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On the Linear Stability of Splitting Methods

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Abstract A comprehensive linear stability analysis of splitting methods is carried out by means of a 2×2 matrix $K(x)$ with polynomial entries (the stability matrix) and the stability polynomial $p(x)$ (the trace of $K(x)$ divided by two). An algorithm is provided for determining the coefficients of all possible time-reversible splitting schemes for a prescribed stability polynomial. It is shown that $p(x)$ carries essentially all the information needed to construct processed splitting methods for numerically approximating the evolution of linear systems. By conveniently selecting the stability polynomial, new integrators with processing for linear equations are built which are orders of magnitude more efficient than other algorithms previously available.

Keywords Splitting methods · Linear stability · Processing technique

AMS Subject Classification 65L05 · 65L20

This paper is dedicated to Arieh Iserles on the occasion of his 60th anniversary.

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1 Introduction

Splitting methods are frequently used in practice to integrate differential equations numerically. They constitute a natural choice when the vector field associated with the differential equation can be split into a sum of two or more parts that are simpler to integrate than the original problem. Suppose we have an ordinary differential equation (ODE) of the form

$$z' = f(z) = f^{[A]}(z) + f^{[B]}(z), \tag{1.1}$$

such that the h-flows $\varphi_h^{[A]}$ and $\varphi_h^{[B]}$ corresponding to $f^{[A]}$ and $f^{[B]}$, respectively, can be either exactly computed or accurately approximated. Then the exact flow φ_h of (1.1) can be approximated by a composition of the flows of the parts

$$\psi_h = \varphi_{b_k h}^{[B]} \circ \varphi_{a_k h}^{[A]} \circ \cdots \circ \varphi_{b_2 h}^{[B]} \circ \varphi_{a_2 h}^{[A]} \circ \varphi_{b_1 h}^{[B]} \circ \varphi_{a_1 h}^{[A]}, \tag{1.2}$$

where the $2k$ coefficients a_i, b_i are chosen as to ensure that ψ_h is a suitable approximation to the exact flow φ_h, typically in such a way that $\psi_h = \varphi_h + \mathcal{O}(h^{p+1})$: then the numerical integrator ψ_h is said to be accurate to order p in the time step h.

Perhaps the most frequently used splitting methods are

$$\psi_{h,1} = \varphi_h^{[B]} \circ \varphi_h^{[A]} \quad \text{and} \quad \psi_{h,2} = \varphi_{h/2}^{[A]} \circ \varphi_h^{[B]} \circ \varphi_{h/2}^{[A]}, \tag{1.3}$$

corresponding to the first-order Lie–Trotter method and the second-order leapfrog (also called Störmer, Verlet, Strang splitting, etc.) method, respectively. Their straightforward implementation and low storage requirements have made them common tools for the numerical treatment of ODEs and partial differential equations (PDEs).

Splitting schemes have proved to be especially useful in the context of *geometric integration*, when the flow of f lies in a particular group of diffeomorphisms. In fact, splitting methods preserve structural features of the flow of f as long as the basic methods $\varphi_h^{[A]}$ and $\varphi_h^{[B]}$ do, but this of course depends on the feature describing the group of diffeomorphisms [25, Sect. 2.1]. Important examples include symplecticity, volume preservation, symmetries, etc. In this sense, schemes (1.3) can be considered as geometric integrators and, as such, they show smaller error growth than standard integrators. It is not surprising, then, that a systematic search for splitting methods of higher order of accuracy has taken place during the last two decades and a large number of them exist in the literature (see [12, 17, 25, 26, 29] and references therein) which have been specifically designed for different families of problems.

Another characteristic of a numerical integration method for differential equations is *stability*. Roughly speaking, the numerical solution provided by a stable numerical integrator does not tend to infinity when the exact solution is bounded. Although important, this feature has received considerably less attention in the specific case of splitting methods.

To test the (linear) stability of the method (1.2), instead of the linear equation $y' = ay$ as in the usual stability analysis for ODE integrators, one considers the harmonic oscillator as a model problem [19, 23],

$$y'' + \lambda^2 y = 0, \quad \lambda > 0, \tag{1.4}$$

with the standard ($(q, p) = (\lambda y, y')$) splitting

$$\begin{Bmatrix} q' \\ p' \end{Bmatrix} = \Bigg[\underbrace{\begin{pmatrix} 0 & \lambda \\ 0 & 0 \end{pmatrix}}_{A} + \underbrace{\begin{pmatrix} 0 & 0 \\ -\lambda & 0 \end{pmatrix}}_{B}\Bigg] \begin{Bmatrix} q \\ p \end{Bmatrix}, \tag{1.5}$$

so that $z = (q, p)^{\mathrm{T}}$ and $f^{[A]}(z) = Az$, $f^{[B]}(z) = Bz$. The idea here is to find the time steps for which all numerical solutions remain bounded. The integrator (1.2) typically will be unstable for $|h\lambda| > x_*$, where the parameter x_* determines the stability threshold of the numerical scheme.

For instance, application of the simple splitting methods (1.3) to (1.5) leads trivially to $\psi_{h,1}(z) = K^{(1)}(x)z$ and $\psi_{h,2}(z) = K^{(2)}(x)z$, where $x \equiv h\lambda$,

$$K^{(1)}(x) = \begin{pmatrix} 1 & x \\ -x & 1 - x^2 \end{pmatrix} \quad \text{and} \quad K^{(2)}(x) = \begin{pmatrix} 1 - \frac{x^2}{2} & x - \frac{x^3}{4} \\ -x & 1 - \frac{x^2}{2} \end{pmatrix}, \tag{1.6}$$

respectively. Now, as both matrices have unit determinant, one concludes that $\psi_{h,1}$ and $\psi_{h,2}$ are (linearly) stable if $\mathrm{tr}(K^{(1)}(x)) = \mathrm{tr}(K^{(2)}(x)) = |2 - x^2| < 2$, or $|x| < 2$ and thus $x_* = 2$. Although one might think at first glance that $\psi_{h,1}$ is more stable per unit work than $\psi_{h,2}$ because the latter involves one more evaluation of the basic flow $\varphi_{h/2}^{[A]}$, this is not so, as the leftmost basic flow of one step of $\psi_{h,2}$ can be concatenated with the rightmost basic flow of the next step. This is perhaps more clearly seen by observing that the composition of n steps of $\psi_{h,2}$ is related with n steps of $\psi_{h,1}$ by $(\psi_{h,2})^n = \varphi_{h/2}^{[A]} \circ (\psi_{h,1})^n \circ (\varphi_{h/2}^{[A]})^{-1}$, which explains why both methods have the same stability properties and the same computational cost.

To take into account the computational cost in the stability analysis of the scheme (1.2), one must compare its stability threshold x_* with the stability limit $2k$ of the concatenation of k steps of length h/k of methods (1.3). This shows that one must consider the value of x_*/k (the *relative stability threshold*) to compare the stability of splitting methods with different numbers of basic compositions. To be more precise, we define the relative stability threshold as x_*/k', where the *(effective) number of stages* of the scheme (1.2) is given as: (i) $k' = k$ if $a_j \neq 0$ and $b_j \neq 0$ for $j = 1, \ldots, k$; and (ii) $k' = k - 1$ if $a_j \neq 0$ and $b_{j-1} \neq 0$ for $j = 2, \ldots, k$, and $a_1 = 0$ and/or $b_k = 0$. For instance, the effective number of stages of both schemes in (1.3) is one, so that the relative stability threshold is 2 for both of them. As a matter of fact, the optimal value for the relative stability threshold of consistent splitting methods is precisely two [9].

In the process of building high-order schemes, linear stability is not usually taken into account, ending sometimes with methods possessing such a small relative stability threshold that they are useless in practice. In contrast, López-Marcos et al. [19] developed a fourth-order integrator with maximal stability interval, whereas in [23] the analysis was generalized to arbitrary order n and stage number k.

The aim of the present paper is two-fold: (i) first, to carry out a detailed theoretical analysis of the linear stability of splitting methods; and (ii) second, to construct schemes with relatively large linear stability intervals (relatively close to the optimal values obtained in [23]) that are highly accurate when applied to the harmonic oscillator.

It is known that the stability of a splitting method is essentially characterized by an even polynomial $p(x)$ with $p(0)=1$ (the so-called stability polynomial [19, 23]), and that it is readily determined from the coefficients a_j, b_j defining the scheme (1.2). Here we give a constructive procedure to obtain all possible splitting schemes having a prescribed $p(x)$ as stability polynomial. This proves to be a very powerful tool in the fulfillment of the second goal enumerated in the preceding paragraph.

The new methods that we present in this work have the special structure

$$\hat{\psi}_h = \pi_h \circ \psi_h \circ \pi_h^{-1}. \tag{1.7}$$

Observe that the second-order method $\psi_{h,2}$ given in (1.3) can be considered as a particular case of $\hat{\psi}_h$, with $\psi_{h,1}$ playing the role of ψ_h. Here ψ_h is referred to as the kernel and π_h^{-1}, π_h are the pre- and post-processors or correctors. Schemes ψ_h and $\hat{\psi}_h$ are said to be *conjugate* in the terminology of dynamical systems. Application of $\hat{\psi}_h$ over n integration steps with constant step size h gives

$$\hat{\psi}_h^n = \pi_h \circ \psi_h^n \circ \pi_h^{-1}. \tag{1.8}$$

One says that ψ_h has effective order p if there exist maps π_h^{-1}, π_h such that $\hat{\psi}_h$ has order p. This processing technique was first introduced by Butcher [8] and later received renewed attention in the context of geometric integration [1, 2, 5–7, 19, 20, 22, 28, 31].

The processing technique presents several advantages in comparison with conventional integration methods. First, the analysis of the order conditions of the method $\hat{\psi}_h$ shows that many of them can be satisfied by the processor π_h, so that the kernel ψ_h must fulfill a much reduced set of restrictions, thus allowing us to build kernels of effective order p involving far fewer function evaluations than a conventional integrator of order p [1, 2, 5, 22, 25]. Second, since the number of order conditions for the kernel is smaller, one can analyze in more detail the set of solutions, even for moderate order, and eventually find very efficient methods [1, 2, 25, 31]. This turns out to be especially relevant for the kind of linear systems we consider here. Third, although the post-processor are usually more expensive than the kernel itself (thus deteriorating the overall efficiency of the method), it has been shown in [1] that π_h can be replaced by a new map $\hat{\pi}_h \simeq \pi_h$ obtained from the intermediate stages in the computation of the kernel. Thus, as a general rule, one evaluates a very accurate pre-processor π_h^{-1} only once to start the integration whereas the post-processor is approximated by $\hat{\pi}_h$ (which is virtually cost-free and only introduces a local error) when output is frequently required. In this way, we can safely state that the cost of $\hat{\psi}_h$ is measured by the cost of the kernel. On the other hand, the stability analysis of such a class of methods is concerned only with the kernel, since the processor does not affect the stability, as evidenced by (1.8).

Obviously, there is not much point in designing new and somewhat sophisticated numerical methods for the harmonic oscillator (1.5). It turns out, however, that splitting methods especially tailored for this system can be of great interest for the numerical treatment of nontrivial problems appearing, for instance, in quantum mechanics, electrodynamics, structural dynamics and for any evolution PDEs that, once spatially discretized, give rise to systems of coupled harmonic oscillators [10, 15, 16, 32]. As a matter of fact, by using the analysis carried out in this work, we are able to build very efficient processed methods of any order of accuracy with an arbitrary number of stages for the linear system

$$q' = Mp, \qquad p' = -Nq, \tag{1.9}$$

with $q \in \mathbb{R}^{d_1}$, $p \in \mathbb{R}^{d_2}$, $M \in \mathbb{R}^{d_1 \times d_2}$ and $N \in \mathbb{R}^{d_2 \times d_1}$.

When constructing processed splitting methods for systems of this form, we have observed the following (and perhaps surprising) features:

- Contrary to the typical situation for general integrators, where increasing the order of accuracy by adding more stages leads to methods that are less stable (and less accurate for values of h near the stability limit), the particular structure of the system (1.9) allows us to construct higher-order methods by increasing the number of stages without deteriorating the stability and accuracy for larger values of h.
- For linear systems of the form (1.9) that can be reduced (by a linear change of variables) to a system of decoupled harmonic oscillators, very efficient second-order methods with a large number of stages can be constructed that outperform high-order methods for a wide range of values of the time step h.

The paper is organized as follows. In Sect. 2 we introduce and characterize the stability matrix of a splitting method as applied to the one-dimensional harmonic oscillator. We show (Sect. 2.1) that any splitting method is uniquely determined by its stability matrix. Furthermore, we prove in a constructive way (Sect. 2.2) that if the trace of the stability matrix (or, equivalently, the stability polynomial $p(x)$) is known, then there exists a finite number of choices for the coefficients of symmetric compositions of the form (1.2) having such stability polynomial. Next we characterize the linear stability of a splitting method and give the formal definition of several relevant parameters related to the stability interval (Sect. 2.3). It is shown that the high-order of accuracy $2n$ requires that $p(x) = \cos x + \mathcal{O}(x^{2n+2})$ as $x \to 0$. What is more important, *the accuracy of a processed splitting method when applied to the harmonic oscillator only depends on how* $p(x)$ *approximates* $\cos x$ *in the stability interval* (Sect. 2.4).

The analysis done in Sect. 2 is applied subsequently in Sect. 3 to systems of the form (1.9). In that case we show that *any partitioned method* (such as splitting methods or partitioned Runge–Kutta schemes) *is indeed conjugate to a non-partitioned method for a sufficiently small time step* h.

In Sect. 4 we particularize the previous treatment to the construction of splitting methods of the form (1.7) with high accuracy and enlarged stability domain for the linear system (1.9). We proceed by first determining a stability polynomial approximating $\cos x$ for some relatively large interval of x. Here two different strategies are pursued. In the first one we consider the even polynomial $p^{n,l}(x)$ with minimal degree among those verifying that $p^{n,l}(x) = \cos x + \mathcal{O}(x^{2n+2})$ as $x \to 0$ and $p^{n,l}(x) - (-1)^j$ has a double zero at $x_j = j\pi$ for $j = 1, \dots, l$. In the second strategy, a polynomial $p^{n,l,m}(x)$ with m additional parameters is introduced, so that, besides the previous conditions, it minimizes in the least square sense the coefficients of the Chebyshev series expansion of the difference $(p(x) - \cos x)/x^{2n+2}$ in the stability interval. In this way, the solution matrix can be accurately approximated for large values of x. As far as we know, this constitutes a novel approach for solving the problem. We also propose a device to monitor the theoretical efficiency of the resulting processed splitting methods based only on their stability polynomial. Then, by applying the results of Sect. 2, the stability matrix and the coefficients of the kernel are obtained. As for the processor, it is constructed as a matrix whose entries are polynomials of sufficiently high degree. We propose, in particular, several representative kernels of effective orders 10 and 16 requiring 19 and 32 stages, respectively, in addition to an extremely efficient second-order kernel with 38 stages previously constructed along these same lines in [3]. As a matter of fact, the main purpose of reference [3] was to show that this class of methods constitutes indeed a very efficient numerical tool to solve evolution problems in quantum mechanics: they are accurate, easy to implement and very stable in comparison with other standard integrators. Here, by contrast, our main goals are, on the one hand, to fill the gap existing in the literature with respect to the linear stability theory of splitting methods and, on the other hand, to provide a sound theoretical analysis justifying such an impressive performance.

The new methods are illustrated in Sect. 5 on some numerical examples aimed:

(a) to verify that the criteria developed in Sect. 4 to show that the relative performance of the stability polynomials when approximating the function $\cos x$ is also reflected in the final splitting methods in practical applications, where the integration of linear systems of the form (1.9) is required;
(b) to show how the new schemes compare with other standard splitting methods; and
(c) to illustrate that the proposed processed splitting schemes can be advantageously used to approximate the time evolution of important classes of semidiscretized linear partial differential equations.

Finally, Sect. 6 contains some conclusions and the outlook of future work.

2 Analysis of Splitting Methods Applied to the Harmonic Oscillator

When applying the splitting method (1.2) to the one-dimensional harmonic oscillator (1.5), we approximate the exact 2×2 solution matrix

$$O(x) = \begin{pmatrix} \cos x & \sin x \\ -\sin x & \cos x \end{pmatrix}, \qquad x = h\lambda, \tag{2.1}$$

by $K(x)$, where

$$K(x) = \begin{pmatrix} 1 & 0 \\ -b_k x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_k x \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ -b_1 x & 1 \end{pmatrix} \begin{pmatrix} 1 & a_1 x \\ 0 & 1 \end{pmatrix}, \tag{2.2}$$

or, alternatively, in terms of the matrices A and B introduced in (1.5),

$$K(x) = \mathrm{e}^{hb_k B} \mathrm{e}^{ha_k A} \cdots \mathrm{e}^{hb_1 B} \mathrm{e}^{ha_1 A}, \tag{2.3}$$

with appropriate coefficients $a_i, b_i \in \mathbb{R}$. The matrix $K(x)$ (the *stability matrix* of the splitting method) has the form

$$K(x) = \begin{pmatrix} K_1(x) & K_2(x) \\ K_3(x) & K_4(x) \end{pmatrix}, \tag{2.4}$$

with elements

$$\begin{aligned} K_1(x) &= 1 + \sum_{i=1}^{k-1} k_{1,i} x^{2i}, \qquad & K_2(x) &= \sum_{i=1}^{k} k_{2,i} x^{2i-1}, \\ K_3(x) &= \sum_{i=1}^{k} k_{3,i} x^{2i-1}, \qquad & K_4(x) &= 1 + \sum_{i=1}^{k} k_{4,i} x^{2i}. \end{aligned} \tag{2.5}$$

In (2.5), $k_{i,j}$ are homogeneous polynomials in the parameters a_i, b_i. In particular, $k_{2,1} = \sum_{j=1}^{k} a_j$, $k_{3,1} = -\sum_{j=1}^{k} b_j$ and $k_{1,1} + k_{4,1} = k_{2,1} k_{3,1}$. Since each individual matrix in the composition (2.2) has unit determinant, it must hold that $\det K(x) \equiv 1$. It is not difficult to check that

$$|d(K_1) - d(K_4)| \le 2, \qquad |d(K_2) - d(K_3)| \le 2, \tag{2.6}$$

where we denote by $d(K_i)$ the degree of each polynomial $K_i(x)$ $(i = 1, \dots, 4)$.

The linear stability analysis of splitting methods is made easier by considering a generalization of the matrix (2.4)–(2.5).

Definition 2.1 By a stability matrix we mean a generic 2×2 matrix

$$K(x) = \begin{pmatrix} K_1(x) & K_2(x) \\ K_3(x) & K_4(x) \end{pmatrix}, \tag{2.7}$$

such that $K_1(x)$ and $K_4(x)$ (respectively, $K_2(x)$ and $K_3(x)$) are even (respectively, odd) polynomials in x and

$$\det K(x) = K_1(x) K_4(x) - K_2(x) K_3(x) \equiv 1, \tag{2.8}$$

$$K_1(0) = K_4(0) = 1. \tag{2.9}$$

We will typically consider stability matrices satisfying, in addition,

$$K_2'(0) = -K_3'(0) = 1 \tag{2.10}$$

since we are interested in consistent methods.

In the application of a splitting method to the harmonic oscillator, an essential role is played by the so-called *stability polynomial*.

Definition 2.2 Given a stability matrix $K(x)$, the corresponding stability polynomial is defined as

$$p(x) = \frac{1}{2} \operatorname{tr} K(x) = \frac{1}{2}\big(K_1(x) + K_4(x)\big).$$

Clearly, the stability polynomial of a consistent splitting method is an even polynomial $p(x)$ satisfying

$$p(x) = 1 - x^2/2 + \mathcal{O}\big(x^4\big) \quad \text{as } x \to 0. \tag{2.11}$$

In particular, for schemes (1.3) one has, from (1.6), $p(x) = 1 - x^2/2$.

2.1 From the Stability Matrix to the Splitting Method

Obviously, analyzing splitting methods through a generic stability matrix is useful as long as one is able to factorize $K(x)$ as (2.2) and determine uniquely the coefficients a_i, b_i of the splitting method from a particular $K(x)$ with polynomial entries. Only in such circumstances could one say that any splitting method of the form (1.2) is completely characterized by the result of applying one step of the method to the harmonic oscillator. What the following result shows precisely is that any splitting method is uniquely determined by its stability matrix.

Proposition 2.3 *Given a stability matrix $K(x)$ as in Definition 2.1, there exists a unique decomposition of $K(x)$ of the form*

$$\begin{pmatrix} 1 & 0 \\ -B_m(x) & 1 \end{pmatrix} \begin{pmatrix} 1 & A_m(x) \\ 0 & 1 \end{pmatrix} \cdots \begin{pmatrix} 1 & 0 \\ -B_1(x) & 1 \end{pmatrix} \begin{pmatrix} 1 & A_1(x) \\ 0 & 1 \end{pmatrix}, \tag{2.12}$$

where $A_j(x)$, $B_j(x)$ $(j = 1, \dots, m)$ are odd polynomials in x satisfying that

$$B_{j-1}(x) \neq 0, \quad A_j(x) \neq 0, \quad j = 2, \dots, m. \tag{2.13}$$

Proof We will first prove the existence of such a decomposition by induction on the sum of the degrees of the two polynomials $K_1(x)$ and $K_4(x)$. In the trivial case, where the sum of their degrees is 0, it holds by assumption that $K_1(x) \equiv K_4(x) \equiv 1$, and since $\det K(x) \equiv 1$, either $K_2(x) \equiv 0$ or $K_3(x) \equiv 0$, so the existence follows trivially.

If $d(K_1) + d(K_4) > 0$, then two possibilities occur:

- $d(K_1) < d(K_2)$. In that case $d(K_3) < d(K_4)$, since $\det K(x) \equiv 1$. Application of polynomial division uniquely determines the odd polynomials $A_1(x)$ and $\hat{K}_2(x)$ such that

$$K_2(x) = K_1(x)A_1(x) + \hat{K}_2(x), \tag{2.14}$$

where $d(K_2) = d(K_1) + d(A_1)$ and $d(\hat{K}_2) < d(K_1)$. Now, we define the even polynomial $\hat{K}_4(x) = K_4(x) - K_3(x)A_1(x)$, so that

$$\begin{pmatrix} K_1(x) & K_2(x) \\ K_3(x) & K_4(x) \end{pmatrix} = \begin{pmatrix} K_1(x) & \hat{K}_2(x) \\ K_3(x) & \hat{K}_4(x) \end{pmatrix} \begin{pmatrix} 1 & A_1(x) \\ 0 & 1 \end{pmatrix}.$$

Clearly, $\hat{K}_4(0) = 1$ and $K_1(x)\hat{K}_4(x) - \hat{K}_2(x)K_3(x) = 1$ which, together with $d(\hat{K}_2) < d(K_1)$, implies that $d(\hat{K}_4) < d(K_3) < d(K_4)$, and the required result follows by induction.

- $d(K_1) > d(K_2)$. Then $d(K_3) > d(K_4)$ because $\det K(x) \equiv 1$, and one similarly obtains the decomposition

$$\begin{pmatrix} K_1(x) & K_2(x) \\ K_3(x) & K_4(x) \end{pmatrix} = \begin{pmatrix} \hat{K}_1(x) & K_2(x) \\ \hat{K}_3(x) & K_4(x) \end{pmatrix} \begin{pmatrix} 1 & 0 \\ B_1(x) & 1 \end{pmatrix},$$

  where the odd polynomials $B_1(x)$ and $\hat{K}_3(x)$ are determined from the polynomial division of $K_3(x)$ by $K_4(x)$, so that $K_3(x) = K_4(x)B_1(x) + \hat{K}_3(x)$, and then $\hat{K}_1(x)$ is determined as $\hat{K}_1(x) = K_1(x) - K_2(x)B_1(x)$. Clearly, $\hat{K}_1(0) = 1$ and $\hat{K}_1(x)K_4(x) - K_2(x)\hat{K}_3(x) = 1$. Since now $d(\hat{K}_3) < d(K_4)$, then $d(\hat{K}_1) < d(K_2) < d(K_1)$ and the required result follows by induction.

This completes the proof of the existence of the decomposition.

To prove the uniqueness, suppose that there are two different decompositions D_1 and D_2 of $K(x)$ of the form (2.12). Then, clearly, the product $D_1 D_2^{-1}$ also has the same structure (2.12) with (2.13) and is equal to the identity matrix. But this cannot be the case, since, as we have seen, if $K(x)$ admits the decomposition (2.12) with (2.13), then $d(K_1) \geq d(K_2)$ and $d(K_3) > d(K_4)$ provided that $A_1(x) \equiv 0$, and $d(K_1) < d(K_2)$ and $d(K_3) \leq d(K_4)$ otherwise, and these inequalities are not satisfied by the identity matrix. □

Remarks 1. Notice from the proof of Proposition 2.3 that $\hat{K}_4(x)$ (respectively, $\hat{K}_1(x)$) can also be obtained as the remainder of the polynomial division of $K_4(x)$ by $K_3(x)$ (respectively, $K_1(x)$ by $K_2(x)$), which (in exact arithmetic) must give the same quotient $A_1(x)$ (respectively, $B_1(x)$) due to the fact that $\det K(x) \equiv 1$.

2. Obviously, the decomposition (2.2) corresponds to (2.12) with $A_j(x) = a_j x$ and $B_j(x) = b_j x$ for $j = 1, \ldots, k$.

Example Let us illustrate this result with two different stability matrices, leading to different types of decomposition. Consider first the matrix

$$K(x) = \begin{pmatrix} 1 - \frac{1}{2}x^2 + \frac{1}{32}x^4 & x - \frac{3}{16}x^3 + \frac{1}{128}x^5 \\ -x + \frac{1}{8}x^3 & 1 - \frac{1}{2}x^2 + \frac{1}{32}x^4 \end{pmatrix}, \tag{2.15}$$

which satisfies conditions (2.6)–(2.10). By applying the constructive proof of Proposition 2.3 it is straightforward to check that $K(x)$ can be decomposed as

$$K(x) = \begin{pmatrix} 1 & \frac{x}{4} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{x}{2} & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{x}{2} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -\frac{x}{2} & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{x}{4} \\ 0 & 1 \end{pmatrix}, \tag{2.16}$$

and this is in fact the only decomposition of the form (2.2) for the matrix (2.15). As a second example, consider now

$$\bar{K}(x) = \begin{pmatrix} 1 - \frac{1}{2}x^2 + \frac{1}{32}x^4 & x - \frac{1}{4}x^3 + \frac{1}{64}x^5 \\ -x + \frac{1}{16}x^3 & 1 - \frac{1}{2}x^2 + \frac{1}{32}x^4 \end{pmatrix} \tag{2.17}$$

with the same stability polynomial as $K(x)$. In this case, although the degrees of the entries coincide with those of (2.15) (and thus condition (2.6) holds), $\bar{K}(x)$ cannot be decomposed in the form (2.2). Instead it admits the unique decomposition

$$\bar{K}(x) = \begin{pmatrix} 1 & \frac{1}{2}x \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -x + \frac{1}{16}x^3 & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{2}x \\ 0 & 1 \end{pmatrix}, \tag{2.18}$$

which is not of the form (2.2).

2.2 From the Stability Polynomial to the Splitting Method

We have seen that, under certain circumstances, the stability matrix $K(x)$ allows us to get the composition (2.2) in a unique way and therefore the values of the coefficients of the splitting method. The question we analyze now is whether something similar can be done starting from the stability polynomial. We show that, *given such a $p(x)$, there exists a finite number of different time-reversible splitting schemes having $p(x)$ as their stability polynomial.*

To begin with, suppose one has an even polynomial $p(x)$ satisfying (2.11). Obviously, there exists an infinite number of splitting methods having such a $p(x)$ as their stability polynomial. Nevertheless, for each arbitrary even polynomial $r(x) \neq p(x)$ with $r(0) = 0$ there exists a *finite* number of consistent splitting methods with stability matrix (2.7) verifying $K_1(x) = p(x) + r(x)$ and $K_4(x) = p(x) - r(x)$ or, equivalently,

$$p(x) = \frac{K_1(x) + K_4(x)}{2}, \qquad r(x) = \frac{K_1(x) - K_4(x)}{2}.$$

The remaining entries of (2.7) are obtained by considering all possible decompositions of the polynomial $p(x)^2 - r(x)^2 - 1$ $(= K_1(x)K_4(x) - 1)$ as the product of two odd polynomials $K_2(x)$ and $K_3(x)$ satisfying (2.10).

Proposition 2.3 then gives a decomposition of the form (2.12) for each choice of the stability matrix $K(x)$. Finally, all possible consistent splitting methods corresponding to the polynomials $p(x)$ and $r(x)$ are obtained by selecting, among the finite number of different decompositions of the form (2.12) obtained in that way, those that are actually of the form (2.2).

With the simplest choice $r(x) \equiv 0$ one has $K_1(x) \equiv K_4(x)$. In that case, the stability matrix verifies the identity $K(x)^{-1} \equiv K(-x)$, and this is precisely the characterization of a time-reversible method [12]. In terms of the composition (2.2) it corresponds to taking either $a_{k+1-i} = a_i$, $b_k = 0$, $b_{k-i} = b_i$ or $a_1 = 0$, $a_{k+1-i} = a_{i+1}$, $b_{k+1-i} = b_i$, $i = 1, 2, \ldots$, which results in a palindromic composition. In this way it is possible to construct explicitly all consistent time-reversible splitting methods with a prescribed stability polynomial $p(x)$ satisfying (2.11).

Example Let us consider the stability polynomial of $K(x)$ and $\bar{K}(x)$ in (2.15) and (2.17), respectively,

$$p(x) = 1 - \frac{1}{2}x^2 + \frac{1}{32}x^4, \quad \text{so that} \quad p(x)^2 - 1 = -x^2\left(1 - \frac{x^2}{16}\right)\left(1 - \frac{x^2}{8}\right)^2. \tag{2.19}$$

There are six different ways of factorizing $p(x)^2 - 1$ as a product of two odd polynomials $K_2(x)$ and $K_3(x)$ with $K_2'(0) = 1 = -K_3'(0)$. The three choices satisfying $d(K_3) < d(K_4)$ are:

(i) $K_3(x) = -x(1-\frac{x^2}{8})$ which gives the stability matrix (2.15), with unique decomposition (2.16);
(ii) $K_3(x) = -x(1-\frac{x^2}{16})$ which gives the stability matrix (2.17) (with unique decomposition (2.18), and thus not corresponding to an splitting method of the form (1.2)); and
(iii) $K_3(x) = -x$ which leads to the stability matrix

$$\tilde{K}(x) = \begin{pmatrix} 1-\frac{1}{2}x^2+\frac{1}{32}x^4 & x-\frac{5}{16}x^3+\frac{x^5}{32}-\frac{x^7}{1024} \\ -x & 1-\frac{1}{2}x^2+\frac{1}{32}x^4 \end{pmatrix}. \tag{2.20}$$

Application of the algorithm used in the proof of Proposition 2.3 allows us to factorize the matrix (2.20) as

$$\tilde{K}(x) = \begin{pmatrix} 1 & \frac{1}{2}x-\frac{1}{32}x^3 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -x & 1 \end{pmatrix}\begin{pmatrix} 1 & \frac{1}{2}x-\frac{1}{32}x^3 \\ 0 & 1 \end{pmatrix}, \tag{2.21}$$

which does not correspond to a splitting method of the form (1.2), as expected because $\tilde{K}(x)$ does not satisfy conditions (2.6). The remaining three stability matrices are obtained by interchanging the roles of the polynomials $K_2(x)$ and $-K_3(x)$.

2.3 Stability

According to the notion of stability given in the Introduction, a splitting method is stable when applied to the harmonic oscillator if $[K(x)]^n$ can be bounded independently of $n \geq 1$. As is well known, if the method is stable for a given $x \in \mathbb{R}$, then $|p(x)| \leq 1$. The converse is not true in general, as shown by the following simple example:

$$K(x) = \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}, \quad \text{so that} \quad [K(x)]^n = \begin{pmatrix} 1 & nx \\ 0 & 1 \end{pmatrix},$$

and thus $K(x)$ is linearly unstable. The following proposition gives a useful characterization of the stability of $K(x)$.

Proposition 2.4 *Let* $K(x)$ *be a* 2×2 *matrix with* $\det K(x) = 1$, *and* $p(x) = \frac{1}{2}\operatorname{tr} K(x)$. *Then, the following statements are equivalent*:

(a) *The matrix* $K(x)$ *is stable.*
(b) *The matrix* $K(x)$ *is diagonalizable with eigenvalues of modulus one.*
(c) $|p(x)| \leq 1$, *and* $K(x)$ *is similar to the matrix*

$$S(x) = \begin{pmatrix} \cos\Phi(x) & \sin\Phi(x) \\ -\sin\Phi(x) & \cos\Phi(x) \end{pmatrix}, \quad \textit{where } \Phi(x) = \arccos p(x). \tag{2.22}$$

Proof This is in fact an elementary consequence of the symplecticity of the matrix $K(x)$. In more detail, let $\lambda_1(x)$ and $\lambda_2(x)$ be the eigenvalues of $K(x)$. The assumption $\det K(x) = 1$ implies that $\lambda_1(x)\lambda_2(x) = 1$. Thus, if $K(x)$ is stable, then $|\lambda_1(x)| = |\lambda_2(x)| = 1$, and $K(x)$ is necessarily diagonalizable, unless $+1$ or -1 is an eigenvalue with multiplicity 2. In both cases, if $K(x)$ is not diagonalizable, then it is linearly unstable. Hence, if $K(x)$ is stable it is diagonalizable with eigenvalues of modulus 1.

The eigenvalues of $K(x)$ are the zeros of $\lambda^2 - (\operatorname{tr} K(x))\lambda + 1$. Thus, if $K(x)$ is diagonalizable with eigenvalues of modulus 1, then $|p(x)| \le 1$, and

$$\lambda_1(x) = \mathrm{e}^{\mathrm{i}\Phi(x)}, \qquad \lambda_2(x) = \mathrm{e}^{-\mathrm{i}\Phi(x)}, \tag{2.23}$$

where $\Phi(x)$ is given by (2.22). In consequence, $K(x)$ is similar to the matrix $S(x)$ given in (2.22), as $S(x)$ is also diagonalizable with eigenvalues (2.23).

Finally, condition (c) clearly implies that the matrices $S(x)$ and $K(x)$ are both stable. □

In the stability analysis, the real parameters x_* and x^* defined next play a crucial role.

Definition 2.5 Given a 2×2 matrix $K(x)$ depending on a real parameter x such that $\det K(x) \equiv 1$, we denote by x_* the largest nonnegative real number such that $K(x)$ is stable for all $x \in (-x_*, x_*)$. We say that x_* is the stability threshold of $K(x)$, and that $(-x_*, x_*)$ is the stability interval of $K(x)$.

Definition 2.6 Let $p(x)$ be an even polynomial in x with $p(0) = 1$. We denote by x^* the largest real nonnegative number such that $|p(x)| \le 1$ for all $x \in [0, x^*]$.

Remarks 1. If $p(x)$ is the stability polynomial of a stability matrix $K(x)$ as given by Definition 2.1, it is clear from the proof of Proposition 2.4 that $[-x^*, x^*]$ is the largest interval including 0 such that $K(x)$ has eigenvalues of modulus 1 and therefore $x_* \le x^*$.

2. If $p''(0) < 0$, then $p(x)^2 - 1 \le 0$ for sufficiently small $|x|$, and in that case x^* is the smallest real positive zero with odd multiplicity of the polynomial $p(x)^2 - 1$ (for this x^*, the sign of the polynomial $p(x)^2 - 1$ does not change in the interval $x \in (-x^*, x^*)$, but it actually does when crossing $x = \pm x^*$).

3. Observe that $S(x)$ can be considered as the stability matrix of a time-reversible method. In consequence, Proposition 2.4 allows us to conclude that *for sufficiently small values of x each matrix $K(x)$ with* $\det K(x) = 1$ *is similar to a time-reversible matrix*, provided that $p''(0) < 0$.

Next we analyze which conditions have to be imposed on $K(x)$ for a given stability polynomial $p(x)$ to get the optimal stability threshold, i.e., to ensure that $x_* = x^*$.

Proposition 2.7 *Assume that a 2×2 matrix $K(x)$ depending on a real parameter x of the form* (2.2) *is such that* $\det K(x) \equiv 1$, *$K_1(x)$ and $K_4(x)$ are even polynomials, $K_2(x)$ and $K_3(x)$ are odd polynomials, $K_1(0) = K_4(0) = 1$, and $K_2'(0)K_3'(0) < 0$. Let $p(x) = \frac{1}{2} \operatorname{tr} K(x)$ be the corresponding stability polynomial and suppose that $0 = x_0 < x_1 < \cdots < x_l$ are the real zeros with even multiplicity of the polynomial $p(x)^2 - 1$ in the interval* $[0, x^*]$. *Then, $x_* = x^*$ if*

$$K_2(x_j) = K_3(x_j) = 0 \tag{2.24}$$

for each $j = 1, \dots, l$. Otherwise, x_* is the smallest x_j that violates condition (2.24).

Proof On the one hand, by differentiating $\det K(x) \equiv 1$ twice, replacing x by 0 and taking into account that $K_1(0) = K_4(0) = 1$ and $K_2'(0)K_3'(0) < 0$, we conclude that $p''(0) = K_1''(0) + K_4''(0) = 2K_2'(0)K_3(0) < 0$, which guarantees that the eigenvalues of $K(x)$ for $x \in (-x^*, x^*)$ have modulus one, and thus $K(x)$ is stable if and only if it is diagonalizable. When $|p(x)| < 1$ the eigenvalues of $K(x)$ are distinct, and thus $K(x)$ is diagonalizable. If $x \in (-x^*, x^*)$ and $|p(x)| = 1$, that is, if $x = x_j$ for some $j = 1, \dots, l$, then $K(x)$ has the double eigenvalue 1 or -1, and in that case, $K(x)$ is diagonalizable if and only if $K(x)$ or $-K(x)$ are the identity matrix I, that is, if and only if (2.24) holds. □

Notice that the assumptions in Proposition 2.7 hold for the stability matrix $K(x)$ of any consistent splitting method (i.e., for the matrix $K(x)$ of Definition 2.1).

Example Consider the polynomial $p(x)$ given in (2.19). Then $l = 1$, $x_1 = 2\sqrt{2}$, and $x^* = 4$. For the stability matrix (2.15) we have $K_2(x_1) = K_3(x_1) = 0$, and thus the corresponding stability threshold is $x_* = x^* = 4$. As for the stability matrices $\bar{K}(x)$ and $\tilde{K}(x)$ in (2.17) and (2.20), respectively, one has $\bar{K}_3(x_1) = -\sqrt{2} \neq 0$ and $\tilde{K}_3(x_1) = -2\sqrt{2} \neq 0$, and thus $x_* = 2\sqrt{2} < 4 = x^*$ in both cases.

The above proposition allows us to build easily a stability matrix corresponding to a time-reversible splitting method with the optimal stability threshold.

Proposition 2.8 *Let $p(x)$ be an even polynomial satisfying* (2.11). *Then there exists a stability matrix of the form*

$$K(x) = \begin{pmatrix} p(x) & K_2(x) \\ K_3(x) & p(x) \end{pmatrix} \tag{2.25}$$

for which $x_* = x^*$.

Proof Let $0 = x_0 < x_1 < \cdots < x_l$ be the real zeros with even multiplicity of the polynomial $p(x)^2 - 1$ in the interval $[0, x^*]$. Then the polynomial $p(x)^2 - 1$ can be decomposed as

$$p(x)^2 - 1 = -x^2 Q(x) \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big)^2,$$

where $Q(x)$ is an even polynomial verifying $Q(0) = 1$. We then choose a decomposition $Q(x) = Q_2(x)Q_3(x)$ of even polynomials such that $Q_2(0) = Q_3(0) = 1$, and determine $K_2(x)$, $K_3(x)$ as

$$\begin{aligned} K_2(x) &= x Q_2(x) \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big), \\ K_3(x) &= -x Q_3(x) \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big). \end{aligned} \tag{2.26}$$

This completes the proof. □

2.4 Accuracy

As mentioned in the Introduction, an accurate high-order method can be useless in practice if it possesses a tiny stability domain. Similarly, a very stable but poorly accurate method is also of no interest in practical applications. In consequence, when designing new integration schemes of the form (2.2) the goal is to achieve the right balance between accuracy and stability. This, of course, is not an easy task in general, although a partial analysis has been done for the harmonic oscillator [10, 23].

Obviously, the accuracy of a splitting method depends on the difference between the matrix $K(x)$ and the exact solution, $O(x)$. Roughly speaking, if $\|K(x) - O(x)\|$ is small, then the eigenvalues of $K(x)$ must be close to the eigenvalues of $O(x)$. According to Proposition 2.4, the stability polynomial $p(x)$ must be an approximation to $\cos x$. In particular, for a splitting method of order $2n$, it necessarily holds that

$$p(x) = \cos x + \mathcal{O}\bigl(x^{2n+2}\bigr) \quad \text{as } x \to 0,$$

i.e., $\Phi(x) = \arccos p(x) = x + \mathcal{O}(x^{2n+1})$ in (2.22). In addition, under the assumptions of Proposition 2.7, if (2.2) is a good approximation to the solution matrix in a large subinterval of the stability interval $(-x_*, x_*)$, say $[-x_k, x_k]$ for some $k \le l$, then $x_j \approx j\pi$ and $p(x_j) = (-1)^j$ for $j = 1, \dots, k$.

It is worth stressing that *if one is interested in processed splitting methods of the form* (1.7), *then*, according to Proposition 2.4, *their accuracy when applied to the harmonic oscillator only depends on the quality of the approximation* $p(x) \approx \cos x$ *of their stability polynomial* $p(x)$ *in the stability interval* $[-x_*, x_*]$.

2.5 Geometric Properties

Consider the application of a consistent splitting method (with stability matrix $K(x)$ and stability polynomial $p(x)$) to the harmonic oscillator (1.4) split as (1.5). According to Proposition 2.4, if $x \equiv h\lambda \in (-x_*, x_*)$, one step of the method is conjugate to the exact h-flow of the modified harmonic oscillator

$$y'' + \tilde{\lambda}(h)^2 y = 0, \tag{2.27}$$

with $\tilde{\lambda}(h) = (1/h)\Phi(h\lambda)$. In other words, there exists a well-defined matrix

$$P(x) = \begin{pmatrix} P_1(x) & P_2(x) \\ P_3(x) & P_4(x) \end{pmatrix} \tag{2.28}$$

(with $\det P(x) = 1$) such that

$$S(x) = P(x) K(x) P^{-1}(x) \tag{2.29}$$

is given in (2.22). In the particular case of time-reversible methods (i.e., satisfying that $K(-x) = K^{-1}(x)$ or, equivalently, $K_4(x) = K_1(x)$), one can choose

$$P(x) = \begin{pmatrix} P_1(x) & 0 \\ 0 & P_4(x) \end{pmatrix}, \tag{2.30}$$

where

$$P_1(x) = \sqrt[4]{\frac{-K_3(x)}{K_2(x)}}, \qquad P_4(x) = \sqrt[4]{\frac{-K_2(x)}{K_3(x)}}. \tag{2.31}$$

Obviously, these expressions are only valid when $K_2(x) \neq 0 \neq K_3(x)$. Otherwise, $K_2(x) = 0 = K_3(x)$ for $x \in (-x_*, x_*)$, and then $P_1(x) = 1 = P_4(x)$.

Although one step of the splitting method is conjugate to the exact flow of (2.27) when $x \in (-x_*, x_*)$, another important issue is for what values of x the modified frequency $\tilde{\lambda}(h)$ may actually be expanded in power series of $x = h\lambda$. This is related of course to the radius of convergence of the function $\Phi(x)$ in Proposition 2.4.

Definition 2.9 We denote by r^* the radius of convergence of the expansion in powers of x of $\Phi(x) = \arccos p(x) = \arcsin \sqrt{1 - p(x)^2}$, that is, the maximum of the modulus of the (nonnecessarily real) zeros of $1 - p(x)^2$ with odd multiplicity.

Notice that $r^* \leq x^*$, but not necessarily $r^* \leq x_*$. It is then clear that, for $|x| < r^*$, one has $\Phi(x) = x + \phi_3 x^3 + \phi_5 x^5 + \cdots$. In addition, one step of the method is conjugate to the exact h-flow of the modified harmonic oscillator (2.27) with

$$\tilde{\lambda}(h) = \lambda + h^2 \phi_3 \lambda^3 + h^4 \phi_5 \lambda^5 + \cdots, \tag{2.32}$$

whenever $|h\lambda| < \min(x_*, r^*)$.

On the other hand, notice that the exact solution $O(x)$ given by (2.1) is an orthogonal matrix. Alternatively, the complex quantity $u = q + \mathrm{i}\, p$ evolves through a unitary operator, i.e., $u(x) = U(x)u(0)$ with $U(x) = \mathrm{e}^{-\mathrm{i}x}$ (since u verifies $\mathrm{i}\, u' = \lambda u$). Although a splitting method of the form (2.2) does not preserve the unitarity of $U(x)$ or, equivalently, the orthogonality of $O(x)$, the previous considerations show that *the average relative errors due to the lack of preservation of unitarity or orthogonality do not grow with time, since the scheme is conjugate* (*when* $|h\lambda| < x_*$) *to orthogonal or unitary methods*.

3 Application of Splitting Methods to Linear Systems

One could reasonably argue that there is not much interest in designing new splitting methods with high accuracy and enlarged stability for the numerical integration of the simple harmonic oscillator. There are, however, at least two different issues to be taken into account in regarding this assertion. First, it is unlikely that a splitting method applied to an arbitrary nonlinear system provides good efficiency if it performs poorly when applied to the harmonic oscillator. In particular, good stability and accuracy for the harmonic oscillator is a necessary condition for a good performance when applied to systems that can be considered as perturbations of harmonic oscillators. Second, there are several PDEs modelling highly relevant physical phenomena that, once spatially discretized, give rise to systems of coupled harmonic oscillators where the previous analysis can be used to build accurate and stable algorithms for their numerical treatment. In the sequel, we briefly review four classes of linear systems for which the results in Sect. 2 are of interest.

(i) As a first instance, we consider the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\nabla^2 + V(x)\right)\psi(x,t), \qquad \psi(x,0) = \psi_0(x), \tag{3.1}$$

where $\psi(x,t) : \mathbb{R}^D \times \mathbb{R} \to \mathbb{C}$ is the wave function associated with the system. A common procedure for numerically solving this problem consists in taking first a discrete spatial representation of the wave function. For simplicity, let us consider the one-dimensional case and a given interval $x \in [x_0, x_d]$ ($\psi(x_0,t) = \psi(x_d,t) = 0$ or it has periodic boundary conditions). The interval is split in d parts of length $\Delta x = (x_d - x_0)/d$ and the vector $u = (u_0, \ldots, u_{d-1})^{\mathrm{T}} \in \mathbb{C}^d$ is formed, with $u_j = \psi(x_j,t)(\Delta x)^{1/2}$ and $x_j = x_0 + j\Delta x$, $j = 0, 1, \ldots, d-1$. The PDE (3.1) is then replaced by the d-dimensional complex linear ODE

$$\mathrm{i}u'(t) = Hu(t), \tag{3.2}$$

where $H \in \mathbb{R}^{d\times d}$ represents the (real symmetric) matrix associated with the Hamiltonian. Complex vectors can be avoided by writing $u = q + \mathrm{i}p$, with $q, p \in \mathbb{R}^d$. Equation (3.2) is then equivalent to [3, 10, 11, 18, 23, 34]

$$q' = Hp, \qquad p' = -Hq. \tag{3.3}$$

In principle, H can be factorized as $H = R^{-1}\Lambda R$, where Λ is the diagonal matrix containing the eigenvalues of H. The system (3.3) can be decoupled, after the change of variables $Q = Rq$, $P = Rp$, into a system of d one-dimensional harmonic oscillators

$$Q' = \Lambda P, \qquad P' = -\Lambda Q. \tag{3.4}$$

In practice, however, $d \gg 1$, so it turns prohibitively expensive to carry out the diagonalization of H. In such circumstances, it is of interest to apply splitting methods to (3.3), since our previous analysis remains valid here. Moreover, due to the nature of this problem, Fourier techniques can be used and the products Hq, Hp can be evaluated with $\mathcal{O}(d \log d)$ operations with the Fast Fourier Transform (FFT) algorithm. Notice that $H = T + \hat{V}$, where $\hat{V}$ is a diagonal matrix with elements $\hat{V}_{jj} = V(x_j)$ and the matrix T (associated to the kinetic energy) can be diagonalized. Thus we have $T = F^{-1}DF$, where F, F^{-1} correspond to the Fourier transform and its inverse, respectively, and D is a diagonal matrix. Therefore (3.3) can be written as

$$q' = \left(F^{-1}DF + \hat{V}\right)p, \qquad p' = -\left(F^{-1}DF + \hat{V}\right)q. \tag{3.5}$$

Thus, numerical methods requiring only the computation of matrix–vector products of the form Hq and Hp may lead to very efficient integration algorithms. This is precisely the case when the splitting method (1.2) is applied to (3.3) with

$$f^{[A]}(z) = (Hp, 0)^{\mathrm{T}}, \qquad f^{[B]}(z) = (0, -Hq)^{\mathrm{T}}, \qquad z = (q,p)^{\mathrm{T}},$$

as the corresponding h-flows $\varphi_h^{[A]}$ and $\varphi_h^{[B]}$ are

$$\varphi^{[A]}(z) = (q + hHp, p), \qquad \varphi^{[B]}(z) = (q, p - hHq).$$

Since, by assumption, H is a symmetric matrix, the solution operator of (3.3) is orthogonal. Equivalently, the vector u associated with the wave function evolves through a unitary operator, and the norm of u is preserved. Then, as we have seen in Sect. 2.5, when a splitting method is applied this property is not exactly preserved, but the averaged errors in the preservation of unitarity do not grow with time (a fact already noticed numerically in [30]).

Let us analyze this issue in more detail. Clearly, applying a splitting method to (3.3) is equivalent, after the change of variables $Q = Rq$, $P = Rp$, to applying the same method to the system (3.4) of decoupled harmonic oscillators. Hence, one step of the method is conjugate to the exact h-flow of harmonic oscillators of the form (2.27) with $\tilde{\lambda}(h) = \Phi(h\lambda)/h$. In consequence, by reversing the change of variables, one step of the method is conjugate to the exact h-flow of the modified system

$$q' = \tilde{H}(h)p, \qquad p' = -\tilde{H}(h)q, \tag{3.6}$$

(or, equivalently, $\mathrm{i}u' = \tilde{H}(h)u$) for values of h such that $|h|\rho(H) < x_*$, where $\rho(H)$ is the spectral radius of H. Here $\tilde{H}(h) = (1/h)R^{-1}\Phi(h\Lambda)R$ (and Φ is applied componentwise to each entry of the diagonal matrix $h\Lambda$). If $|h|\rho(H) < \min(r^*, x_*)$, we have

$$\tilde{H}(h) = H + h^2\phi_3 H^3 + h^4\phi_5 H^5 + \cdots. \tag{3.7}$$

Notice that $\tilde{H}(h)$ is obviously a symmetric matrix, provided that H is also symmetric.

(ii) Another system which can also be decoupled into a number of one-dimensional harmonic oscillators is

$$y'' + Ky = 0, \tag{3.8}$$

where $y \in \mathbb{R}^d$ and the matrix $K \in \mathbb{R}^{d\times d}$ is diagonalizable with real positive eigenvalues (K can be, in particular, a real symmetric positive definite matrix). Systems of this form arise after a semidiscretization of some parabolic PDEs whose linear part has to be efficiently computed (see Chap. XIII of [12] and references therein).

In this case, one can use a change of variables of the form $P = \Lambda^{-1}Ry'$, $Q = Ry$ (where Λ is the diagonal matrix such that $K = R^{-1}\Lambda^2 R$) to show that the application of one step of size h of a splitting method to the system (3.8) is, provided that $|h|\sqrt{\rho(K)} < x_*$, conjugate to the exact h-flow of the modified system

$$y'' + \tilde{K}(h)y = 0,$$

with $\tilde{K}(h)$ a perturbation of K defined in terms of Φ. In particular, $\tilde{K}(h) = K + h^2\phi_3 K^2 + h^4\phi_5 K^3 + \cdots$ whenever $|h|\sqrt{\rho(K)} < \min(r^*, x_*)$.

(iii) A more general class of problems which can be reduced to a system of decoupled harmonic oscillators is the following:

$$q' = Mp, \qquad p' = -Nq. \tag{3.9}$$

Here $q \in \mathbb{R}^{d_1}$, $p \in \mathbb{R}^{d_2}$, $M \in \mathbb{R}^{d_1\times d_2}$ and $N \in \mathbb{R}^{d_2\times d_1}$, with the additional constraint that either MN or NM is diagonalizable with real positive eigenvalues. Notice that this class includes both (3.3) and (3.8) as particular instances, with $M = N = H$ in the first case and $M = I$, $N = K$ in the second one.

Systems of the form (3.9) arise, for example, after spacial discretization of the Maxwell equations, of relevant interest in physics and engineering [13, 27, 32].

The relation of (3.9) with (3.8) becomes clear by observing that the solution of (3.9) can be obtained by solving either

$$q'' + MNq = 0, \qquad p' = -Nq,$$

or

$$p'' + NMp = 0, \qquad q' = Mp.$$

As a matter of fact, a splitting method applied to (3.9) is conjugate, for sufficiently small h, to the solution of the modified system

$$q' = \tilde{M}(h)p, \qquad p' = -\tilde{N}(h)q, \tag{3.10}$$

with

$$\begin{aligned}\tilde{M}(h) &= M\big(I + \phi_3 h^2 (NM) + \phi_5 h^4 (NM)^2 + \cdots\big)\\ &= \big(I + \phi_3 h^2 (MN) + \phi_5 h^4 (MN)^2 + \cdots\big)M, \end{aligned}\tag{3.11}$$

$$\begin{aligned}\tilde{N}(h) &= N\big(I + \phi_3 h^2 (MN) + \phi_5 h^4 (MN)^2 + \cdots\big)\\ &= \big(I + \phi_3 h^2 (NM) + \phi_5 h^4 (NM)^2 + \cdots\big)N. \end{aligned}\tag{3.12}$$

This can be established, as in the cases (i) and (ii) previously, in two particular situations:

(a) The matrix MN is diagonalizable with positive eigenvalues and, in addition, M and N are square matrices and M is invertible. In that case, let MN be decomposed as $MN = R^{-1}\Lambda^2 R$, where Λ is a diagonal matrix. Then the system (3.9) is decoupled as (3.4) with the transformation $P = \Lambda^{-1}RMp$, $Q = Rq$. A similar argument to that used in (i) leads to the required result whenever $|h|\sqrt{\rho(MN)} < \min(r^*, x_*)$.

(b) The matrix NM is diagonalizable with positive eigenvalues and, in addition, M and N are square matrices and N is invertible. Then a similar argument leads to the required result whenever $|h|\sqrt{\rho(NM)} < \min(r^*, x_*)$.

In general, we will next show that there exists $r_* > 0$ (satisfying that $r_* \leq \min(r^*, x_*)$), depending on the parameters a_j, b_j of the splitting method such that the approximate solution of (3.9) obtained is conjugate to the solution of the modified system (3.10)–(3.12) whenever $|h|\sqrt{\rho_{M,N}} < r_*$, where

$$\rho_{M,N} = \min\big(\rho(NM), \rho(MN)\big). \tag{3.13}$$

As this assertion can be proved for arbitrary matrices N and M (without any constraint about the square matrices NM and MN), it is worth considering a more general class of systems.

(iv) Let us examine now a linear system of the form (3.9) with arbitrary matrices N and M. One step of the splitting method (1.2) applied to that system with

$$f^{[A]}(z) = (Mp, 0)^{\mathrm{T}}, \qquad f^{[B]}(z) = (0, -Nq)^{\mathrm{T}}, \qquad z = (q, p)^{\mathrm{T}},$$

gives $\psi_h(z) = \mathbf{K}(h)z$, where

$$\mathbf{K}(h) = \begin{pmatrix} I & 0 \\ -b_k N & I \end{pmatrix} \begin{pmatrix} I & a_k M \\ 0 & I \end{pmatrix} \cdots \begin{pmatrix} I & 0 \\ -b_1 N & I \end{pmatrix} \begin{pmatrix} I & a_1 M \\ 0 & I \end{pmatrix}. \tag{3.14}$$

Studying the application of splitting methods to the system (3.9) is of interest, for instance, when considering the linearization around a stationary point of a Hamiltonian system with Hamiltonian function of the form $H(q,p) = T(p) + V(q)$.

Clearly, $\mathbf{K}(h)$ can be rewritten in the form

$$\mathbf{K}(h) = \begin{pmatrix} I_{d_1} + \sum_{j\ge 1} k_{1,j} h^{2j} (MN)^j & \sum_{j\ge 1} k_{2,j} h^{2j-1} M (NM)^{j-1} \\ \sum_{j\ge 1} k_{3,j} h^{2j-1} N (MN)^{j-1} & I_{d_2} + \sum_{j\ge 1} k_{4,j} h^{2j} (NM)^j \end{pmatrix}. \tag{3.15}$$

Here the coefficients $k_{i,j}$ are those of the polynomial entries (2.5) of the stability matrix (2.7) of the splitting method. It is worth noting that one step $\psi_h(z)$ of an arbitrary partitioned Runge–Kutta (PRK) method applied to the partitioned system (3.9) has also the form $\psi_h(z) = \mathbf{K}(h)z$, where the matrix $\mathbf{K}(h)$ is of the form (3.15). For implicit PRK methods there is an infinite number of nonzero coefficients $k_{i,j}$, and the expressions

$$\begin{aligned} K_1(x) &= 1 + \sum_{j\ge 1} k_{1,j} x^{2j}, & K_2(x) &= \sum_{j\ge 1} k_{2,j} x^{2j-1}, \\ K_3(x) &= \sum_{j\ge 1} k_{3,j} x^{2j-1}, & K_4(x) &= 1 + \sum_{j\ge 1} k_{4,j} x^{2j}, \end{aligned} \tag{3.16}$$

are obtained by expanding in series of powers of x certain rational functions (the entries of the stability matrix $K(x)$ of the method). For explicit PRK methods, $K_1(x)$, $K_2(x)$, $K_3(x)$, $K_4(x)$ are polynomial functions.

The next result shows that *any partitioned method* (*splitting methods, PRK methods*) *applied to the system* (3.9) *is, for a sufficiently small step size h, conjugate to a nonpartitioned method* (defined as a power series expansion).

Proposition 3.1 *Let us consider a* 2×2 *matrix* (2.7) *depending on the variable* x *whose entries are defined as power series* (3.16) *with nonzero radius of convergence. For arbitrary matrices* $M \in \mathbb{R}^{d_1 \times d_2}$, $N \in \mathbb{R}^{d_2 \times d_1}$, *consider the square matrix of dimension* $(d_1 + d_2)$ *given by* (3.15).

Then there exists $r > 0$ *and a power series* $\sum_{j\ge 1} s_j x^j$ *such that the matrix* $\mathbf{K}(h)$ *given by* (3.15) *is, provided that* $|h|\sqrt{\rho_{M,N}} < r$, *similar to*

$$\mathbf{S}(h) = I_{d_1+d_2} + \sum_{j\ge 1} s_j h^j \begin{pmatrix} 0 & M \\ -N & 0 \end{pmatrix}^j. \tag{3.17}$$

In addition, if $\det K(x) \equiv 1$ (*in particular, if* $K(x)$ *is the stability matrix of a splitting method*), *then* $\mathbf{S}(h)$ *is the exponential of the matrix*

$$h \begin{pmatrix} 0 & \tilde{M}(h) \\ -\tilde{N}(h) & 0 \end{pmatrix},$$

where $\tilde{M}(h)$ *and* $\tilde{N}(h)$ *are given by* (3.11)–(3.12), *and* $x + \phi_3 x^3 + \phi_5 x^5 + \cdots$ *is the power series expansion of*

$$\Phi(x) = \arccos \frac{K_1(x) + K_4(x)}{2} = \arcsin \sqrt{1 - \left(\frac{K_1(x) + K_4(x)}{2}\right)^2}.$$

Proof We first show that there exist $r > 0$ and a 2×2 matrix (2.28) whose entries are defined as power series

$$P_1(x) = 1 + \sum_{j\geq 1} p_{1,j} x^{2j}, \qquad P_2(x) = \sum_{j\geq 1} p_{2,j} x^{2j-1},$$
$$P_3(x) = \sum_{j\geq 1} p_{3,j} x^{2j-1}, \qquad P_4(x) = 1 + \sum_{j\geq 1} p_{4,j} x^{2j},$$

with nonzero radius of convergence, such that, for $|x| < r$, $P(x)K(x)P(x)^{-1}$ is well-defined and has the form

$$S(x) = \begin{pmatrix} S_1(x) & S_2(x) \\ -S_2(x) & S_1(x) \end{pmatrix}, \tag{3.18}$$

where

$$S_1(x) = 1 + \sum_{j\geq 1} (-1)^j s_{2j} x^{2j}, \qquad S_2(x) = \sum_{j\geq 1} (-1)^{j-1} s_{2j-1} x^{2j-1}. \tag{3.19}$$

Once this is proven, it is straightforward to check that, for the square matrix $\mathbf{P}(h)$ of dimension $(d_1 + d_2)$,

$$\mathbf{P}(h) = \begin{pmatrix} I_{d_1} + \sum_{j\geq 1} p_{1,j} h^{2j} (MN)^j, & \sum_{j\geq 1} p_{2,j} h^{2j-1} M(NM)^{j-1} \\ \sum_{j\geq 1} p_{3,j} h^{2j-1} N(MN)^{j-1} & I_{d_2} + \sum_{j\geq 1} p_{4,j} h^{2j} (NM)^j \end{pmatrix}, \tag{3.20}$$

the matrix $\mathbf{P}(h)\mathbf{K}(h)\mathbf{P}(h)^{-1}$ coincides, whenever $|h|\sqrt{\rho_{M,N}} < r$, with

$$\begin{pmatrix} I_{d_1} + \sum_{j\geq 1} (-1)^j s_{2j} h^{2j} (MN)^j, & \sum_{j\geq 1} (-1)^{j-1} s_{2j-1} h^{2j-1} M(NM)^{j-1} \\ \sum_{j\geq 1} (-1)^j s_{2j-1} h^{2j-1} N(MN)^{j-1} & I_{d_2} + \sum_{j\geq 1} (-1)^j s_{2j} h^{2j} (NM)^j \end{pmatrix},$$

which is precisely (3.17).

Indeed, one can directly check that $P(x)K(x)P(x)^{-1} = S(x)$ with

$$\begin{aligned} S_1(x) &= \frac{K_1(x)+K_4(x)}{2}, \qquad & S_2(x) &= \sqrt{\det(K(x)) - S_1(x)^2}, \\ P_1(x) &= \sqrt{\frac{-K_3(x)}{S_2(x)}}, \qquad & P_2(x) &= \frac{K_1(x)-K_4(x)}{2S_2(x)P_1(x)}, \\ P_3(x) &= 0, \qquad & P_4(x) &= \frac{1}{P_1(x)}, \end{aligned} \tag{3.21}$$

and r can be taken as the minimum among the radii of convergence of the series $K_j(x), S_j(x), P_j(x)$. According to (3.19), $S_1(x) + \mathrm{i}S_2(x) = \sum s_j(\mathrm{i}x)^j$, and thus $\sum s_j x^j$ is the series expansion of $S_1(-\mathrm{i}x) + \mathrm{i}S_2(-\mathrm{i}x)$ where $S_1(x)$ and $S_2(x)$ are given by (3.21). If $\det K(x) \equiv 1$ (in particular, if $K(x)$ is the stability matrix of a splitting method), we have that

$$S_1(x) = \frac{K_1(x)+K_4(x)}{2} = \cos(\Phi(x)), \qquad S_2(x) = \sqrt{1 - S_1(x)^2} = \sin(\Phi(x)),$$

where

$$\Phi(x) = \arccos S_1(x) = \arcsin \sqrt{1 - S_1(x)^2},$$

and therefore $\sum s_j x^j$ is the series expansion of $\exp(\mathrm{i}\Phi(-\mathrm{i}x))$. If $x + \phi_3 x^3 + \phi_5 x^5 + \cdots$ is the power series expansion of $\Phi(x)$, it is clear that $\mathrm{i}\Phi(-\mathrm{i}x) = x - \phi_3 x^3 + \phi_5 x^5 - \cdots$ and a simple calculation shows that $\mathbf{S}(h)$ is the exponential of

$$\mathrm{i}\Phi\left(-\mathrm{i}h\begin{pmatrix} 0 & M \\ -N & 0 \end{pmatrix}\right) = h\begin{pmatrix} 0 & \tilde{M}(h) \\ -\tilde{N}(h) & 0 \end{pmatrix},$$

thus completing the proof. □

Notice that, in the proof above, there are other choices for $P(x)$. For instance, we could have required that $P_2(x) = 0$, $P_4(x) = 1/P_1(x)$. Different choices for $P(x)$ in general will give a different value of r.

Definition 3.2 Let us denote as r_* the maximal r for which the statement of Proposition 3.1 holds.

For splitting methods, we always have that $r_* \le r^*$ and $r_* \le x_*$. The following generalization of Proposition 2.8 will be useful in the next section.

Proposition 3.3 *Suppose we have an even polynomial $p(x)$ satisfying* (2.11), *so that $0 < r^* \le x^*$. Then, there exists a time-reversible stability matrix of the form*

$$K(x) = \begin{pmatrix} p(x) & K_2(x) \\ K_3(x) & p(x) \end{pmatrix} \tag{3.22}$$

for which $x_* = x^*$ and $r_* = r^*$.

Proof According to Definition 2.9, $r^* > 0$ is the maximum of the modulus of the zeros of $1 - p(x)^2$ with odd multiplicity. Now let $0, \pm x_1, \ldots, \pm x_l$ be all the zeros with even multiplicity of the polynomial $1 - p(x)^2$ with modulus $|x_j| < r^*$. Then the polynomial $1 - p(x)^2$ can be decomposed as

$$1 - p(x)^2 = x^{2m_0} Q(x) \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big)^{2m_j},$$

where each $m_0, m_1, \ldots, m_l$ is the multiplicity of the zeros $0, \pm x_1, \ldots, \pm x_l$, respectively, and $Q(x)$ is an even polynomial satisfying that $Q(0) = 1$ and has no zeros with even multiplicity. We thus have that

$$\begin{aligned}
\Phi(x) &= \arccos\big(p(x)\big) \\
&= \arcsin\Big(\sqrt{1 - p(x)^2}\Big) \\
&= \arcsin\left(\sqrt{Q(x)} x^{m_0} \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big)^{m_j}\right),
\end{aligned}$$

so that r^* is the maximum of the modulus of the zeros of $Q(x)$. We then choose a decomposition $Q(x) = Q_2(x) Q_3(x)$ of even polynomials such that $Q_2(0) = Q_3(0) = 1$, and determine $K_2(x), K_3(x)$ as

$$\begin{aligned}
K_2(x) &= x^{m_0} Q_2(x) \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big)^{m_j}, \\
K_3(x) &= -x^{m_0} Q_3(x) \prod_{j=1}^{l} \big((x/x_j)^2 - 1\big)^{m_j}.
\end{aligned} \tag{3.23}$$

This completes the proof, since, according to (2.31), $P_1(x) = \sqrt[4]{Q_3(x)/Q_2(x)}$ and $P_4(x) = \sqrt[4]{Q_2(x)/Q_3(x)}$, and the radius of convergence of their powers series expansions is precisely the maximum of the modulus of the zeros of $Q(x) = Q_2(x) Q_3(x)$, that is, r^*. □

4 Construction of Processed Splitting Methods with Enlarged Stability Domain and High Accuracy

The theoretical analysis done in the previous sections shows, in particular, that the stability polynomial $p(x)$ carries all the information needed to construct processed splitting methods for numerically approximating the evolution of the harmonic oscillator. Our aim in this section is precisely to use this analysis to obtain efficient processed splitting methods to solve numerically the linear system (3.9). In other words, our goal is to approximate the exponential

$$\exp\left[t \begin{pmatrix} 0 & M \\ -N & 0 \end{pmatrix}\right] \tag{4.1}$$

by means of

$$\mathbf{S}(h)^m = \mathbf{P}(h)[\mathbf{K}(h)]^m \mathbf{P}(h)^{-1},$$

where $h = t/m$ is sufficiently small, the kernel $\mathbf{K}(h)$ is given by (3.14) (which can be rewritten as (3.15)), and $\mathbf{P}(h)$ is defined in terms of power series expansions as in the proof of Proposition 3.1 provided that $h\sqrt{\rho_{M,N}} < r_*$, where $\rho_{M,N}$ is given by (3.13).

We will concentrate ourselves in the case where either NM or MN is diagonalizable with positive eigenvalues, so that the performance of the method will be directly related to the accuracy and stability of the method when applied to the harmonic oscillator.

In practice, $\mathbf{P}(h)$ and $\mathbf{P}(h)^{-1}$ will be approximated by polynomials, and one will be able to approximate the action of the exponential (4.1) on the vector $(q, p)^{\mathrm{T}}$ by means of matrix–vector products of the form Mp and Nq.

Taking previous considerations into account, we consider a composition of the form (3.14) whose stability polynomial $p(x)$ fulfills the following requirements:

- C.1. $p(x) = \cos x + \mathcal{O}(x^{2n+2})$ as $x \to 0$ for certain $n \geq 1$ (thus achieving effective order $q = 2n$).
- C.2. There exist $l \geq 1$ and $x_j \in \mathbb{R}$, $j = 1, \ldots, l$, such that $0 < x_1 < \cdots < x_l$, each x_j is a double zero of the polynomial $p(x) - (-1)^j$, and all the (perhaps complex) zeros of odd multiplicity of the polynomial $(p(x)^2 - 1)$ have modulus greater than x_l (so that $x^* \geq r^* > x_l$).
- C.3. For each $j = 1, \ldots, l$, $x_j = j\pi$.

Once the polynomial $p(x)$ is fixed, there still remains to determine a stability matrix $K(x)$. In general, we have that $x_* \leq x^*$ and $r_* \leq r^*$. *The optimal case is achieved when $x_* = x^*$ and $r_* = r^*$, and any processed method for which these two equalities hold are equivalent*. The proof of Proposition 3.3 provides a procedure to obtain all stability matrices $K(x)$ for which $x_* = x^*$ and $r_* = r^*$. For each such a stability matrix $K(x)$, we follow the algorithm described in the proof of Proposition 2.3 to obtain its decomposition (2.12), and we choose among them a stability matrix $K(x)$ whose decomposition is of the form (2.2). This will give us the coefficients a_i, b_i for kernel of the processed method given by the composition (3.14). In Subsection 4.3 we provide a simple procedure to obtain pre- and post-processors from the polynomials $K_i(x)$.

It is important to keep in mind that the cost of a composition method with polynomial stability $p(x)$ is proportional to the degree of $p(x)$. We can always improve both the stability and the accuracy of $p(x)$ by increasing its degree, but this makes sense only if the improvement compensates for the extra computational cost required.

4.1 Construction of Stability Polynomials

According to the previous requirements, we take as candidates for $p(x)$ polynomials in the following family. For each $n, l \geq 0$ we consider the even polynomial $p^{n,l}(x)$ with minimal degree among those satisfying: (i) $p^{n,l}(x) = \cos x + \mathcal{O}(x^{2n+2})$ as $x \to 0$; and (ii) for each $1 \leq j \leq l$, $x_j = j\pi$ is a double zero of $p^{n,l}(x) - (-1)^j$.

For arbitrary $n, l \geq 1$ we take $p^{n,l}(x)$ as

$$p^{n,l}(x) = 1 + \sum_{j=1}^{n} (-1)^j \frac{x^{2j}}{(2j)!} + x^{2n} \sum_{j=1}^{2l} d_j x^{2j}, \tag{4.2}$$

where the coefficients d_j are uniquely determined by the requirement that

$$p(j\pi) = (-1)^j, \quad p'(j\pi) = 0, \quad j = 1, \dots, l, \tag{4.3}$$

holds for $p(x) = p^{n,l}(x)$. Notice the interpolatory nature of $p^{n,l}(x)$ (as $\cos(j\pi) = (-1)^j$ and $\cos'(j\pi) = -\sin(j\pi) = 0$). By using a symbolic algebra package one gets the numerical values of d_j, $j = 1, \dots, 2l$, with the desired accuracy and for any value of l of practical interest.

With the polynomial $p^{n,l}(x)$ it is possible to get an estimate of the relative performance of the splitting methods which can be obtained from it. Since a k-stage method has a stability polynomial of degree $2k$ we can take the degree of $p^{n,l}(x)$ $(d(p^{n,l}) = 2(n + 2l))$ as twice the number of stages needed for the composition methods. The accuracy can be measured by evaluating the error function $\mathcal{E}_{n,l}(x) \equiv |\arccos p^{n,l}(x) - x|$ for different values of $x \in [0, x^*]$. Figure 1(a) shows $\mathcal{E}_{n,l}(x)$ versus COST$= (n + 2l)/x$ (to measure the accuracy at a given cost, where x plays the role of the time step) for $n = 5$, $l = 3, 5, 7$ and $n = 10$, $l = 6, 10, 14$ corresponding to approximations of order 10 and 20. Each choice for $p^{n,l}(x)$ is denoted by $(n, l, 0)$ in the figure. The curves which stay below in the same figure show the highest performance, i.e., they give the smallest error at a given cost. From the figures we observe the surprising fact that *the performance seems to improve with l for each fixed value of n*, and for most values of COST. This occurs for nearly all values of n and l checked, up to $(n + 2l) = 50$, corresponding to methods with up to 50 stages. Figure 1(b) shows the results for $(n, l) = (5, 7), (8, 12), (10, 14)$ which would correspond to methods with 19, 32 and 38 stages, respectively.

On the other hand, if one is interested in approximating the solution matrix $O(x)$ accurately for $x \in (-x_*, x_*)$ with $|x|$ as large as possible, we may require, in addition to C.1–C.3 above:

C.4. For a relatively low effective order $q = 2n$, the stability polynomial $p(x)$ approximates $\cos(x)$ with acceptable precision for all $x \in (-x_l, x_l)$.

With the purpose of fulfilling this goal, we propose considering the following polynomials as candidates for the stability polynomial $p(x)$. For each $n, l, m \geq 0$, we take

$$p^{n,l,m}(x) = \sum_{j=1}^{n} (-1)^j \frac{x^{2j}}{(2j)!} + x^{2n} \sum_{j=1}^{2l} d_j x^{2j} + x^{2n} \prod_{j=1}^{l} \bigl(x^2 - (j\pi)^2\bigr)^2 \sum_{i=1}^{m} e_i x^{2i}, \tag{4.4}$$

satisfying (4.3) for $p(x) = p^{n,l,m}(x)$, so that the coefficients d_j $(1 \leq j \leq 2l)$ verify the same conditions as before (and thus they are uniquely determined). We have now

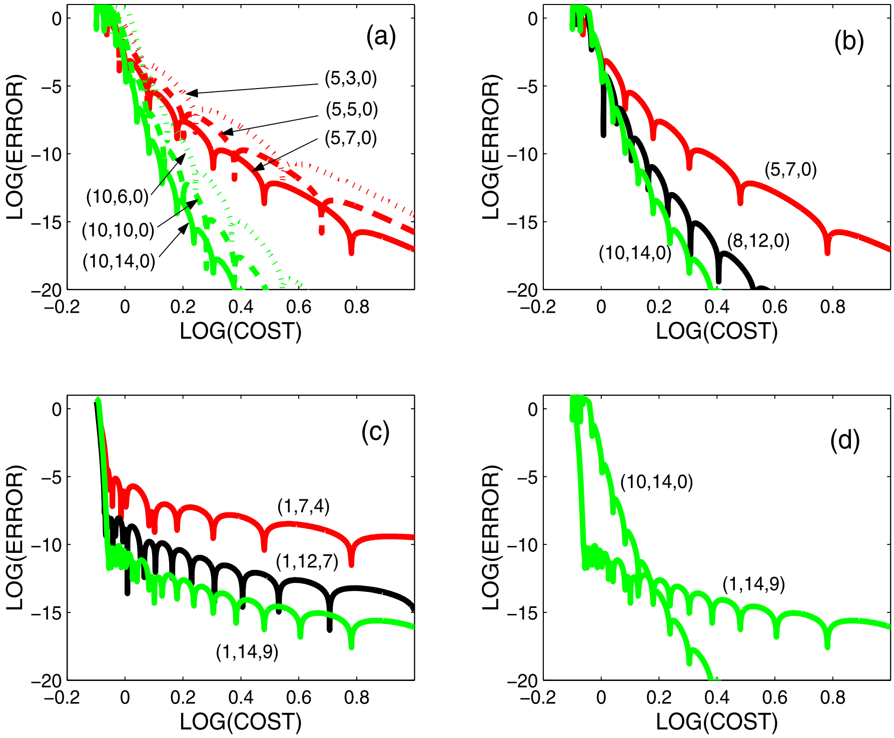

Fig. 1 Error $\mathcal{E}_{n,l,m}$ given by (4.6) versus COST $= (n+2l+m)/x$ in double logarithmic scale: **a** for stability polynomials $p^{n,l}(x)$ with $n=5,10$ (corresponding to approximations of order 10 and 20 and $m=0$) and different values of l, which are denoted by $(n,l,0)$; **b** for $(n,l)=(5,7),(8,12),(10,14)$; **c** the same for $p^{n,l,m}(x)$ with $(n,l,m)=(1,7,4),(1,12,7),(1,14,9)$ corresponding to polynomials of the same degree as in (b); and **d** comparison of the most efficient stability polynomials

the free parameters e_i $(1 \le i \le m)$, which we propose to determine in such a way that

$$\int_{-l\pi}^{l\pi} \left(1-\left(\frac{x}{l\pi}\right)^2\right)^{-1/2} \left(\frac{p^{n,l,m}(x)-\cos x}{x^{2n+2}}\right)^2 \mathrm{d}x \tag{4.5}$$

is minimized. Notice that this is equivalent to minimizing in the least square sense the coefficients of the Chebyshev series expansion of $(p^{n,l,m}(x)-\cos x)/(x^{2n+2})$, which depend linearly on e_i $(1 \le i \le m)$, and thus the values of e_i can be exactly determined. In practice, this can be done conveniently with the help of some symbolic algebra program.

By following this approach we have analyzed stability polynomials with up to $(n+2l+m)=50$ (corresponding to methods up to 50 stages) for different values of n,l,m. Analogously, to measure their relative performances, we compare the error

$$\mathcal{E}_{n,l,m}(x) \equiv \left|\arccos\, p^{n,l,m}(x) - x\right| \tag{4.6}$$

versus COST $= (n+2l+m)/x$ for different real values of x. In Fig. 1(c) we show the results obtained for some representative choices of $p^{n,l,m}(x)$, denoted by (n,l,m), corresponding to polynomials of the same degree as those shown in Fig. 1(b).

In all cases, the performance apparently improves with the number of stages. Figure 1(d) compares the performance of the best stability polynomial of each family (both correspond to polynomials of degree 76 and associated to 38-stage methods). It seems that, up to a very high accuracy, the best performance corresponds to the second-order method $(1,14,9)$. The fact that second-order schemes requiring a large number of stages perform better than higher-order integrators in this setting is perhaps surprising. We should bear in mind, however, that the new methods have been designed precisely by following the strategy stated in the Introduction and pursued in Sects. 2 and 3: we select the coefficients in such a way that the error coefficients (beyond second-order) are sufficiently small to get high accuracy in practice *and* the stability interval is not seriously deteriorated in comparison with a concatenation of leapfrog methods.

4.2 Construction of the Stability Matrix

Once a polynomial $p(x)$ satisfying conditions C.1–C.3 (and possibly C.4) is determined, the next step is choosing the remaining entries of the stability matrix (3.22). As previously stated, two different k-stage palindromic compositions are considered for the kernel:

$$\mathrm{e}^{ha_{k+1}A}\mathrm{e}^{hb_k B}\mathrm{e}^{ha_k A}\cdots\mathrm{e}^{hb_1 B}\mathrm{e}^{ha_1 A}, \tag{4.7}$$

with $a_{k+2-i}=a_i$, $b_{k+1}=0$, $b_{k+1-i}=b_i$, $i=1,2,\dots,$ and

$$\mathrm{e}^{hb_{k+1}B}\mathrm{e}^{ha_{k+1}A}\mathrm{e}^{hb_k B}\mathrm{e}^{ha_k A}\cdots\mathrm{e}^{hb_1 B}, \tag{4.8}$$

with $a_1=0$, $a_{k+2-i}=a_{i+1}$, $b_{k+2-i}=b_i$, $i=1,2,\dots.$

In both cases $p(x)$ has degree $2k$. With respect to the entries of the corresponding stability matrix $K(x)$, we have $K_1(x)=K_4(x)=p(x)$, and $(K_2(x), K_3(x))$ have degree $(2k-1, 2k+1)$ for (4.7) and degree $(2k+1, 2k-1)$ for (4.8). The polynomials $(K_2(x), K_3(x))$ are such that

$$\begin{aligned} p(x)^2-1 &= K_2(x)K_3(x),\\ K_2'(0) &= -K_3'(0)=1,\\ K_2(x_j) &= K_3(x_j)=0, \qquad j=1,\dots,l, \end{aligned}$$

and they satisfy (2.26), thus assuring that $\det K(x)=1$, $K(x)$ is a consistent approximation to (2.1), $x_*=x^*$ and $r_*=r^*$. Clearly, there is a finite number of different choices of such pairs $(K_2(x), K_3(x))$, and among them, we choose a pair such that the corresponding matrix $K(x)$ admits a decomposition of the form (2.2).

For convenience, we denote by $\mathrm{P}_k 2n$ a processed method of order $2n$ whose kernel is a k-stage composition of the form (2.2).

As representative of the methods which can be obtained by applying this procedure, in Table 1 we show the coefficients a_i, b_i for the kernel of a pair of processed

Table 1 Coefficients for a 19-stage and a 32-stage time-reversible kernels corresponding to processed methods of orders 10, $P_{19}10$, and 16, $P_{32}16$, respectively

$P_{19}10$	
$a_1 = 0.0432386502874358427757883618871$	$b_1 = 0.0874171140239240929444597874709$
$a_2 = 0.0891872116514875241139576575882$	$b_2 = 0.0895405507537538756041132269850$
$a_3 = 0.0874015611733434678704032626168$	$b_3 = 0.0864066075260518454826592764125$
$a_4 = 0.0954273508490522988798690279811$	$b_4 = 0.140834736382004911175445238602$
$a_5 = -0.0753249126916028783286798309378$	$b_5 = -0.0137118117308991304396120981534$
$a_6 = 0.202523451531452141504790651968$	$b_6 = 0.541807462991626392685440183001$
$a_7 = -0.000603437796174370985636258252420$	$b_7 = -0.461545568134225404224525737926$
$a_8 = 0.141029942275295351245992767342$	$b_8 = 0.414574847635699390317333308406$
$a_9 = 0.000076451609282844443214456109750 9$	$b_9 = -0.417468813318454485878866802863$
$a_{10} = \frac{1}{2} - (a_1 + \cdots + a_9)$	$b_{10} = 1 - 2(b_1 + \cdots + b_9)$
$a_{21-i} = a_i, \quad i = 1, \ldots, 10$	$b_{20-i} = b_i, \quad i = 1, \ldots, 9$
$P_{32}16$	
$a_1 = 0$	$b_1 = 0.0246666504515374580138379933112$
$a_2 = 0.0503626559561541491851284108304$	$b_2 = 0.0526269985834362938158150887511$
$a_3 = 0.0546948611952386879984253468680$	$b_3 = 0.0557559872576229997353176147790$
$a_4 = 0.0554620390434566637065911933769$	$b_4 = 0.0537116878888677727588921080438$
$a_5 = 0.0516143924380795892137585965956$	$b_5 = 0.0519896869988046163617507304275$
$a_6 = 0.0568363649879098885339104529672$	$b_6 = 0.0666959676117604242374885628805$
$a_7 = 0.0939589227273508162683355424334$	$b_7 = -0.102796651142514055780607785308$
$a_8 = -0.00445692008047188584894138698734$	$b_8 = 0.182323867085459132242253779621$
$a_9 = 0.0817426743654653601759083129289$	$b_9 = -0.00542617878109449520635361125714$
$a_{10} = -0.0366714030328452540070009347543$	$b_{10} = 0.0593919899010186971711928695894$
$a_{11} = 0.0620267535945808302363559446459$	$b_{11} = 0.0462313377171662707918171716453$
$a_{12} = -0.0316075550822111219959097903622$	$b_{12} = -0.0137171722415664093079656810822$
$a_{13} = 0.0518562640986284507641256284631$	$b_{13} = 0.582408428792399942617750550408$
$a_{14} = -0.000737830036206379685982463916033$	$b_{14} = -0.562094520697629270991481101437$
$a_{15} = 0.0536217552433463298408750165913$	$b_{15} = -0.0180034629218910159228722367539$
$a_{16} = 0.0150674488859324181502166600981$	$b_{16} = 0.00990593102843635080330651455161$
$a_{17} = \frac{1}{2} - (a_1 + \cdots + a_{16})$	$b_{17} = 1 - 2(b_1 + \cdots + b_{16})$
$a_{34-i} = a_{i+1}, \quad i = 1, \ldots, 16$	$b_{34-i} = b_i, \quad i = 1, \ldots, 16$

methods. The first set of coefficients corresponds to $P_{19}10$, given by the composition (4.7) with $k = 19$, whereas the second belongs to $P_{32}16$, given by the composition (4.8) with $k = 32$. Coefficients for a method $P_{38}2$ can be found in [3].

It is worth noticing here a distinctive pattern observed in the coefficients of the methods we have obtained. Let us consider, in particular, the scheme $P_{32}16$ from Table 1. The coefficients $a_i, b_i,\ i = 1, \ldots, 6$, are very close to a sequence of leapfrog stages $\psi_{\alpha_i h,2} = \varphi_{\alpha_i h/2}^{[B]} \circ \varphi_{\alpha_i h}^{[A]} \circ \varphi_{\alpha_i h/2}^{[B]}$ with $\alpha_i \approx 0.05$ (this value is only slightly larger than that corresponding to a full sequence of leapfrog stages with $\alpha_i = 1/32,\ i = 1, \ldots, 32$, and is also closely related to the rule of thumb proposed by McLachlan

[24]). There are some coefficients, like b_{13} and b_{14}, with considerably larger values, but these appear in a very particular sequence. Notice that the composition

$$K(b_i, a_i, b_{i-1}) \equiv \mathrm{e}^{hb_i B}\mathrm{e}^{ha_i A}\mathrm{e}^{hb_{i-1} B} = \begin{pmatrix} 1 - h^2 a_i b_{i-1} & ha_i \\ -h(b_i + b_{i-1}) + h^3 a_i b_i b_{i-1} & 1 - h^2 a_i b_i \end{pmatrix}$$

gives in this case

$$K(b_{14}, a_{14}, b_{13}) \approx \begin{pmatrix} 1 - 4.1 \cdot 10^{-5} h^2 & -7.3 \cdot 10^{-5} h \\ -0.02h + 2.4 \cdot 10^{-5} h^3 & 1 + 4.3 \cdot 10^{-5} h^2 \end{pmatrix},$$

i.e., $\mathrm{e}^{hb_{14}B}\mathrm{e}^{ha_{14}A}\mathrm{e}^{hb_{13}B} \approx \mathrm{e}^{hB/50}$. We also find this pattern (a very small coefficient between two relatively large coefficients of opposite sign and similar magnitude) in the method $\mathrm{P}_{19}10$ in Table 1 for $K(b_7, a_7, b_6)$ and $K(b_9, a_9, b_8)$. This provides an illustration of the fact that, in some cases, many-stage methods with large coefficients can also lead to very accurate and stable integrators.

4.3 Construction of the Processor

As for the processor, since the kernel is time-reversible, it can be chosen as (2.30). Recall that, for their practical implementation, $P_1(x)$ and $P_4(x)$ must be replaced by polynomial approximations, say

$$P_1(x) = \sum_{i=0}^{s} c_i x^{2i}, \qquad P_4(x) = \sum_{i=0}^{s} d_i x^{2i}, \tag{4.9}$$

for a given s. In this way, the constraint $P_4 = P_1^{-1}$ is relaxed to $P_4 = P_1^{-1} + \mathcal{O}(x^{2s+2})$.

If we assume that $S(x) = P(x)K(x)P(x)^{-1}$ with $S(x)$ given by (2.22), then the coefficients c_i, d_i in (4.9) can be obtained, for instance, by truncating the Taylor expansion of the expressions (2.31). Note that by construction, the radius of convergence of the series $P_1(x)$ and $P_4(x)$ is $r_* = r^* > x_l$. Coefficients c_i, d_i for $\mathrm{P}_{38}2$ can be found in [3].

There are many other ways to approximate the processor which might be more convenient for a given problem. For instance, one may consider even polynomials $\tilde{P}_j(x)$ of degree $2(n+m)$ such that $P_j(x) - \tilde{P}_j(x) = \mathcal{O}(x^{2n+2})$ as $x \to 0$, which minimize

$$\int_{-l\pi}^{l\pi} \left(1 - \left(\frac{x}{l\pi}\right)^2\right)^{-1/2} \left(\frac{\tilde{P}_j(x) - P_j(x)}{x^{2n+2}}\right)^2 \mathrm{d}x.$$

There is still another procedure which may be suitable in case the output is frequently required. The post-processor can be virtually cost free if approximated using the intermediate stages obtained during the computation of the kernel (see [1] for more details).

Table 2 Relevant parameters for the selected new processed splitting methods

Method	(n, l, m)	x_*/k	r_*/k
$P_{19}10$	(5, 7, 0)	1.11974	1.10487
$P_{32}16$	(8, 12, 0)	1.11308	1.06485
$P_{38}20$	(10, 14, 0)	1.09686	1.04713
$P_{19}2$	(1, 7, 4)	1.2463	1.20186
$P_{32}2$	(1, 12, 7)	1.24978	1.15949
$P_{38}2$	(1, 14, 9)	1.23292	1.14573

5 Numerical Examples

We have analyzed the relative performance of the stability polynomials when approximating the function $\cos x$. This study has allowed us to choose some representative stability polynomials among those showing the best performance and subsequently we have built processed splitting methods from them. It is then important to check whether this relative performance still takes place in practical applications for the splitting methods obtained.

For the numerical tests carried out here we have selected the following representative k-stage processed methods of order $2n$, $P_k 2n$, built in this paper:

(i) the high-order processed methods $P_{19}10$, $P_{32}16$ and $P_{38}20$ obtained using the stability polynomial $p^{n,l}(x)$ in (4.2) with $(n, l) = (5, 7), (8, 12), (10, 14)$, respectively, where $k = n + 2l$; and
(ii) the second-order processed schemes $P_{19}2$, $P_{32}2$ and $P_{38}2$, obtained from the stability polynomial $p^{n,l,m}(x)$ in (4.4) with $(n, l, m) = (1, 7, 4), (1, 12, 7), (1, 14, 9)$, respectively, where $k = n + 2l + m$, and optimized by minimizing (4.5).

In Table 2 the relative stability threshold x_*/k of our selected processed splitting methods are displayed. We also include for each method the parameter r_*/k, where r_* has been introduced in Sect. 3.

The following standard nonprocessed splitting methods from the literature are chosen for comparison:

- The 1-stage second-order leapfrog method, $\psi_{h,2}$, given in (1.3) and denoted by $LF_1 2$.
- The well-known 3-stage fourth-order time-reversible method ($YS_3 4$) [33], and the 17-stage eighth-order time-reversible method ($M_{17}8$) [21, 25] (very similar performances are attained with the eighth-order method given in [12, 14]). Both methods are used with $\psi_{h,2}$ as the basic scheme.
- The m-stage mth-order nonsymmetric methods ($GM_m m$) with $m = 4, 6, 8, 10, 12$ given in [10], and specifically designed for the harmonic oscillator.

We have also considered as a reference the standard 4-stage fourth-order nonsymplectic Runge–Kutta method, $RK_4 4$.

The corresponding stability parameters x_*/k and r_*/k of all the splitting methods of reference considered in the numerical comparisons are displayed in Table 3.

Table 3 Stability parameters for the splitting methods of reference used for comparison

Method	x_*/k	r_*/k
$\mathrm{LF}_1 2$	2	2
$\mathrm{YS}_3 4$	0.524467	0.524467
$\mathrm{M}_{17} 8$	0.181596	0.181596
$\mathrm{GM}_4 4$	0.80954	0.80954
$\mathrm{GM}_6 6$	0.521821	0.521821
$\mathrm{GM}_8 8$	0.392691	0.392691
$\mathrm{GM}_{10} 10$	0.314159	0.314159

5.1 The Harmonic Oscillator

As a first example we consider again the one-dimensional harmonic oscillator

$$\begin{Bmatrix} q' \\ p' \end{Bmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{Bmatrix} q \\ p \end{Bmatrix}.$$

This trivial example is well suited as a test bench for the following purposes:

(i) to check that all coefficients of the kernel and post-processor are correct with sufficient accuracy;
(ii) to see whether the relative performance shown by the stability polynomials is still valid for the processed splitting methods obtained from them; and
(iii) to compare the performance of the new processed methods with other well-established methods from the literature.

We take as initial conditions $(q,p)=(1,1)$ and integrate for $t \in [0, 2000\pi]$ using different (constant) time steps. The largest time step corresponds to the stability threshold (we have repeated the experiment by increasing the time step until an overflow appeared). We measure the average error in the Euclidean norm of (q,p) versus the total number of exponentials $\mathrm{e}^{ha_i A}$, $\mathrm{e}^{hb_i B}$ required, NE (for processed methods, this number corresponds to the kernel, so that $\mathrm{NE} = 2000\pi(n+2l+m)/h$). Figure 2(a) shows the results obtained for the standard nonprocessed methods from the literature ($\mathrm{LF}_1 2$, $\mathrm{YS}_3 4$, $\mathrm{GM}_4 4$, $\mathrm{M}_{17} 8$, $\mathrm{GM}_{10} 10$, $\mathrm{GM}_{12} 12$). We clearly see that $\mathrm{LF}_1 2$ is the most stable and $\mathrm{GM}_{12} 12$ is the most efficient if accurate results are desired (recall that this is a method designed for the harmonic oscillator), so that they are chosen to compare with the new processed schemes. Figure 2(b) shows the results obtained with the high-order processed methods $\mathrm{P}_{19} 10$, $\mathrm{P}_{32} 16$ and $\mathrm{P}_{38} 20$, while Fig. 2(c) repeats the experiments for the second-order processed schemes $\mathrm{P}_{19} 2$, $\mathrm{P}_{32} 2$ and $\mathrm{P}_{38} 2$. Finally, Fig. 2(d) illustrates the performance achieved by the most efficient methods in each case. The superiority of $\mathrm{P}_{38} 2$ is clear when accurate results are desired.

For the processor we have considered (2.30)–(2.31), where P_1, P_4 are approximated using (4.9) and the coefficients c_i, d_i, $i = 1, \dots, s$, are obtained from the Taylor series expansion. The error introduced by the processor is of local character and does not propagate with time. For most problems it is enough to take for the pre-processor $s = k$ for $2k$-stage methods. With respect to the post-processor, we can take either the same value of s or a smaller one (depending on the accuracy required

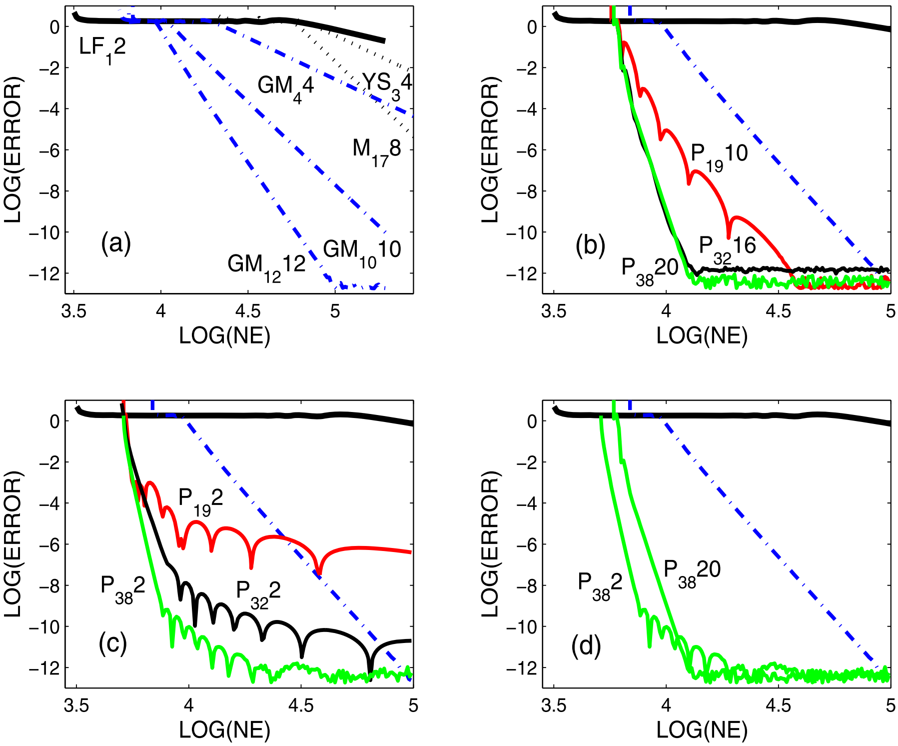

Fig. 2 Error in phase space versus the total number of exponentials in double logarithmic scale for the simple harmonic oscillator: **a** obtained with the 2nd- to 12th-order nonprocessed methods, $LF_1 2$, $YS_3 4$, $GM_4 4$, $M_{17} 8$, $GM_{10} 10$, $GM_{12} 12$; **b** obtained with $LF_1 2$ and $GM_{12} 12$ in comparison with the processed methods $P_{19} 10$, $P_{32} 16$ and $P_{38} 20$ built from $p^{n,l,m}(x)$ with $(n,l,m) = (5,7,0)$, $(8,12,0)$, and $(10,14,0)$, respectively; **c** the same for $P_{19} 2$, $P_{32} 2$ and $P_{38} 2$, corresponding to $(n,l,m) = (1,7,4)$, $(1,12,7)$ and $(1,14,9)$, respectively; and **d** comparison of the most efficient processed methods with the most efficient nonprocessed ones

at intermediate outputs or the length of the integration interval) because this error does not propagate. If the output is required frequently we can always approximate the post-processor using the intermediate stages obtained during the computation of the kernel [1].

Finally, it is important to notice the agreement between the relative performance shown by the processed methods given in Fig. 2 and the results obtained for the stability polynomials in Fig. 1. To better compare the curves of both figures, notice that in Fig. 1, $\mathrm{COST} = (n + 2l + m)/x$, whereas in Fig. 2, $\mathrm{NE} = 2000\pi\,\mathrm{COST}$, since $x = h$ in this case.

5.2 The Schrödinger Equation

As a second example we now consider the one-dimensional time-dependent Schrödinger equation (3.1) with the Morse potential $V(x) = D(1 - \mathrm{e}^{-\alpha x})^2$. We fix the parameters to the following values in adimensional units (a.u.): $\mu = 1745$ a.u.,

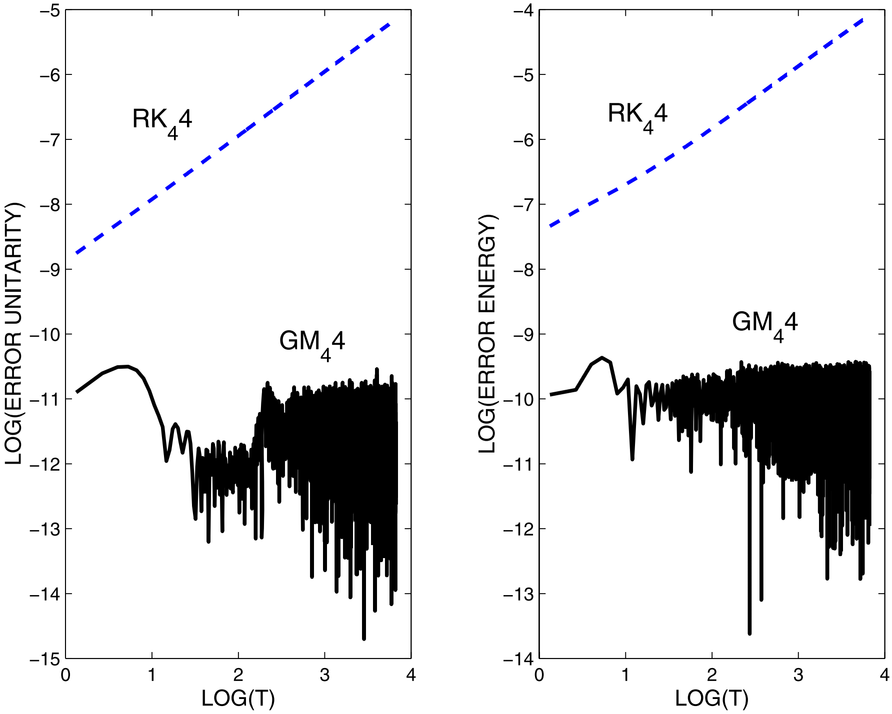

Fig. 3 Error in the preservation of unitarity and energy as a function of time in double logarithmic scale for the nonsymplectic RK$_4$4 and symplectic splitting GM$_4$4 methods applied to the Schrödinger equation. Both 4-stage explicit fourth-order methods are used with the same time step

$D = 0.2251$ a.u. and $\alpha = 1.1741$ a.u., which are frequently used for modelling the HF molecule. As initial conditions we take the Gaussian wave function $\psi(x,t) = \rho \exp(-\beta(x-\bar{x})^2)$, with $\beta = \sqrt{k\mu}/2$, $k = 2D\alpha^2$, $\bar{x} = -0.1$, and ρ is a normalizing constant. Assuming that the system is defined in the interval $x \in [-0.8, 4.32]$, we split it into $d = 128$ parts of length $\Delta x = 0.04$, take periodic boundary conditions and integrate along the interval $t \in [0, 20 \cdot 2\pi/w_0]$ with $w_0 = \alpha\sqrt{2D/\mu}$ (see [3] for more details on the implementation of the splitting methods to this particular problem).

As we have seen, the splitting methods considered in this work preserve symplecticity but not unitarity. In Fig. 3 we show the error in the preservation of unitarity, $|q^{\mathrm{T}}(t)q(t) + p^{\mathrm{T}}(t)p(t) - 1|$, and the relative error in energy $(|(E(t) - E(0))/E(0)|$, where $E(t) = u^{\mathrm{T}}(t)Hu(t) = q^{\mathrm{T}}(t)Hq(t) + p^{\mathrm{T}}(t)Hp(t))$ for the 4-stage fourth-order methods RK$_4$4 and GM$_4$4. Both methods require the same number of FFT calls per step (GM$_4$4 has less storage requirements) and they are used with the same time step $h = (2\pi/w_0)/250$. The error in energy does not grow secularly in time for the scheme GM$_4$4, as expected from a symplectic integrator, whereas the error for the nonsymplectic scheme RK$_4$4 grows linearly. A similar behaviour is observed for the error in unitarity, in agreement with the results presented in this work.

Figure 4 shows the error in the Euclidean norm of the vector solution at the end of the integration versus the number of FFT calls in double logarithmic scale. The

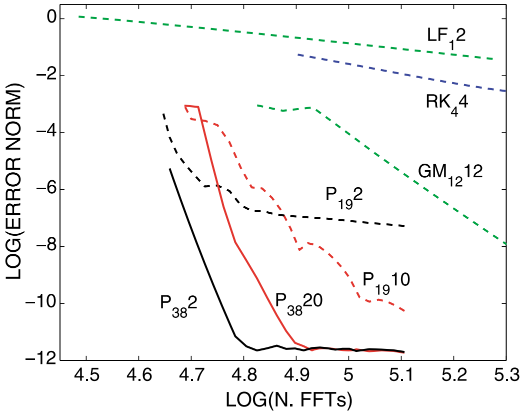

Fig. 4 Error of the vector solution for the Schrödinger equation versus the number of FFT calls in double logarithmic scale for the 2nd- and 12th-order nonprocessed methods, $LF_1 2$, $GM_{12} 12$, the standard $RK_4 4$ and for the processed methods $P_{19} 2$, $P_{19} 10$, $P_{38} 2$ and $P_{38} 20$

integrations are done starting from a sufficiently small time step and repeating the computation by slightly increasing the time step until an overflow occurs, which we identify with the stability limit. We present the results for the 2nd- and 12th-order nonprocessed splitting methods chosen from the previous example (the results corresponding to the remaining methods also stay between them). For the processed methods we take the 19- and 38-stage methods both of order 2 ($P_{19} 2$ and $P_{38} 2$) and of order 10 ($P_{19} 10$) and 20 ($P_{38} 20$), respectively. We observe that these methods have a relative performance similar to that obtained from the study of the harmonic oscillator or the corresponding stability polynomials. For reference, we have also included the results for the $RK_4 4$ method.

It is worth stressing that in the above figures only the computational cost required to evaluate the kernel has been taken into consideration, but the use of a processed method means that the processor has to be applied whenever output is needed. As we have mentioned, if it is frequently required the efficiency of the algorithm can be reduced. In that case, though, the post-processor can be approximated by a linear combination of the internal stages of the kernel by following the strategy developed in [1].

6 Concluding Remarks

Linear stability of splitting methods, that is, their stability when applied to the simple harmonic oscillator, is of great relevance for their application to the numerical integration of linear systems of the form (1.9), and of nonlinear systems that can be considered, in a neighbourhood of the trajectory, a small perturbation of a linear system of that form.

In this paper we have analyzed in detail the linear stability of splitting methods by considering the stability matrix $K(x)$, which describes the application of a splitting method to the harmonic oscillator, and the stability polynomial $p(x) = \frac{1}{2}\operatorname{tr}(K(x))$. We have shown that $K(x)$ uniquely determines the actual coefficients a_j, b_j of the scheme (1.2), and that there exists a finite number of different time-reversible splitting schemes having a given polynomial stability.

We have also studied the application of splitting methods (actually, a more general class of integrators which embrace splitting methods) to linear systems of the form (1.9), of interest in many physical applications. A backward error analysis has been carried out, showing that the numerical flow of any splitting method is, for a small enough time step h, conjugate to the exact flow of a system of the form (1.9) with perturbed matrices M and N. Moreover, we have proved that any partitioned method is conjugate to a nonpartitioned method for a sufficiently small h.

The performance of a processed splitting method when applied to equation (1.9) is essentially determined by the stability polynomial $p(x)$. This feature allows us to construct extraordinarily efficient processed integrators for the linear system (1.9) with kernels (1.2) involving a large number of stages k: we first judiciously select the stability polynomial $p(x)$, and then choose a set of coefficients a_j, b_j of a time-reversible scheme with that stability polynomial among all the possible choices computed by the procedure developed in Sect. 2.

It is worth stressing that the new processed methods thus constructed are more accurate for the harmonic oscillator than any previous splitting scheme, while being nearly as stable as the methods with optimal relative stability threshold proposed in [23]. Achieving at the same time excellent stability and accuracy may be surprising if one considers what is the typical situation in the construction of splitting methods for more general systems. In our case, this has been possible because the interpolatory nature of conditions (4.3) imposed on the stability polynomial $p(x)$ contributes both to have good stability *and* good accuracy. We recall that, for processed methods, accuracy (for the harmonic oscillator) means that $p(x)$ is a good approximation to $\cos(x)$. In the case of the optimal stability methods designed in [23], the interpolation nodes $j\pi$ in (4.3) are replaced by free parameters x_j which are then used to maximize the relative stability threshold. However, the quality of the approximation $p(x) \approx \cos(x)$ deteriorates as the nodes x_j are moved far enough from the interpolatory values $j\pi$.

We have also constructed methods of second-order of accuracy that are very accurate, and even outperform our new class of high-order methods. Needless to say, our new high-order integrators are more accurate for sufficiently small values of the step size h, but the actual value of h where this occurs has to be very small indeed. This is quite uncommon in the field of numerical integration of ODEs, where low-order methods are usually less efficient than high-order methods for relatively larger values of the step size h. The main difference is that in the case of the application of splitting methods to the harmonic oscillator, the relative efficiency of two processed splitting methods with roughly the same relative stability threshold, only depends on how the stability polynomials $p(x)$ approximate $\cos(x)$ in their stability interval $x \in [-x_*, x_*]$. A possible measure of the quality of that approximation for methods of order 2 or higher, that is, methods with stability polynomial $p(x)$ satisfying that $p(x) - \cos(x) = x^4 e(x)$ could be

$$\sup_{x \in [-x_*, x_*]} |e(x)|. \tag{6.1}$$

Compared to the stability polynomials $p^{n,l,0}(x)$ of our high-order methods (which in the particular case $l = 0$ are the truncated Taylor expansions of $\cos(x)$), the stability polynomials $p^{1,l,n-1}(x)$ of our second-order methods are better approximations in the sense that they have a smaller value of (6.1). It is worth mentioning that the situation is reversed if one considers $|e(x)|$ for complex values of x satisfying $|x| < x_*$ (or rather $|x| < \rho^*$), as would be the case if one were interested in applying splitting methods to systems (1.4) with arbitrary complex values of λ. This is related to the fact that near-to-optimal polynomial approximations of a function in a real interval are obtained with truncated Chebyshev series, whereas truncated Taylor series give near-to-optimal approximations in a disk of the complex plane.

One might think at first that the processed methods proposed here are difficult to implement in order to numerically integrate a given problem, since the kernel involves a large number of stages and the processor requires evaluating the polynomial approximations (4.9). But this is not the case, actually, since the whole method only requires the computation of matrix–vector products of the form Nq and Mp. To minimize the number of matrix–vector products, Horner's rule can be used to evaluate the action of P_1 and P_4 in the processor on both q and p, whereas the implementation of the kernel is exactly the same as that of schemes (1.3). In reference [3] an actual algorithm is provided for the case (3.3), whereas in [1] a virtually cost-free procedure is designed to approximate P by a linear combination of the internal stages of the kernel. This is particularly suitable when the output is frequently required.

We would like to emphasize again that splitting methods which show a high efficiency when applied to the harmonic oscillator can also be useful as a first step in the construction of efficient methods for certain classes of nonlinear systems, such as nonlinear perturbations of equation (1.9), or linear systems of the form (1.9) with time-dependent matrices N and M [4] (arising, in particular, when the time-dependent Schrödinger equation is spatially discretized). In this last instance, splitting methods with processing are not particularly well suited, and thus designing nonprocessed splitting methods for linear problems is a relevant issue by itself. This turns out to be a more difficult problem, however, since one needs to solve quadratic systems of algebraic equations of high dimension. The design of very efficient nonprocessed splitting schemes when applied to the harmonic oscillator thus constitutes a subject well worth further research.

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