward* symplectic algorithm with only ≈ 2 evaluations). These symplectic integrators steadily improves from FR, to M, to Mag, 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

$$q_{4B}(t) = t - t^2 + \frac{t^3}{2} - 0.1635t^4 + 0.0397t^5 - 0.0070t^6 + 0.0009t^7 \cdots , \qquad (92)$$

with the correct third-order coefficient and comparable higher order coefficients as the exact solution (88). By contrast, the FR algorithm, which is well know to have rather large errors, has the expansion,

$$q_{FR}(t) = t - t^2 - 0.1942t^3 + 3.528t^4 - 2.415t^5 + 0.5742t^6 - 0.0437t^7 \cdots , \quad (93)$$

with terms of the wrong signs beyond t^2.

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

$$f(t) = t^2 - 3, \quad (94)$$

and exact ground state solution

$$q(t) = t\mathrm{e}^{-t^2/2} = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{t^{11}}{3840} + \cdots , \quad (95)$$

the multi-product expansion now gives,

$$\begin{aligned} q_2(t) &= t - \frac{3t^3}{4} + \frac{t^5}{16} \\ q_4(t) &= t - \frac{t^3}{2} + \frac{29t^5}{192} + \cdots \\ q_6(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{13t^7}{576} + \cdots \\ q_8(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{20803t^9}{7741440} + \cdots \\ q_{10}(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{50977t^{11}}{193536000} + \cdots , \end{aligned} \quad (96)$$

and matches the Taylor expansion up to the claimed order, as it is in the previous case of (69).

A fourth-order Magnus algorithm is given by

$$\mathcal{T}_4(\Delta t) = \mathrm{e}^{c_3 \Delta t (V_2 - V_1)} \mathrm{e}^{\Delta t (T + \frac{1}{2}(V_1 + V_2))} \mathrm{e}^{-c_3 \Delta t (V_2 - V_1)} \quad (97)$$

where

$$c_1 = 1/2 - \sqrt{3}/6, \qquad c_2 = 1/2 + \sqrt{3}/6, \qquad c_3 = \sqrt{3}/12$$

and

$$V_1 = V(t + c_1 \Delta t), \qquad V_2 = V(t + c_2 \Delta t).$$

Normally, one would need to further split the central exponential in (97) to fourth-order. In the general case, this would require at least three force evaluations. However, because it is an harmonic oscillator, it can be splitted to fourth-order via

$$\mathrm{e}^{\Delta t (T + \frac{1}{2}(V_1 + V_2))} = \mathrm{e}^{c_e \Delta t \frac{1}{2}(V_1 + V_2))} \mathrm{e}^{c_m \Delta t T} \mathrm{e}^{c_e \Delta t \frac{1}{2}(V_1 + V_2)} \quad (98)$$

where

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

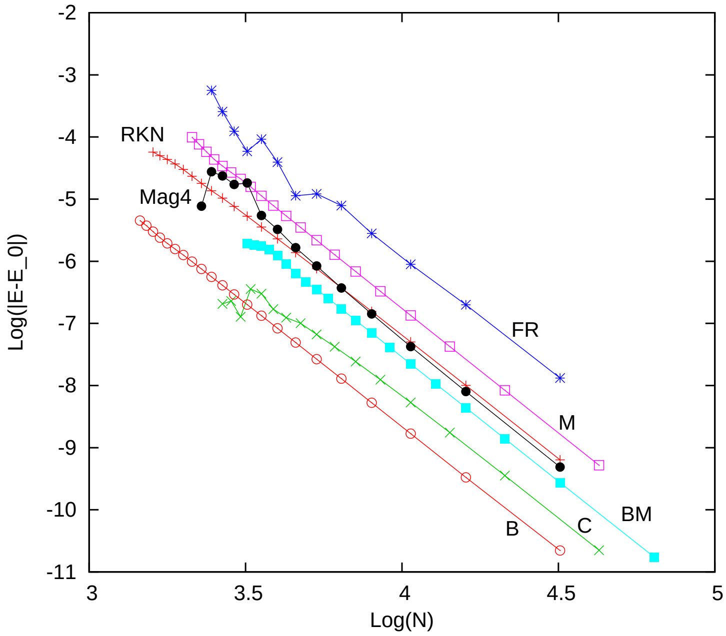

Fig. 3. Comparison between Magnus expansion and Suzuki's expansion.

where $f_a = \frac{1}{2}[f(t + c_1 \Delta t, E) + f(t + c_2 \Delta t, E)]$. Thus the entire algorithm (97) only needs two evaluations of the potential in $f(t, E)$. In Fig.1, algorithm B also only requires two evaluations of the potential.

In Figure 3, we present the comparison between Magnus and Suzuki's method.

The radial Schrödinger equation is know to be highly nonlinear and therefore an optimal example to compare our methods.

While we apply an improved Magnus expansion due to the commutator free scheme, the underlying Suzuki's method that can be done with only applying extrapolation schemes. We have reductions in computing exponential matrices for both methods.

One the one hand Magnus expansion achieve his accuracy while applying a composition method based on optimal choose of quadrature points to the time-dependent matrices, while Suzuki's expansion apply multiplications of one standard matrix.

Here we see the benefit of the Suzuki's method, while dealing with only one matrix type, where on the other hand Magnus expansion has to compute multiple time-points for each matrix.

6 Conclusions and Discussions

We have presented time-dependent splitting methods, based on Magnus and Suzuki's ideas. Numerical examples confirm the applications to Schrödinger equations. We present 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 the 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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