"High-order actions and their applications" to honor our friend and collaborator Siu A. Chin Universitat Politecnica de Catalunya, Barcelona, Spain Lecture: Magnus Expansion and Suzuki's Method

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Outline of the talk

0) Time Decomposition methods: Magnus Expansion - Suzuki's Expansion
1) Multi product Expansion: Theory and Analysis
2) Comparisons
3) Numerical Results

Introduction

Timedependent decomposition methods are important algorithms to solve Hamiltonian problems (e.g., Schrödinger equations, harmonic oscillators, etc.) so hyperbolic problems. Here Magnus expansion has been widely studied, see some of the recent literature, e.g.,

1. The Magnus expansion and some of its applications, see [Blanes, Casas, Oteo, Ros 2008] ;
2. Convergence of Magnus series, see [Moan, Niesen 2008] ;
3. Commutator free Magnus expansion, see [Blanes, Moan 2006] ;

Introduction

Some delicate computational work is to do in the Magnus expansion:

- time-integrals
- nested commutators to obtain higher order methods

Derivation of higher orders beyond sixth-order are consuming.

Introduction

An alternative algorithm is a multiproduct expansion with Suzuki's method to provide a simpler ways of a higher order method for time-dependent problems.
Suzuki's method has been studied in different applications, see some of the recent literature, e.g.,

1. General decomposition theory of ordered exponentials, see [Suzuki 1993] ;
2. Gradient symplectic algorithms for solving the Schrödinger equation, see [Chin, Chen 2002] ;
3. Multiproduct splitting and Runge-Kutta-Nyström integrators, see [Chin 2008] ;

Introduction

We concentrate on solving linear evolution equations, such as the time-dependent Schrödinger equation,

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

where A can be an unbounded and time-dependent operator. For solving Hamiltonian problems, it is often the case that $A(t) = T + V(t)$, where only the potential operator $V(t)$ is time-dependent and T is the linear operator (e.g., spatial dependent: diffusion operator).

Exponential Splitting based on Magnus Integrator

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

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

with solution

$$Y(t) = \exp(\Omega(t))Y(0) \; . \qquad (3)$$

This can be expressed as:

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

where the time-ordering operator $\mathcal{T}$, see [Dyson 1976].
The Magnus expansion is defined as:

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

where the first few terms are:

$$\Omega_1(t) = \int_0^t dt_1 A_1, \quad \Omega_2(t) = \frac{1}{2} \int_0^t dt_1 \int_0^{t_1} dt_2 [A_1, A_2],$$
$$\Omega_3(t) = \frac{1}{6} \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 ([A_1, [A_2, A_3] + [[A_1, A_2], A_3]),$$
$$\cdots\cdots \qquad \text{etc.} \qquad (6)$$

For practical reasons, it is more useful to define the *n*th order Magnus operator

$$\Omega^{[n]}(t) = \Omega(t) + O(t^{n+1}) \tag{7}$$

such that

$$Y(t) = \exp\left[\Omega^{[n]}(t)\right] Y(0) + O(t^{n+1}). \tag{8}$$

Thus the second-order Magnus operator is

$$\Omega^{[2]}(t) = \int_0^t dt_1 A(t_1) = tA\left(\frac{1}{2}t\right) + O(t^3) \tag{9}$$

Example: A fourth-order Magnus operator [Blanes 2008] is given as

$$\Omega^{[4]}(t) = \frac{1}{2}t(A_1 + A_2) - c_3 t^2 [A_1, A_2] \tag{10}$$

where $A_1 = A(c_1 t)$, $A_2 = A(c_2 t)$ and

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \qquad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}, \qquad c_3 = \frac{\sqrt{3}}{12}. \tag{11}$$

To apply Magnus integrators one have to evaluate nested commutators, which makes Magnus integrators beyond the fourth-order rather complex.
Example:

$$A(t) = T + V(t), \tag{12}$$

one has

$$\begin{aligned} e^{\Omega^{[2]}(t)} &= e^{t[T+V(t/2)]} \\ &= e^{\frac{1}{2}tT} e^{tV(t/2)} e^{\frac{1}{2}tT} + O(t^3) \end{aligned} \tag{13}$$

and

$$e^{\Omega^{[4]}(t)} = e^{c_3 t(V_2 - V_1)} e^{t(T + \frac{1}{2}(V_1 + V_2))} e^{-c_3 t(V_2 - V_1)} \tag{14}$$

where

$$V_1 = V(c_1 t), \qquad V_2 = V(c_2 t). \tag{15}$$

Remark

1.) General operator case: Magnus expansion generates more terms in the exponential, more complex splittings are necessary.
2.) Example: Central exponential in (14) must be further splitted to fourth-order method, to maintain the fourth-order character of the overall algorithm (e.g., fourth order integration formula)

Suzuki's time-ordered exponential and multi-product splitting

Instead of the Magnus series (5) expanding the time-dependent problems, we directly implement the time-ordered exponential as suggested by Suzuki [Suzuki 1993]:

$$Y(t+\Delta t) = \mathcal{T}\left(\exp \int_t^{t+\Delta t} A(s) ds\right) Y(t), \tag{16}$$

aside from the conventional expansion

$$\mathcal{T}\left(\exp \int_t^{t+\Delta t} A(s) ds\right) \tag{17}$$
$$= 1 + \int_t^{t+\Delta t} A(s_1) ds_1 + \int_t^{t+\Delta t} ds_1 \int_t^{s_1} ds_2 A(s_1) A(s_2) + \cdots ,$$

Time-ordered exponential can also interpreted as (use Trotter product formula)

$$\mathcal{T}\left(\exp \int_t^{t+\Delta t} A(s)ds\right) = \lim_{n\to\infty} \mathcal{T}\left(\mathrm{e}^{\frac{\Delta t}{n}\sum_{i=1}^{n} A(t+i\frac{\Delta t}{n})}\right), \tag{18}$$

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

Further Suzuki introduces the *forward time derivative* operator

$$D = \frac{\overleftarrow{\partial}}{\partial t} \tag{19}$$

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

$$F(t)\mathrm{e}^{\Delta t D}G(t) = F(t+\Delta t)G(t). \tag{20}$$

Trotter's formula then gives

$$\exp[\Delta t(A(t) + D)] = \lim_{n\to\infty} \left(\mathrm{e}^{\frac{\Delta t}{n} A(t)} \mathrm{e}^{\frac{\Delta t}{n} D} \right)^n, \tag{21}$$
$$= \lim_{n\to\infty} \mathrm{e}^{\frac{\Delta t}{n} A(t+\Delta t)} \cdots \mathrm{e}^{\frac{\Delta t}{n} A(t+\frac{2\Delta t}{n})} \mathrm{e}^{\frac{\Delta t}{n} A(t+\frac{\Delta t}{n})},$$

where property (20) has been applied repeatedly and accumulatively. Comparing (19) with (22) yields Suzuki's decomposition of the time-ordered exponential:

$$\mathcal{T}\left(\exp \int_t^{t+\Delta t} A(s)ds\right) = \exp[\Delta t(A(t) + D)]. \tag{22}$$

Thus time-ordering can be achieve by splitting an additional operator D.

Idea: Transforms of any existing splitting algorithms into integrators of explicit time-dependent problems.
For example, we have the following second order splittings

$$\mathcal{T}_2(\Delta t) = \mathrm{e}^{\frac{1}{2}\Delta t D}\mathrm{e}^{\Delta t A(t)}\mathrm{e}^{\frac{1}{2}\Delta t D} = \mathrm{e}^{\Delta t A(t+\frac{1}{2}\Delta t)}. \qquad (23)$$

The choice of symmetric products is important, because one then has only odd powers of Δt

$$\mathcal{T}_2(\Delta t) = \mathrm{e}^{\Delta t(A(t)+D)+\Delta t^3 E_3+\Delta t^5 E_5+\cdots} \qquad (24)$$

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 $t + \Delta t$. For example,

$$\mathcal{T}_2(\Delta t)\mathcal{T}_2(\Delta t) = \mathrm{e}^{\Delta t A(t+\frac{3}{2}\Delta t)}\mathrm{e}^{\Delta t A(t+\frac{1}{2}\Delta t)}. \qquad (25)$$

Problem:
Higher order factorization of (22) into a single product form

$$\exp[\Delta t(A(t) + D)] = \Pi_i \mathrm{e}^{a_i \Delta t A(t)} \mathrm{e}^{d_i \Delta t D} \tag{26}$$

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

Benefits of the MPE algorithm:
Higher order algorithms can be built from the multi-product expansion, see [Chin 2008] of (22), with only quadratically growing number of exponentials at high orders.
For example,

$$\mathcal{T}_4(\Delta t) = -\frac{1}{3}\mathcal{T}_2(\Delta t) + \frac{4}{3}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) \tag{27}$$

$$\mathcal{T}_6(\Delta t) = \frac{1}{24}\mathcal{T}_2(\Delta t) - \frac{16}{15}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) + \frac{81}{40}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right) \tag{28}$$

$$\mathcal{T}_8(\Delta t) = -\frac{1}{360}\mathcal{T}_2(\Delta t) + \frac{16}{45}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) - \frac{729}{280}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right) + \frac{1024}{315}\mathcal{T}_2^4\left(\frac{\Delta t}{4}\right) \quad (29)$$

$$\mathcal{T}_{10}(\Delta t) = \frac{1}{8640}\mathcal{T}_2(\Delta t) - \frac{64}{945}\mathcal{T}_2^2\left(\frac{\Delta t}{2}\right) + \frac{6561}{4480}\mathcal{T}_2^3\left(\frac{\Delta t}{3}\right) - \frac{16384}{2835}\mathcal{T}_2^4\left(\frac{\Delta t}{4}\right) + \frac{390625}{72576}\mathcal{T}_2^5\left(\frac{\Delta t}{5}\right).. \quad (30)$$

Derivation of the closed form: For a given set of n distinct whole numbers $\{k_1, k_2, ...k_n\}$, one can form a $2n$-order approximation of $\mathrm{e}^{\Delta t(A+D)}$ via

$$\mathrm{e}^{\Delta t(A+D)} = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i} \left(\frac{\Delta t}{k_i} \right) + e_{2n+1}(h^{2n+1} E_{2n+1}). \quad (31)$$

with *closed form* solutions

$$c_i = \prod_{j=1(\neq i)}^{n} \frac{k_i^2}{k_i^2 - k_j^2} \quad (32)$$

and error coefficient,

$$e_{2n+1} = (-1)^{n-1} \prod_{i=1}^{n} \frac{1}{k_i^2}. \quad (33)$$

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

$$\begin{pmatrix} 1 & 1 & 1 & \ldots & 1 \\ k_1^{-2} & k_2^{-2} & k_3^{-2} & \ldots & k_n^{-2} \\ k_1^{-4} & k_2^{-4} & k_3^{-4} & \ldots & k_n^{-4} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ k_1^{-2(n-1)} & k_2^{-2(n-1)} & k_3^{-2(n-1)} & \ldots & k_n^{-2(n-1)} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \ldots \\ c_n \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \ldots \\ 0 \end{pmatrix} \quad (34)$$

Since

$$\mathcal{T}_2^{k_i}\left(\frac{\Delta t}{k}_i\right) = \exp\left(\Delta t(A(t)+D) + \frac{\Delta t^3}{k_i^2}E_3 + \frac{\Delta t^5}{k_i^4}E_5 + \cdots\right), \tag{35}$$

the coefficients c_i so determined by (34), guarantees that all error terms in (24) and (35) when expanded from the exponential, including cross-terms, vanish up to order $2n$. That is, the extrapolation acts correctly on the entire exponential and not just on the exponent. The above explicit form corresponds to the harmonic sequence $\{k_1, k_2, k_3, \ldots\} = \{1, 2, 3, \ldots\}$.

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

$$\mathcal{T}_2(\Delta t) = \mathrm{e}^{\Delta t A(t+\frac{1}{2}\Delta t)} = \mathrm{e}^{\frac{1}{2}\Delta t T}\mathrm{e}^{\Delta t V(t+\Delta t/2)}\mathrm{e}^{\frac{1}{2}\Delta t T} + O(\Delta t^3). \quad (36)$$

Proposition

An error estimates is given as:

$$\mathrm{e}^{\frac{1}{2}\Delta t T}\mathrm{e}^{\Delta t V}\mathrm{e}^{\frac{1}{2}\Delta t T} = \mathrm{e}^{\Delta t(T+V)+\Delta t^3 E_3+\Delta t^5 E_5+\ldots}, \ \textit{with} \quad (37)$$

$$E_3 = -\frac{1}{24}[TTV] - \frac{1}{12}[VTV],$$

$$E_5 = \frac{7}{5760}[T^4 V] + \frac{1}{480}[T^2 VTV] + \frac{1}{360}[VT^3 V] + \frac{1}{120}[VTVTV],$$

where $[T^2 V] = [T, [T, V]]$ *and* $[T^4 V] = [T, [T, [T, [T, V]]]]$ *etc., denote nested commutators, where* $[VVTV] = 0$.

The estimation of the error terms are given as:

$$
\begin{aligned}
||E_3|| &= || - \frac{1}{24}[TTV] - \frac{1}{12}[VTV]|| \qquad (38) \\
&\leq \frac{1}{24}||T^2||||V|| + \frac{1}{12}||T||||V^2||, \\
||E_5|| &= ||\frac{7}{5760}[TTTTV] + \frac{1}{480}[TTVTV] \qquad (39) \\
&+\frac{1}{360}[VTTTV] + \frac{1}{120}[VTVTV]|| \\
&\leq \frac{7}{5760}||T^4||||V|| + \frac{7}{1440}||T^3||||V^2|| + \frac{1}{120}||T^2||||V^3||
\end{aligned}
$$

General:
Magnus expansion and the exponential-splitting scheme require exponentially growing number of operators at higher orders.
Suzuki's rule of incorporating time-ordering operators reduce this fundamental requirement of exponentially growing.
Currently, only MPE, which systematically removes each odd-order error term by extrapolation, limits the growth of operators quadratically.

Error analysis of the Multi-product expansion

The convergence analysis is based on the restriction to exponential splitting, our proof of convergence based on the general framework of [Ostermann, Hansen 2008].
We assume small h, the second-order decomposition is bounded as follow:

$$||\mathcal{T}_2(h)|| = || \exp(\frac{1}{2} hD) \exp(hA(t)) \exp(\frac{1}{2} hD)|| \leq \exp(c\omega h), \tag{40}$$

with c only depends on the coefficients of the method and ω is a constant. We can then derive the following convergence results for the multi-product expansion.

Theorem

For the numerical solution of (2), we consider our MPE method (31) of order $2n+1$ *and we apply Assumption (40), then we have:*

$$|| \left(S^m - \exp(mh(A(t)+D))\right) u_0|| \leq CO(h^{2n+1}), mh \leq T, \quad (41)$$

where $S = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i})$ *and C is to be chosen uniformly on bounded time intervals and independent of m and h for sufficient small h.*

Proof.

We apply the telescopic identity and obtain:

$$\left(S^m - \exp(mh(A(t) + D))\right) u_0 = \tag{42}$$

$$\sum_{\nu=0}^{m-1} S^{m-\nu-1}(S - \exp(h(A(t) + D))) \exp(\nu h(A(t) + D))u_0.$$

where $S = \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i})$

We apply assumption (40) and yield to the stability:

$$|| \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i})|| \leq \exp(c\omega h). \tag{43}$$

□

We assume that the consistency is bound:

$$|| \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i}) - \exp(h(A + D))|| \leq O(h^{2n+1}) \qquad (44)$$

is valid, we have the following error bound:

$$|| \left(S^m - \exp(mh(A(t) + D))\right) u_0|| \leq CO(h^{2n+1}), mh \leq T, \quad (45)$$

The consistency is derived in the following theorem.

Theorem

For the numerical solution of (2), we have the following consistency:

$$|| \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}(\frac{h}{k_i}) - \exp(h(A+D)) || \leq O(h^{2n+1}). \quad (46)$$

Proof.

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

$$\sum_{k=1}^{n} c_k \mathcal{T}_2^k(\frac{h}{k}) \tag{47}$$

$$= \sum_{k=1}^{n} c_k \left(\exp((A+B)h) - (k^{-2} h^3 E_3 + k^{-4} h^5 E_5 + \ldots) \right),$$

$$= \sum_{k=1}^{n} c_k \left(\exp((A+B)h) - \sum_{i}^{n} k^{-2i} h^{2i+1} E_{2i+1} \right),$$

□

$$
\begin{aligned}
&= \left(\exp((A+B)h) - \sum_{k=1}^{n} c_k \sum_{i}^{n} k^{-2i} h^{2i+1} E_{2i+1} \right), \\
&= O(h^{2n+1}). \qquad (48)
\end{aligned}
$$

Lemma

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

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 h.

□

Theorem

We assume T_2 is non-singular, see previous Lemma. If T_2 is non-singular, then the entire MPE is non-singular and we have a uniform convergence.

Proof.

Since

$$T_2 = \exp(hA(t + h/2)), \tag{49}$$

for sufficient small $h << 1$, we have

$$T_2 = 1 + h\, A(t). \tag{50}$$

Thus if $||A(t)||$ is bounded in $0 \leq t \leq T$, then T_2 is nonsingular and bounded, and we have uniform convergence in $[0, T]$. see [Yoshida 1980].

Numerical Experiments

Example 1: The non-singular matrix case
To assess the convergence of the Multi-product expansion with that of the Magnus series, consider the well known example [moan 2008] of

$$A(t) = \begin{pmatrix} 2 & t \\ 0 & -1 \end{pmatrix}. \tag{51}$$

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

$$Y(t) = \begin{pmatrix} \mathrm{e}^{2t} & f(t) \\ 0 & \mathrm{e}^{-t} \end{pmatrix}, \tag{52}$$

with

$$f(t) = \frac{1}{9}\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1 - 3t) \tag{53}$$

$$= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13t^{11}}{178200} \tag{54}$$

For the Magnus expansion, one has the series

$$\Omega(t) = \begin{pmatrix} 2t & g(t) \\ 0 & -t \end{pmatrix}, \qquad (55)$$

with, up to the 10th order,

$$\begin{aligned} g(t) &= \frac{1}{2}t^2 - \frac{1}{4}t^3 + \frac{3}{80}t^5 - \frac{9}{1120}t^7 + \frac{81}{44800}t^9 + \cdots \\ &\rightarrow \frac{t(\mathrm{e}^{3t} - 1 - 3t)}{3(\mathrm{e}^{3t} - 1)}. \end{aligned} \qquad (56)$$

Exponentiating (55) yields (52) with

$$\begin{aligned} f(t) &= t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1)\left(\frac{1}{6} - \frac{1}{12}t + \frac{1}{80}t^3 - \frac{3}{1120}t^5 + \frac{27}{44800}t^7 + \cdots\right) \\ &\rightarrow t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1)\left(\frac{1}{9t} - \frac{1}{3(\mathrm{e}^{3t} - 1)}\right) \end{aligned} \qquad (57)$$

The multi-product expansion suffers no such drawbacks. From (23), by setting $\Delta t = t$ and $t = 0$, we have

$$\mathcal{T}_2(t) = \exp\left[t\begin{pmatrix} 2 & \frac{1}{2}t \\ 0 & -1 \end{pmatrix}\right] = \begin{pmatrix} \mathrm{e}^{2t} & f_2(t) \\ 0 & \mathrm{e}^{-t} \end{pmatrix} \tag{58}$$

with

$$f_2(t) = \frac{1}{6}t\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1). \tag{59}$$

This is identical to first term of the Magnus series (57) 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

$$f_4(t) = t\mathrm{e}^{-t}\left(\frac{\mathrm{e}^{3t} - 5}{18} + \frac{2\mathrm{e}^{3t/2}}{9}\right) \tag{60}$$

$$f_6(t) = t\mathrm{e}^{-t}\left(\frac{11\mathrm{e}^{3t} - 109}{360} + \frac{9}{40}(\mathrm{e}^{2t} + \mathrm{e}^{t}) - \frac{8}{45}\mathrm{e}^{3t/2}\right) \tag{61}$$

$$f_8(t) = t\mathrm{e}^{-t}\left(\frac{151\mathrm{e}^{3t} - 2369}{7560} + \frac{256}{945}(\mathrm{e}^{9t/4} + \mathrm{e}^{3t/4}) - \frac{81}{280}(\mathrm{e}^{2t} + \mathrm{e}^{t}) + \frac{104}{315}\mathrm{e}^{3t/2}\right) \quad (62)$$

$$f_{10}(t) = t\mathrm{e}^{-t}\left(\frac{15619\mathrm{e}^{3t} - 347261}{1088640} + \frac{78125}{217728}(\mathrm{e}^{12t/5} + \mathrm{e}^{9t/5} + \mathrm{e}^{6t/5} + \mathrm{e}^{3t/5}) - \frac{4096}{8505}(\mathrm{e}^{9t/4} + \mathrm{e}^{3t/4}) + \frac{729}{4480}(\mathrm{e}^{2t} + \mathrm{e}^{t}) - \frac{4192}{8505}\mathrm{e}^{3t/2}\right). \quad (63)$$

When expanded, the above yields

$$
\begin{aligned}
f_2(t) &= \frac{t^2}{2} + \frac{t^3}{4} + \cdots \\
f_4(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{5t^5}{192} + \cdots \\
f_6(t) &= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{384} + \cdots
\end{aligned} \tag{64}
$$

$$f_8(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{1307t^9}{8601600} + \cdots \qquad (65)$$

$$f_{10}(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \frac{13099t^{11}}{232243200} + \cdots \qquad (66)$$

and agree with the exact solution to the claimed order.

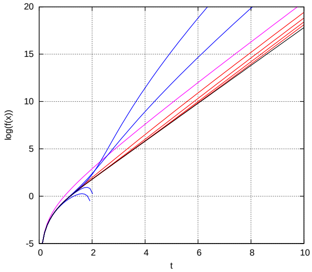

Figure: The black line is the exact result (53). The blue lines are the Magnus fourth to tenth order results (57), which diverge from the exact result beyond $t > 2$. The red lines are the multi-product expansions. The purple line is their common second order result.

Results:
The Magnus series (56) and (57) only converge for $|t| < \frac{2}{3}\pi$ due to the pole at $t = \frac{2}{3}\pi i$.
The MPE series convergences uniform for all t.

Experiment 2: The radial Schödinger equation
We consider the radial Schrödinger equation

$$\frac{\partial^2 u}{\partial r^2} = f(r, E)u(r) \tag{67}$$

where

$$f(r, E) = 2V(r) - 2E + \frac{l(l+1)}{r^2} \ , \tag{68}$$

By relabeling $r \to t$ and $u(r) \to q(t)$, (67) can be viewed as harmonic oscillator with a time dependent spring constant

$$k(t, E) = -f(t, E) \tag{69}$$

and Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}k(t, E)q^2. \tag{70}$$

Thus any eigenfunction of (67) is an exact time-dependent solution of (70). For example, the ground state of the hydrogen atom with $l = 0$, $E = -1/2$ and

$$V(r) = -\frac{1}{r} \tag{71}$$

yields the exact solution

$$q(t) = t \exp(-t) \tag{72}$$

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

Denoting

$$Y(t) = \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}, \tag{73}$$

the time-dependent oscillator (70) now corresponds to

$$A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} \equiv T + V(t), \tag{74}$$

with

$$f(t) = (1 - \frac{2}{t}). \tag{75}$$

In this case, the second-order midpoint algorithm is

$$\begin{aligned} \mathcal{T}_2(h,t) &= \mathrm{e}^{\frac{1}{2}hT}\mathrm{e}^{hV(t+h/2)}\mathrm{e}^{\frac{1}{2}hT} \\ &= \begin{pmatrix} 1+\frac{1}{2}h^2 f(t+\frac{1}{2}h) & h+\frac{1}{4}h^3 f(t+\frac{1}{2}h) \\ hf(t+\frac{1}{2}h) & 1+\frac{1}{2}h^2 f(t+\frac{1}{2}h), \end{pmatrix} \end{aligned} \quad (76)$$

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

$$q_2(t) = t + \frac{1}{4}t^3 f(\frac{1}{2}t) = t - t^2 + \frac{1}{4}t^3. \quad (77)$$

Higher order multi-product expansions, using (76), then yield

$$\begin{aligned} q_4(t) &= t - t^2 + \frac{7t^3}{18} - \frac{t^4}{9} + \frac{t^5}{96} \\ q_6(t) &= t - t^2 + \frac{211t^3}{450} - \frac{31t^4}{225} + \frac{17t^5}{600} + \cdots \\ q_8(t) &= t - t^2 + \frac{32233t^3}{66150} - \frac{5101t^4}{33075} + \frac{3139t^5}{88200} + \cdots \\ q_{10}(t) &= t - t^2 + \frac{88159t^3}{1786050} - \frac{143177t^4}{893025} + \frac{91753t^5}{2381400} + \cdots \end{aligned} \quad (78)$$

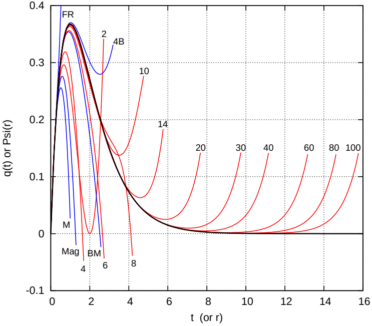

Figure: The uniform convergence of the multi-product expansion in solving for the hydrogen ground state wave function. (Black line: exact ground state wave function, The numbers indicates the order of the MPE. Blue lines: various fourth-order algorithms.

Remarks:
While wel-known higher order splitting method, as FR (Forest-Ruth 1990, 3 force-evaluations), M (McLachlan 1995, 4 force-evaluations), BM (Blanes-Moan 2002, 6 force-evaluations), Mag4 (Magnus integrator, see below, ≈ 2.5 force-evaluations) leaks with the accuracy, MPE series up to the 100th order, matches against the exact solution and 4B [Chin 2006] (a *forward* symplectic algorithm with only ≈ 2 evaluations).

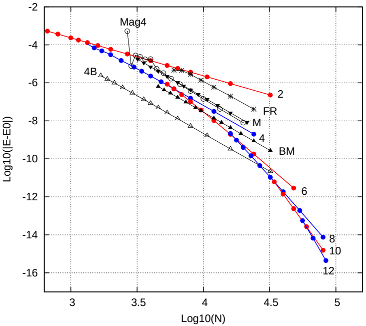

Figure: A precision-effort comparison of various fourth-order algorithms with that of MPE for computing the ground state of a spiked harmonic oscillator. N is the number of force-evaluations.

Conclusions

We present an alternative method: MPE of operators together with Suzuki's rule of incorporating the time-ordered exponential. We have compared the MPE method with that of the Magnus expansion and found that in cases where the Magnus expansion has a finite radius of convergence, the MPE converges uniformly.

Moreover, MPE requires far less operators at higher orders than either the Magnus series or conventional exponential-splitting. In the future we will focus on applying MPE method for solving nonlinear differential equations.