Effective approximation for the linear time-dependent Schrödinger equation

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July 16, 2012

Abstract

The computation of the linear Schrödinger equation presents major challenges because of the presence of a small parameter. Assuming periodic boundary conditions, the standard approach consists of semi-discretisation with a spectral method, followed by an exponential splitting. In this paper we sketch an alternative strategy. Our analysis commences from the investigation of the free Lie algebra generated by differentiation and by multiplication with the interaction potential: it turns out that this algebra possesses structure that renders it amenable to a very effective form of *asymptotic splitting:* exponential splitting where consecutive terms are scaled by increasing powers of the small parameter. This leads to methods that attain high spatial and temporal accuracy and whose cost scales like $\mathcal{O}(N)$ or $\mathcal{O}(N \log N)$, where N is the number of degrees of freedom.

1 Introduction

The linear Schrödinger equation plays central role in a wide range of applications and is the fundamental model of quantum mechanics (Griffiths 2004). Its computation presents numerous enduring challenges (Jin, Markowich & Sparber 2011) which form the centrepiece of this paper.

We consider the standard *linear Schrödinger equation* in a single space variable,

$$\mathrm{i}\hbar\frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 u}{\partial x^2} - \tilde{V}(x)u, \qquad t \geq 0, \quad x \in [-(2m)^{-1/2}, (2m)^{-1/2}], \tag{1.1}$$

where $u = u(x,t)$, given with an initial condition and periodic boundary conditions, where the *interaction potential* $\tilde{V}$ is a periodic function and m is the mass of the

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underlying particle. We note, that the important case of unbounded potentials can also be included in this setting, when we propagate bounded states inside a sufficiently large interval. The parameter $\hbar$, the *reduced Planck constant*, is truly minute, $\hbar \approx 1,05457168 \cdot 10^{-34}$ Joule secs, while m is a small quantity, although substantially larger than $\hbar$. However, since physical interest is in fairly small spatial and temporal 'windows', it is usual to rescale $x = \tilde{x}\hbar/\varepsilon/\sqrt{2m}$ and $t = \tilde{t}\hbar/\varepsilon$ so that (1.1) is replaced with

$$\mathrm{i}\varepsilon\frac{\partial u}{\partial t} = -\varepsilon^2\frac{\partial^2 u}{\partial x^2} - V(x)u, \qquad t \geq 0, \quad x \in [-1,1], \tag{1.2}$$

$V(x) = \tilde{V}((2m)^{-1/2}x\hbar/\varepsilon)$, where $\varepsilon > 0$ is a small parameter: it is useful to keep in mind the range $10^{-8} \leq \varepsilon \leq 10^{-4}$.

The equation (1.2) is a univariate model for the considerably more important multivariate linear Schrödinger equation,

$$\mathrm{i}\varepsilon\frac{\partial u}{\partial t} = -\varepsilon^2 E\nabla^2 u - V(\boldsymbol{x})u, \qquad t \geq 0, \quad \boldsymbol{x} \in [-1,1]^d, \tag{1.3}$$

where $u = u(t,\boldsymbol{x})$ and E is a diagonal matrix, with periodic boundary conditions. This equation models the evolution of a system of particles in (typically) $\mathbb{R}^3$. The methodology of this paper lends itself to straightforward generalisation to (1.3) provided that the dimension d is moderate. Large values of d require combining our approach with other computational techniques, an area under current investigation.

The small size of ε is a source of substantial difficulties in the numerical discretization of (1.2) because, using a naive approach, rapid oscillations require a spatial resolution of $\mathcal{O}(\varepsilon)$ which is often impractical or, at best, exceedingly expensive. This is the motivation to pursue alternative approaches, based in the main on the concept of *exponential splittings* (Faou 2012, Jin et al. 2011, Lubich 2008, McLachlan & Quispel 2002).

The construction of exponential splitting methods typically commences from space discretization. Rewriting (1.2) in the form

$$\frac{\partial u}{\partial t} = \mathrm{i}\omega^{-1}\frac{\partial^2 u}{\partial x^2} + \mathrm{i}\omega V(x)u, \qquad t \geq 0, \qquad x \in [-1,1], \tag{1.4}$$

where $\omega = \varepsilon^{-1} \gg 1$, we let the vector $\boldsymbol{u}(t) \in \mathbb{C}^N$ represent an approximation to the solution at time t: typically, the components of $\boldsymbol{u}$ are either approximations to the values of u on a grid or to Fourier coefficients of this function. Replacing the second derivative operator by a matrix $\mathcal{K}$ (thus, replacing an infinite-dimensional linear operator by a finite-dimensional one), we obtain the ODE system

$$\boldsymbol{u}' = \mathrm{i}(\omega^{-1}\mathcal{K} + \omega\mathcal{D})\boldsymbol{u}, \qquad t \geq 0, \tag{1.5}$$

where $\boldsymbol{u}(0)$ is derived from the initial conditions and $\mathcal{D}$ represents a multiplication by the interaction potential V in the finite-dimensional space.

The exact solution of (1.5) is of course

$$\boldsymbol{u}(t) = \exp\left(\mathrm{i}t(\omega^{-1}\mathcal{K} + \omega\mathcal{D})\right)\boldsymbol{u}(0)$$

and a natural temptation is to approximate it (using small time steps) by any of many methods to compute the matrix exponential, $\boldsymbol{u}((n+1)\Delta t) \approx \mathrm{e}^{\mathrm{i}\Delta t(\omega^{-1}\mathcal{K}+\omega\mathcal{D})}\boldsymbol{u}(n\Delta t)$, $n \in \mathbb{Z}_+$. This is generally accepted as a poor idea, because the vastly different scales of $\omega^{-1}\mathcal{K}$ and $\omega\mathcal{D}$ require either very small time step Δt or exceedingly expensive methods to approximate the exponential (e.g. Krylov subspace methods of dimension $\approx N$) to attain reasonable accuracy. The alternative is to separate scales by means of an exponential splitting. The starting point is usually the *Strang splitting*

$$\mathrm{e}^{\mathrm{i}t(\omega^{-1}\mathcal{K}+\omega\mathcal{D})} = \mathrm{e}^{\frac{1}{2}\mathrm{i}t\omega^{-1}\mathcal{K}}\mathrm{e}^{\mathrm{i}t\omega\mathcal{D}}\mathrm{e}^{\frac{1}{2}\mathrm{i}t\omega^{-1}\mathcal{K}} + \mathcal{O}\big(t^3\big)\,. \tag{1.6}$$

This has the clear virtue of separating scales. Moreover, usually each individual exponential can be computed very affordably: e.g., once we semidiscretise (1.4) with a spectral method, $\mathcal{K}$ is diagonal and $\mathcal{D}$ a circulant, therefore $\mathrm{e}^{\frac{1}{2}\mathrm{i}t\omega^{-1}\mathcal{K}}$ is a diagonal matrix, while $\mathrm{e}^{\mathrm{i}t\omega\mathcal{D}}$ can be approximated in $\mathcal{O}(N\log N)$ operations with FFT. Yet the order of approximation is unacceptably low. The standard generalisation of the Strang splitting bears the form

$$\mathrm{e}^{\mathrm{i}\alpha_1 t\omega^{-1}\mathcal{K}}\mathrm{e}^{\mathrm{i}\beta_1 t\omega\mathcal{D}}\mathrm{e}^{\mathrm{i}\alpha_2 t\omega^{-1}\mathcal{K}}\cdots\mathrm{e}^{\mathrm{i}\alpha_r t\omega^{-1}\mathcal{K}}\mathrm{e}^{\mathrm{i}\beta_r t\omega\mathcal{D}}\mathrm{e}^{\mathrm{i}\alpha_r t\omega^{-1}\mathcal{K}}\cdots\mathrm{e}^{\mathrm{i}\alpha_2 t\omega^{-1}\mathcal{K}}\mathrm{e}^{\mathrm{i}\beta_1 t\omega\mathcal{D}}\mathrm{e}^{\mathrm{i}\alpha_1 t\omega^{-1}\mathcal{K}}.$$

The palindromic form of this splitting (it reads the same from the left and from the right), which is referred to as symmetric splitting in much of the literature, is not accidental, since it guarantees higher order. The coefficients α_i and β_i are typically chosen to ensure either higher order (because of palindromy, the order is always even) or smaller error constants or both (Blanes, Casas & Murua 2006, McLachlan & Quispel 2002).

This approach retains the main virtues of (1.6), namely separation of scales and the ease of computation of individual exponentials. However, a inordinately large number of exponentials is required to attain significant order. The simplest means toward a high-order splitting, the *Yošida method* (McLachlan & Quispel 2002, Yošida 1990), calls for $r = 3^{p-1}$ (which translates to $2\cdot 3^{p-1}+1$ exponentials) to attain order $2p$. Our aim in this paper is to present splittings that require far fewer exponentials to attain given order: we wish the number of exponentials to grow linearly, rather than exponentially, with order. Moreover, once the number of exponentials becomes large, ideally we do not want all of them to fit into the same two scales but wish for them to become increasingly smaller: to have an *asymptotic splitting*.

In this paper we introduce a family of exponential splittings with these favourable features. More specifically, we introduce and analyse exponential splittings of the form

$$\mathrm{e}^{\mathrm{i}\Delta t(\omega^{-1}\mathcal{K}+\omega\mathcal{D})} = \mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\cdots\mathrm{e}^{\mathcal{R}_s}\mathrm{e}^{\mathcal{T}_{s+1}}\mathrm{e}^{R_s}\cdots\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0} = \mathcal{O}\Big(\varepsilon^{s+3/2}\Big)\,, \tag{1.7}$$

where

$$\begin{aligned}\mathcal{R}_k &= \mathcal{R}_k(\Delta t,\varepsilon,\mathcal{K},\mathcal{D}) = \mathcal{O}\Big(\varepsilon^{k-1/2}\Big)\,, \qquad k=0,1,\dots,s,\\ \mathcal{T}_{s+1} &= \mathcal{T}_{s+1}(\Delta t,\varepsilon,\mathcal{K},\mathcal{D}) = \mathcal{O}\Big(\varepsilon^{s+1/2}\Big)\end{aligned}$$

(recall that $\omega = \varepsilon^{-1}$) and variations on this theme. Note a number of critical differences between (1.7) and standard exponential splittings.

Firstly, we quantify the error not in terms of the step-size Δt but of the small parameter ε. Of course, there are three small quantities at play: $\varepsilon, \Delta t$ and $1/M$ (where M is the number of degrees of freedom in the semidiscretisation). By letting power laws govern the relationship between ε and the choices of Δt and M, we express the error in the single quantity ε.

Secondly, the number of individual terms in (1.7) is remarkably small and it grows *linearly* with s – compare with the exponential growth, as a function of order, in the number of components of standard splittings. The reason is that the arguments of the exponentials in (1.7) decay increasingly more rapidly in ε.

Thirdly, each of these exponentials can be computed rapidly. Some of the $\mathcal{R}_k$s are diagonal matrices, whereby computing the exponential is trivial. Other are circulants and can be computed with FFT. Finally, because of the minute size of the arguments for sufficiently large k, the remaining exponentials can be evaluated up to $\mathcal{O}\big(\varepsilon^{s+3/2}\big)$ using a *very* low-dimensional Krylov subspace method.

The asymptotic splitting (1.7) is possible because we have deliberately breached the consensus in the design of exponential splittings: the terms $\mathcal{R}_k$ and $\mathcal{T}_{s+1}$ contain nested commutators. The use of commutators is usually frowned upon because of their cost, and also because they are believed to increase in norm. However, as we demonstrate in Section 2, in the current setting the use of commutators, appropriately handled, is benign. The first idea is to forego the standard steps of first semidiscretising like in (1.5) and then splitting the exponential: we semidiscretise only once the splitting has been done! Thus, the entire narrative take place within the *free Lie algebra* $\mathfrak{F} = \mathrm{FLA}\{\partial_x^2, V\}$, where $\partial_x = \frac{\mathrm{d}}{\mathrm{d}x}$ and V is the operation of multiplying with the interaction potential: since we have not yet discretised, both are infinite-dimensional linear operators. We demonstrate in Section 2 that $\mathfrak{F}$ can be embedded in a larger Lie algebra $\mathfrak{G}$, where the commutation has simple, straightforward interpretation. To all intents and purposes, commutators are replaced by simple linear combinations of powers of ∂_x. Moreover – and this is what lets all this procedure work in a beneficial manner – these are smaller powers of ∂_x then naively expected. Section 2 also describes two Lie-algebraic concepts which are at the heart of our methodology, the symmetric BCH formula and the Zassenhaus splitting.

In Section 3 we introduce – still working in an infinite-dimensional operatorial setting – our exponential splitting. This requires a recursive procedure, based upon repeated application of the symmetric BCH formula in $\mathfrak{G}$, working in the Hall basis. Although the underlying algebra is time consuming, it needs be done just once and the outcome is fairly simple.

Section 4 is concerned with semidiscretisation. We consider several alternatives, finally concluding that finite differences of appropriately high order are not just the simplest but the most appropriate option, since they lend themselves to very rapid calculation of matrix exponentials.

The computation of matrix exponentials is the theme of Section 5. Most exponentials in (1.7) are trivial to calculate because the underlying matrix is either diagonal or a circulant. The one exception are matrices of size $\mathcal{O}(\varepsilon^{\alpha})$ for sufficiently large $\alpha > 0$. Therefore, once they are calculated by Krylov subspace methods, the price tag is very small.

In Section 6 we present a number of preliminary numerical results, while Section 7

is devoted to brief conclusions and pointers for future research.

2 A Lie-algebraic setting

2.1 An algebra of operators

The vector field in the linear Schrödinger equation (1.5) is a linear combination of the action of two operators, ∂_x^2 and the multiplication by the interaction potential V. Since the calculation of exponential splittings entails nested commutation, the focus of our interest is on the free Lie algebra

$$\mathfrak{F} = \mathrm{FLA}\{\partial_x^2, V\},$$

i.e. the linear-space closure of all nested commutators generated by ∂_x^2 and V. The elements of $\mathfrak{F}$ are operators, acting on the initial value of (1.5): for the purpose of this paper and for simplicity sake we assume that the initial value, hence the solution of (1.5) for moderate values of $t \geq 0$, is a periodic function in $\mathrm{C}^\infty[-1,1]$, but our results extend in a straightforward manner to functions of lower smoothness.

To compute commutators we need in principle to describe their action on functions, e.g.

$$[V, \partial_x^2]u = V(\partial_x^2 u) - \partial_x^2(Vu) = -(\partial_x^2 V)u - 2(\partial_x V)\partial_x u$$

implies that $[V, \partial_x^2] = -(\partial_x^2 V) - 2(\partial_x V)\partial_x$. We list the lowest order further commutators that form a so called Hall basis (Reutenauer 1993) of the free Lie-algebra $\mathfrak{F}$ in Table 1. "Grade" therein refers to the number of "letters" V and ∂_x^2 in the expression, while χ_j is the coefficient of this term in the symmetric BCH formula, cf. Subsection 2.2.

Table 1: The terms of the Hall basis of $\mathfrak{F}$ of grade ≤ 4.

j	Nested commutator	χ_j	grade
H_1	∂_x^2	1	1
H_2	V	1	1
H_3	$[V, \partial_x^2]$	0	2
H_4	$[[V, \partial_x^2], \partial_x^2]$	$-\frac{1}{24}$	3
H_5	$[[V, \partial_x^2], V]$	$-\frac{1}{12}$	3
H_6	$[[[V, \partial_x^2], \partial_x^2], \partial_x^2]$	0	4
H_7	$[[[V, \partial_x^2], \partial_x^2], V]$	0	4
H_8	$[[[V, \partial_x^2], V], V]$	0	4

Computing the commutators H_j, $j = 3, 4, \ldots, 8$ explicitly, we have

$$\begin{aligned}
H_3 &= -(\partial_x^2 V) - 2(\partial_x V)\partial_x,\\
H_4 &= (\partial_x^4 V) + 4(\partial_x^3 V)\partial_x + 4(\partial_x^2 V)\partial_x^2,\\
H_5 &= -2(\partial_x V)^2,\\
H_6 &= -(\partial_x^6 V) - 6(\partial_x^5 V)\partial_x - 12(\partial_x^4 V)\partial_x^2 - 8(\partial_x^3 V)\partial_x^3,\\
H_7 &= 4[(\partial_x V)(\partial_x^3 V) + (\partial_x^2 V)^2] + 8(\partial_x V)(\partial_x^2 V)\partial_x,\\
H_8 &= 0.
\end{aligned}$$

We note that all the terms belong to the set

$$\mathfrak{G} = \left\{ \sum_{k=0}^{n} y_k(x)\partial_x^k \,:\, n \in \mathbb{Z}_+,\ y_0, \ldots, y_n \in \mathrm{C}^\infty[-1,1] \text{ periodic with period } 2 \right\}.$$

It is trivial to observe that $\mathfrak{G}$ is itself a Lie algebra.

There are numerous cancellations, similar to $H_8 = 0$, because of the special structure induced by the letters ∂_x^2 and $V(x)$, nevertheless, for our exposition it is more appropriate to operate in the larger Lie-algebra $\mathfrak{G}$, where all cancellations will be taken care of by simple computation of the commutators, according to

$$\begin{aligned}
\left[\sum_{i=0}^{n} f_i(x)\partial_x^i, \sum_{j=0}^{m} g_j(x)\partial_x^j \right] = &\sum_{i=0}^{n}\sum_{j=0}^{m}\sum_{\ell=0}^{i} \binom{i}{\ell} f_i(x) \left(\partial_x^{i-\ell} g_j(x)\right) \partial_x^{\ell+j}\\
&- \sum_{j=0}^{m}\sum_{i=0}^{n}\sum_{\ell=0}^{j} \binom{j}{\ell} g_j(x) \left(\partial_x^{j-\ell} f_i(x)\right) \partial_x^{\ell+i}. \qquad (2.1)
\end{aligned}$$

2.2 The symmetric BCH formula

Let X and Y be two terms in a Lie algebra $\mathfrak{g}$. The *symmetric Baker–Campbell–Hausdorff formula* (usually known in an abbreviated form as the symmetric BCH formula) is

$$\mathrm{e}^{\frac{1}{2}X}\mathrm{e}^{Y}\mathrm{e}^{\frac{1}{2}X} = \mathrm{e}^{\mathrm{sBCH}(X,Y)}, \qquad (2.2)$$

where

$$\begin{aligned}
&\mathrm{sBCH}(tX,tY) \qquad (2.3)\\
&= t(X+Y) - t^3(\tfrac{1}{24}[[Y,X],X] - \tfrac{1}{12}[[Y,X],Y]) + t^5(\tfrac{7}{5760}[[[[Y,X],X],X],X]\\
&\quad + \tfrac{7}{1440}[[[[Y,X],X],X],Y] + \tfrac{1}{180}[[[[Y,X],X],Y],Y]\\
&\quad + \tfrac{1}{720}[[[[Y,X],Y],Y],Y] + \tfrac{1}{480}[[[Y,X],X],[Y,X]]\\
&\quad - \tfrac{1}{360}[[[Y,X],Y],[Y,X]]) + t^7(-\tfrac{31}{967680}[[[[[[Y,X],X],X],X],X],X]\\
&\quad - \tfrac{31}{161280}[[[[[[Y,X],X],X],X],X],Y] - \tfrac{13}{30240}[[[[[[Y,X],X],X],X],Y],Y]\\
&\quad - \tfrac{53}{120960}[[[[[[Y,X],X],X],Y],Y],Y] - \tfrac{1}{5040}[[[[[[Y,X],X],Y],Y],Y],Y]\\
&\quad - \tfrac{1}{30240}[[[[[[Y,X],Y],Y],Y],Y],Y] - \tfrac{53}{161280}[[[[[Y,X],X],X],X],[Y,X]]\\
&\quad - \tfrac{11}{12096}[[[[[Y,X],X],X],Y],[Y,X]] - \tfrac{3}{4480}[[[[[Y,X],X],Y],Y],[Y,X]]\\
&\quad - \tfrac{1}{10080}[[[[[Y,X],Y],Y],Y],[Y,X]] - \tfrac{1}{4032}[[[[Y,X],X],[Y,X]],[Y,X]]\\
&\quad - \tfrac{1}{6720}[[[[Y,X],Y],[Y,X]],[Y,X]] - \tfrac{19}{80640}[[[[Y,X],X],X],[[Y,X],X]]\\
&\quad - \tfrac{1}{10080}[[[[Y,X],X],Y],[[Y,X],X]] + \tfrac{17}{40320}[[[[Y,X],Y],Y],[[Y,X],X]]\\
&\quad - \tfrac{53}{60480}[[[[Y,X],X],X],[[Y,X],Y]] - \tfrac{19}{13440}[[[[Y,X],X],Y],[[Y,X],Y]]\\
&\quad - \tfrac{1}{5040}[[[[Y,X],Y],Y],[[Y,X],Y]]) + \mathcal{O}\big(t^9\big)\,.
\end{aligned}$$

The expansion (2.3) can be computed to an arbitrary power of t using an algorithm from (Casas & Murua 2009). (Because (2.3) is palindromic, only odd powers of t feature in the expansion.) An observant reader would have noticed that the coefficients are the numbers χ_j from Table 1. This is not accidental: once we let $X = \partial_x^2$ and $Y = V$, the table lists the coefficients up to $\mathcal{O}\big(t^4\big)$.

2.3 The Zassenhaus splitting

Unless X and Y commute, it is in general not true that $\mathrm{e}^{t(X+Y)} = \mathrm{e}^{tX}\mathrm{e}^{tY}$. The *Zassenhaus splitting* (Oteo 1991)

$$\mathrm{e}^{t(X+Y)} = \mathrm{e}^{tX}\mathrm{e}^{tY}\mathrm{e}^{t^2U_2(X,Y)}\mathrm{e}^{t^3U_3(X,Y)}\mathrm{e}^{t^4U_4(X,Y)}\cdots\,, \qquad (2.4)$$

where

$$\begin{aligned}
U_2(X,Y) &= \tfrac{1}{2}[Y,X],\\
U_3(X,Y) &= \tfrac{1}{3}[[Y,X],Y] + \tfrac{1}{6}[[Y,X],X],\\
U_4(X,Y) &= \tfrac{1}{24}[[[Y,X],X],X] + \tfrac{1}{8}[[[Y,X],X],Y] + \tfrac{1}{8}[[[Y,X],Y],Y],
\end{aligned}$$

quantifies this discrepancy. (More terms can be generated using the – non-symmetric – BCH formula.)

The splitting (2.4) is not well known and seldom used in computation, for the perfectly valid reason that it is not palindromic. The natural temptation is thus to *symmetrize* it and consider a palindromic splitting of the form

$$\mathrm{e}^{t(X+Y)} = \cdots\mathrm{e}^{t^5Q_5(X,Y)}\mathrm{e}^{t^3Q_3(X,Y)}\mathrm{e}^{\frac{1}{2}tX}\mathrm{e}^{tY}\mathrm{e}^{\frac{1}{2}tX}\mathrm{e}^{t^3Q_3(X,Y)}\mathrm{e}^{t^5Q_5(X,Y)}\cdots \qquad (2.5)$$

where we can deduce by inspection of (2.3), that

$$Q_3(X,Y) = \tfrac{1}{48}[[Y,X],X] + \tfrac{1}{24}[[Y,X],Y].$$

Rather than engaging in increasingly tedious calculations to compute Q_5, we replace (2.5) by a more computation-friendly splitting. We commence from the symmetric BCH formula (2.3),

$$\mathrm{e}^{-\frac{1}{2}tX}\mathrm{e}^{t(X+Y)}\mathrm{e}^{-\frac{1}{2}tX} = \mathrm{e}^{\mathrm{sBCH}(-tX,t(X+Y))},$$

which we rewrite in the form

$$\mathrm{e}^{t(X+Y)} = \mathrm{e}^{\frac{1}{2}tX}\mathrm{e}^{\mathrm{sBCH}(-tX,t(X+Y))}\mathrm{e}^{\frac{1}{2}tX}. \tag{2.6}$$

It follows from (2.3) that

$$\mathrm{sBCH}(-tX,t(X+Y)) = \mathcal{W}^{[1]} = tY + \mathcal{O}\big(t^3\big)\,,$$

and we note that we have extracted the outer term tX from the inner exponent. We iterate (2.6) over the resulting term and continue to symmetrically pull-out the lowest order terms, one by one, until the central exponent reaches the desired high order,

$$\begin{aligned}\exp t(X+Y) &= \mathrm{e}^{\frac{1}{2}tX}e^{\mathrm{sBCH}(-tX,t(X+Y))}\mathrm{e}^{\frac{1}{2}tX}\\ &= \mathrm{e}^{\frac{1}{2}tX}e^{\frac{1}{2}tY}\mathrm{e}^{\mathrm{sBCH}(-tY,\mathrm{sBCH}(-tX,t(X+Y)))}\mathrm{e}^{\frac{1}{2}tY}e^{\frac{1}{2}tX}.\end{aligned}$$

Notice that by pulling-out, we essentially subtract a term and add higher order corrections. It is important to observe that the order of the exponent given by the sBCH formula (2.6) is never decreased by this procedure[1] and thus we can easily control the order of the approximation error when truncating the BCH formula. With the notation

$$\mathcal{W}^{[k+1]} = \mathrm{sBCH}(-W^{[k]},\mathcal{W}^{[k]}), \quad \mathcal{W}^{[0]} = t(X+Y), \tag{2.7}$$

the result after s steps can be written as

$$\exp t(X+Y) = \mathrm{e}^{\frac{1}{2}W^{[0]}}e^{\frac{1}{2}W^{[1]}}\cdots\mathrm{e}^{\frac{1}{2}W^{[s]}}\mathrm{e}^{\mathcal{W}^{[s+1]}}\mathrm{e}^{\frac{1}{2}W^{[s]}}\cdots\mathrm{e}^{\frac{1}{2}W^{[1]}}\mathrm{e}^{\frac{1}{2}W^{[0]}}.$$

We emphasise that, in principle, we can freely choose the elements $W^{[k]}$ that we want to extract. A first idea is to choose the $W^{[k]} = \mathcal{O}\big(t^{2k-1}\big)$ for $k > 0$ and $W^{[0]} = \mathcal{O}(t)$, which yields a separation of powers, analogous to (2.5), and thus for s stages and approximating $\mathcal{W}^{[s+1]} = W^{[s+1]} + \mathcal{O}\big(t^{2s+3}\big)$, we obtain a symmetric Zassenhaus splitting of order $2s+2$.

We have almost established the splitting (1.7) – 'almost' because of yet another consideration. In standard splittings, e.g. in the context of a numerical solution of Hamiltonian ordinary differential equations, there is usually a single small parameter, Δt (the time step), and it makes perfect sense to expand in its powers. However, once we contemplate the discretization of (1.4), we have *three* small parameters to reckon with:

[1] Unless a non-existing term is subtracted and thus newly introduced instead of removed.

1. The built-in small parameter $\varepsilon = \omega^{-1}$;
2. The time step Δt;
3. $1/M$, where M is the number of degrees of freedom in the spatial semidiscretisation.

Although we derive our splitting *before* the infinite-dimensional operator ∂_x^2 has been discretised, we must keep the eventual discretisation at the back of our mind. In other words, sooner or later (more specifically, in Section 4) we replace ∂_x^2 with a *differentiation matrix* acting on an appropriate M-dimensional space: M might be the number of nodal values or of Fourier modes. It is elementary that the norm of a differentiation matrix corresponding to ∂_x^n scales like $\mathcal{O}(M^n)$, $n \in \mathbb{N}$. Therefore, we must employ in our analysis the shorthand $\partial_x^2 \sim \mathcal{O}\big(M^2\big)$.

We propose to deal with three small parameters in unison by converting them into a single currency. More specifically, we assume that our choice of Δt and M is governed by the *scaling laws*

$$M \sim \mathcal{O}(\omega^\rho) = \mathcal{O}\big(\varepsilon^{-\rho}\big)\,, \qquad \Delta t \sim \mathcal{O}\big(\omega^{-\sigma}\big) = \mathcal{O}(\varepsilon^\sigma)\,, \tag{2.8}$$

where $\rho, \sigma > 0$ are given. More specifically, we assume that each ∂_x^n scales like $\mathcal{O}(\varepsilon^{-n\rho})$.

The simplest and most obvious choice of parameters in (2.8) is $\rho = \sigma = \frac{1}{2}$ and this is what we assume in the next section.

3 An asymptotic splitting

3.1 Towards an asymptotic splitting

Recalling that $\rho = \sigma = \frac{1}{2}$, we commence in in this section with an asymptotic splitting (1.7) with $s = 2$, i.e. bearing the error of $\mathcal{O}\big(\varepsilon^{7/2}\big)$. Given that $\varepsilon > 0$ is very small, this presents a method which is very accurate – arguably, of higher accuracy than required in standard numerical computations. We will expand the commutators in powers of ε and successively remove them from the core of our expansion, aiming for $W^{[j]} = \mathcal{O}\big(\varepsilon^{j-1/2}\big)$. Our next observation is that Δt is always multiplied by i, therefore it is handy to let

$$\tau = \mathrm{i}\Delta t = \mathcal{O}\Big(\varepsilon^{1/2}\Big)\,.$$

Note that $\tau\omega^{-1}\delta_x^2 = \mathcal{O}\big(\varepsilon^{1/2}\big)$ and $\tau\omega V = \mathcal{O}\big(\varepsilon^{-1/2}\big)$, or more generally

$$\tau^\ell \omega^m \partial_x^n = \mathcal{O}\Big(\varepsilon^{\ell/2-m-n/2}\Big)\,, \qquad \varepsilon \to 0. \tag{3.1}$$

We can now commence the algorithm (2.7), setting

$$\mathcal{W}^{[0]} = \tau\omega V + \tau\omega^{-1}\delta_x^2, \qquad W^{[0]} = W^{[0]} = \tau\omega V.$$

With the help of (2.3), we compute the commutators in $\mathcal{W}^{[1]} = \mathrm{sBCH}(-W^{[0]}, \mathcal{W}^{[0]})$ according to (2.1). This task faces us with long and tedious algebra, but can, however be automatized with a computer algebra programme. It is worth pointing out, that all

simplifications, such as $[V,\partial_x^2],V]=0$ are automatically performed once we work in the larger Lie algebra $\mathfrak{S}$ with differential operators and scalar functions. Likewise, there is no need for a tedious representation of expansion elements in, say the Hall basis, because this is done automatically in $\mathfrak{G}$.

Substituting and aggregating terms of the same order of magnitude, we obtain

$$\begin{aligned}\mathcal{W}^{[1]} = {} & \overbrace{\tau\omega^{-1}\partial_x^2+\tfrac{1}{12}\tau^3\omega(\partial_x V)^2}^{\mathcal{O}(\varepsilon^{1/2})} \\ & + \overbrace{\tfrac{1}{60}\tau^5\omega(\partial_x^2V)(\partial_xV)^2-\tfrac{1}{3}\tau^3\omega^{-1}(\partial_x^2V)\partial_x^2}^{\mathcal{O}(\varepsilon^{3/2})} - \overbrace{\tfrac{1}{3}\tau^3\omega^{-1}(\partial_x^3V)\partial_x}^{\mathcal{O}(\varepsilon^{2})} \\ & + \overbrace{\tau^3\omega^{-1}\tfrac{1}{12}(\partial_x^4V)+\tau^5\omega^{-1}\{-\tfrac{1}{90}(\partial_x^3V)(\partial_xV)+\tfrac{4}{45}(\partial_x^2V)^2\}\partial_x^2}^{\mathcal{O}(\varepsilon^{5/2})} \\ & + \overbrace{\tau^7\omega\{\tfrac{1}{840}(\partial_x^3V)(\partial_xV)^3+\tfrac{1}{945}(\partial_x^2V)^2(\partial_xV)^2\}}^{\mathcal{O}(\varepsilon^{5/2})} \\ & + \overbrace{\tau^5\omega^{-1}\{\tfrac{1}{6}(\partial_x^4V)(\partial_xV)-\tfrac{1}{90}(\partial_x^3V)(\partial_x^2V)\}\partial_x}^{\mathcal{O}(\varepsilon^{3})} + \mathcal{O}\Big(\varepsilon^{7/2}\Big).\end{aligned} \tag{3.2}$$

Unfortunately, (3.2) contains terms of order $\mathcal{O}\big(\varepsilon^2\big)$ and $\mathcal{O}\big(\varepsilon^3\big)$ that are both due to the presence of odd powers of ∂_x. This presence is worrisome for an important reason, namely *stability*. Both ∂_x^2 and multiplication by V are Hermitian operators, therefore $\tau(\omega^{-1}\partial_x^2+\omega V)$ is a skew-Hermitian operator: its exponential is thus unitary. This survives under eventual discretisation, because any reasonable approximation of ∂_x^2 preserves Hermitian structure. However, ∂_x (and, in general, odd powers of ∂_x) is a skew-symmetric operator and so are its reasonable approximations. Therefore, the introduction of odd powers of ∂_x is fraught with loss of unitarity and stability. An extra ingredient is required in our algorithm!

3.2 An intermezzo: getting even

Let y be a C^1 function. The starting point for our current construction is the identity

$$y(x)\partial_x = -\tfrac{1}{2}\int_{x_0}^x y(\xi)\,\mathrm{d}\xi\partial_x^2 - \tfrac{1}{2}\partial_x y(x) + \tfrac{1}{2}\partial_x^2\left[\int_{x_0}^x y(\xi)\,\mathrm{d}\xi\,\cdot\right], \tag{3.3}$$

where x_0 is arbitrary: its direct proof is trivial. Note that, while we have ∂_x on the left, the right-hand side features ∂_x^0 and ∂_x^2, both even powers of the differentiation operator. Since in principle we might be interested in expanding beyond $\mathcal{O}\big(\varepsilon^{7/2}\big)$ or employ different values of ρ and σ, we wish to cater not just for ∂_x but for all its odd powers. The challenge is thus to generalise (3.3) and express $y(x)\partial_x^{2s+1}$, $s\in\mathbb{Z}_+$, solely by means of even derivatives.

Theorem 1 *Let $s \in \mathbb{Z}_+$, define the real sequence $\{\beta_k\}_{k\geq 0}$ by*

$$\sum_{k=0}^{\infty} \frac{(-1)^k \beta_k}{(2k+1)!} T^k = \frac{1}{T}\left(1 - \frac{T^{1/2}}{\sinh T^{1/2}}\right)$$

and set

$$Q_k(x) = (-1)^{s-k+1}\beta_{s-k}\binom{2s+1}{2k}\partial_x^{2s-2k+1} y(x), \qquad k = 0, 1, \ldots, s, \tag{3.4}$$

$$Q_{s+1}(x) = \frac{1}{2s+2}\int_{x_0}^{x} y(\xi)\,\mathrm{d}\xi, \tag{3.5}$$

$$P_k(x) = -\sum_{\ell=k}^{s+1}\binom{2\ell}{2k}\partial_x^{2\ell-2k} Q_\ell(x), \qquad k = 1, 2, \ldots, s+1. \tag{3.6}$$

Then

$$y(x)\partial_x^{2s+1} = \sum_{k=0}^{s+1} P_k(x)\partial_x^{2k} + \sum_{k=0}^{s+1}\partial_x^{2k}[Q_k(x)\cdot\,]. \tag{3.7}$$

Proof We act on the second sum on the right of (3.7) with the Leibnitz rule, whereby

$$\begin{aligned} y\partial_x^{2s+1} &= \sum_{k=1}^{s+1} P_k\partial_x^{2k} + \sum_{\ell=0}^{s+1}\sum_{k=0}^{2\ell}\binom{2\ell}{k}(\partial_x^{2\ell-k}Q_\ell)\partial_x^k \\ &= \sum_{k=1}^{s+1} P_k\partial_x^{2k} + \sum_{k=0}^{s+1}\left[\sum_{\ell=k}^{s+1}\binom{2\ell}{2k}(\partial_x^{2(\ell-k)}Q_\ell)\right]\partial_x^{2k} \\ &\quad + \sum_{k=0}^{s}\left[\sum_{\ell=k+1}^{s+1}\binom{2\ell}{2k+1}(\partial_x^{2(\ell-k)-1}Q_\ell)\right]\partial_x^{2k+1}. \end{aligned}$$

Equating powers of ∂_x on both sides, we obtain (3.5), (3.6) and the equations

$$\sum_{\ell=k+1}^{s+1}\binom{2\ell}{2k+1}\partial_x^{2(\ell-k)-1}Q_\ell = 0, \qquad k = s-1, s-2, \ldots, 0. \tag{3.8}$$

Our contention is that there exist coefficients $\{\beta_k\}_{k\geq 0}$ such that (3.4) is true. Indeed, substituting (3.4) in (3.8) yields, after simple algebra, the triangular linear system

$$\sum_{\ell=k+1}^{s}(-1)^{s-\ell}\binom{2s-2k}{2s+1-2\ell}\beta_{s-\ell} = \frac{1}{2s-2k+1}, \qquad k = 0, 1, \ldots, s-1.$$

We deduce that

$$\sum_{\ell=0}^{k-1}(-1)^{\ell}\binom{2k}{2\ell+1}\beta_\ell = \frac{1}{2k+1}, \qquad k \in \mathbb{N}.$$

Finally, we multiply the last equation by $T^{k-1}/(2k)!$ and sum up for $k \in \mathbb{N}$. On the left we have

$$\begin{aligned}\sum_{k=1}^{\infty} \frac{1}{(2k)!} \sum_{\ell=0}^{k-1} (-1)^{\ell} \binom{2k}{2\ell+1} \beta_{\ell} T^{k-1} &= \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell}\beta_{\ell}}{(2\ell+1)!} \sum_{\ell=k+1}^{\infty} \frac{T^{k-1}}{(2k-2\ell-1)!} \\ &= \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell}\beta_{\ell}}{(2\ell+1)!} T^{\ell} \sum_{k=0}^{\infty} \frac{T^{k}}{(2k+1)!} \\ &= \frac{\sinh T^{1/2}}{T^{1/2}} \sum_{\ell=0}^{\infty} \frac{(-1)^{\ell}\beta_{\ell}}{(2\ell+1)!} T^{\ell},\end{aligned}$$

while on the right we obtain

$$\sum_{k=1}^{\infty} \frac{T^{k-1}}{(2k+1)!} = \frac{1}{T} \left(\frac{\sinh T^{1/2}}{T^{1/2}} - 1 \right).$$

This confirms (3.4) and completes the proof. □

First few values are $\beta_0 = \frac{1}{6}$, $\beta_1 = \frac{7}{60}$, $\beta_2 = \frac{31}{126}$, $\beta_3 = \frac{127}{120}$, $\beta_4 = \frac{511}{66}$, $\beta_5 = \frac{1414477}{16380}$ and $\beta_6 = \frac{8191}{6}$. Practically, just

$$\begin{aligned}y\partial_x &= -\tfrac{1}{2} \int_0^x y(\xi)\,\mathrm{d}\xi \partial_x^2 - \tfrac{1}{2}\partial_x y + \tfrac{1}{2}\partial_x^2 \left[\int_0^x y(\xi)\,\mathrm{d}\xi\, \cdot \right], \\ y\partial_x^3 &= -(\partial_x y)\partial_x^2 - \tfrac{1}{4} \int_0^x y(\xi)\,\mathrm{d}\xi \partial_x^4 + \tfrac{1}{4}\partial_x^3 y - \tfrac{1}{2}\partial_x^2[(\partial_x y)\,\cdot\,] + \tfrac{1}{4}\partial_x^4 \left[\int_0^x y(\xi)\,\mathrm{d}\xi\, \cdot \right], \\ y\partial_x^5 &= \tfrac{4}{3}(\partial_x^3 y)\partial_x^2 - \tfrac{5}{3}(\partial_x y)\partial_x^4 - \tfrac{1}{6} \int_0^x y(\xi)\,\mathrm{d}\xi \partial_x^6 - \tfrac{1}{2}\partial_x^5 y + \tfrac{7}{6}\partial_x^2[(\partial_x^3 y)\,\cdot\,] \\ &\quad - \tfrac{5}{6}\partial_x^4[(\partial_x y)\,\cdot\,] + \tfrac{1}{6}\partial_x^6 \left[\int_0^x y(\xi)\,\mathrm{d}\xi\, \cdot \right].\end{aligned}$$

are ever likely to be needed in practical computation.

3.3 An asymptotic splitting

Now, all necessary tools are available and we dedicate this subsection to illustrate how to compute the splitting (1.7) with the algorithm in Table 2. Using (3.3) to replace

Symmetric Zassenhaus Algorithm

$s := 0; \quad \mathcal{W}^{[0]} := \tau(\omega^{-1}\partial_x^2 + \omega V(x)); \quad W^{[0]} := \tau\omega V(x)$
do
  $s := s + 1$
  compute $\mathcal{W}^{[s]} := \mathrm{sBCH}(-W^{[s-1]}, \mathcal{W}^{[s-1]})$
  rewrite $\mathcal{W}^{[s]}$ in even derivatives, cf. (3.7)
  expand result in powers of ε
  define $W^{[s]} := \mathcal{O}\big(\varepsilon^{s-1/2}\big)$, s.t. $W^{[s]} - \mathcal{W}^{[s]} = \mathcal{O}\big(\varepsilon^{s+1/2}\big)$
while $s <$ desired order $s_{\max}$
Resulting method:
$\mathrm{e}^{\mathcal{W}^{[0]}} = \mathrm{e}^{W^{[0]}/2}\mathrm{e}^{W^{[1]}/2}\cdots\mathrm{e}^{W^{[s_{\max}]}}\cdots\mathrm{e}^{W^{[1]}/2}\mathrm{e}^{W^{[0]}/2} + \mathcal{O}\big(\varepsilon^{s_{\max}+1/2}\big)$

Table 2: Symmetric Zassenhaus splitting of the first kind in even order derivatives

all the occurrences of ∂_x in (3.2), we express $\mathcal{W}^{[1]}$ in the form

$$\begin{aligned}\mathcal{W}^{[1]} = {} & \overbrace{\tau\omega^{-1}\partial_x^2 + \tfrac{1}{12}\tau^3\omega(\partial_x V)^2}^{\varepsilon^{1/2}} \\ & + \overbrace{\tfrac{1}{60}\tau^5\omega(\partial_x^2 V)(\partial_x V)^2 - \tfrac{1}{6}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2 V)\,\cdot\,] + (\partial_x^2 V)\partial_x^2\}}^{\varepsilon^{3/2}} \\ & + \overbrace{\tfrac{1}{12}\tau^3\omega^{-1}(\partial_x^4 V)}^{\varepsilon^{5/2}} \\ & + \overbrace{\tfrac{1}{180}\tau^5\omega^{-1}\{-\partial_x^2[(\partial_x^3 V)(\partial_x V)\,\cdot\,] + 8\partial_x^2[(\partial_x^2 V)^2\,\cdot\,] - (\partial_x^3 V)(\partial_x V)\partial_x^2 + 8(\partial_x^2 V)^2\partial_x^2\}}^{\varepsilon^{5/2}} \\ & + \overbrace{\tfrac{1}{7560}\tau^7\omega\{9(\partial_x^3 V)(\partial_x V)^3 + 8(\partial_x^2 V)^2(\partial_x V)^2\}}^{\varepsilon^{5/2}} + \mathcal{O}\Big(\varepsilon^{7/2}\Big)\,.\end{aligned}$$

Recall that we have started the algorithm with

$$\mathcal{R}_0 = \tfrac{1}{2}W^{[0]} = \tfrac{1}{2}\tau\omega V$$

and, to progress to the second stage, we choose to eliminate the lowest ε-order term,

$$\mathcal{R}_1 = \tfrac{1}{2}W^{[1]} = \tfrac{1}{2}\tau\omega^{-1}\partial_x^2 + \tfrac{1}{24}\tau^3\omega(\partial_x V)^2$$

from $\mathcal{W}^{[1]}$.

Although the new $W^{[1]}$ and $\mathcal{W}^{[1]}$ are more complicated, the computations are now much simpler. The main reason is that the ε-order behaves under commutation like

$$[\tau^{i_1}\omega^{j_1}f(x)\partial_x^{k_1}, \tau^{i_2}\omega^{j_2}g(x)\partial_x^{k_2}] = \mathcal{O}\big(\tau^{i_1+i_2}\omega^{j_1+j_2}\partial_x^{k_1+k_2-1}\big)\,,$$

and thus, the order increases under very general assumptions. The first commutators then become,

$$[W^{[1]}, \mathcal{W}^{[1]}] = \mathcal{O}\big(\varepsilon^2\big) \text{ and } [[\mathcal{W}^{[1]}, W^{[1]}], W^{[1]}],\ [[\mathcal{W}^{[1]}, W^{[1]}], \mathcal{W}^{[1]}] = \mathcal{O}\Big(\varepsilon^{7/2}\Big)\,.$$

Subsequent commutators are even smaller and we obtain

$$\begin{aligned}\mathcal{W}^{[2]} &= \mathrm{sBCH}(-W^{[1]},\mathcal{W}^{[1]}) = -W^{[1]}+\mathcal{W}^{[1]}+\mathcal{O}\Big(\varepsilon^{7/2}\Big)\\ &= \overbrace{\tfrac{1}{60}\tau^5\omega(\partial_x^2V)(\partial_xV)^2-\tfrac{1}{6}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2V)\cdot]+(\partial_x^2V)\partial_x^2\}}^{\varepsilon^{3/2}}\\ &\quad+\overbrace{\tfrac{1}{12}\tau^3\omega^{-1}(\partial_x^4V)}^{\varepsilon^{5/2}}\\ &\quad+\overbrace{\tfrac{1}{180}\tau^5\omega^{-1}\{-\partial_x^2[(\partial_x^3V)(\partial_xV)\cdot]+8\partial_x^2[(\partial_x^2V)^2\cdot]-(\partial_x^3)(\partial_xV)\partial_x^2+8(\partial_x^2V)^2\partial_x^2\}}^{\varepsilon^{5/2}}\\ &\quad+\overbrace{\tfrac{1}{7560}\tau^7\omega\{9(\partial_x^3V)(\partial_xV)^3+8(\partial_x^2V)^2(\partial_xV)^2\}}^{\varepsilon^{5/2}}+\mathcal{O}\Big(\varepsilon^{7/2}\Big).\end{aligned}$$

In the next iteration, we pull out the $\mathcal{O}\big(\varepsilon^{3/2}\big)$ term,

$$2\mathcal{R}_2 = W^{[2]} = \tfrac{1}{60}\tau^5\omega(\partial_x^2V)(\partial_xV)^2-\tfrac{1}{6}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2V)\cdot]+(\partial_x^2V)\partial_x^2\}$$

and need to compute $\mathcal{W}^{[3]}$. Because of $[W^{[2]},\mathcal{W}^{[2]}]=\mathcal{O}\big(\varepsilon^4\big)$, again, commutators can be disregarded to obtain $\mathcal{T}_3=\mathcal{W}^{[3]}=\mathcal{O}\big(\varepsilon^{5/2}\big)$: the asymptotic splitting is therefore

$$\mathcal{S}^{[1]}_{(\frac12,\frac12),2} = \mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{T}_3}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0}. \tag{3.9}$$

where

$$\begin{aligned}\mathcal{R}_0 &= \tfrac12\tau\omega V = \mathcal{O}\Big(\varepsilon^{-1/2}\Big), \qquad (3.10)\\ \mathcal{R}_1 &= \tfrac12\tau\omega^{-1}\partial_x^2+\tfrac{1}{24}\tau^3\omega(\partial_xV)^2 = \mathcal{O}\Big(\varepsilon^{1/2}\Big),\\ \mathcal{R}_2 &= -\tfrac{1}{12}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2V)\cdot]+(\partial_x^2V)\partial_x^2\}+\tfrac{1}{120}\tau^5\omega(\partial_x^2V)(\partial_xV)^2 = \mathcal{O}\Big(\varepsilon^{3/2}\Big),\\ \mathcal{T}_3 &= \tfrac{1}{12}\tau^3\omega^{-1}(\partial_x^4V)\\ &\quad+\tfrac{1}{180}\tau^5\omega^{-1}\{-\partial_x^2[(\partial_x^3V)(\partial_xV)\cdot]+8\partial_x^2[(\partial_x^2V)^2\cdot]-(\partial_x^3)(\partial_xV)\partial_x^2\\ &\qquad+8(\partial_x^2V)^2\partial_x^2\}+\tfrac{1}{7560}\tau^7\omega\{9(\partial_x^3V)(\partial_xV)^3+8(\partial_x^2V)^2(\partial_xV)^2\} = \mathcal{O}\Big(\varepsilon^{5/2}\Big)\end{aligned}$$

The notation $\mathcal{S}^{[1]}_{(\frac12,\frac12),2}$ is mostly self-explanatory: $(\frac12,\frac12)$ refers to the values of ρ and σ, while $s=2$. The superscript $^{[1]}$ stands for an asymptotic splitting *of the first kind:* in Subsection 3.5 we consider an alternative splitting (with initial $W^{[0]}$ equalling $-\tau\omega^{-1}\partial_x^2$), which we designate as an asymptotic splitting of the second kind.

Once we replace derivatives by differentiation matrices, the evaluation of a single time step $\boldsymbol{u}^{n+1}=\tilde{\mathcal{S}}^{[1]}_{(\frac12,\frac12),2}\boldsymbol{u}^n$ requires in principle 7 exponentials. However, we note that, once we use nodal values in semidiscretisation, the discretised matrix $\mathcal{R}_0$ is diagonal and the computation of its exponential can be accomplished in $\mathcal{O}(M)$ operations.[2] This is an important point because $\mathcal{R}_0$ is the largest matrix present. All other

[2]Using a Fourier basis the cost is $\mathcal{O}(M\log M)$.

matrices are $\mathcal{O}\big(\varepsilon^{1/2}\big)$ or less and, as will be clear in Section 5, their computation with Krylov subspace methods is very affordable.

3.4 Stability

The convergence of classical methods for initial-value partial differential equations is governed by the Lax equivalence theorem: convergence equals consistency plus stability (Iserles 2008). Our method is clearly consistent but the question is whether, once derivatives are replaced by differentiation matrices, the ensuing finite-dimensional operator is stable in the sense of Lax. Within our formalism this is equivalent to

$$\lim_{\varepsilon\to 0}\limsup_{n\to\infty}\|(\tilde{\mathcal{S}}^{[1]}_{(\frac{1}{2},\frac{1}{2}),2})^n\|<\infty, \tag{3.11}$$

where $\tilde{\mathcal{S}}^{[1]}_{(\frac{1}{2},\frac{1}{2}),2}$ is the finite-dimensional discretisation of $\mathcal{S}^{[1]}_{(\frac{1}{2},\frac{1}{2}),2}$. Here $\|\cdot\|$ is the standard Euclidean norm.

The condition (3.11) is clearly implied by $\tilde{\mathcal{S}}^{[1]}_{(\frac{1}{2},\frac{1}{2}),2}$ being a unitary matrix for all (sufficiently small) $\varepsilon>0$, in other words by the discretisation method being *unitary*. This has the added virtue of the discretisation method mimicking the unitarity of the infinite-dimensional operator $\exp(\mathrm{i}t(\omega^{-1}\partial_x^2+\omega V))$. (The latter follows because both $\mathrm{i}\partial_x^2$ and multiplication by $\mathrm{i}V$ are skew-Hermitian.) Consequently, in that case we obtain a *geometric integrator* in the sense of (Faou 2012, Hairer, Lubich & Wanner 2006, Lubich 2008).

Suppose that $\mathcal{R}_0,\mathcal{R}_1,\mathcal{R}_2$ and $\mathcal{T}_3$ are all unitary matrices. Then, by (3.9), so is $\mathcal{S}^{[1]}_{(\frac{1}{2},\frac{1}{2}),2}$. But are they?

The discretisation of ∂_x^2 is the subject of Section 4. Here we preempt the discussion by identifying two options. Either we choose the unknowns as nodal values (e.g. by using finite differences, spectral collocation or a pseudo-spectral method) or as Fourier coefficients (using a spectral method). In the first case ∂_x^2 is approximated by a *symmetric circulant* $\mathcal{K}$ and multiplication with V by a *diagonal matrix* $\mathcal{D}$. In the second case all is reversed: ∂_x^2 is approximated by a diagonal matrix and multiplication by V by a symmetric circulant. In either case $\mathrm{i}\mathcal{K},\mathrm{i}\mathcal{D}\in\mathfrak{su}_M(\mathbb{C})$, the Lie algebra of $M\times M$ complex skew-Hermitian matrices. It follows at once that $\tilde{\mathcal{R}}_0,\tilde{\mathcal{R}}_1\in\mathfrak{su}_M(\mathbb{C})$, consequently $\mathrm{e}^{\tilde{\mathcal{R}}_0},\mathrm{e}^{\tilde{\mathcal{R}}_1}\in\mathrm{U}_M(\mathbb{C})$.[3] However,

$$\tilde{\mathcal{R}}_2=-\tfrac{1}{12}\tau^3\omega^{-1}(\mathcal{K}\mathcal{D}_{\partial_x^2V}+\mathcal{D}_{\partial_x^2V}\mathcal{K})+\tfrac{1}{120}\tau^5\omega\mathcal{D}_{(\partial_x^2V)(\partial_xV)^2},$$

where $\mathcal{D}_f$ is the discretisation of a multiplication by f, may seem problematic: $\mathrm{i}\mathcal{K},\mathrm{i}\mathcal{D}\in\mathfrak{su}_M(\mathbb{C})$ need not imply that $\mathrm{i}\mathcal{K}\mathcal{D},\mathrm{i}\mathcal{D}\mathcal{K}\in\mathfrak{su}_M(\mathbb{C})$.[4] Fortunately, it is trivial to verify that $\mathrm{i}(\mathcal{K}\mathcal{D}+\mathcal{D}\mathcal{K})\in\mathfrak{su}_M(\mathbb{C})$ and this proves that $\tilde{\mathcal{R}}_2\in\mathfrak{su}_M(\mathbb{C})$. Examining carefully (3.10), we observe that so does $\tilde{\mathcal{T}}_3$. We deduce that $\mathrm{e}^{\tilde{\mathcal{R}}_2},\mathrm{e}^{\tilde{\mathcal{T}}_3}\in\mathrm{U}_M(\mathbb{C})$ and stability (3.11) follows.

[3] As before, a tilde denotes a discretisation.

[4] All powers of τ are odd, because of the palindromy of the symmetric BCH formula. Since $\tau=\mathrm{i}\Delta t$, this means that they always contribute a multiple of $\pm\mathrm{i}$.

The unitarity of $\mathcal{S}^{[1]}_{(\frac{1}{2},\frac{1}{2}),2}$ is not accidental and we do not need to repeat our analysis on a case-by-case basis for different values of ρ, σ and s or for the asymptotic splittings of the second kind from the next subsection.

Theorem 2 *Supposing that the splitting (1.7) has been derived by the symmetric Zassenhaus algorithm of Table 2, it is true that* $W^{[i]} \in \mathfrak{su}(\mathbb{C})$ *for all* $i \geq 0$ *and thus also* $\mathcal{R}_0, \mathcal{R}_1, \ldots, \mathcal{R}_s, \mathcal{T}_{s+1} \in \mathfrak{su}(\mathbb{C})$.

Proof The algorithm starts from a skew-symmetric operator $\mathcal{W}^{[0]}$ and, in each step, pulls out a term $W^{[j]}$ via the symmetric BCH formula (2.3). Assume, that $W^{[j]}$ is skew-symmetric, then so will $\mathcal{W}^{[j+1]}$ because skew-symmetry is preserved under commutation. What remains to be shown is that at each step, the lowest order ε terms in $\mathcal{W}^{[j]}$ after the 'odd to even' substitution (3.3), namely $W^{[j]}$, are indeed skew-symmetric. Recall that, by assumption, $\mathcal{W}^{[j]}$ is skew-symmetric and since the substitution is exact, it will still be. For this reason, it is clear that its summands are either skew-symmetric or come in skew-symmetric pairs $\mathrm{i}(\mathcal{K}^l\mathcal{D} + \mathcal{D}\mathcal{K}^l)$, where $\mathcal{K}^k$ is a symmetric discretisation of ∂_x^{2k}. The algorithm groups terms with the same scaling and since $\mathcal{D}\mathcal{K}^k = \mathcal{O}\big(\varepsilon^{-k}\big) = \mathcal{K}^k\mathcal{D}$, the pair will not be split and thus $W^{[j]} \in \mathfrak{su}(\mathbb{C})$. □

3.5 An asymptotic splitting of the second kind

It is natural to commence the symmetric Zassenhaus splitting from the largest term, $\tau\omega V$. However, natural need not be the best: as it turns out, there is an advantage to start from the *smaller* term, $\tau\omega^{-1}\partial_x^2$. Although this leads to a larger number of terms, we will demonstrate in this subsection that this procedure leads to exponentials which are easier to compute.

Revisiting the narrative of Subsection 3.1, while proceeding faster and sparing the reader many details of algebraic computations, we start from

$$2\mathcal{R}_{-1} = W^{[0]} = \tau\omega^{-1}\partial_x^2, \qquad \mathcal{W}^{[0]} = \tau\omega^{-1}\partial_x^2 + \tau\omega V$$

This results in

$$\mathcal{W}^{[1]} = \mathrm{sBCH}(-W^{[0]}, \mathcal{W}^{[0]}) = \sum_{j=-1}^{\infty} \mathcal{W}_j^{[1]}, \qquad \text{where} \qquad \mathcal{W}_j^{[1]} = \mathcal{O}\Big(\varepsilon^{j+1/2}\Big),$$

and

$$\begin{aligned}
\mathcal{W}_{-1}^{[1]} &= \tau\omega V,\\
\mathcal{W}_{0}^{[1]} &= -\tfrac{1}{6}\tau^3\omega(\partial_x V)^2\\
\mathcal{W}_{1}^{[1]} &= \tfrac{1}{12}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2 V)\cdot\,] + (\partial_x^2 V)\partial_x^2\} + \tfrac{2}{45}\tau^5\omega(\partial_x^2 V)(\partial_x V)^2\\
\mathcal{W}_{2}^{[1]} &= -\tfrac{1}{24}\tau^3\omega^{-1}(\partial_x^4 V) - \tau^5\omega^{-1}\{\tfrac{1}{30}\partial_x^2[(\partial_x^3 V)(\partial_x V)\cdot\,] + \tfrac{1}{30}(\partial_x^3 V)(\partial_x V)\partial_x^2\\
&\quad -\tfrac{1}{60}\partial_x^2[(\partial_x^2 V)^2\cdot\,] - \tfrac{1}{60}(\partial_x^2 V)^2\partial_x^2\} - \tau^7\omega\{\tfrac{1}{630}(\partial_x^3 V)(\partial_x V)^3\\
&\quad +\tfrac{19}{945}(\partial_x^2 V)^2(\partial_x V)^2\}.
\end{aligned}$$

We next remove $2\mathcal{R}_0 = W^{[1]} = \mathcal{W}_{-1}^{[1]} = \mathcal{O}\big(\varepsilon^{1/2}\big)$ and obtain, with the short hand $X = -W^{[1]}$, $Y = \mathcal{W}^{[1]}$,

$$\mathcal{W}^{[2]} = \mathrm{sBCH}(X,Y) = X + Y - \tfrac{1}{24}[[Y,X],X] - \tfrac{1}{12}[[Y,X],Y] + \mathcal{O}\Big(\varepsilon^{7/2}\Big) = \sum_{j=0}^{\infty} \mathcal{W}_j^{[2]},$$

where

$$\begin{aligned}
\mathcal{W}_0^{[2]} &= -\tfrac{1}{6}\tau^3\omega(\partial_x V)^2,\\
\mathcal{W}_1^{[2]} &= \tfrac{1}{12}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2 V)\cdot] + (\partial_x^2 V)\partial_x^2\} + \tfrac{7}{120}\tau^5\omega(\partial_x^2 V)(\partial_x V)^2,\\
\mathcal{W}_2^{[2]} &= -\tfrac{1}{24}\tau^3\omega^{-1}(\partial_x^4 V) - \tau^5\omega^{-1}\{\tfrac{1}{30}\partial_x^2[(\partial_x^3 V)(\partial_x V)\cdot] + \tfrac{1}{30}(\partial_x^3 V)(\partial_x V)\partial_x^2\\
&\quad - \tfrac{1}{60}\partial_x^2[(\partial_x^2 V)^2\cdot] - \tfrac{1}{60}(\partial_x^2 V)^2\partial_x^2\} - \tau^7\omega\{\tfrac{1}{140}(\partial_x^3 V)(\partial_x V)^3\\
&\quad + \tfrac{17}{840}(\partial_x^2 V)^2(\partial_x V)^2.
\end{aligned}$$

Next,

$$\mathcal{R}_1 = \tfrac{1}{2}W^{[2]} = \tfrac{1}{2}\mathcal{W}_0^{[2]} = -\tfrac{1}{12}\tau^3\omega(\partial_x V)^2,$$

and we deduce that the relevant terms of $\mathcal{W}^{[3]} = \sum_{j=1}^{\infty}\mathcal{W}_j^{[3]}$ are

$$\begin{aligned}
\mathcal{W}_1^{[3]} &= \tfrac{1}{12}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2 V)\cdot] + (\partial_x^2 V)\partial_x^2\} + \tfrac{7}{120}\tau^5\omega(\partial_x^2 V)(\partial_x V)^2,\\
\mathcal{W}_2^{[3]} &= -\tfrac{1}{24}\tau^3\omega^{-1}(\partial_x^4 V) - \tau^5\omega^{-1}\{\tfrac{1}{30}\partial_x^2[(\partial_x^3 V)(\partial_x B)\cdot] + \tfrac{1}{30}(\partial_x^3 V)(\partial_x V)\partial_x^2 -\\
&\quad \tfrac{1}{60}\partial_x^2[(\partial_x^2 V)^2\cdot] - \tfrac{1}{60}(\partial_x^2 V)^2\partial_x^2\} - \tau^7\omega\{\tfrac{1}{140}(\partial_x^3 V)(\partial_x V)^3\\
&\quad + \tfrac{17}{840}(\partial_x^2 V)^2(\partial_x V)^2.
\end{aligned}$$

And, finally,

$$\mathcal{R}_2 = \tfrac{1}{2}\mathcal{W}_1^{[3]}, \qquad \mathcal{T}_3 = \mathcal{W}_2^{[3]}.$$

The outcome is the splitting

$$\mathcal{S}^{[2]}_{(\frac{1}{2},\frac{1}{2}),2} = \mathrm{e}^{\mathcal{R}_{-1}}\mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{T}_3}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_0}\mathrm{e}^{\mathcal{R}_{-1}}, \tag{3.12}$$

where

$$\begin{aligned}
\mathcal{R}_{-1} &= \tfrac{1}{2}\tau\omega^{-1}\partial_x^2,\\
\mathcal{R}_0 &= \tfrac{1}{2}\tau\omega V,\\
\mathcal{R}_1 &= -\tfrac{1}{12}\tau^3\omega(\partial_x V)^2,\\
\mathcal{R}_2 &= \tfrac{1}{24}\tau^3\omega^{-1}\{\partial_x^2[(\partial_x^2 V)\cdot] + (\partial_x^2 V)\partial_x^2\} + \tfrac{7}{240}\tau^5\omega(\partial_x^2 V)(\partial_x V)^2,\\
\mathcal{T}_3 &= -\tfrac{1}{24}\tau^3\omega^{-1}(\partial_x^4 V) - \tau^5\omega^{-1}\{\tfrac{1}{30}\partial_x^2[(\partial_x^3 V)(\partial_x V)\cdot] + \tfrac{1}{30}(\partial_x^3 V)(\partial_x V)\partial_x^2 -\\
&\quad \tfrac{1}{60}\partial_x^2[(\partial_x^2 V)^2\cdot] - \tfrac{1}{60}(\partial_x^2 V)^2\partial_x^2\} - \tau^7\omega\{\tfrac{1}{140}(\partial_x^3 V)(\partial_x V)^3\\
&\quad + \tfrac{17}{840}(\partial_x^2 V)^2(\partial_x V)^2.
\end{aligned}$$

Compare (3.12) with (3.9): we have presently 9 exponentials in place of 7. However, $\tilde{\mathcal{R}}_{-1}$ is either a circulant (once we use nodal values) or a diagonal matrix (in case we

employ a Fourier expansion), while both $\tilde{\mathcal{R}}_0$ and $\tilde{\mathcal{R}}_1$ are then either diagonal matrices or circulants – the opposite of $\tilde{\mathcal{R}}_{-1}$. Therefore the cost of computing $\tilde{\mathcal{R}}_i$, $i=-1,0,1$, is $\mathcal{O}(M\log M)$ operations. This leaves $\tilde{\mathcal{R}}_2=\mathcal{O}\big(\varepsilon^{3/2}\big)$ and $\tilde{\mathcal{T}}_3=\mathcal{O}\big(\varepsilon^{5/2}\big)$, which need be computed with Krylov subspace methods. The small magnitude of both these matrices means that their exponentials can be computed in ridiculously small number of Krylov iterations, cf. Section 5.

Note that the palindromic property allows us to further reduce the number of exponentials if no output at intermediate steps is required. This so-called First-Same-As-Last (FSAL) property, together with the observation that $[\mathcal{R}_0,\mathcal{R}_1]=0$, hence that $\mathrm{e}^{\mathcal{R}_0+\mathcal{R}_1}$ can be computed easily, effectively yield a method

$$\tilde{\mathcal{S}}(\alpha)^{[2]}_{(\frac12,\frac12),2}=\mathrm{e}^{\mathcal{R}_0+\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{T}_3}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{R}_1+\mathcal{R}_0}\mathrm{e}^{\alpha\mathcal{R}_{-1}}, \tag{3.13}$$

where the first step has to be calculated with $\alpha=1$, and further steps with $\alpha=2$. Whenever output is required, we apply $\mathrm{e}^{\mathcal{R}_{-1}}$, and initialise the method by letting $\alpha=1$ for the next step. All in all, we only need to compute six exponentials each step, two of which are of diagonal matrices, $\mathcal{R}_1$ is circulant and the remaining ones can be approximated cheaply by Krylov methods.

4 The semidiscretisation

The asymptotic splittings (3.9) and (3.12) are expressed in operatorial terms: to render them into proper computational algorithms we must replace ∂_x^2 with an appropriate differentiation matrix, acting on an M-dimensional space.

It is common in the numerical solution of the Schrödinger equation to use *spectral* discretization (Faou 2012, Jin et al. 2011). Thus, the unknowns are the Fourier coefficients of u, $\mathcal{K}$ is a diagonal matrix, $\mathcal{K}_{j,j}=-\pi^2j^2$, $j=1,2,\dots,M$ (note that indeed $\|\mathcal{K}\|=\mathcal{O}\big(M^2\big)=\mathcal{O}\big(\varepsilon^{-1}\big)$) and the operator of a multiplication by f is discretised a circulant $\mathcal{D}_f$, composed of the Fourier coefficients of f. We deduce that, for any $\boldsymbol{v}\in\mathbb{C}^M$, the computation of $\mathcal{K}\boldsymbol{v}$ costs $\mathcal{O}(M)$ operations, while the price tag of $\mathcal{D}_f\boldsymbol{v}$, computed with FFT, is $\mathcal{O}(M\log M)$. The main appeal of spectral methods is that they exhibit *spectral convergence:* for sufficiently large M the error decays faster than $M^{-\alpha}=\mathcal{O}\big(\varepsilon^{\alpha/2}\big)$ for any $\alpha>0$. In classical terms, the method is of an infinite order.

Alternative methods of discretisation are all based on *nodal values.* In all such methods a multiplication by a function f discretises into a diagonal matrix. Since it is compelling in the presence of period boundary conditions to use equispaced points, the unknowns are thus $u_m\approx u(m/(N+\frac12))$, $|m|\le N$, where $M=2N+1$. We prefer to use nodal values because, as evident in (3.9) and (3.12), more $\mathcal{R}_\ell$s are multiples of a function than multiples of ∂_x^2, therefore we are keen for multiplication by a function to discretise into a diagonal matrix.

We consider the following three types of nodal methods:

1. *Symmetric finite differences*

$$u''(\tfrac{m}{N+\frac12})\approx\frac{1}{(\Delta x)}\sum_{k=-r}^{r}\alpha_{r,k}u_{m+k} \tag{4.1}$$

where $r \le N$, $\Delta x = 1/(N+\frac{1}{2})$ and

$$a_{r,k} = a_{r,-k} = \frac{2(-1)^{k-1} r!^2}{k^2 (r-k)!(r+k)!}, \quad 1 \le k \le r, \qquad a_{r,0} = -2\sum_{k=1}^{r} a_{r,k}.$$

Once $m+k$ in (4.1) is outside the range $\{-N, -N+1, \dots, N\}$, we wrap around using periodicity. The method (4.1) is of order $2r$, i.e. its error behaves like $\mathcal{O}\big((\Delta x)^{2r+1}\big) = \mathcal{O}\big(\varepsilon^{r+1/2}\big)$.

In this case $\mathcal{K}$ is a banded circulant, $\mathcal{K}_{j,\ell} = a_{r,|j-\ell| \bmod N}$.

2. *Spectral collocation* (Hesthaven, Gottlieb & Gottlieb 2007) The idea here is to interpolate the solution at the nodal values using a trigonometric polynomial. Since a trigonometric interpolation can be written as a convolution with the values of the scaled *Dirichlet kernel*

$$D_N(x) = \frac{\sin((N+\frac{1}{2})\pi x)}{(2N+1)\sin(\frac{1}{2}\pi x)}$$

– in other words, $\sum_{\ell=-N}^{N} D_N(x - \ell/(N+\frac{1}{2}))u_\ell$ is an Nth-order trigonometric polynomial that equals u_m at $m/(N+\frac{1}{2})$ – therefore $\mathcal{K}_{j,\ell} = D_N''((j-\ell)/(N+\frac{1}{2}))$ is a circulant.

Like spectral methods, spectral collocation exhibits spectral convergence.

3. *Pseudo-spectral methods* (Fornberg 1998). There is nothing to prevent us from taking $r \ge N+1$ in (4.1): all it means is that we wrap around a number of times, while making the order as large as we want. Indeed, we may allow $r \to \infty$, resulting in spectral convergence, except that numerical experimentation indicates a law of diminishing returns: after several wrap-arounds any further improvement is marginal.

The differentiation matrix $\mathcal{K}$ is again a dense circulant. For example, letting $r = 2N+1$, we have $\mathcal{K}_{j,j} = a_{2N+1,0}$ and, for $j \ne \ell$, $\mathcal{K}_{j,\ell} = a_{2N+1,|j-\ell| \bmod N} + a_{2N+1,|N+1-j+\ell| \bmod N}$.

Faced with this embarrassment of riches, we opt for the simplest: a finite difference method (4.1) of adequately high order. The main reason is that there is little point in gaining spectral accuracy in space discretisation and commit an $\mathcal{O}\big(\varepsilon^{7/2}\big)$ in the time discretisation. Instead, we exploit the fact that for finite difference methods $\mathcal{K}$ is a banded circulant. Therefore, inasmuch as we can multiply $\mathcal{K}\boldsymbol{v}$ with FFT in $\mathcal{O}(M \log M)$ operations, we can do so in $\mathcal{O}(M)$ operations in a naive matrix-vector product exploiting sparsity!

Our method of choice is $r = 4$, namely

$$u_m'' \approx \frac{1}{(\Delta x)^2}\left(-\frac{1}{560}u_{m-4} + \frac{8}{315}u_{m-3} - \frac{1}{5}u_{m-2} + \frac{8}{5}u_{m-1} - \frac{205}{72}u_m + \frac{8}{5}u_{m+1} - \frac{1}{5}u_{m+2} + \frac{8}{315}u_{m+3} - \frac{1}{560}u_{m+4}\right), \qquad |m| \le N. \tag{4.2}$$

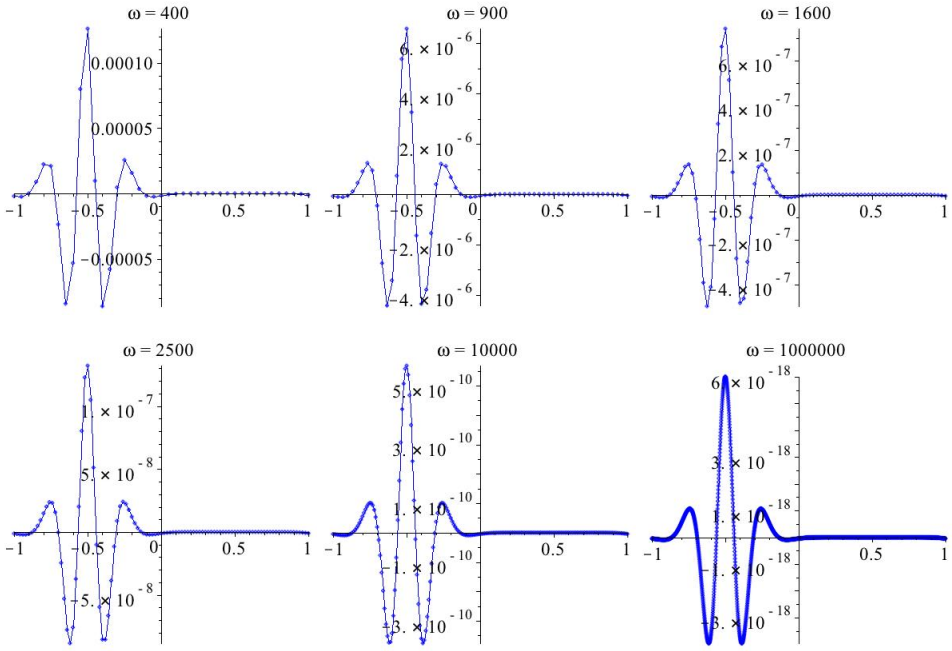

Figure 4.1: The error committed in approximating u'' using the finite difference method (4.2), $u(x) = 1/(2 + \sin \pi x)$ and $N = \omega^{1/2}$.

Therefore, $\mathcal{K}$ is a 9-diagonal circulant.

How good is (4.2)? In Figs 4.1 and 4.2 we display the error committed by (4.2) in approximating the second derivative of two functions: $1/(2 + \sin \pi x)$ and $\mathrm{e}^{\cos \pi x}$, both analytic and periodic in $[-1, 1]$. We have taken $M = 2N + 1 = \mathcal{O}\big(\varepsilon^{-1/2}\big)$ to its logical conclusion, setting $N = \omega^{1/2} = \varepsilon^{-1/2}$. It is evident that the error decreases as ω increases – little surprise, because $\Delta x = 1/(N + \frac{1}{2})$. The rate of decrease, however, is exceedingly rapid.

To quantify this rate of decrease in the error we examine the two figures more closely. The first conclusion is that, at variance with the expected situation with spectral (and spectral-type) methods, the rate of decrease is roughly the same for both functions, although the first is meromorphic and the second entire in the complex plane. More interestingly, perhaps, it is compelling that the error in each figure lives on (or exceedingly near) a scaled curve. To identify this curve, thereby predicting the size of the error and rate of its decay as ε decreases, we recall that, being of order $2r$, the coefficients of (4.1) satisfy the equation

$$\sum_{m=-r}^{r} a_m \cos m\theta = -\theta^2 + c_r \theta^{2r+2} + \mathcal{O}\big(\theta^{2r+4}\big), \qquad \theta \to 0,$$

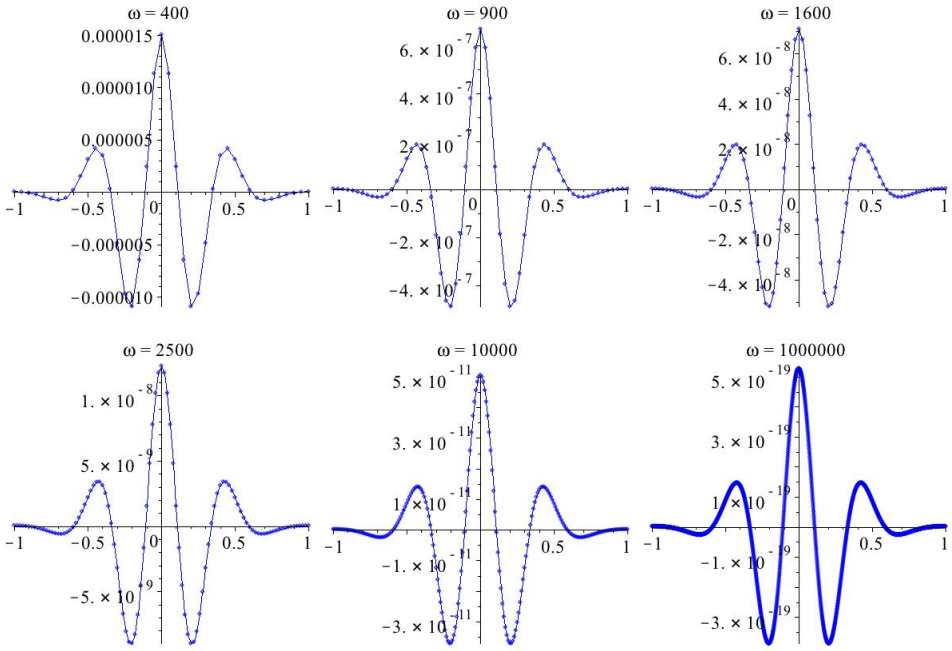

Figure 4.2: The error committed in approximating u'' using the finite difference method (4.2), $u(x) = \mathrm{e}^{\cos \pi x}$ and $N = \omega^{1/2}$.

for some c_r and its error, once (1.1) acts on a function $u \in \mathrm{C}^\infty[-1, 1]$, is

$$c_r(\Delta x)^{2r} u^{(2r+2)}(x) + \mathcal{O}\big((\Delta x)^{2r+2}\big)$$

(Iserles, Munthe-Kaas, Nørsett & Zanna 2000). In the present case $c_4 = -\frac{1}{3150}$ and we thus deduce that the local error is

$$-\tfrac{1}{3150} \frac{1}{(N + \frac{1}{2})^8} u^{(10)}(x) + \mathcal{O}\big(N^{-10}\big)\,. \tag{4.3}$$

Numerical experimentation confirms that, even for moderate values of ω, the leading term in (4.3) represents a very good approximation to the error, well in excess of what is typically expected from discretisation methods for partial differential equations of evolution.

How well does the finite difference method (4.2) compare with spectrally-convergent methods? The error for $1/(2 + \sin \pi x)$ and $\mathrm{e}^{\cos \pi x}$ is displayed in Figs 4.3 and 4.4 respectively. The error in Fig. 4.3 is a vast improvement on the top row of Fig. 4.1: although the spectacular performance of spectrally-convergent methods is hardly surprising, it is amazing nonetheless. The difference between Fig. 4.2 and Fig. 4.4 is even more striking: the reason spectral convergence for $\mathrm{e}^{\cos \pi x}$ is so fast – super-exponential, compared to exponential convergence for $1/(2 + \sin \pi x)$ – is because the first function is entire, while the second has a polar singularity at $\mathrm{i}(\sqrt{3} - 2)$. However, the sort

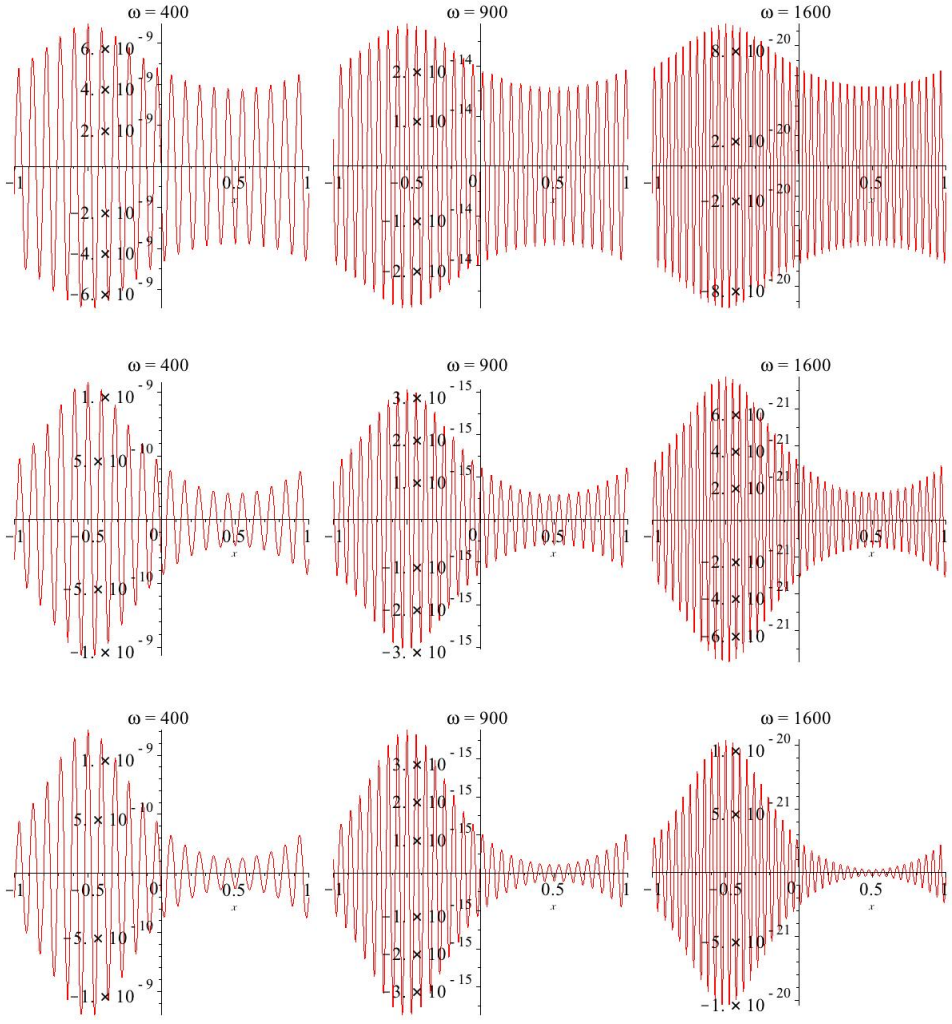

Figure 4.3: The error in approximating u'' committed by the Fourier method (top row), spectral collocation (middle row) and a pseudo-spectral method with 20 'wrap arounds' for the function $u(x) = 1/(2 + \sin \pi x)$ and $N = \omega^{1/2}$.

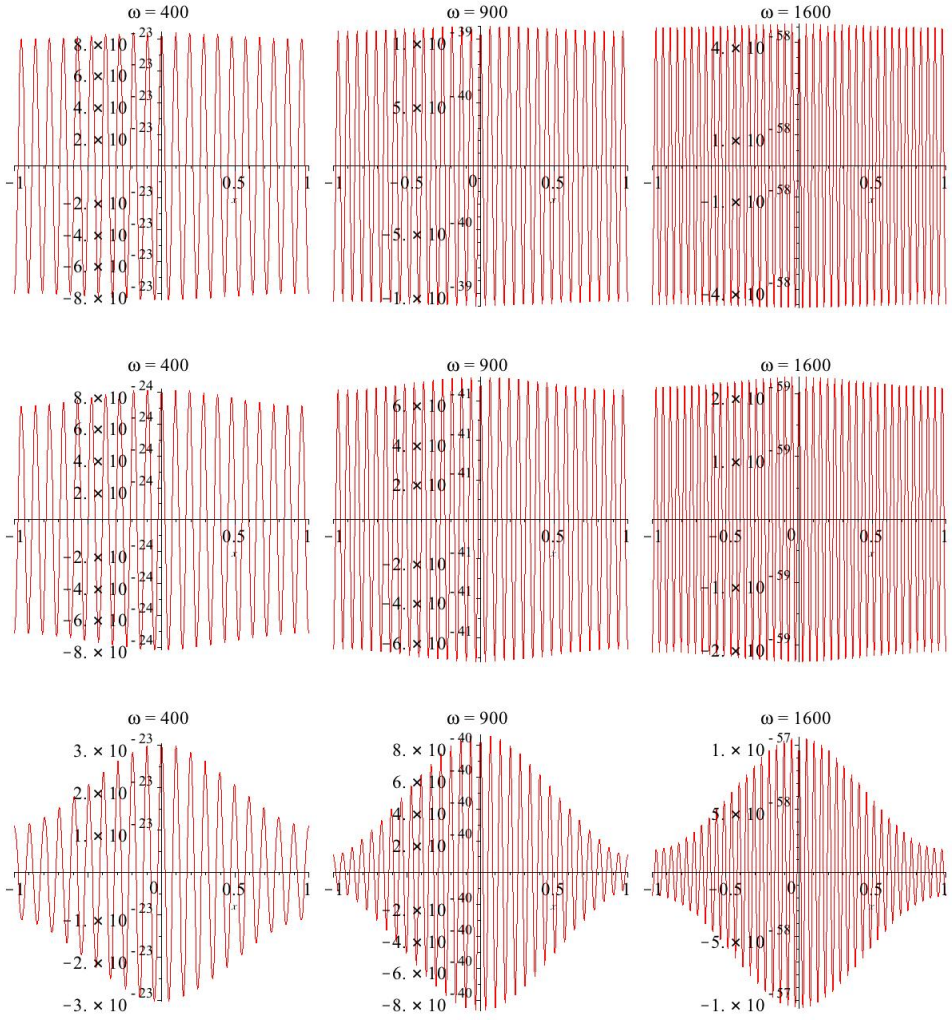

Figure 4.4: The error in approximating u'' committed by the Fourier method (top row), spectral collocation (middle row) and a pseudo-spectral method with 20 'wrap arounds' for the function $u(x) = \mathrm{e}^{\cos \pi x}$ and $N = \omega^{1/2}$.

of accuracy exhibited in Figs 4.3–4 is clearly in excess of $\mathcal{O}\big(\varepsilon^{7/2}\big)$, the error committed in the course of time discretisation. Therefore, after all, there is little advantage in using spectrally-convergent methods to discretise in space, while using the finite-difference method (4.2) has the virtue of cheaper linear algebra in the evaluation of matrix exponentials.

We need accompany our choice of a finite-difference method by an important caveat. Once u oscillates, the size of its derivatives increases rapidly. In particular, if u oscillates (as it will often do) like $\sin(\omega^{1/2}t)$ then (4.3) implies that $N=\mathcal{O}\big(\omega^{1/2}\big)$ is insufficient for reasonable accuracy. On the other hand, spectral-type methods cope well with high oscillation for $N>c\omega^{1/2}$ and $c>1$ sufficiently large. In that case, keen to use nodal values, we recommend either a pseudo-spectral method or spectral collocation.

5 The computation of exponentials

Considering splitting of the second kind (3.10), each step forward in time calls for the computation of

$$\boldsymbol{u}^{n+1}=\mathrm{e}^{\mathcal{R}_{-1}}\mathrm{e}^{\mathcal{R}_0+\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{T}_3}\mathrm{e}^{\mathcal{R}_2}\mathrm{e}^{\mathcal{R}_0+\mathcal{R}_1}\mathrm{e}^{\mathcal{R}_{-1}}\boldsymbol{u}^n, \tag{5.1}$$

where $\boldsymbol{u}^n$ is the initial value at t_n, say, while $\boldsymbol{u}^{n+1}$ approximates $u(\,\cdot\,,t_{n+1})$, where $t_{n+1}=t_n+\Delta t_n$. The matrices $\mathcal{R}_k$ and $\mathcal{T}_3$ depend on Δt_n and we aggregate $\mathcal{R}_0+\mathcal{R}_1$ consistently with the discussion by the end of Section 3. We recall that, using finite differences, spectral collocation of a pseudo-spectral method, $\boldsymbol{u}^n$ is made out of equally-distributed function values, $\mathcal{R}_{-1}$ is a Toeplitz circulant and $\mathcal{R}_0+\mathcal{R}_1$ is diagonal. However, once we use a spectral method, the entries of $\boldsymbol{u}^n$ consist of Fourier coefficients, $\mathcal{R}_{-1}$ is diagonal and $\mathcal{R}_0+\mathcal{R}_1$ is a circulant. One way or the other, we need to calculate (or approximate up to $\mathcal{O}\big(\varepsilon^{7/2}\big)$) the vector $\mathrm{e}^{\mathcal{S}}\boldsymbol{v}$ for $\boldsymbol{v}\in\mathbb{C}^M$ and three types of $M\times M$ skew-Hermitian matrices $\mathcal{S}$: (a) diagonal, (b) Toeplitz circulant, and (c) neither, yet small: $\mathcal{R}_2=\mathcal{O}\big(\varepsilon^{3/2}\big)$ and $\mathcal{T}_3=\mathcal{O}\big(\varepsilon^{5/2}\big)$. Note that we must keep in mind three prerogatives: not just error of $\mathcal{O}\big(\varepsilon^{7/2}\big)$ and low cost but also maintenance of unitarity.

Cases (a) and (b) are straightforward. The exponential of a diagonal matrix is itself diagonal and can be computed in $\mathcal{O}(M)=\mathcal{O}\big(\varepsilon^{-1/2}\big)$ operations, while $\mathrm{e}^{\mathcal{S}}\boldsymbol{v}$ for a circulant $\mathcal{S}$ can be calculated by two FFTs, at the price tag of $\mathcal{O}(M\log_2 M)=\mathcal{O}\big(-\varepsilon^{-1/2}\log\varepsilon\big)$ operations. Since both calculations are exact (up to machine accuracy), unitarity is maintained. Finally, to deal with case (c) we use a *Krylov subspace method.* Such methods have undergone many enhancements since the pioneering work of Tal Ezer & Kosloff (1984): in the current paper we adopt the approach in (Hochbruck & Lubich 1997).

Given an $M\times M$ matrix $\mathcal{A}$ and $\boldsymbol{v}\in\mathbb{C}^M$, the mth Krylov subspace is

$$\boldsymbol{K}_m(\mathcal{A},\boldsymbol{v})=\mathrm{span}\,\{\boldsymbol{v},\mathcal{A}\boldsymbol{v},\mathcal{A}^2\boldsymbol{v},\ldots,\mathcal{A}^{m-1}\boldsymbol{v}\},\qquad m\in\mathbb{N}.$$

It is well known that $\dim\boldsymbol{K}_{m-1}(\mathcal{A},\boldsymbol{v})\le\dim\boldsymbol{K}_m(\mathcal{A},\boldsymbol{v})\le\min\{m,M\}$ and we refer to (Golub & Van Loan 1996) for other properties of Krylov subspaces. The main idea is to approximate

$$\mathrm{e}^{\mathcal{A}}\boldsymbol{v}\approx\mathcal{V}_m\mathrm{e}^{\mathcal{H}_m}\mathcal{V}_m^*\boldsymbol{v}, \tag{5.2}$$

where $\mathcal{V}_m$ and $\mathcal{H}_m$ are $M \times m$ and $m \times m$ respectively and $m \ll M$. In addition, the columns of $\mathcal{V}_m$ are orthonormal vectors which form a basis of $\boldsymbol{K}_m(\mathcal{A}, \boldsymbol{v})$, while $\mathcal{H}_m$ is upper Hessenberg.

The matrices $\mathcal{V}_m$ and $\mathcal{H}_m$ are generated by the *Arnoldi process*

The Arnoldi process

$\boldsymbol{v}_1 = \boldsymbol{v}/\|\boldsymbol{v}\|_2$
for $j = 1, \ldots, m-1$ **do**
  $\boldsymbol{t} = \mathcal{A}\boldsymbol{v}_j$
  for $i = 1, \ldots, j$ **do**
    $h_{i,j} = \boldsymbol{v}_i^* \boldsymbol{t}, \qquad \boldsymbol{t} = \boldsymbol{t} - h_{i,j}\boldsymbol{v}_i$
  end for
$h_{j+1,j} = \|\boldsymbol{t}\|_2; \qquad \boldsymbol{v}_{j+1} = \boldsymbol{t}/h_{j+1,j}$
end for

(Golub & Van Loan 1996, Hochbruck & Lubich 1997). Note that, once $\mathcal{A} \in \mathfrak{su}_M(\mathbb{C})$, it follows that $\mathcal{H}_m \in \mathfrak{su}_m(\mathbb{C})$. Therefore, the columns of $\mathcal{V}_m$ being orthonormal, unitarity is conserved. Moreover, since $\mathcal{V}_m^* \boldsymbol{v} = \|\boldsymbol{v}\|_2 \boldsymbol{e}_1$, where $\boldsymbol{e}_1 \in \mathbb{C}^m$ is the first unit vector, it follows that $\mathrm{e}^{\mathcal{H}_m}\mathcal{V}_m^*\boldsymbol{v}$ is merely the first column of $\mathrm{e}^{\mathcal{H}_m}$, scaled by $\|\boldsymbol{v}\|_2$. To compute the approximation (5.2) we thus need to evaluate a *small* exponential and calculate a single matrix–vector product, at overall cost of $\mathcal{O}(mM)$ operations.

The question of an appropriate value of m is answered by the inequality

$$\|\mathrm{e}^{\mathcal{A}}\boldsymbol{v} - \mathcal{V}_m \mathrm{e}^{\mathcal{H}_m}\mathcal{V}_m^*\boldsymbol{v}\|_2 \le 12\mathrm{e}^{-\rho^2/(4m)}\left(\frac{\mathrm{e}\rho}{2m}\right)^m, \qquad m \ge \rho, \tag{5.3}$$

where $\rho = \rho(\mathcal{A})$ (Hochbruck & Lubich 1997). We know that $\mathcal{R}_3 = \mathcal{O}\big(\varepsilon^{3/2}\big)$ and assume, with very minor loss of generality, that $\rho(\mathcal{R}_3) \le c\varepsilon^{3/2}$ for some $c > 0$. We thus deduce from (5.3) that

$$\|\mathrm{e}^{\mathcal{R}_3}\boldsymbol{v} - \mathcal{V}_m \mathrm{e}^{\mathcal{H}_m}\mathcal{V}_m^*\boldsymbol{v}\|_2 \le 12\left(\frac{\mathrm{e}c}{2m}\right)^m \varepsilon^{3m/2}, \qquad m \ge \rho,$$

and $m = 3$ is sufficient to reduce the error to $\mathcal{O}\big(\varepsilon^{9/2}\big)$, well under the $\mathcal{O}\big(\varepsilon^{7/2}\big)$ error of our symmetric Zassenhaus algorithm. This is true provided that $\rho \le 3$, i.e. $\varepsilon \le (3/c)^{2/3}$: since we expect $\varepsilon > 0$ to be very small, this is not much in a way of restriction. Likewise, $\mathcal{T}_4 = \mathcal{O}\big(\varepsilon^{5/2}\big)$ and the inequality $\rho(\mathcal{T}_4) \le \tilde{c}\varepsilon^{5/2}$ implies that

$$\|\mathrm{e}^{\mathcal{T}_4}\boldsymbol{v} - \mathcal{V}_m \mathrm{e}^{\mathcal{H}_m}\mathcal{V}_m^*\boldsymbol{v}\|_2 \le 12\left(\frac{\mathrm{e}\tilde{c}}{2m}\right)^m \varepsilon^{5m/2}, \qquad m \ge \rho$$

and for $\varepsilon \le (2/\tilde{c})^{2/5}$ we need just $m = 2$. Altogether, we deduce that the computation (consistent with the error of $\mathcal{O}\big(\varepsilon^{7/2}\big)$) of $\mathrm{e}^{\mathcal{R}_3}\boldsymbol{v}$ (twice) and $\mathrm{e}^{\mathcal{T}_4}\boldsymbol{v}$ in each step (5.1) cost just $\mathcal{O}(M)$ operations.

Fig. 5.1 presents the ℓ_2 error committed in approximating $\mathrm{e}^{\mathcal{R}_3}\boldsymbol{v}$, where we have combined the semidiscretisation (4.2) with $V(x) = 10^{-2}\mathrm{e}^{-20\sin^2(\pi x/4)}$ and $v(x) = \mathrm{e}^{-4[\sin^2(5\pi x/2)+\sin^2(\pi x/2)]}$, both discretised at nodal values with $N = \lfloor \omega^{1/2} \rfloor$. Although we have used just $m = 3$ (i.e., approximated the $(2N+1) \times (2N+1)$ exponential by

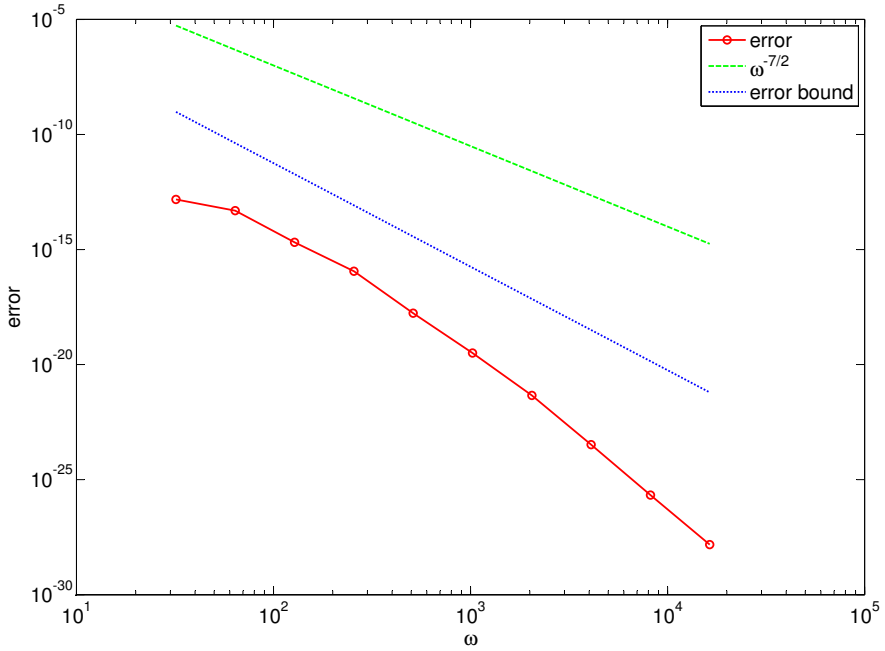

Figure 5.1: The error, compared to the error bound and the line $\omega^{-7/2} = \varepsilon^{7/2}$, in computing $\mathrm{e}^{\mathcal{R}_3}\boldsymbol{v}$.

an 3×3 one) the error is truly minuscule, well below our upper bound. Moreover, consistently with our theory (but not with conventional numerical intuition) it decreases when ω grows. Indeed, the sort of accuracies we obtain for significant values of ω are well in excess of what is required in realistic numerical computations.

In Fig. 5.2 we display identical information for $\mathrm{e}^{\mathcal{T}_4}\boldsymbol{v}$. Again, everything is consistent with our analysis: note that in this case we approximate with just a 2×2 exponential!

The slope of the error bound is steeper than $\omega^{-7/2}$ in both figures and this should cause no surprise. The error for $\mathrm{e}^{\mathcal{R}_3}\boldsymbol{v}$ decays like $\mathcal{O}\big(\omega^{-9/2}\big)$ and for $\mathrm{e}^{\mathcal{T}_4}\boldsymbol{v}$ like $\mathcal{O}\big(\omega^{-5}\big)$, both faster than required.

6 Conclusions

In this paper we have presented a methodology for the computation of the linear Schrödinger equation (1.4) with large values of ω. It has led to asymptotic exponential splitting *á la* (3.9) and (3.12), where each consecutive argument (except perhaps for one) is progressively smaller. Moreover, these arguments are skew-Hermitian (hence stability and unitarity) and the underlying exponentials are easy to compute. All this has been accomplished by creating a Lie-algebraic framework that uses nested

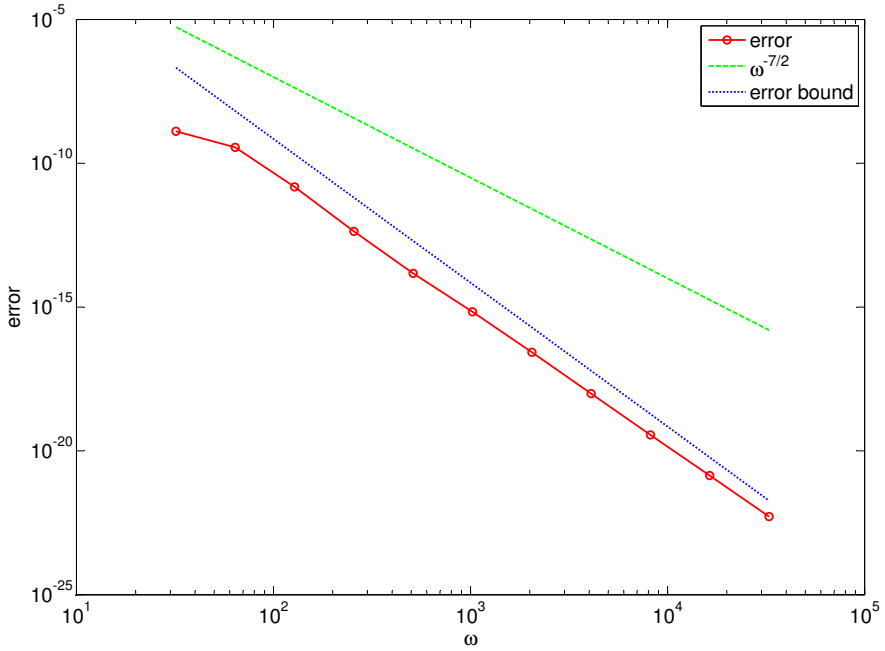

Figure 5.2: The error, compared to the error bound and the line $\omega^{-7/2} = \varepsilon^{7/2}$, in computing $\mathrm{e}^{\mathcal{T}_4}\boldsymbol{v}$.

commutators, yet avoids their expensive computation, combined with a repeated use of the symmetric BCH formula to form a symmetric Zassenhaus splitting. We have also discussed the choice of semidiscretisation and of effective means to approximate matrix exponentials.

We do not view the work of this paper as a finished and complete endeavour: it is more in the nature of an initial foray into a broad and fascinating subject area. There is a wide range of issues that our work raises. Some are already subject to active investigation, others more speculative:

1. *Asymptotic splittings with different values of ρ and σ.* Setting $\rho = \sigma = \frac{1}{2}$ is the first, perhaps the most obvious choice but, if there is one lesson of this work, it is that obvious choice need not be optimal. A great deal of further experimentation is required, not just with different values of ρ and σ but also of $s \geq 1$. Ideally, such work should avoid the error-prone tedium of human algebra: the authors are in the process of experimenting with symbolic algebra routines to this end.

2. *A time-dependent interaction potential.* In place of (1.4) we can consider the non-autonomuos equation

$$\frac{\partial u}{\partial t} = \mathrm{i}\omega^{-1}\frac{\partial^2 u}{\partial x^2} + \mathrm{i}\omega V(x,t)u, \qquad t \geq 0, \quad x \in [-1,1],$$

again with periodic boundary conditions. To this end we need to combine our methodology – algebra of operators, symmetric Zassenhaus – with Magnus expansions (Iserles et al. 2000). Preliminary work indicates that, inasmuch as this leads to considerably more complicated framework, it can fit into our narrative. Specifically, different Magnus terms can be written in a form consistent with the Lie algebra $\mathfrak{G}$. We expect to report on this work in the near future.

3. *A multivariate setting.* An effective numerical discretisation of the equation (1.3), evolving in a torus in $\mathbb{C}^d$, is the ultimate goal of this work. Insofar as small $d \geq 1$ is concerned, this is a fairly straightforward exercise but matters are more complicated when d becomes large and the cost of $\mathcal{O}\big(N^d \log N\big)$ becomes unsustainable. It is clear that, for our methodology to be scaleable to large dimensions, it must be combined with other approaches, e.g. sparse grids (Bungartz & Griebel 2004).

4. *The nonlinear Schrödinger equation.* A major challenge is to apply our methodology in a nonlinear setting, e.g. to the nonlinear Schrödinger equation

$$\mathrm{i}\varepsilon\frac{\partial u}{\partial t} = -\frac{\varepsilon^2}{2m}\frac{\partial^2 u}{\partial x^2} - V(x)u + \lambda|u|^2 u.$$

Preliminary investigation seems to indicate that a naive generalisation does not work, because we are not enjoying the reduction of positive powers of $\omega = \varepsilon^{-1}$ after commutation with Lie-derivatives corresponding to $|u|^2$.

5. *Symmetric Zassenhaus in other settings.* Exponential splittings have reached their apogee in the context of symplectic integrators for Hamiltonian ordinary differential equations (Hairer et al. 2006, McLachlan & Quispel 2002). Can symmetric Zassenhaus be used in this setting? The idea seems particularly appealing in the context of Hamiltonian functions of the form

$$H(\boldsymbol{p},\boldsymbol{q}) = H_1(\boldsymbol{p},\boldsymbol{q}) + \varepsilon H_2(\boldsymbol{p},\boldsymbol{q}),$$

where $0 < |\varepsilon| \ll 1$. Such systems occur often in celestial mechanics and many-body problems once there exists large disparity of masses and it is tempting to use an asymptotic splitting. However, in general we cannot employ in this context the formalism of Subsection 2.1, computing commutators easily. The computation of commutators in this context (in which they become Poisson brackets) is frowned upon because it is expensive. However, for special Hamiltonian functions this approach might be feasible.

Similar reasoning applies to volume-conserving geometric integrators based on splittings (McLachlan, Munthe-Kaas, Quispel & Zanna 2008).

The symmetric Zassenhaus formula might be also relevant within the realm of partial differential equations in the presence of a small parameter, e.g. the Klein–Gordon equation

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = \nabla^2 u + \frac{m^2 c^2}{\hbar^2}u.$$

This, again, is matter for further research.

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