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Multi-product operator splitting as a general method of solving autonomous and nonautonomous equations

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Prior to the recent development of symplectic integrators, the time-stepping operator $e^{h(A+B)}$ was routinely decomposed into a sum of products of e^{hA} and e^{hB} in the study of hyperbolic partial differential equations. In the context of solving Hamiltonian dynamics, we show that such a decomposition gives rise to both *even*- and *odd*-order Runge–Kutta and Nyström integrators. By the use of Suzuki's forward-time derivative operator to enforce the time-ordered exponential, we show that the same decomposition can be used to solve nonautonomous equations. In particular, odd-order algorithms are derived on the basis of a highly nontrivial *time-asymmetric* kernel. Such an operator approach provides a general and unified basis for understanding structure nonpreserving algorithms and is especially useful in deriving very high-order algorithms via *analytical* extrapolations. In this work algorithms up to 100th order are tested by integrating the ground-state wave function of the hydrogen atom. For such a singular Coulomb problem, the multi-product expansion shows uniform convergence and is free of poles usually associated with structure-preserving methods. Other examples are also discussed.

Keywords: general exponential splitting; nonautonomous equations; Runge–Kutta–Nyström integrators; operator extrapolation methods.

1. Introduction

In the course of devising numerical algorithms for solving the prototype linear hyperbolic equation

$$\partial_t u = Au_x + Bu_y, \quad u(0) = u_0, \tag{1.1}$$

where A and B are noncommuting matrices, Strang (1968) proposed two second-order algorithms corresponding to approximating

$$\mathcal{T}(h) = e^{h(A+B)} \tag{1.2}$$

either as

$$S(h) = \frac{1}{2}(e^{hA}\, e^{hB} + e^{hB}\, e^{hA}) \tag{1.3}$$

or as

$$S_{AB}(h) = \mathrm{e}^{(h/2)B}\,\mathrm{e}^{hA}\,\mathrm{e}^{(h/2)B}. \tag{1.4}$$

Following up on Strang's work, Burstein & Mirin (1970) suggested that Strang's approximations can be generalized to higher orders in the form of a multi-product expansion (MPE),

$$\mathrm{e}^{h(A+B)} = \sum_k c_k \prod_i \mathrm{e}^{a_{ki}hA}\mathrm{e}^{b_{ki}hB}, \tag{1.5}$$

and gave two third-order approximations

$$D(h) = \frac{4}{3}\left(\frac{S_{AB}(h)+S_{BA}(h)}{2}\right) - \frac{1}{3}S(h), \tag{1.6}$$

where S_{BA} is just S_{AB} with A and B interchanged, and

$$B_{AB}(h) = \frac{9}{8}\mathrm{e}^{(h/3)A}\,\mathrm{e}^{(2h/3)B}\,\mathrm{e}^{(2h/3)A}\,\mathrm{e}^{(h/3)B} - \frac{1}{8}\mathrm{e}^{hA}\,\mathrm{e}^{hB}. \tag{1.7}$$

They credited J. Dunn for finding the decomposition $D(h)$ and noted that the weights c_k are no longer positive beyond second order. Thus, the stability of the entire algorithm can no longer be inferred from the stability of each component product.

Since (1.3), (1.4), (1.6) and (1.7) are approximations for the exponential of two general operators, they can be applied to problems unrelated to solving hyperbolic partial differential equations. For example, the evolution of any dynamical variable $u(\mathbf{q},\mathbf{p})$ (including $\mathbf{q}$ and $\mathbf{p}$ themselves) is given by the Poisson bracket

$$\partial_t u(\mathbf{q},\mathbf{p}) = \left(\frac{\partial u}{\partial \mathbf{q}}\cdot\frac{\partial H}{\partial \mathbf{p}} - \frac{\partial u}{\partial \mathbf{p}}\cdot\frac{\partial H}{\partial \mathbf{q}}\right) = (A+B)u(\mathbf{q},\mathbf{p}). \tag{1.8}$$

For a separable Hamiltonian

$$H(\mathbf{p},\mathbf{q}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}), \tag{1.9}$$

A and B are Lie operators or vector fields

$$A = \mathbf{v}\cdot\frac{\partial}{\partial \mathbf{q}}, \quad B = \mathbf{a}(\mathbf{q})\cdot\frac{\partial}{\partial \mathbf{v}}, \tag{1.10}$$

where we have abbreviated $\mathbf{v} = \mathbf{p}/m$ and $\mathbf{a}(\mathbf{q}) = -\nabla V(\mathbf{q})/m$. The exponential operators e^{hA} and e^{hB} are then just shift operators, with $S(h)$ giving the second-order Runge–Kutta integrator

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{1}{2}h^2\mathbf{a}(\mathbf{q}_0) \equiv \mathbf{q}_1, \tag{1.11}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{2}[\mathbf{a}(\mathbf{q}_0) + \mathbf{a}(\mathbf{q}_0 + h\mathbf{v}_0)], \tag{1.12}$$

and $S_{AB}(h)$ giving the symplectic Verlet or leap-frog algorithm

$$\mathbf{q} = \mathbf{q}_1, \tag{1.13}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{2}[\mathbf{a}(\mathbf{q}_0) + \mathbf{a}(\mathbf{q})]. \tag{1.14}$$

More interestingly, Dunn's decomposition $D(h)$ gives

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{6}\left[\mathbf{a}(\mathbf{q}_0) + 2\mathbf{a}\left(\mathbf{q}_0 + \frac{h}{2}\mathbf{v}_0\right)\right], \tag{1.15}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{6}\left[\mathbf{a}(\mathbf{q}_0) + 4\mathbf{a}\left(\mathbf{q}_0 + \frac{h}{2}\mathbf{v}_0\right) + 2\mathbf{a}(\mathbf{q}_1) - \mathbf{a}\left(\mathbf{q}_1 - \frac{1}{2}h^2\mathbf{a}(\mathbf{q}_0)\right)\right]. \tag{1.16}$$

Since

$$2\mathbf{a}(\mathbf{q}_1) - \mathbf{a}\left(\mathbf{q}_1 - \frac{1}{2}h^2\mathbf{a}(\mathbf{q}_0)\right) = \mathbf{a}\left(\mathbf{q}_1 + \frac{1}{2}h^2\mathbf{a}(\mathbf{q}_0)\right) + \mathrm{O}(h^4), \tag{1.17}$$

it remains correct to third order to write

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{6}\left[\mathbf{a}(\mathbf{q}_0) + 4\mathbf{a}\left(\mathbf{q}_0 + \frac{h}{2}\mathbf{v}_0\right) + \mathbf{a}\left(\mathbf{q}_0 + h\mathbf{v}_0 + h^2\mathbf{a}(\mathbf{q}_0)\right)\right]. \tag{1.18}$$

One recognizes that (1.15) and (1.18) are *precisely* Kutta's third-order algorithm (Hildebrand, 1956) for solving a second-order differential equation. Burstein and Mirin's approximation $B_{AB}(h)$ directly gives, without any change,

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{4}[\mathbf{a}(\mathbf{q}_0) + \mathbf{a}(\mathbf{q}_{2/3})], \tag{1.19}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{4}[\mathbf{a}(\mathbf{q}_0) + 3\mathbf{a}(\mathbf{q}_{2/3})], \tag{1.20}$$

with

$$\mathbf{q}_{2/3} \equiv \mathbf{q}_0 + \frac{2}{3}h\mathbf{v}_0 + \frac{2}{9}h^2\mathbf{a}(\mathbf{q}_0), \tag{1.21}$$

which is Nyström's third-order algorithm requiring only two force evaluations (Nyström, 1925; Battin, 1999). Since Burstein and Mirin's approximation is not symmetric, $B_{BA}(h)$ produces a different algorithm, namely,

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{2}\mathbf{a}_{1/3}, \tag{1.22}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{4}\left[3\mathbf{a}_{1/3} + \frac{3}{2}\mathbf{a}\left(\mathbf{q}_0 + h\mathbf{v}_0 + \frac{4}{9}h^2\mathbf{a}_{1/3}\right) - \frac{1}{2}\mathbf{a}(\mathbf{q}_0 + h\mathbf{v}_0)\right], \tag{1.23}$$

where $\mathbf{a}_{1/3} = \mathbf{a}(\mathbf{q}_0 + h\mathbf{v}_0/3)$. Again, since

$$\frac{3}{2}\mathbf{a}\left(\mathbf{q}_0 + h\mathbf{v}_0 + \frac{4}{9}h^2\mathbf{a}_{1/3}\right) - \frac{1}{2}\mathbf{a}(\mathbf{q}_0 + h\mathbf{v}_0) = \mathbf{a}\left(\mathbf{q}_0 + h\mathbf{v}_0 + \frac{2}{3}h^2\mathbf{a}_{1/3}\right) + \mathrm{O}(h^4), \tag{1.24}$$

(1.23) can be rewritten as

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{4}\left[3\mathbf{a}_{1/3} + \mathbf{a}\left(\mathbf{q}_0 + h\mathbf{v}_0 + \frac{2}{3}h^2\mathbf{a}_{1/3}\right)\right]. \tag{1.25}$$

Equations (1.22) and (1.25) are a new third-order algorithm with two force evaluations but without evaluating the force at the starting position. More recently, Chin (2010) has shown that Nyström's fourth-order algorithm (Battin, 1999) with three force evaluations and Albrecht's sixth-order algorithm (Albrecht, 1955) with five force evaluations can all be derived from operator expansions of the form (1.5).

Just as symplectic integrators (Neri, 1987; Forest & Ruth, 1990) can be derived from a *single-product* splitting

$$\mathrm{e}^{h(A+B)} = \prod_i \mathrm{e}^{a_i hA}\,\mathrm{e}^{b_i hB}, \tag{1.26}$$

these examples clearly show that the *multi-product* splitting (1.5) is the fundamental basis for deriving nonsymplectic Nyström-type algorithms. (These are not fully Runge–Kutta algorithms because the operator B in (1.10) would not be a simple shift operator if $\mathbf{a}(\mathbf{q})$ becomes dependent on $\mathbf{v}$. On the other hand, Nyström-type algorithms are all that are necessary for the study of most Hamiltonian systems.) As illustrated above, one goal of this work is to show that all traditional results on Nyström integrators can be much more simply derived and understood on the basis of multi-product splitting. In fact, we have the following theorem.

THEOREM 1. Every decomposition of $\mathrm{e}^{h(A+B)}$ in the form of

$$\sum_k c_k \prod_i \mathrm{e}^{a_{ki} hA}\,\mathrm{e}^{b_{ki} hB} = \mathrm{e}^{h(A+B)} + \mathrm{O}(h^{n+1}), \tag{1.27}$$

where A and B are noncommuting operators, with real coefficients $\{c_k, a_{ki}, b_{ki}\}$ and finite indices k and i, produces an nth-order Nyström integrator.

Note that the order n of the integrator is defined with respect to the error in approximating the operator $(A+B)$, and therefore the error in the time-stepping operator is one order higher. The resulting integrator, however, may not be optimal. As illustrated above, at low orders, some force evaluations can be combined without affecting the order of the integrator. However, such a force consolidation is increasingly unlikely at higher orders. This theorem produces both the traditional Nyström integrators, where the force is always evaluated initially, and non-FASL (First as Last) integrators, where the force is never evaluated initially, as in (1.22) and (1.25).

The advantage of a single-product splitting is that the resulting algorithms are structure preserving (Hairer et al., 2002), such as being symplectic, unitary or remaining within the group manifold. However, single-product splittings beyond second order require an exponentially growing number of operators with unavoidable negative coefficients (Sheng, 1989; Suzuki, 1991) and cannot be applied to time-irreversible or semigroup problems. Even for time-reversible systems, where negative time steps are not a problem, the exponential growth on the number of force evaluations renders high-order symplectic integrators difficult to derive and expensive to use. For example, it has been found empirically that symplectic algorithms of orders 4, 6, 8 and 10 required a minimum of 3, 7, 15 and 31 force evaluations, respectively (Chin, 2010). Here we show that *analytically* extrapolated algorithms of *odd* orders 3, 5, 7 and 9 only require 2, 4, 7 and 11 force evaluations and algorithms of *even* orders 4, 6, 8 and 10 only require 3, 5, 10 and 15 force evaluations. Thus, at 10th order, an extrapolated MPE integrator only requires half the computational effort of a symplectic integrator. Or, for 28 force evaluations, one can use a 14th-order MPE integrator instead. This is a great advantage in many practical calculations where long-term accuracy and structure preserving is not an issue. The advantage is greater still beyond 10th order, where no symplectic integrators and very few Runge–Kutta–Nyström algorithms are known. Here we demonstrate the working of MPE algorithms up to 100th order.

By the use of the Suzuki (1993) method of implementing the time-ordered exponential, Chin and Chen (2002) this work shows that the MPE (1.27) can be easily adopted to solve the nonautonomous equation

$$\partial_t Y(t) = A(t)Y(t), \quad Y(0) = Y_0. \tag{1.28}$$

In even-order cases, this method reproduces the classical result of Gragg (1965) in just a few lines. In odd-order cases, this method demonstrates a highly nontrivial extrapolation of a *time-asymmetric* kernel that has never been observed before. Finally, we show that the MPE (1.27) converges uniformly, in contrast to structure-preserving methods such as the Magnus expansion, which generally has a finite radius of convergence. The convergence of (1.27) is verified in various analytical and numerical examples up to 100th order.

The paper is outlined as follows. In Section 2 we derive key results of MPEs, including the extrapolation of odd-order algorithms. In Section 3 we show how Suzuki's method can be used to transform any splitting scheme for solving nonautonomous equations. In Section 4 we present an error and convergence analysis of the multi-product splitting based on extrapolation. Numerical examples and a comparison with the Magnus expansion are given in Section 5. In Section 6 we briefly summarize our results.

2. Multi-product decomposition

The multi-product decomposition (1.5) is obviously more complicated than the single-product splitting (1.26). Fortunately, 19 years after Burstein & Mirin (1970), Sheng (1989) proved their observation that, beyond second order, a_{ki}, b_{ki} and c_k cannot all be positive. This negative result, surprisingly, can be used to completely determine a_{ki}, b_{ki} and c_k to all orders. This is because, for general applications, including solving time-irreversible problems, one must have a_{ki} and b_{ki} positive. Therefore, every single product in (1.5) can be at most second order (Sheng, 1989; Suzuki, 1991). But such a product is easy to construct because every left–right symmetric single product *is* second order. Let $\mathcal{T}_S(h)$ be such a product with $\sum_i a_{ki} = 1$ and $\sum_i b_{ki} = 1$. Then $\mathcal{T}_S(h)$ is time symmetric by construction, that is,

$$\mathcal{T}_S(-h)\mathcal{T}_S(h) = 1, \tag{2.1}$$

which implies that it has only odd powers of h, that is,

$$\mathcal{T}_S(h) = \exp(h(A + B) + h^3 E_3 + h^5 E_5 + \cdots), \tag{2.2}$$

and is therefore correct to second order. (The error terms E_i are nested commutators of A and B depending on the specific form of $\mathcal{T}_S$.) This immediately suggests that the kth power of $\mathcal{T}_S$ at step size h/k must have the form

$$\mathcal{T}_S^k(h/k) = \exp(h(A + B) + k^{-2}h^3 E_3 + k^{-4}h^5 E_5 + \cdots) \tag{2.3}$$

and can serve as a basis for the MPE (1.5). The simplest such symmetric product is

$$\mathcal{T}_2(h) = S_{AB}(h) \quad \text{or} \quad \mathcal{T}_2(h) = S_{BA}(h). \tag{2.4}$$

If one naively assumes that

$$\mathcal{T}_2(h) = \mathrm{e}^{h(A+B)} + Ch^3 + Dh^4 + \cdots, \tag{2.5}$$

then a Richardson extrapolation would only give

$$\frac{1}{k^2-1}[k^2\mathcal{T}_2^k(h/k)-\mathcal{T}_2(h)]=\mathrm{e}^{h(A+B)}+\mathrm{O}(h^4), \tag{2.6}$$

a third-order (Schatzman, 1994) algorithm. However, because the error structure of $\mathcal{T}_2(h/k)$ is actually given by (2.3), one has

$$\mathcal{T}_2^k(h/k)=\mathrm{e}^{h(A+B)}+k^{-2}h^3E_3+\frac{1}{2}k^{-2}h^4[(A+B)E_3+E_3(A+B)]+\mathrm{O}(h^5), \tag{2.7}$$

and *both* the third- and fourth-order errors can be eliminated simultaneously, yielding a fourth-order algorithm. Similarly, the leading $(2n+1)$th- and $(2n+2)$th-order errors are multiplied by k^{-2n} and can be eliminated at the same time. Thus, for a given set of n whole numbers $\{k_i\}$, one can have a $2n$th-order approximation

$$\mathrm{e}^{h(A+B)}=\sum_{i=1}^{n}c_i\mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right)+\mathrm{O}(h^{2n+1}), \tag{2.8}$$

provided that c_i satisfy the following simple Vandermonde equation:

$$\begin{pmatrix} 1 & 1 & 1 & \dots & 1 \\ k_1^{-2} & k_2^{-2} & k_3^{-2} & \dots & k_n^{-2} \\ k_1^{-4} & k_2^{-4} & k_3^{-4} & \dots & k_n^{-4} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ k_1^{-2(n-1)} & k_2^{-2(n-1)} & k_3^{-2(n-1)} & \dots & k_n^{-2(n-1)} \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{pmatrix}=\begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \tag{2.9}$$

Surprisingly, this equation has the following closed form solutions (Chin, 2010) for all n:

$$c_i=\prod_{j=1(\neq i)}^{n}\frac{k_i^2}{k_i^2-k_j^2}. \tag{2.10}$$

The natural sequence $\{k_i\}=\{1,2,3,\dots,n\}$ produces a $2n$th-order algorithm with the minimum $n(n+1)/2$ evaluations for $\mathcal{T}_2(h)$. For orders four to ten, one has explicitly

$$\mathcal{T}_4(h)=-\frac{1}{3}\mathcal{T}_2(h)+\frac{4}{3}\mathcal{T}_2^2\left(\frac{h}{2}\right), \tag{2.11}$$

$$\mathcal{T}_6(h)=\frac{1}{24}\mathcal{T}_2(h)-\frac{16}{15}\mathcal{T}_2^2\left(\frac{h}{2}\right)+\frac{81}{40}\mathcal{T}_2^3\left(\frac{h}{3}\right), \tag{2.12}$$

$$\mathcal{T}_8(h)=-\frac{1}{360}\mathcal{T}_2(h)+\frac{16}{45}\mathcal{T}_2^2\left(\frac{h}{2}\right)-\frac{729}{280}\mathcal{T}_2^3\left(\frac{h}{3}\right)+\frac{1024}{315}\mathcal{T}_2^4\left(\frac{h}{4}\right), \tag{2.13}$$

$$\mathcal{T}_{10}(h)=\frac{1}{8640}\mathcal{T}_2(h)-\frac{64}{945}\mathcal{T}_2^2\left(\frac{h}{2}\right)+\frac{6561}{4480}\mathcal{T}_2^3\left(\frac{h}{3}\right)-\frac{16384}{2835}\mathcal{T}_2^4\left(\frac{h}{4}\right)+\frac{390625}{72576}\mathcal{T}_2^5\left(\frac{h}{5}\right). \tag{2.14}$$

As shown in Chin (2010), $\mathcal{T}_4(h)$ reproduces Nyström's fourth-order algorithm with three force evaluations and $\mathcal{T}_6(h)$ yields a new sixth-order Nyström-type algorithm with five force evaluations.

REMARK 2.1 It is easy to show that the Verlet algorithm (1.13) and (1.14) corresponding to $S_{AB}(h)$ produces the same trajectory as Stömer's second-order scheme

$$\mathbf{q}_1 - 2\mathbf{q}_0 + \mathbf{q}_{-1} = h^2\mathbf{a}(\mathbf{q}_0). \tag{2.15}$$

However, it is extremely difficult to deduce from (2.15) that the underlying error structure is basically (2.2) and allows for an h^2-extrapolation. This is the great achievement of Gragg (1965). Nevertheless, the power of the present operator approach is that we can reproduce his results in a few lines. The error structure here, (2.2), is a simple consequence of the symmetric character of the product and allows us to bypass Gragg's lengthy proof on the asymptotic errors of (2.15). Moreover, this h^2-extrapolation can be applied to any $\mathcal{T}_S(h)$, not necessarily restricted to (2.15). For example, the use of $S_{BA}(h)$ produces an entirely different sequence of extrapolations (Chin, 2010), distinct from that based on (2.15).

REMARK 2.2 In the original work of Gragg, the use of (2.15) as the basis for his extrapolation is a matter of default, as (2.15) is a well-known second-order solution. Here, in extrapolating operators, the use of $S_{AB}(h)$ or $S_{BA}(h)$ is for the specific purpose that they can be applied to time-irreversible problems. While all positive time steps algorithms can be made fourth order (Suzuki, 1996; Chin, 1997) by including the operator $[B, [A, B]]$, MPE is currently the only way of producing sixth- and higher-order algorithms in solving the imaginary time Schrödinger equation (Chin *et al.*, 2009) and in doing path integral Monte Carlo simulations (Zillich *et al.*, 2010). The fact that MPE is no longer norm preserving nor even strictly positive does not affect higher-order convergence in these applications. These nonstructure preserving elements are within the error noise of the algorithm. MPE is less useful in solving real-time Schrödinger equation, where unitarity is of critical importance.

REMARK 2.3 The explicit coefficients c_i coincide with the diagonal elements of the Richardson–Aitken–Neville extrapolation (Hairer *et al.*, 1993) table. This is not surprising since they are coefficients of extrapolation. As shown in Chin (2010), $c_i = L_i(0)$, where $L_i(x)$ are the Lagrange interpolating polynomials with the interpolation points $x_i = k_i^{-2}$. What is novel here is that the c_i are known analytically and a simple routine calling them repeatedly to execute $\mathcal{T}_2(h)$ will generate an arbitrary even-order algorithm without any table construction. The resulting algorithm is extremely portable and compact and can serve as a benchmark by which all integrators of the same order can be compared. In Chin (2010) the only algorithm that outperformed MPE was the 12th-order integrator of Dormand *et al.* (1987), as given in Brankin *et al.* (1989).

Having the explicit solutions c_i now suggests new ways of solving old problems. Suppose one wishes to integrate the system to time t. One may begin by using a second-order algorithm and iterate it m times at the time step $h = t/m$, that is,

$$\mathcal{T}_{2,m}(h) = \mathcal{T}_2^m(t/m). \tag{2.16}$$

Every position on the trajectory will then be correct to second order in h. However, if one were only interested in the final position at time t, then one can correct this *final position* to fourth order by simply computing *one* more $\mathcal{T}_2(t)$ and modify (2.16) via

$$\mathcal{T}_{4,m}(h) = \frac{m^2}{m^2 - 1^2}\mathcal{T}_2^m(t/m) - \frac{1^2}{m^2 - 1^2}\mathcal{T}_2(t) \tag{2.17}$$

or correct it to sixth order via

$$\mathcal{T}_{6,m}(h) = \frac{m^4\mathcal{T}_2^m(t/m)}{(m^2-1^2)(m^2-2^2)} + \frac{2^4\mathcal{T}_2^2(t/2)}{(2^2-1^2)(2^2-m^2)} + \frac{1^4\mathcal{T}_2(t)}{(1^2-2^2)(1^2-m^2)}, \tag{2.18}$$

and so on, to any even order. The expansion coefficients are given by $\{k_i\}$ and are equal to $\{m, 1\}$, $\{m, 2, 1\}$, $\{m, 3, 2, 1\}$, etc. This is similar to the idea of process algorithms (Blanes *et al.*, 1999b), but is far simpler. The process for correcting (2.16) beyond fourth order can be quite complex if the entire algorithm were to remain symplectic. Here, for Nyström integrators, the extrapolation coefficient is known to all even orders. Alternatively, one can view the above as correcting every mth step of the basic algorithm $\mathcal{T}_2(t/m)$ over a short time interval of t. Thus, knowing c_i allows great flexibility in designing algorithms that run the gamut from being correct to arbitrary high order at every time step, every other time step, every third time step, etc. to only at the final time step. With MPE, one can easily produce versatile adaptive algorithms by varying both the time step size h and the order of the algorithm.

REMARK 2.4 Since MPE is an extrapolation, it is expected to be more prone to round-off errors. Thus, if n is too large in (2.17), then the second term may be too small and the correction is lost to round-off errors. However, as seen in (1.17) and (1.24), the required subtractions are sometimes well defined and the round-off errors are within the error noise of the algorithm. As will be shown in Section 5, the round-off errors are sometimes less severe than expected.

REMARK 2.5 The idea of extrapolating symplectic algorithms has been previously considered by Blanes *et al.* (1999a) and Chan & Murus (2000). They studied the case of extrapolating a $2n$th-order symplectic integrator. They did not obtain analytical forms for their expansion coefficients, but noted that extrapolating a $2n$th-order symplectic integrator will preserve the symplectic character of the algorithm to order $4n+1$. While this is more general, such an extrapolation cannot be applied to time-irreversible systems for $n > 1$.

Finally, we note that

$$e^{h(A+B)} = \lim_{n\to\infty} \sum_{i=1}^{n} c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right). \tag{2.19}$$

In principle, for any countable sets of $\{k_i\}$, we have achieved an exact decomposition, with known coefficients. This is in contrast to the structure preserving but impractical Zassenhaus formula.

The above derivation of even-order algorithms is at most an elaboration on Gragg's seminal work. Below, we will derive arbitrary *odd-order* Nyström algorithms that have not been observed in any classical study. Since

$$\mathcal{T}_1(h) = e^{hA}\, e^{hB} = \exp[h(A+B) + h^2F_2 + h^3F_3 + h^4F_4 + \cdots] \tag{2.20}$$

contain errors of all orders (the $\{F_i\}$ are nested commutators of the usual Baker–Campbell–Hausdorff formula), extrapolations based on $\mathcal{T}_1^k(h/k)$ will not yield an h^2-order scheme. However, there is an h^2-order basis hidden in Burstein and Mirin's original decomposition (1.7). For $n = 1, 2, 3, \ldots$ the basis

$$\mathcal{U}_n(h) = e^{\frac{h}{2n-1}A}\left(e^{\frac{2h}{2n-1}B}\, e^{\frac{2h}{2n-1}A}\right)^{n-1} e^{\frac{h}{2n-1}B} \tag{2.21}$$

has the remarkable property that it *effectively* behaves as if

$$\mathcal{U}_n(h) = \exp[h(A+B) + x^{-2}(h^2F_2 + h^3F_3) + x^{-4}(h^4F_4 + h^5F_5) + \cdots], \tag{2.22}$$

where $x = (2n-1)$. (By 'effectively', we mean that $\mathcal{U}_n(h)$ actually has the form

$$\mathcal{U}_n(h) = \exp[h(A+B) + x^{-2}(h^2F_2 + h^3F_3) + (x^{-2} - x^{-4})h^4F_4' + x^{-4}(h^4F_4 + h^5F_5) + \cdots], \tag{2.23}$$

where F_4' are additional commutators not present in (2.20). However, this is essentially (2.22) with altered F_i but without changing the crucial power pattern of x^{-2k}.) In this case (2.22) (as well as (2.23)) can be extrapolated similarly as in the even-order case, namely,

$$\mathrm{e}^{h(A+B)} = \sum_{i=1}^{n} \tilde{c}_i \mathcal{U}_i(h) + \mathrm{O}(h^{2n}), \tag{2.24}$$

where $\tilde{c}_i$ satisfies the same Vandermonde equation (2.9), with the same solution (2.10), but with $\{k_i\}$ consisting of only *odd* whole numbers. The first few odd-order decompositions corresponding to $\{k_i\}$ being $\{1, 3\}$, $\{1, 3, 5\}$, $\{1, 3, 5, 7\}$ and $\{1, 3, 5, 7, 9\}$ are

$$\mathcal{T}_3(h) = -\frac{1}{8}\mathcal{U}_1(h) + \frac{9}{8}\mathcal{U}_2(h), \tag{2.25}$$

$$\mathcal{T}_5(h) = \frac{1}{192}\mathcal{U}_1(h) - \frac{81}{128}\mathcal{U}_2(h) + \frac{625}{384}\mathcal{U}_3(h), \tag{2.26}$$

$$\mathcal{T}_7(h) = -\frac{1}{9216}\mathcal{U}_1(h) + \frac{729}{5120}\mathcal{U}_2(h) - \frac{15625}{9216}\mathcal{U}_3(h) + \frac{117649}{46080}\mathcal{U}_4(h), \tag{2.27}$$

$$\mathcal{T}_9(h) = \frac{1}{737280}\mathcal{U}_1(h) - \frac{729}{40960}\mathcal{U}_2(h) + \frac{390625}{516096}\mathcal{U}_3(h) - \frac{5764801}{1474560}\mathcal{U}_4(h) + \frac{4782969}{1146880}\mathcal{U}_5(h). \tag{2.28}$$

The splitting $\mathcal{T}_3(h)$ explains the original form of Burstein and Mirin's decomposition and Nyström's third-order algorithm. The splitting $\mathcal{T}_5(h)$ again produces, without any adjustment, Nyström's fifth-order integrators (Battin, 1999) with four force evaluations as follows:

$$\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{192}[23\mathbf{a}_0 + 75\mathbf{a}_{2/5} - 27\mathbf{a}_{2/3} + 25\mathbf{a}_{4/5}], \tag{2.29}$$

$$\mathbf{v} = \mathbf{v}_0 + \frac{h}{192}[23\mathbf{a}_0 + 125\mathbf{a}_{2/5} - 81\mathbf{a}_{2/3} + 125\mathbf{a}_{4/5}], \tag{2.30}$$

where we have defined $\mathbf{a}_{i/k} = \mathbf{a}(\mathbf{q}_{i/k})$ with

$$\mathbf{q}_{2/5} = \mathbf{q}_0 + \frac{2}{5}h\mathbf{v}_0 + \frac{2}{25}h^2\mathbf{a}_0,$$
$$\mathbf{q}_{4/5} = \mathbf{q}_0 + \frac{4}{5}h\mathbf{v}_0 + \frac{4}{25}h^2(\mathbf{a}_0 + \mathbf{a}_{2/5}), \tag{2.31}$$

and where $\mathbf{q}_{2/3}$ has been given earlier in (1.21). (An interchange of A and B in $\mathcal{T}_5(h)$ will also yield a fifth-order algorithm, but since the final force evaluations can only be combined as in (1.24) to order

$O(h^4)$, such a force consolidation cannot be used for a fifth-order algorithm. The algorithm will then require six force evaluations, which is undesirable. We shall therefore ignore this alternative case from now on.) With three more force evaluations at

$$\begin{aligned}
\mathbf{q}_{2/7} &= \mathbf{q}_0 + \frac{2}{7}h\mathbf{v}_0 + \frac{2}{49}h^2\mathbf{a}_0,\\
\mathbf{q}_{4/7} &= \mathbf{q}_0 + \frac{4}{7}h\mathbf{v}_0 + \frac{4}{49}h^2(\mathbf{a}_0 + \mathbf{a}_{2/7}),\\
\mathbf{q}_{6/7} &= \mathbf{q}_0 + \frac{6}{7}h\mathbf{v}_0 + \frac{2}{49}h^2(3\mathbf{a}_0 + 4\mathbf{a}_{2/7} + 2\mathbf{a}_{4/7}),
\end{aligned} \tag{2.32}$$

$\mathcal{T}_7(h)$ produces the following seventh-order algorithm with seven force evaluations, which has never been derived before:

$$\begin{aligned}
\mathbf{q} = \mathbf{q}_0 + h\mathbf{v}_0 + \frac{h^2}{23040}[1682\mathbf{a}_0 + 729\mathbf{a}_{2/3} - 3125(3\mathbf{a}_{2/5} + \mathbf{a}_{4/5})\\
+ 2401(5\mathbf{a}_{2/7} + 3\mathbf{a}_{4/7} + \mathbf{a}_{6/7})],
\end{aligned} \tag{2.33}$$

$$\begin{aligned}
\mathbf{v} = \mathbf{v}_0 + \frac{h}{23040}[1682\mathbf{a}_0 + 2167\mathbf{a}_{2/3} - 15625(\mathbf{a}_{2/5} + \mathbf{a}_{4/5})\\
+ 16807(\mathbf{a}_{2/7} + \mathbf{a}_{4/7} + \mathbf{a}_{6/7})].
\end{aligned} \tag{2.34}$$

These analytical derivations are, of course, unnecessary in practical applications. As in the even-order case, both the coefficients c_k and the algorithm corresponding to $\mathcal{U}_n(h)$ can be called repeatedly to generate any odd-order integrators.

Since each $\mathcal{U}_n(h)$ requires n force evaluations, but have the initial force in common, each $(2n-1)$th-order algorithm requires $\frac{1}{2}n(n-1)+1$ force evaluations. Thus, for odd orders 3, 5, 7 and 9, the number of force evaluations required is 2, 4, 7 and 11. As alluded to earlier, for even order 4, 6, 8 and 10, the number of force evaluations required are 3, 5, 10 and 15. These sequences of extrapolated algorithms therefore provide a natural explanation for the order barrier in Nyström algorithms. For order $p < 7$, the number of force evaluations can be $p-1$, but, for $p > 7$, the number of force evaluations must be greater than p.

REMARK 2.6 In general, we have the following order notation for the even and odd algorithms.

- The order of the even algorithm is $2n$, and its decomposition error is $2n+1$.
- The order of the odd algorithm is $2n-1$, and its decomposition error is $2n$.

3. Solving nonautonomous equations

The solution to the nonautonomous equation (1.28) can be formally written as

$$Y(t+h) = \mathcal{T}\left(\exp\int_t^{t+h} A(s)\mathrm{d}s\right)Y(t), \tag{3.1}$$

where, instead of the conventional expansion

$$\mathcal{T}\left(\exp\int_t^{t+h} A(s)\mathrm{d}s\right) = 1 + \int_t^{t+h} A(s_1)\mathrm{d}s_1 + \int_t^{t+h}\mathrm{d}s_1\int_t^{s_1}\mathrm{d}s_2 A(s_1)A(s_2) + \cdots, \tag{3.2}$$

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

$$\mathcal{T}\left(\exp\int_t^{t+h} A(s)\mathrm{d}s\right) = \lim_{n\to\infty}\mathcal{T}\left(\mathrm{e}^{\frac{h}{n}\sum_{i=1}^{n} A\left(t+i\frac{h}{n}\right)}\right), \tag{3.3}$$

$$= \lim_{n\to\infty}\mathrm{e}^{\frac{h}{n}A(t+h)}\cdots\mathrm{e}^{\frac{h}{n}A\left(t+\frac{2h}{n}\right)}\mathrm{e}^{\frac{h}{n}A\left(t+\frac{h}{n}\right)}. \tag{3.4}$$

The time ordering is trivially accomplished in going from (3.3) to (3.4). To enforce the latter equation Suzuki (1993) introduced the *forward time derivative* operator, also called the super-operator, as follows:

$$D = \frac{\overleftarrow{\partial}}{\partial t} \tag{3.5}$$

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

$$F(t)\,\mathrm{e}^{hD}G(t) = F(t+h)G(t). \tag{3.6}$$

If $F(t) = 1$, then we have

$$1\,\mathrm{e}^{hD}G(t) = \mathrm{e}^{hD}G(t) = G(t). \tag{3.7}$$

Trotter's formula then gives

$$\begin{aligned}\exp[h(A(t)+D)] &= \lim_{n\to\infty}\left(\mathrm{e}^{\frac{h}{n}A(t)}\mathrm{e}^{\frac{h}{n}D}\right)^n\\ &= \lim_{n\to\infty}\mathrm{e}^{\frac{h}{n}A(t+h)},\ldots,\mathrm{e}^{\frac{h}{n}A\left(t+\frac{2h}{n}\right)}\mathrm{e}^{\frac{h}{n}A\left(t+\frac{h}{n}\right)},\end{aligned} \tag{3.8}$$

where property (3.7) has been applied repeatedly and accumulatively. Comparing (3.4) with (3.8) yields Suzuki's decomposition of the time-ordered exponential (Suzuki, 1993)

$$\mathcal{T}\left(\exp\int_t^{t+h} A(s)\mathrm{d}s\right) = \exp[h(A(t)+D)]. \tag{3.9}$$

Thus, time ordering can be achieved by splitting an additional operator D. This is extremely useful and transforms any existing splitting algorithms into integrators of nonautonomous equations. For example, one has the following symmetric splitting:

$$\mathcal{T}_2(h) = \mathrm{e}^{\frac{1}{2}hD}\,\mathrm{e}^{hA(t)}\,\mathrm{e}^{\frac{1}{2}hD} = \mathrm{e}^{hA(t+\frac{1}{2}h)}, \tag{3.10}$$

which is the second-order mid-point approximation. Every occurrence of the operator $\mathrm{e}^{d_i hD}$, from right to left, updates the current time t to $t + d_i h$. If t is the time at the start of the algorithm, then, after the first occurrence of $\mathrm{e}^{\frac{1}{2}hD}$, the time is $t+\frac{1}{2}h$. After the second $\mathrm{e}^{\frac{1}{2}hD}$, the time is $t+h$. Thus, the leftmost $\mathrm{e}^{\frac{1}{2}hD}$ is not without effect. It correctly updates the time for the next iteration. Thus, the iterations of $\mathcal{T}_2(h)$ implicitly imply that

$$\begin{aligned}\mathcal{T}_2^2(h/2) &= \mathrm{e}^{\frac{1}{2}hA\left(t+\frac{3}{4}h\right)}\mathrm{e}^{\frac{1}{2}hA\left(t+\frac{1}{4}h\right)},\\ \mathcal{T}_2^3(h/3) &= \mathrm{e}^{\frac{1}{3}hA\left(t+\frac{5}{6}h\right)}\mathrm{e}^{\frac{1}{3}hA\left(t+\frac{1}{2}h\right)}\mathrm{e}^{\frac{1}{3}hA\left(t+\frac{1}{6}h\right)},\\ &\ \ \vdots\end{aligned} \tag{3.11}$$

For the odd-order basis, we have

$$\begin{aligned}
\mathcal{U}_1(h) &= \mathrm{e}^{hD}\mathrm{e}^{hA(t)} = \mathrm{e}^{hA(t)},\\
\mathcal{U}_2(h) &= \mathrm{e}^{\frac{1}{3}hD}\,\mathrm{e}^{\frac{2}{3}hA(t)}\,\mathrm{e}^{\frac{2}{3}hD}\mathrm{e}^{\frac{1}{3}hA(t)} = \mathrm{e}^{\frac{2}{3}hA\left(t+\frac{2}{3}h\right)}\mathrm{e}^{\frac{1}{3}hA(t)},\\
\mathcal{U}_3(h) &= \mathrm{e}^{\frac{2}{5}hA\left(t+\frac{4}{5}h\right)}\mathrm{e}^{\frac{2}{5}hA\left(t+\frac{2}{5}h\right)}\mathrm{e}^{\frac{1}{5}hA(t)},\\
&\ \ \vdots
\end{aligned} \tag{3.12}$$

REMARK 3.1 The recent work by Wiebe *et al.* (2010) suggests that Suzuki's decomposition (3.9) only holds if $A(t)$ is sufficiently smooth. In cases where the derivatives of $A(t)$ cease to exist, high-order integrators based on (3.9) may be degraded to lower orders.

For $A(t) = T + V(t)$, since $[D, T] = 0$, the second-order algorithm can be obtained as follows:

$$\begin{aligned}
\mathcal{T}_2(h) &= \mathrm{e}^{\frac{1}{2}h(T+D)}\mathrm{e}^{hV(t)}\mathrm{e}^{\frac{1}{2}h(T+D)}\\
&= \mathrm{e}^{\frac{1}{2}hT}\,\mathrm{e}^{\frac{1}{2}hD}\,\mathrm{e}^{hV(t)}\mathrm{e}^{\frac{1}{2}hD}\,\mathrm{e}^{\frac{1}{2}hT}\\
&= \mathrm{e}^{\frac{1}{2}hT}\,\mathrm{e}^{hV(t+h/2)}\mathrm{e}^{\frac{1}{2}hT}.
\end{aligned} \tag{3.13}$$

For odd-order algorithms, we now have the following sequence of basis products:

$$\begin{aligned}
\mathcal{U}_1(h) &= \mathrm{e}^{hT}\mathrm{e}^{hV(t)},\\
\mathcal{U}_2(h) &= \mathrm{e}^{\frac{1}{3}hT}\,\mathrm{e}^{\frac{2}{3}hV\left(t+\frac{2}{3}h\right)}\mathrm{e}^{\frac{2}{3}hT}\,\mathrm{e}^{\frac{1}{3}hV(t)},\\
\mathcal{U}_3(h) &= \mathrm{e}^{\frac{1}{5}hT}\mathrm{e}^{\frac{2}{5}hV\left(t+\frac{4}{5}h\right)}\mathrm{e}^{\frac{2}{5}hT}\,\mathrm{e}^{\frac{2}{5}hV\left(t+\frac{2}{5}h\right)}\mathrm{e}^{\frac{2}{5}hT}\,\mathrm{e}^{\frac{1}{5}hV(t)},\\
&\ \ \vdots
\end{aligned} \tag{3.14}$$

While any power of $\mathcal{T}_2(h)$ is time symmetric, each $\mathcal{U}_n(h)$ is *time asymmetric*, that is,

$$\mathcal{U}_n(-h)\mathcal{U}_n(h) \neq 1. \tag{3.15}$$

4. Errors and convergence of the MPE

While extrapolation methods are well known in the study of differential equations, virtually no work has been done in the context of operators. Here we extend the method of extrapolation to the decomposition of two operators, which is the basis of the MPE method. Working at the operator level, rather than at the solution level, allows the extrapolation method to be widely applied to many time-dependent equations. In particular, we will use the constructive details in Chin (2010) to prove convergence results for the MPE. While this work is restricted to exponential splitting, our proof of convergence is based on the general framework of Hansen & Ostermann (2009).

4.1 *Analysis of the even-order kernel $\mathcal{T}_2$*

We will assume that, at sufficiently small h, the Strang splitting is bounded as follows:

$$\|\mathcal{T}_2(h)\| = \left\|\exp\left(\frac{1}{2}hD\right)\exp(hA(t))\exp\left(\frac{1}{2}hD\right)\right\| \leqslant \exp(c\omega h), \tag{4.1}$$

with c only depending on the coefficients of the method (see the work on convergence analysis for this splitting by Jahnke & Lubich (2000)). We can then derive the following convergence results for the MPE.

THEOREM 2. For the numerical solution of (1.28), we consider the MPE algorithm (2.8) of order $2n$. Further, we assume that the error estimate in equation (4.1) holds. Then we have the following convergence result:

$$\|(S^m - \exp(mh(A(t)+D)))u_0\| \leqslant CO(h^{2n+1}), \quad mh \leqslant t_{\mathrm{end}}, \tag{4.2}$$

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

Proof. We apply the telescopic identity and obtain

$$(S^m - \exp(mh(A(t)+D)))u_0 = \sum_{\nu=0}^{m-1} S^{m-\nu-1}(S - \exp(h(A(t)+D)))\exp(\nu h(A(t)+D))u_0, \tag{4.3}$$

where $S = \sum_{i=1}^n c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right)$. We apply the error estimate in (4.1) to obtain the stability requirement

$$\left\|\sum_{i=1}^n c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right)\right\| \leqslant \exp(c\omega h). \tag{4.4}$$

Assuming the consistency of

$$\left\|\sum_{i=1}^n c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right) - \exp(h(A+D))\right\| \leqslant CO(h^{2n+1}), \tag{4.5}$$

we have the following error bound:

$$\|(S^m - \exp(mh(A(t)+D)))u_0\| \leqslant CO(h^{2n+1}), \quad mh \leqslant t_{\mathrm{end}}. \tag{4.6}$$

The consistency of the error bound is derived in the following theorem. □

THEOREM 3. For the numerical solution of (1.28) we have the following consistency:

$$\left\|\sum_{i=1}^n c_i \mathcal{T}_2^{k_i}\left(\frac{h}{k_i}\right) - \exp(h(A+D))\right\| \leqslant CO(h^{2n+1}). \tag{4.7}$$

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

$$\sum_{k=1}^{n} c_k \mathcal{T}_2^k\left(\frac{h}{k}\right) = \sum_{k=1}^{n} c_k(\exp((A+D)h) - (k^{-2}h^3E_3 + k^{-4}h^5E_5 + \cdots)) \tag{4.8}$$

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

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

$$= \mathrm{O}(h^{2n+1}), \tag{4.9}$$

where the coefficients are given in (2.10). □

LEMMA 1 We assume that $\|A(t)\|$ is bounded in the interval $t \in (0, t_{\mathrm{end}})$. Then $\mathcal{T}_2$ is nonsingular for sufficiently small h.

Proof. We use our assumption that $\|A(t)\|$ is be bounded in the interval $0 < t < t_{\mathrm{end}}$. Thus we can find $\|A(t)\| < C$ for $0 < t < t_{\mathrm{end}}$, where $C \in \mathbb{R}^+$ is a bound of the operator $A(t)$ that is independent of t. Therefore, $\mathcal{T}_2$ is always nonsingular for sufficiently small h. □

REMARK 4.4 Based on these results, the kernel $\mathcal{T}_2$ is also uniformly convergent.

The same argument can be applied to the MPE formula, for which all operators are convergent, and the sum of all operators is also bounded and convergent (see Dvoretzky & Rogers, 1950; Eggleston, 1953).

REMARK 4.5 For higher kernels (e.g., fourth order) there also exist error bounds so that uniformly convergent results can be derived (see, e.g., Geiser, 2008). Such kernels can also be used for the MPE method to achieve higher-order accuracy with uniformly convergent series. But, as we noted earlier, these cannot be applied to time-irreversible problems.

4.2 *Analysis of the odd-order kernel $\mathcal{U}_n$*

LEMMA 2 We will assume that, for sufficiently small h, the Burstein and Mirin decomposition is bounded as follows:

$$\|\mathcal{U}_n(h)\| = \left\| \mathrm{e}^{\frac{h}{2n-1}A(t)} \left(\mathrm{e}^{\frac{2h}{2n-1}D}\mathrm{e}^{\frac{2h}{2n-1}A(t)}\right)^{n-1} \mathrm{e}^{\frac{h}{2n-1}D} \right\| \leqslant \exp(c\omega h) \quad \forall\, t \geqslant 0, \tag{4.10}$$

with c only dependent on the coefficients of the method.

Proof. The proof follows by rewriting equation (4.10) as a product of the Strang and the $A-B$ splitting schemes. Equation (4.10) can be rewritten as follows:

$$\mathrm{e}^{\frac{h}{2n-1}A(t)} \left(\mathrm{e}^{\frac{2h}{2n-1}D}\,\mathrm{e}^{\frac{2h}{2n-1}A(t)}\right)^{n-1} \mathrm{e}^{\frac{h}{2n-1}D} = \left(\mathrm{e}^{\frac{h}{2n-1}A(t)}\mathrm{e}^{\frac{2h}{2n-1}D}\,\mathrm{e}^{\frac{h}{2n-1}A(t)}\right)^{n-1} \mathrm{e}^{\frac{h}{2n-1}A(t)}\mathrm{e}^{\frac{h}{2n-1}D} \quad \forall\, t \geqslant 0. \tag{4.11}$$

The error bound and the underlying convergence analysis for both the Strang and the $A - B$ splitting have been previously studied by Jahnke & Lubich (2000). □

We assume the following derivation of the higher-order MPE.

ASSUMPTION 1 We assume the following higher-order decomposition:

$$\mathrm{e}^{h(A+D)} = \sum_{i=1}^{n} \tilde{c}_i \mathcal{U}_i(h) + \mathrm{O}(h^{2n}), \tag{4.12}$$

where the $\tilde{c}_i$ are derived based on the Vandermonde equation (2.9) with $\{k_i\}$ being a set of odd whole numbers.

We can then derive the following convergence results for the MPE.

THEOREM 4. For the numerical solution of (1.28), we consider the Assumption 1 with order $2n - 1$ and we apply Lemma 2. Then we have a convergence result that is given as follows:

$$\|(S^m - \exp(mh(A(t) + D)))u_0\| \leqslant C\mathrm{O}(h^{2n}), \quad mh \leqslant t_{\mathrm{end}}, \tag{4.13}$$

with $n = 1, 2, 3, \ldots$, and where $S = \sum_{i=1}^{n} \tilde{c}_i \mathcal{U}_i(h)$ and C is to be chosen uniformly on bounded time intervals and is independent of m and h for sufficiently small h.

Proof. The same proof ideas can be followed as for the proof of Theorem 2. The consistency of the error bound is derived in the following theorem. □

THEOREM 5. For the numerical solution of (1.28), we have the following consistency:

$$\left\| \sum_{i=1}^{n} \tilde{c}_i \mathcal{U}_i(h) - \exp(h(A + D)) \right\| \leqslant C\mathrm{O}(h^{2n}). \tag{4.14}$$

Proof. The same proof ideas can be followed as for the proof of Theorem 3. □

REMARK 4.10 The same proof idea can be used to generalize the higher-order schemes.

5. Analytical and numerical verifications

In this section we seek to verify and assess the convergence of both the even- and odd-order MPE algorithms. For a single-product splitting, there are no known splittings that are exact in the limit of a large number of operators. Even in the case of the Zassenhaus formula, it is nontrivial to compute the higher-order products, not to mention evaluating them. For this purpose, we turn to the much studied Magnus expansion, where the exact limit can be computed in simple cases.

The Magnus expansion (Blanes *et al.*, 2009) solves (1.28) in the form

$$Y(t) = \exp(\Omega(t))Y(0), \quad \Omega(t) = \sum_{n=1}^{\infty} \Omega_n(t), \tag{5.1}$$

where the first few terms are

$$\begin{aligned}
\Omega_1(t) &= \int_0^t \mathrm{d}t_1 A_1,\\
\Omega_2(t) &= \frac{1}{2}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 [A_1, A_2],\\
\Omega_3(t) &= \frac{1}{6}\int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 ([A_1,[A_2,A_3]] + [[A_1,A_2],A_3]),\\
&\vdots
\end{aligned} \tag{5.2}$$

with $A_n \equiv A(t_n)$. In practice, it is more useful to define the nth-order Magnus operator

$$\Omega^{[n]}(t) = \Omega(t) + \mathrm{O}(t^{n+1}) \tag{5.3}$$

such that

$$Y(t) = \exp\big[\Omega^{[n]}(t)\big]Y(0) + \mathrm{O}(t^{n+1}). \tag{5.4}$$

Thus, the second-order Magnus operator is

$$\begin{aligned}
\Omega^{[2]}(t) &= \int_0^t \mathrm{d}t_1 A(t_1)\\
&= tA\left(\frac{1}{2}t\right) + \mathrm{O}(t^3)
\end{aligned} \tag{5.5}$$

and a fourth-order Magnus operator (Blanes *et al.*, 2009) is

$$\Omega^{[4]}(t) = \frac{1}{2}t(A_1 + A_2) - c_3 t^2 [A_1, A_2], \tag{5.6}$$

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

$$c_1 = \frac{1}{2} - \frac{\sqrt{3}}{6}, \quad c_2 = \frac{1}{2} + \frac{\sqrt{3}}{6}, \quad c_3 = \frac{\sqrt{3}}{12}. \tag{5.7}$$

For the ubiquitous case of

$$A(t) = T + V(t), \tag{5.8}$$

one has

$$\begin{aligned}
\mathrm{e}^{\Omega^{[2]}(t)} &= \mathrm{e}^{t[T+V(t/2)]}\\
&= \mathrm{e}^{\frac{1}{2}tT}\,\mathrm{e}^{tV(t/2)}\mathrm{e}^{\frac{1}{2}tT} + \mathrm{O}(t^3)
\end{aligned} \tag{5.9}$$

and

$$\mathrm{e}^{\Omega^{[4]}(t)} = \mathrm{e}^{c_3 t(V_2 - V_1)}\mathrm{e}^{t\left(T + \frac{1}{2}(V_1+V_2)\right)}\mathrm{e}^{-c_3 t(V_2 - V_1)} + \mathrm{O}(t^5), \tag{5.10}$$

where

$$V_1 = V(c_1 t), \quad V_2 = V(c_2 t). \tag{5.11}$$

The Magnus expansion (5.4) is automatically structure preserving because it is a *single exponential operator* approximation. However, since one must further split $\Omega^{[n]}$ into computable parts, the expansion is as complex, if not more so, than a single-product splitting. In the following, the comparison is not strictly equitable because the MPE is *not* structure preserving. Nevertheless it is useful to know that, perhaps for that reason, the MPE can be uniformly convergent.

5.1 *The nonsingular matrix case*

To assess the convergence of the MPE with that of the Magnus series, consider the well-known example (Moan & Niesen, 2008) of

$$A(t) = \begin{pmatrix} 2 & t \\ 0 & -1 \end{pmatrix}. \tag{5.12}$$

The exact solution to (1.28) with $Y(0) = I$ is

$$Y(t) = \begin{pmatrix} e^{2t} & f(t) \\ 0 & e^{-t} \end{pmatrix}, \tag{5.13}$$

with

$$f(t) = \frac{1}{9}e^{-t}(e^{3t} - 1 - 3t) \tag{5.14}$$

$$= \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{13t^{10}}{403200} + \cdots . \tag{5.15}$$

For the Magnus expansion one has the series

$$\Omega(t) = \begin{pmatrix} 2t & g(t) \\ 0 & -t \end{pmatrix}, \tag{5.16}$$

with, up to 10th order,

$$g(t) = \frac{1}{2}t^2 - \frac{1}{4}t^3 + \frac{3}{80}t^5 - \frac{9}{1120}t^7 + \frac{81}{44800}t^9 + \cdots \tag{5.17}$$

$$\to \frac{t(e^{3t} - 1 - 3t)}{3(e^{3t} - 1)}. \tag{5.18}$$

Taking the exponential of (5.16) yields (5.13) with

$$f(t) = t\,e^{-t}(e^{3t} - 1)\left(\frac{1}{6} - \frac{1}{12}t + \frac{1}{80}t^3 - \frac{3}{1120}t^5 + \frac{27}{44800}t^7 + \cdots\right) \tag{5.19}$$

$$\to t\,e^{-t}(e^{3t} - 1)\left(\frac{1}{9t} - \frac{1}{3(e^{3t} - 1)}\right). \tag{5.20}$$

Whereas the exact solution (5.14) is an entire function of t, the Magnus series (5.17) and (5.19) only converge for $|t| < \frac{2}{3}\pi$ due to the pole at $t = \frac{2}{3}\pi\,\mathrm{i}$. The Magnus series (5.19) is plotted in Fig. 1 as dotted lines. The pole at $|t| = \frac{2}{3}\pi \approx 2$ is clearly visible.

For the even-order MPE, from (3.10), by setting $h = t$ and $t = 0$, we have

$$\mathcal{T}_2(t) = \exp\left[t\begin{pmatrix} 2 & \frac{1}{2}t \\ 0 & -1 \end{pmatrix}\right] = \begin{pmatrix} \mathrm{e}^{2t} & f_2(t) \\ 0 & \mathrm{e}^{-t} \end{pmatrix}, \tag{5.21}$$

and we compute $\mathcal{T}_2^2(t)$ according to (3.11) as

$$\mathcal{T}_2^2(t/2) = \exp\left[\frac{t}{2}\begin{pmatrix} 2 & \frac{3}{4}t \\ 0 & -1 \end{pmatrix}\right]\begin{pmatrix} \mathrm{e}^{t} & f_2(t/2) \\ 0 & \mathrm{e}^{-\frac{t}{2}} \end{pmatrix} \tag{5.22}$$

with

$$f_2(t) = \frac{1}{6}t\,\mathrm{e}^{-t}(\mathrm{e}^{3t} - 1). \tag{5.23}$$

This is identical to the first term of the Magnus series (5.19) and is an entire function of t. Since a higher-order MPE uses only powers of $\mathcal{T}_2$, higher-order MPE approximations are also entire functions

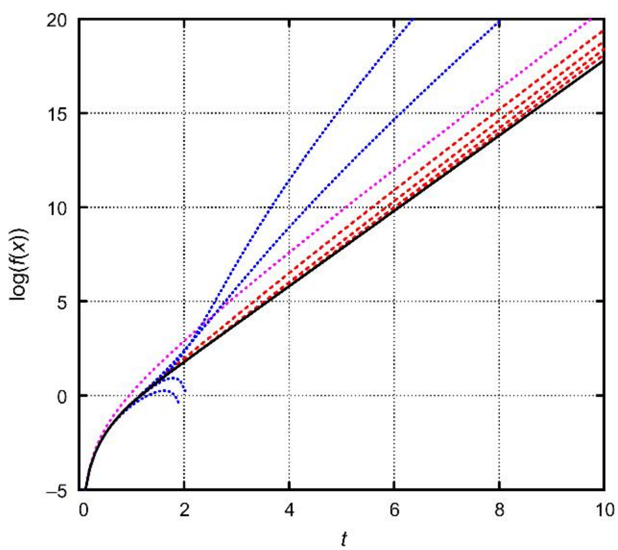

FIG. 1. The solid line is the exact result (5.14). The dotted lines are the Magnus fourth- to 10th-order results (5.19), which diverge from the exact result beyond $t > 2$. The dashed lines are the MPE. The dot–dashed line is their common second-order result.

of t. Thus, up to 10th order, one finds

$$f_4(t) = t\,\mathrm{e}^{-t}\left(\frac{\mathrm{e}^{3t}-5}{18}+\frac{2\mathrm{e}^{3t/2}}{9}\right), \tag{5.24}$$

$$f_6(t) = t\,\mathrm{e}^{-t}\left(\frac{11\mathrm{e}^{3t}-109}{360}+\frac{9}{40}(\mathrm{e}^{2t}+\mathrm{e}^{t})-\frac{8}{45}\mathrm{e}^{3t/2}\right), \tag{5.25}$$

$$f_8(t) = t\,\mathrm{e}^{-t}\left(\frac{151\mathrm{e}^{3t}-2369}{7560}+\frac{256}{945}\left(\mathrm{e}^{9t/4}+\mathrm{e}^{3t/4}\right)-\frac{81}{280}(\mathrm{e}^{2t}+\mathrm{e}^{t})+\frac{104}{315}\mathrm{e}^{3t/2}\right), \tag{5.26}$$

$$\begin{aligned} f_{10}(t) = t\,\mathrm{e}^{-t}\Bigg(&\frac{15619\,\mathrm{e}^{3t}-347261}{1088640}+\frac{78125}{217728}\left(\mathrm{e}^{12t/5}+\mathrm{e}^{9t/5}+\mathrm{e}^{6t/5}+\mathrm{e}^{3t/5}\right) \\ &-\frac{4096}{8505}\left(\mathrm{e}^{9t/4}+\mathrm{e}^{3t/4}\right)+\frac{729}{4480}(\mathrm{e}^{2t}+\mathrm{e}^{t})-\frac{4192}{8505}\mathrm{e}^{3t/2}\Bigg). \end{aligned} \tag{5.27}$$

These even-order approximations are plotted as dashed lines in Fig. 1. The convergence is uniform for all t.

When expanded, the above yield

$$\begin{aligned} f_2(t) &= \frac{t^2}{2}+\frac{t^3}{4}+\cdots, \\ f_4(t) &= \frac{t^2}{2}+\frac{t^4}{8}+\frac{5t^5}{192}+\cdots, \\ f_6(t) &= \frac{t^2}{2}+\frac{t^4}{8}+\frac{t^5}{60}+\frac{t^6}{80}+\frac{t^7}{384}+\cdots, \\ f_8(t) &= \frac{t^2}{2}+\frac{t^4}{8}+\frac{t^5}{60}+\frac{t^6}{80}+\frac{t^7}{420}+\frac{31t^8}{40320}+\frac{1307t^9}{8601600}+\cdots, \\ f_{10}(t) &= \frac{t^2}{2}+\frac{t^4}{8}+\frac{t^5}{60}+\frac{t^6}{80}+\frac{t^7}{420}+\frac{31t^8}{40320}+\frac{t^9}{6720} \\ &\quad+\frac{13t^{10}}{403200}+\frac{13099t^{11}}{232243200}+\cdots, \end{aligned} \tag{5.28}$$

and these agree with the exact solution to the claimed order. Similarly, the m-step extrapolated algorithms $\mathcal{T}_{2,m}$, $\mathcal{T}_{4,m}$, etc. are also correct up to the claimed order.

For odd orders, by again setting $h = t$ and $t = 0$, the basis defined in (3.12) now reads as follows:

$$\begin{aligned} \mathcal{U}_1(t) &= \exp\left[t\begin{pmatrix}2 & 0\\ 0 & -1\end{pmatrix}\right] = \begin{pmatrix}\mathrm{e}^{2t} & 0\\ 0 & \mathrm{e}^{-t}\end{pmatrix}, \\ \mathcal{U}_2(t) &= \exp\left[\frac{2}{3}t\begin{pmatrix}2 & \frac{2}{3}t\\ 0 & -1\end{pmatrix}\right]\exp\left[\frac{1}{3}t\begin{pmatrix}2 & 0\\ 0 & -1\end{pmatrix}\right] \end{aligned} \tag{5.29}$$

$$= \begin{pmatrix} e^{2t} & \frac{2}{9}t(e^{t} - e^{-t}) \\ 0 & e^{-t} \end{pmatrix},$$

$$\vdots$$

and the MPE (2.25)–(2.28) gives

$$f_3(t) = \frac{t^2}{2} + \frac{t^4}{12} + \cdots,$$

$$f_5(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{11t^6}{1000} + \cdots,$$

$$f_7(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{18299t^8}{24696000} \cdots,$$

$$f_9(t) = \frac{t^2}{2} + \frac{t^4}{8} + \frac{t^5}{60} + \frac{t^6}{80} + \frac{t^7}{420} + \frac{31t^8}{40320} + \frac{t^9}{6720} + \frac{1577t^{10}}{49392000} + \cdots. \tag{5.30}$$

Results (5.28) and (5.30) constitute an analytical verification of the even- and odd-order MPEs (2.11)–(2.14) and (2.25)–(2.28).

5.2 *The singular matrix case*

Consider the radial Schrödinger equation

$$\frac{\partial^2 u}{\partial r^2} = f(r, E)u(r), \tag{5.31}$$

where

$$f(r, E) = 2V(r) - 2E + \frac{l(l+1)}{r^2}. \tag{5.32}$$

By relabelling such that $r \to t$ and $u(r) \to q(t)$, (5.31) can be viewed as a harmonic oscillator with a time-dependent spring constant

$$k(t, E) = -f(t, E) \tag{5.33}$$

and Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{2}k(t, E)q^2. \tag{5.34}$$

Thus, any eigenfunction of (5.31) is an exact time-dependent solution of (5.34). For example, the ground state of the hydrogen atom with $l = 0$, $E = -1/2$ and

$$V(r) = -\frac{1}{r} \tag{5.35}$$

yields the exact solution

$$\begin{aligned} q(t) &= t\exp(-t) \\ &= t - t^2 + \frac{t^3}{2} - \frac{t^4}{6} + \frac{t^5}{24} - \frac{t^6}{120} + \frac{t^7}{720} - \frac{t^8}{5040}\cdots \\ &= t - t^2 + \frac{t^3}{2} - 0.1667t^4 + 0.0417t^5 - 0.0083t^6\cdots, \end{aligned} \tag{5.36}$$

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

$$Y(t) = \begin{pmatrix} q(t) \\ p(t) \end{pmatrix}, \tag{5.37}$$

the time-dependent harmonic oscillator (5.34) now corresponds to

$$A(t) = \begin{pmatrix} 0 & 1 \\ f(t) & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ f(t) & 0 \end{pmatrix} \equiv T + V(t), \tag{5.38}$$

with a singular matrix element

$$f(t) = 1 - \frac{2}{t}. \tag{5.39}$$

The second-order midpoint algorithm is

$$\begin{aligned} \mathcal{T}_2(h,t) &= \mathrm{e}^{\frac{1}{2}hT}\,\mathrm{e}^{hV(t+h/2)}\mathrm{e}^{\frac{1}{2}hT} \\ &= \begin{pmatrix} 1 + \frac{1}{2}h^2 f\left(t + \frac{1}{2}h\right) & h + \frac{1}{4}h^3 f\left(t + \frac{1}{2}h\right) \\ hf\left(t + \frac{1}{2}h\right) & 1 + \frac{1}{2}h^2 f\left(t + \frac{1}{2}h\right) \end{pmatrix}, \end{aligned} \tag{5.40}$$

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

$$q_2(t) = t + \frac{1}{4}t^3 f\left(\frac{1}{2}t\right) = t - t^2 + \frac{1}{4}t^3. \tag{5.41}$$

The even-order MPEs (2.11)–(2.14) then yield

$$\begin{aligned} q_4(t) &= t - t^2 + 0.3889t^3 - 0.1111t^4 + 0.0104t^5, \\ q_6(t) &= t - t^2 + 0.4689t^3 - 0.1378t^4 + 0.0283t^5 - 0.0043t^6, \\ q_8(t) &= t - t^2 + 0.4873t^3 - 0.1542t^4 + 0.0356t^5 - 0.0062t^6\cdots, \\ q_{10}(t) &= t - t^2 + 0.4936t^3 - 0.1603t^4 + 0.0385t^5 - 0.0073t^6\cdots, \end{aligned} \tag{5.42}$$

where we have converted fractions to their decimal form for easier comparison with the exact solution (5.36). One sees that the 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. (If one naively calculates a Taylor expansion about $t = 0$ starting with $q(0) = 0$ and $p(0) = 1$, then every term beyond the initial values would either be divergent or undefined.)

Since $A(t)$ is now singular at $t = 0$, the previous proof of uniform convergence no longer holds. Nevertheless, from the exact solution (5.36), one sees that the force (or acceleration)

$$\lim_{t\to 0} f(t)q(t) = -2 \tag{5.43}$$

remains finite. It seems that this is sufficient for uniform convergence as the coefficients of t^n do approach their correct value with increasing order.

For an odd-order MPE, each term $\mathrm{e}^{(h/x)V(t)}$ of the basis product in (3.14) is singular at $t = 0$, but, because of (5.43), we have

$$\lim_{t\to 0} \mathrm{e}^{(h/x)V(t)} \begin{pmatrix} q(t) \\ p(t) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 - 2h/x \end{pmatrix}. \tag{5.44}$$

Interpreting the action of the first operator this way, the basis products of (3.14) then yield, according to the MPEs (2.25)–(2.28),

$$\begin{aligned} q_3(t) &= t - t^2 + \frac{t^3}{2} - 0.1111t^4, \\ q_5(t) &= t - t^2 + \frac{t^3}{2} - 0.1458t^4 + 0.0333t^5 - 0.0033t^6, \\ q_7(t) &= t - t^2 + \frac{t^3}{2} - 0.1628t^4 + 0.0382t^5 - 0.0067t^6 \cdots, \\ q_9(t) &= t - t^2 + \frac{t^3}{2} - 0.1655t^4 + 0.0406t^5 - 0.0078t^6 \cdots. \end{aligned} \tag{5.45}$$

Now $q_3(t)$ is correct to third order, but higher-order algorithms are still down-graded and only approach the exact solution asymptotically, but uniformly.

To see this uniform convergence, we show in Fig. 2 how higher-order MPEs, both even and odd, up to 100th order, compare with the exact solution. The calculation is done numerically rather than by evaluating the analytical expressions such as (5.42) or (5.45). The orders of the MPE algorithms are indicated by numbers. For odd-order algorithms, we do not even bother to incorporate (5.44), but just avoid the singularity by starting the algorithm at $t = 10^{-6}$. Also shown are the following well-known fourth-order symplectic algorithms: FR (Forest & Ruth, 1990; three force evaluations), M (McLachlan, 1995; four force evaluations), BM (Blanes & Moan, 2002; six force evaluations), Mag4 (Magnus integrator; four force evaluations) and 4B (Chin & Anisimov, 2006) (a *forward* symplectic algorithm with approximately 2 evaluations). These symplectic integrators steadily improve from FR to M, to Mag4, to BM and to 4B. The 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

$$q_{4\mathrm{B}}(t) = t - t^2 + \frac{t^3}{2} - 0.1635t^4 + 0.0397t^5 - 0.0070t^6 + 0.0009t^7 \cdots, \tag{5.46}$$

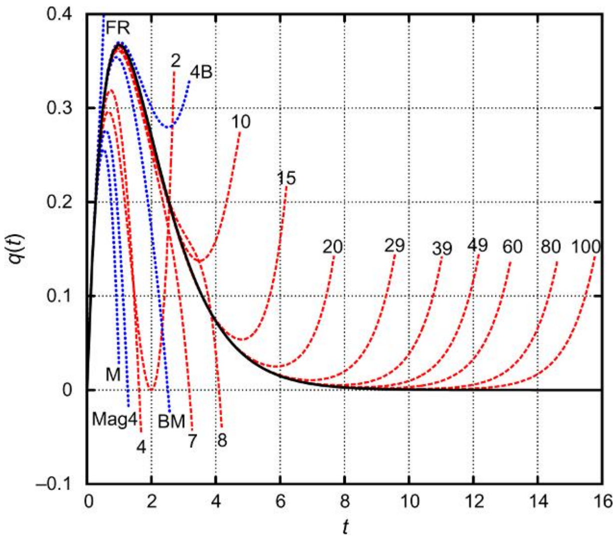

FIG. 2. The uniform convergence of the MPE in solving for the hydrogen ground-state wave function (dashed line). The solid line is the exact ground-state wave function. The numbers denote the order of the MPE. The dotted lines denote results of various fourth-order algorithms.

with the correct third-order coefficient and higher-order coefficients that are comparable to the exact solution (5.36). In contrast, the FR algorithm, which is well known to have rather large errors, has the expansion

$$q_{\mathrm{FR}}(t) = t - t^2 - 0.1942t^3 + 3.528t^4 - 2.415t^5 + 0.5742t^6 - 0.0437t^7 \cdots, \tag{5.47}$$

with terms of the wrong sign 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.* (2010). However, their findings do 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 issue.

In Fig. 2, results for orders 60, 80 and 100 are computed using quadruple precision. If one uses only double precision, then the effect of round-off errors on limited precision is as shown in Fig. 3. For this calculation, the round-off errors are not very noticeable even at orders as high as 40 or 49, which is rather surprising. The round-off errors are noticeable only at orders greater than approximately 60.

For nonsingular potentials such as the radial harmonic oscillator with

$$f(t) = t^2 - 3, \tag{5.48}$$

and exact ground-state solution

$$q(t) = t\,\mathrm{e}^{-t^2/2} = t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{t^{11}}{3840} + \cdots, \tag{5.49}$$

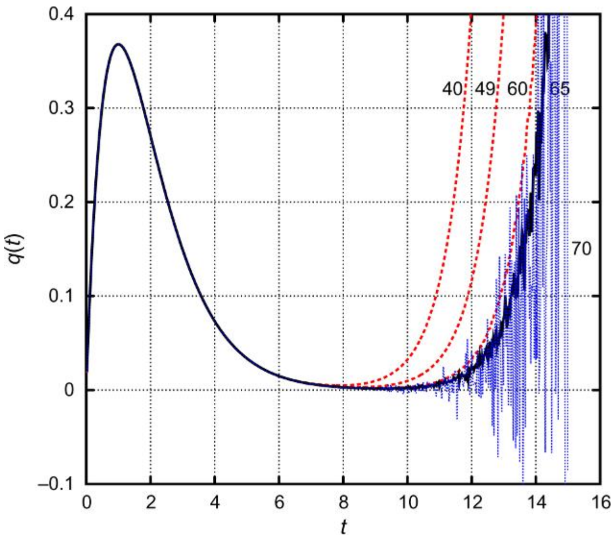

FIG. 3. The MPE results for the hydrogen ground-state wave function using only double-precision arithmetic (dashed lines). The effect of limited precision begins to show at order 60. The results for order 65 and 70 are indicated by dotted lines, respectively.

the MPE has no problem in reproducing the exact solution to the claimed order as follows:

$$\begin{aligned}
q_6(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{13t^7}{576} + \cdots,\\
q_7(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{1082t^9}{385875} + \cdots,\\
q_8(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{20803t^9}{7741440} + \cdots,\\
q_9(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{341t^{11}}{1224720} + \cdots,\\
q_{10}(t) &= t - \frac{t^3}{2} + \frac{t^5}{8} - \frac{t^7}{48} + \frac{t^9}{384} - \frac{50977t^{11}}{193536000} + \cdots .
\end{aligned} \tag{5.50}$$

In this case the odd-order algorithms have the advantage of being correct to one order higher.

6. Concluding summary and discussion

In this work we have shown that the most general framework for deriving Nyström-type algorithms for solving autonomous and nonautonomous equations is multi-product splitting. By expanding on a suitable basis of operators, the resulting MPE can not only reproduce conventional extrapolated integrators of even order but can also yield new odd-order algorithms. By the use of Suzuki's rule for incorporating the time-ordered exponential, any multi-product splitting algorithm can be adopted for solving explicitly time-dependent problems. The analytically known expansion coefficients c_i allow great flexibility in designing adaptive algorithms. Unlike structure-preserving methods such as the Magnus expansion, which has a finite radius of convergence, our MPE converges uniformly. Moreover, MPE requires far less operators at higher orders than either the Magnus expansion or conventional single-product splittings. The general-order condition for multi-product splitting is not known and should be developed. In the future we will focus on applying MPE methods for solving nonlinear differential equations and time-irreversible or semigroup problems.

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