# Splitting methods for non-autonomous linear systems

Sergio Blanes[1*]      Fernando Casas[2†]      Ander Murua[3‡]

**Abstract**

We present splitting methods for numerically solving a certain class of explicitly time-dependent linear differential equations. Starting from an efficient method for the autonomous case and making use of the formal solution obtained with the Magnus expansion, we show how to get the order conditions for the non-autonomous case. We also build a family of sixth-order integrators whose performance is clearly superior to previous splitting methods on several numerical examples.

[1]Instituto de Matemática Multidisciplinar, Universidad Politécnica de Valencia, E-46022 Valencia, Spain.

[2]Departament de Matemàtiques, Universitat Jaume I, E-12071 Castellón, Spain.

[3]Konputazio Zientziak eta A.A. saila, Informatika Fakultatea, EHU/UPV, Donostia/San Sebastián, Spain.

## 1   Introduction

Composition methods constitute a widespread procedure to integrate numerically differential equations, especially in the context of geometric integration. In this work we consider a particular case of partitioned linear systems which frequently appear when discretising many PDEs. Specifically,

$$x' = M(t)y, \qquad y' = -N(t)x, \tag{1}$$

with $x(t_0) = x_0 \in \mathbb{R}^{d_1}$, $y(t_0) = y_0 \in \mathbb{R}^{d_2}$, $M : \mathbb{R} \longrightarrow \mathbb{R}^{d_1 \times d_2}$ and $N : \mathbb{R} \longrightarrow \mathbb{R}^{d_2 \times d_1}$. Systems of the form

$$\bar{x}' = \bar{M}(t)\bar{y} + f(t), \qquad \bar{y}' = -\bar{N}(t)\bar{x} + g(t), \tag{2}$$

*Email: serblaza@imm.upv.es
†Email: Fernando.Casas@uji.es
‡Email: Ander.Murua@ehu.es

are also of type (1), since the solution $(\bar{x}(t), \bar{y}(t))$ of (2) corresponds to the solution $x(t) = (\bar{x}(t)^T, 1)^T$, $y(t) = (\bar{y}(t)^T, 1)^T$ of an enlarged system (1) with

$$M(t) = \begin{pmatrix} \bar{M}(t) & f(t) \\ 0^T & 0 \end{pmatrix}, \qquad N(t) = \begin{pmatrix} \bar{N}(t) & -g(t) \\ 0^T & 0 \end{pmatrix} \qquad (3)$$

and initial conditions $x(t_0) = (\bar{x}(t_0)^T, 1)^T$, $y(t_0) = (\bar{y}(t_0)^T, 1)^T$. Similarly, the second order differential equation

$$x'' = D(t)x + g(t) \qquad (4)$$

with $D : \mathbb{R} \longrightarrow \mathbb{R}^{d \times d}$, $f : \mathbb{R} \longrightarrow \mathbb{R}^d$, can be considered as a special case of (1) with

$$M(t) = \begin{pmatrix} I_d & 0 \\ 0^T & 0 \end{pmatrix}, \qquad N(t) = \begin{pmatrix} -D(t) & -g(t) \\ 0^T & 0 \end{pmatrix}. \qquad (5)$$

Equation (1) describes the evolution of many relevant physical systems. In particular, the space discretization of the Schrödinger equation can be reformulated as an $N$-degrees of freedom classical linear Hamiltonian system with Hamiltonian equations of the form (1) [7, 8, 18] and also the time-dependent Maxwell equations can be expressed in this way [16]. On the other hand, the numerical integration of some nonlinear PDEs (such as the nonlinear Schrödinger equation) is frequently done by solving separately the linear component, which in many cases can be written as (1) and constitutes the most problematic part of the procedure.

Denoting $z = (x, y)^T$, one may write (1) as

$$z' = \Lambda(t)z, \qquad \text{where} \qquad \Lambda(t) = A(t) + B(t), \qquad (6)$$

and

$$A(t) = \begin{pmatrix} 0 & M(t) \\ 0 & 0 \end{pmatrix}, \qquad B(t) = \begin{pmatrix} 0 & 0 \\ -N(t) & 0 \end{pmatrix}. \qquad (7)$$

This system can be numerically solved by using, for instance, Magnus integrators [13, 11, 5]. These methods require computing the exponential of matrices of dimension $(d_1 + d_2) \times (d_1 + d_2)$. If $(d_1 + d_2) \gg 1$ then the exponentiation can be prohibitively costly. For this reason, new methods which only involve matrix-vector products of the form $M(t)y$ and $N(t)x$ are highly desirable.

The purpose of the present work is to adapt to equation (1) the procedure presented in [1] in a more general setting. The approach combines the Magnus expansion with efficient splitting methods for autonomous problems. Here we summarize the main ideas involved and illustrate the technique by constructing several integrators for equations (6)–(7) which outperform previous algorithms.

The new methods have the form (for a time step of size $h$)

$$z(t + h) \approx e^{A_m(t,h)} e^{B_m(t,h)} \cdots e^{A_1(t,h)} e^{B_1(t,h)} z(t), \qquad (8)$$

where the matrices $A_i(t, h)$ and $B_i(t, h)$ are given by

$$A_i(t, h) = h \sum_{j=1}^{k} \rho_{ij} A(t + c_j h), \qquad B_i(t, h) = h \sum_{j=1}^{k} \sigma_{ij} B(t + c_j h), \qquad (9)$$

with appropriately chosen real parameters $c_i, \rho_{ij}, \sigma_{ij}$. Since in our case

$$\mathrm{e}^{A_i(t,h)} = \begin{pmatrix} I & M_i(t, h) \\ 0 & I \end{pmatrix}, \qquad \mathrm{e}^{B_i(t,h)} = \begin{pmatrix} I & 0 \\ -N_i(t, h) & I \end{pmatrix},$$

then (8) can be written as $z(t + h) \approx K(t, h)z(t)$, where

$$\begin{aligned} K(t, h) &= \mathrm{e}^{A_m(t,h)}\mathrm{e}^{B_m(t,h)} \cdots \mathrm{e}^{A_1(t,h)}\mathrm{e}^{B_1(t,h)} \qquad (10) \\ &= \begin{pmatrix} I & M_m \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_m & I \end{pmatrix} \cdots \begin{pmatrix} I & M_1 \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -N_1 & I \end{pmatrix}, \end{aligned}$$

and obviously

$$M_i = h \sum_{j=1}^{k} \rho_{ij} M(t + c_j h), \qquad N_i = h \sum_{j=1}^{k} \sigma_{ij} N(t + c_j h). \qquad (11)$$

Notice that when $M(t)$ and $N(t)$ are constant, then $K(t, h)$ reduces to

$$K(h) = \mathrm{e}^{h a_m A}\mathrm{e}^{h b_m B} \quad \cdots \quad \mathrm{e}^{h a_1 A}\mathrm{e}^{h b_1 B} = \qquad (12)$$
$$\begin{pmatrix} I & a_m hM \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_m hN & I \end{pmatrix} \quad \cdots \quad \begin{pmatrix} I & a_1 hM \\ 0 & I \end{pmatrix} \begin{pmatrix} I & 0 \\ -b_1 hN & I \end{pmatrix},$$

where

$$a_i = \sum_{j=1}^{k} \rho_{ij}, \qquad b_i = \sum_{j=1}^{k} \sigma_{ij}, \qquad i = 1, \ldots, m. \qquad (13)$$

In the autonomous case there exists an extensive list of splitting methods for separable systems in the literature (see [9, 12, 14, 15, 17] and references therein). In addition, for partitioned linear systems extremely efficient methods can be constructed due to the special structure of the system [7, 2, 3]. Our goal here is to start from a set of coefficients $a_i, b_i$ ($i = 1, \ldots, m$) which provides an efficient method for the autonomous case, and then to find appropriate values for $c_i, \rho_{ij}, \sigma_{ij}$ such that (13) holds and (10) leads to a good method for the non-autonomous system (1).

For the convenience of the reader (and potential user of the new class of integration methods) we collect in table 1 two algorithms implementing schemes (12) and (10) for the numerical integration of equation (1) in the autonomous and the non-autonomous case, respectively. In the last situation, the proposed algorithm requires to compute and store $M(t + c_j h), N(t + c_j h)$, $j = 1, \ldots, k$ at each step. We assume that the linear combination (11) is efficiently computed. This is the case, in particular, when $M(t) = \sum_{i=1}^{l} f_i(t)M^{[i]}$ with $M^{[i]}$ constant matrices and $f_i(t)$ scalar functions, for a small value of $l$ (and similarly for $N(t)$).

Table 1: Algorithms for the numerical integration of (1) using $J$ steps of length $h = t/J$: (Algorithm 1) with scheme (12) for the autonomous case, and (Algorithm 2) with scheme (10) for the non-autonomous case.

| Algorithm 1: autonomous | Algorithm 2: non-autonomous |
|---|---|
| $x_0 = x(0);$  $y_0 = y(0)$  <br> **do**  $n = 1, J$  <br>  **do**  $i = 1, m$  <br>   $y_i = y_{i-1} - b_i h N x_{i-1}$  <br>   $x_i = x_{i-1} + a_i h M y_i$  <br>  **enddo**  <br>  $x_0 = x_m;$  $y_0 = y_m$  <br>  **If** (**output**) **then**  <br>  $x_{out}(t_n) = x_0;$  $y_{out}(t_n) = y_0$  <br>  **endif**  <br> **enddo** | $x_0 = x(0);$  $y_0 = y(0);$  $t_n = t_0$  <br> **do**  $n = 1, J$  <br>  **do**  $i = 1, k$  <br>   $M_i = M(t_n + c_i h);$  $N_i = N(t_n + c_i h)$  <br>  **enddo**  <br>  **do**  $i = 1, m$  <br>   $\hat{M} = \rho_{i1} M_1 + \cdots + \rho_{ik} M_k$  <br>   $\hat{N} = \sigma_{i1} N_1 + \cdots + \sigma_{ik} N_k$  <br>   $y_i = y_{i-1} - h \hat{N} x_{i-1}$  <br>   $x_i = x_{i-1} + h \hat{M} y_i$  <br>  **enddo**  <br>  $x_0 = x_m;$  $y_0 = y_m;$  $t_n = t_n + h$  <br>  **If** (**output**) **then**  <br>  $x_{out}(t_n) = x_0;$  $y_{out}(t_n) = y_0$  <br>  **endif**  <br> **enddo** |

## 2  Order conditions

One possible approach for deriving the conditions to be satisfied by the coefficients $c_i, \rho_{ij}, \sigma_{ij}$ of a method of order, say, $p$, is to formally build a solution of equation (6) with the Magnus expansion.

It is well known that $z(t)$ can be formally written as

$$z(t + h) = e^{\Omega(t,h)} z(t), \tag{14}$$

where $\Omega(t, h) = \sum_{k=1}^{\infty} \Omega_k(t, h)$ and each $\Omega_k(t, h)$ is a multiple integral of combinations of nested commutators containing $k$ matrices $\Lambda(t)$ [13]. This constitutes the so-called Magnus expansion of the solution. An important feature of this expansion is that, when the solution of (6) evolves in a Lie group $\mathcal{G}$, then $e^{\Omega(t,h)}$ stays on $\mathcal{G}$ even if the series is truncated, provided that $\Lambda(t)$ belongs to the Lie algebra associated with $\mathcal{G}$ [10].

It is possible to get explicitly $\Omega_k(t, h)$ by inserting into the recurrence defining the Magnus expansion a Taylor series of the matrices $A(t)$ and $B(t)$. In fact, to take advantage of the time-symmetry property of the solution, which implies that

$$\Omega(t + h, -h) = -\Omega(t, h), \tag{15}$$

it is more convenient to expand around $t + h/2$. More specifically, if we denote

$$\alpha_i = \frac{1}{(i-1)!} \left. \frac{d^{i-1} A(s)}{ds^{i-1}} \right|_{s=t+\frac{h}{2}}, \qquad \beta_i = \frac{1}{(i-1)!} \left. \frac{d^{i-1} B(s)}{ds^{i-1}} \right|_{s=t+\frac{h}{2}}$$

so that

$$
\begin{aligned}
A(t + \tfrac{h}{2} + \tau) &= \alpha_1 + \alpha_2 \tau + \alpha_3 \tau^2 + \cdots, \\
B(t + \tfrac{h}{2} + \tau) &= \beta_1 + \beta_2 \tau + \beta_3 \tau^2 + \cdots
\end{aligned}
\tag{16}
$$

then $\Omega(t,h)$ in (14) can be expanded as

$$
\Omega(t,h) = \sum_{n \geq 1} h^n \sum_{k=1}^{n} \Omega_{k,n}(t,h),
\tag{17}
$$

where each $\Omega_{k,n}(t,h)$ is a linear combination of terms of the form $[\mu_{i_1}, \mu_{i_2} \ldots, \mu_{i_k}]$ with $\mu_j = \alpha_{i_j}$ or $\mu_j = \beta_{i_j}$ for each $j = 1, \ldots, k$, and $i_1 + \cdots + i_k = n$. Furthermore, $\Omega_{n,k}(t,h) = 0$ for even values of $n$, $\Omega_{k,k}(t,h) = 0$ for $k > 1$ and $\Omega_{1,1}(t,h) = \alpha_1 + \beta_1$.

In particular, up to order $h^6$ one has [5]

$$
\Omega = h\Omega_{1,1} + h^3(\Omega_{1,3} + \Omega_{2,3}) + h^5(\Omega_{1,5} + \Omega_{2,5} + \Omega_{3,5} + \Omega_{4,5}) + \mathcal{O}(h^7),
\tag{18}
$$

where (for simplicity, we omit the arguments $(t,h)$)

$$
\begin{aligned}
\Omega_{1,1} &= \alpha_1 + \beta_1, \quad \Omega_{1,3} = \frac{1}{12}(\alpha_3 + \beta_3), \quad \Omega_{2,3} = \frac{1}{12}\big([\alpha_2, \beta_1] + [\beta_2, \alpha_1]\big), \\
\Omega_{1,5} &= \frac{1}{80}(\alpha_5 + \beta_5), \quad \Omega_{2,5} = \frac{1}{240}\big([\alpha_2, \beta_3] + [\beta_2, \alpha_3]\big) + \frac{1}{80}\big([\alpha_4, \beta_1] + [\beta_4, \alpha_1]\big), \\
\Omega_{3,5} &= \frac{1}{360}\big(-[\alpha_1, \beta_3, \alpha_1] + [\alpha_1, \beta_1, \alpha_3] - [\beta_1, \alpha_3, \beta_1] + [\beta_1, \alpha_1, \beta_3]\big) \\
&\quad + \frac{1}{240}\big([\alpha_1, \beta_2, \alpha_2] - [\alpha_2, \beta_1, \alpha_2] + [\beta_1, \alpha_2, \beta_2] - [\beta_2, \alpha_1, \beta_2]\big), \\
\Omega_{4,5} &= \frac{1}{720}\big([\alpha_1, \beta_1, \alpha_1, \beta_2] - [\beta_1, \alpha_1, \beta_2, \alpha_1] + [\beta_1, \alpha_1, \beta_1, \alpha_2] - [\alpha_1, \beta_1, \alpha_2, \beta_1]\big).
\end{aligned}
$$

If, on the other hand, one applies the Baker–Campbell–Hausdorff (BCH) formula repeatedly in (8), it is possible to write $K(t,h)$ formally as the exponential of only one operator, $K(t,h) = \exp(\tilde{\Omega}(t,h))$, depending on $A_i(t,h)$, $B_i(t,h)$ $(i = 1, \ldots, m)$ and nested commutators of these matrices. The numerical scheme will be of order $p$ if

$$
\tilde{\Omega}(t,h) - \Omega(t,h) = \mathcal{O}(h^{p+1}) \qquad \text{as } h \to 0.
$$

One can then obtain explicitly the order conditions as follows. First, we expand $A_i(t,h)$, $B_i(t,h)$ in terms of $\alpha_j$, $\beta_j$,

$$
A_i(t,h) = \sum_{n \geq 1} h^n a_i^{(n)} \alpha_n, \qquad B_i(t,h) = \sum_{n \geq 1} h^n b_i^{(n)} \beta_n,
\tag{19}
$$

where

$$
a_i^{(n)} = \sum_{j=1}^{k} \rho_{ij}(c_j - \tfrac{1}{2})^{n-1}, \qquad b_i^{(n)} = \sum_{j=1}^{k} \sigma_{ij}(c_j - \tfrac{1}{2})^{n-1},
\tag{20}
$$

for each $i = 1, \ldots, m$, $n \geq 1$.

Then, we substitute the expressions (19) in the corresponding $\tilde{\Omega}(t, h)$, thus obtaining an expansion of the form

$$\tilde{\Omega}(t, h) = \sum_{n \geq 1} h^n \sum_{k=1}^n \tilde{\Omega}_{k,n}(t, h), \tag{21}$$

where each $\tilde{\Omega}_{k,n}(t, h)$ is a linear combination of terms $[\mu_{i_1}, \mu_{i_2} \ldots, \mu_{i_k}]$ with $i_1 + \cdots + i_k = n$ and $\mu_j = \alpha_{i_j}$ or $\mu_j = \beta_{i_j}$ for $j = 1, \ldots, k$. Finally, we compare the truncated (up to $n = p$) expansion (21) with the corresponding expression (17) for $\Omega(t, h)$, so that the numerical scheme is of order $p$ if

$$\sum_{k=1}^n \tilde{\Omega}_{k,n} = \sum_{k=1}^n \Omega_{k,n} \qquad \text{for } n = 1, \ldots, p. \tag{22}$$

A usual assumption imposed to the scheme (8) that simplifies considerably the analysis (and also leads to integrators with better preservation of qualitative properties) is the time-symmetry of the composition (10). That is, $K(t + h, -h) = K(t, h)^{-1}$, or equivalently, $\tilde{\Omega}(t + h - h) = -\tilde{\Omega}(t, h)$, which implies that $\tilde{\Omega}_{k,n}(t, h) = 0$ for even values of $n$.

This symmetry is automatically satisfied (and thus all order conditions at even orders) if either

$$A_{m+1-i}(t+h, -h) = -A_i(t, h), \quad B_{m-i}(t+h, -h) = -B_i(t, h), \quad B_m(t, h) = 0, \tag{23}$$

or

$$B_{m+1-i}(t+h, -h) = -B_i(t, h), \quad A_{m-i}(t+h, -h) = -A_i(t, h), \quad A_m(t, h) = 0, \tag{24}$$

for $i = 1, 2, \ldots, m$. In the first case, the scheme will be said to be of type ABA, whereas in the second, of type BAB. For our problem, $A$ and $B$ play the same role and they can be interchanged so, without loss of generality, we only consider ABA schemes. Since the first (or last) exponential is cancelled and one exponential can be concatenated in two consecutive steps, these symmetric schemes are referred as $(m-1)$-stage methods. The symmetry (23) is achieved if

$$c_{k-j+1} = 1 - c_j, \quad \rho_{m+1-i,k-j+1} = \rho_{ij}, \quad \sigma_{m+1-i,k-j+1} = \sigma_{ij}, \tag{25}$$

for $j = 1, \ldots, k$, $i = 1, 2, \ldots, m$, which implies that

$$a_{m+1-i}^{(n)} = (-1)^{n+1} a_i^{(n)}, \qquad b_{m-i}^{(n)} = (-1)^{n+1} b_i^{(n)}, \qquad b_m^{(n)} = 0, \tag{26}$$

for $n \geq 1$, $i = 1, 2, \ldots, m$,

If in addition to the time-symmetry, we assume that the method is of order at least six for the autonomous case (that is, $K(h)$ in (12) is such that $K(h) = e^{h(A+B)+\mathcal{O}(h^7)}$) then, by applying the above procedure, we get $\tilde{\Omega}(t, h)$ as

$$\tilde{\Omega} = h\tilde{\Omega}_{1,1} + h^3(\tilde{\Omega}_{1,3} + \tilde{\Omega}_{2,3}) + h^5(\tilde{\Omega}_{2,5} + \tilde{\Omega}_{3,5} + \tilde{\Omega}_{4,5}) + \mathcal{O}(h^7), \tag{27}$$

6

where

$$\tilde{\Omega}_{1,1} = \alpha_1 + \beta_1, \qquad\qquad\qquad \tilde{\Omega}_{1,3} = \lambda_3\alpha_3 + \mu_3\beta_3,$$
$$\tilde{\Omega}_{2,3} = \lambda_{21}[\alpha_2,\beta_1] + \mu_{21}[\beta_2,\alpha_1], \qquad \tilde{\Omega}_{1,5} = \lambda_5\alpha_5 + \mu_5\beta_5,$$
$$\tilde{\Omega}_{2,5} = \lambda_{23}[\alpha_2,\beta_3] + \mu_{23}[\beta_2,\alpha_3] + \lambda_{41}[\alpha_4,\beta_1] + \mu_{41}[\beta_4,\alpha_1],$$
$$\tilde{\Omega}_{3,5} = \lambda_{131}[\alpha_1,\beta_3,\alpha_1] + \lambda_{113}[\alpha_1,\beta_1,\alpha_3] + \mu_{131}[\beta_1,\alpha_3,\beta_1] + \mu_{113}[\beta_1,\alpha_1,\beta_3]$$
$$\qquad + \lambda_{122}[\alpha_1,\beta_2,\alpha_2] + \lambda_{212}[\alpha_2,\beta_1,\alpha_2] + \mu_{122}[\beta_1,\alpha_2,\beta_2] + \mu_{212}[\beta_2,\alpha_1,\beta_2],$$
$$\tilde{\Omega}_{4,5} = \lambda_{1112}[\alpha_1,\beta_1,\alpha_1,\beta_2] + \lambda_{1121}[\beta_1,\alpha_1,\beta_2,\alpha_1] + \mu_{1112}[\beta_1,\alpha_1,\beta_1,\alpha_2]$$
$$\qquad + \mu_{1121}[\alpha_1,\beta_1,\alpha_2,\beta_1], \tag{28}$$

and the coefficients $\lambda_{i_1\cdots i_l}$, $\mu_{i_1\cdots i_l}$, are polynomials in $a_i^{(n)}$, $b_i^{(n)}$, $i = 1,\ldots,m$, $n = 1,\ldots,5$. Their explicit expressions are collected in the appendix.

Since in the autonomous case $\alpha_j = \beta_j = 0$, $j > 1$, we take $a_i^{(1)} = a_i$, $b_i^{(1)} = b_i$ (the coefficients of the splitting method we have previously chosen). The coefficients $a_i^{(n)}$, $b_i^{(n)}$, $n = 2,\ldots,5$, $i = 1,\ldots,m$, must be chosen in such a way that the time-symmetry assumption (26) holds and the following 22 additional order conditions are satisfied:

$$\lambda_3 = \mu_3 = \tfrac{1}{12}, \qquad \lambda_{21} = \mu_{21} = \tfrac{1}{12}, \qquad \lambda_{23} = \mu_{23} = \tfrac{1}{240}, \tag{29}$$
$$\lambda_{131} = \mu_{131} = -\tfrac{1}{360}, \qquad \lambda_{113} = \mu_{113} = \tfrac{1}{360}, \qquad \lambda_{122} = \mu_{122} = \tfrac{1}{240}, \tag{30}$$
$$\lambda_{212} = \mu_{212} = -\tfrac{1}{240}, \qquad \lambda_{1112} = \mu_{1112} = \tfrac{1}{720}, \qquad \lambda_{1121} = \mu_{1121} = -\tfrac{1}{720}, \tag{31}$$
$$\lambda_5 = \mu_5 = \tfrac{1}{80}, \qquad \lambda_{41} = \mu_{41} = \tfrac{1}{80}. \tag{32}$$

Once a set of values for $a_i^{(n)}, b_i^{(n)}$, $n = 2,\ldots,5$, $i = 1,\ldots,m$, satisfying the symmetry condition (26) and the order conditions (29)–(32) is chosen, a sixth order time-symmetric scheme (8)–(9) with $k = 5$ will be obtained for each set of arbitrarily fixed values of the nodes $c_1 < c_2 < c_3 = \frac{1}{2} < c_4 = 1-c_2 < c_5 = 1-c_1$ by determining the coefficients $\rho_{ij}$, $\sigma_{ij}$ uniquely from the linear equations (20).

However, for $k < 5$ and an arbitray set of nodes $c_1 < \cdots < c_k$ satisfying the symmetry condition (25), no sixth order scheme exists, unless the nodes $c_1 < \cdots < c_k$ correspond to a quadrature rule of order 6 for the interval $[0,1]$, that is, unless

$$0 = \int_0^1 t(t-c_1)\cdots(t-c_k)dt. \tag{33}$$

In that case, $\lambda_5 = \mu_5 = 1/80$ automatically hold if the remaining order conditions in (29)–(32) are imposed. For $k = 3$ one has that (33) holds if and only if

$$c_1 = \frac{1}{2} - \frac{\sqrt{15}}{10}, \quad c_2 = \frac{1}{2}, \quad c_3 = \frac{1}{2} + \frac{\sqrt{15}}{10}, \tag{34}$$

i.e., if they are the nodes of the Gaussian quadrature rule. Now the four conditions (32) are automatically satisfied if the eighteen conditions (29)–(31) hold.

Thus, a sixth order time-symmetric scheme (8)–(9) with Gaussian nodes (34) can be constructed by first obtaining a solution of the conditions (29)–(31) for the unknowns $a_i^{(n)}, b_i^{(n)}$, $n = 2, 3$, $i = 1, \ldots, m$ (satisfying the symmetry condition (26)), and then determining the coefficients $\rho_{ij}, \sigma_{ij}$ from (20), or equivalently, from

$$
\begin{pmatrix} \rho_{i1} & \sigma_{i1} \\ \rho_{i2} & \sigma_{i2} \\ \rho_{i3} & \sigma_{i3} \end{pmatrix} = \begin{pmatrix} 0 & -\frac{\sqrt{15}}{3} & \frac{10}{3} \\ 1 & 0 & -\frac{20}{3} \\ 0 & \frac{\sqrt{15}}{3} & \frac{10}{3} \end{pmatrix} \begin{pmatrix} a_i^{(1)} & b_i^{(1)} \\ a_i^{(2)} & b_i^{(2)} \\ a_i^{(3)} & b_i^{(3)} \end{pmatrix}.
$$

More generally, it can be seen [5, 1] that, if the nodes $c_1 < \cdots < c_k$ correspond to a sixth order symmetric quadrature rule with weights $d_i$, then, given $a_i^{(n)}, b_i^{(n)}$, $n = 2, 3$, $i = 1, \ldots, m$, satisfying the symmetry condition (26) and the 18 order conditions (29)–(31), the coefficients $\rho_{ij}, \sigma_{ij}$ of the scheme (8)–(9) can be explicitly determined as

$$
\rho_{ij} = \sum_{n=1}^{3} \sum_{l=1}^{3} a_i^{(n)} r_{nl} d_j (c_j - \frac{1}{2})^{l-1}, \qquad \sigma_{ij} = \sum_{n=1}^{3} \sum_{l=1}^{3} b_i^{(n)} r_{nl} d_j (c_j - \frac{1}{2})^{l-1}, \tag{35}
$$

where

$$
(r_{n,l}) = \begin{pmatrix} \frac{9}{4} & 0 & -15 \\ 0 & 12 & 0 \\ -15 & 0 & 180 \end{pmatrix}. \tag{36}
$$

# 3 Construction of methods of order six

The first step in the construction of new 6th-order methods for equation (1) is to choose symmetric splitting methods which perform efficiently in the autonomous case. This simplifies the search for coefficients and usually leads to efficient methods also for the non-autonomous problem. We must bear in mind, however, that the most efficient method for the autonomous problem does not necessarily shows the best performance on the non-autonomous case. For equation (1) in the time-independent case, a good starting point is the family of splitting methods proposed in [7]. These are $m$-stage schemes of order $m$ for $m = 4, 6, 8, 10, 12$, and are denoted by $\Phi_m(h)$. They are not time-symmetric, so that to apply the above procedure, we have to build symmetrized versions by composing half step of the method with half step of its adjoint (the same composition, but in the reverse order), $\Psi_{2m-1}(h) = \Phi_m(h/2) \circ \Phi_m^*(h/2)$. This also allows saving one stage and, as a result, we have $(2m - 1)$-stage methods of order $m$ for the same values of $m$.

We have analysed the order conditions associated to the methods $\Psi_{2m-1}(h)$ for $m = 6, 8, 10, 12$ and found several sets of solutions (except for $m = 6$ where no real coefficients have been located). Among them, we have chosen those $a_i^{(n)}$, $b_i^{(n)}$, $n = 2, 3$, $i = 1, \ldots, m$ with the smallest absolute values.

Although the schemes $\Psi_{2m-1}(h)$ perform quite satisfactorily in the autonomous case, it is still possible to design other symmetric splitting methods which

are even more efficient in a wide range of time steps values [4]. Here, for the sake of illustration, we consider an 11-stage sixth-order integrator of this new family and build the corresponding scheme for the non-autonomous problem (1).

In the next section we show how the new methods behave in practice by applying them to several numerical examples. In all cases the $\Psi_{2m-1}(h)$ method with $m = 8$ and the new sixth-order integrator show the best performance. For completeness, we collect the coefficients of the method based on $\Psi_{15}(h)$ in Table 2, whereas those corresponding to the new scheme are available from the authors upon request. Notice that the coefficients $a_i^{(1)}$, $b_i^{(1)}$ for the scheme $\Psi_{15}(h)$ are taken from [7] for $\Phi_8(h)$ and are divided by two because $\Psi_{15}(h) = \Phi_8(h/2) \circ \Phi_8^*(h/2)$.

Table 2: Coefficients $a_i^{(j)}$, $b_i^{(j)}$ for the method SGM$_8$.

| | | |
|---|---|---|
| $a_1^{(1)} = 0.0406820423192522/2$ | $a_1^{(2)} = -0.009222020674782949$ | $a_1^{(3)} = 0.042062087251634246$ |
| $b_1^{(1)} = a_8^{(1)}$ | $b_1^{(2)} = -0.027214664019007236$ | $b_1^{(3)} = 0.01203916935966199523$ |
| $a_2^{(1)} = 0.1895126902355599/2$ | $a_2^{(2)} = -0.043751041846595763$ | $a_2^{(3)} = -0.043165966713163549$ |
| $b_2^{(1)} = a_7^{(1)}$ | $b_2^{(2)} = -0.046523437710806227$ | $b_2^{(3)} = 0.018721555200024248$ |
| $a_3^{(1)} = 0.3242803211745088/2$ | $a_3^{(2)} = -0.048031113572426925$ | $a_3^{(3)} = 0.046527834673773506$ |
| $b_3^{(1)} = a_6^{(1)}$ | $b_3^{(2)} = 0.027749195139632094$ | $b_3^{(3)} = -0.007127646651729842$ |
| $a_4^{(1)} = -0.0394120731572997/2$ | $a_4^{(2)} = 0.006708367822842748$ | $a_4^{(3)} = -0.003757288545577531$ |
| $b_4^{(1)} = a_5^{(1)}$ | $b_4^{(2)} = -0.057311963541271888$ | $b_4^{(3)} = 0.018033588758710264$ |
| $a_5^{(1)} = 0.2560570296317553/2$ | $a_5^{(2)} = -0.03179575697272915$ | $a_5^{(3)} = 0$ |
| $b_5^{(1)} = a_4^{(1)}$ | $b_5^{(2)} = -0.0010873106336788798$ | $b_5^{(3)} = 0$ |
| $a_6^{(1)} = -0.1376837011836700/2$ | $a_6^{(2)} = 0.017021775197289018$ | $a_6^{(3)} = 0$ |
| $b_6^{(1)} = a_3^{(1)}$ | $b_6^{(2)} = -0.015640480519270482$ | $b_6^{(3)} = 0$ |
| $a_7^{(1)} = 0.2474725260224518/2$ | $a_7^{(2)} = -0.014452573126795444$ | $a_7^{(3)} = 0$ |
| $b_7^{(1)} = a_2^{(1)}$ | $b_7^{(2)} = 0$ | $b_7^{(3)} = 0$ |
| $a_8^{(1)} = 1/2 - (a_1^{(1)} + \cdots + a_7^{(1)})$ | $a_8^{(2)} = -0.001311755029957398$ | $a_8^{(3)} = 0$ |
| $b_8^{(1)} = 2a_1^{(1)}$ | $b_8^{(2)} = 0$ | $b_8^{(3)} = 0$ |
| $a_{8+i}^{(1)} = a_{9-i}^{(1)}$ | $a_{8+i}^{(2)} = -a_{9-i}^{(2)}$ | $a_{8+i}^{(3)} = a_{9-i}^{(3)}$ |
| $b_{8+i}^{(1)} = b_{8-i}^{(1)}$ | $b_{8+i}^{(2)} = -b_{8-i}^{(2)}$ | $b_{8+i}^{(3)} = b_{8-i}^{(3)}$ |
| $i = 1, \ldots, 8$ | | |

# 4   Numerical examples

Here we compare the new especially adapted splitting methods for partitioned linear systems with standard splitting methods for separable systems on some relatively simple problems.

It is known that the system (1) can be written as an autonomous nonlinear separable system [18]

$$\hat{x}' = f^{[A]}(\hat{y}), \qquad \hat{y}' = f^{[B]}(\hat{x}) \tag{37}$$

with $\hat{x} = (x, x_t)^T \in \mathbb{R}^{d_1+1}$, $\hat{y} = (y, y_t)^T \in \mathbb{R}^{d_2+1}$ and $f^{[A]}(\hat{y}) = (M(y_t)y, 1)^T$, $f^{[B]}(\hat{x}) = (-N(x_t)x, 1)^T$. Equation (37) is separable in solvable parts, but since $N(x_t)$ and $M(y_t)$ are in general nonlinear functions of $x_t$ and $y_t$, respectively, the schemes presented in [7] are not appropriate. On the other hand, standard splitting methods can be used in a straightforward way. We consider the 6-stage fourth-order method (BM$_4$) and the 10-stage sixth-order method (BM$_6$) designed in [6] for general separable systems (the coefficients are also collected in [1, 12, 14, 15]). We can also build a second order symmetric method, say $S_2(h) = \Phi^{[A]}(h/2) \circ \Phi^{[B]}(h) \circ \Phi^{[A]}(h/2)$, where $\Phi^{[A]}(t), \Phi^{[B]}(t)$ denote the $t$-flow associated to $f^{[A]}$ and $f^{[B]}$, respectively. Then, by composing $S_2$ with different time steps, it is possible to build methods of order $m > 2$, denoted here by $S_m^{(2)}$. We can find in the literature schemes with up to 35 stages to build methods up to order 10 [9, 14, 19, 21]. We choose the 5-stage fourth order, the 9-stage sixth-order, the 17-stage eighth-order and the 35-stage tenth-order methods whose coefficients are collected in [9].

We denote by SGM$_m$ with $m = 8, 10, 12$ the symmetrized methods $\Psi_{2m-1}(h)$ adapted to the non-autonomous case, whereas the new symmetric 11-stage sixth-order integrator is referred to as S$_6$. In all the examples the sixth order Gaussian quadrature rule has been chosen, since it minimizes the number of evaluations of $M(t)$ and $N(t)$.

The computational cost of the methods is measured by the number of stages required. It is important to mention, however, that this number is, for the new methods, several times higher than the number of time-dependent function evaluations (using the sixth-order Gaussian quadrature only three evaluations per step are required).

**Perturbed Harmonic Oscillators**. Time dependent linear harmonic oscillators constitute a very simple example where the preceding integrators can be tested.

(i) First we consider the time-dependent Hamiltonian

$$H(q, p, t) = e^{-\epsilon t} \frac{1}{2} p^2 + e^{\epsilon t} \left( \frac{1}{2} q^2 - \delta \cos(\omega t) q \right), \tag{38}$$

$q, p \in \mathbb{R}$, with associated equations of motion

$$q' = e^{-\epsilon t} p, \qquad p' = -e^{\epsilon t} (q - \delta \cos(\omega t)), \tag{39}$$

(or equivalently $q'' + \epsilon q' + q = \delta \cos(\omega t)$) . This system corresponds to a modification of the well known Duffing oscillator. We take as initial conditions $q(0) = 1.75$, $p(0) = 0$, integrate up to $t = 40\,\pi/\omega$ and measure the average error in phase space (at $t = 2\pi/\omega, 4\pi/\omega, \ldots, 40\pi/\omega$) in terms of the number of force evaluations for different time steps (in logarithmic scale).

In Fig. 1(a) we show the results achieved by standard splitting methods for the autonomous case ($\epsilon = \delta = 0$) in order to choose the most efficient integrators in this case. The curves correspond to the schemes BM$_4$, BM$_6$ (dashed lines) and S$_m^{(2)}$, $m = 4, 6, 8, 10$ (solid lines). The order of the method can be easily identified with the slope of the respective curve. For comparison with

10

the schemes proposed in this paper we choose those showing the best efficiency: $BM_4$, $BM_6$ and $S_{10}^{(2)}$ (dashed lines from now on). In Figure 1(b) we collect, in addition, the results achieved with $SGM_8$ (lines with circles), $SGM_{10}$ (lines with $\times$), $SGM_{12}$ (lines with $+$) and $S_6$ (thick solid lines) also in the autonomous case. Figures 1(c) and 1(d), finally, show the results for $\delta = \omega = 1/2$ with $\epsilon = 2 \cdot 10^{-5}$ and $\epsilon = 2 \cdot 10^{-2}$. In the last case, the curves obtained $SGM_{10}$ and $SGM_{12}$ are not included, because now these methods are less efficient than $SGM_8$.
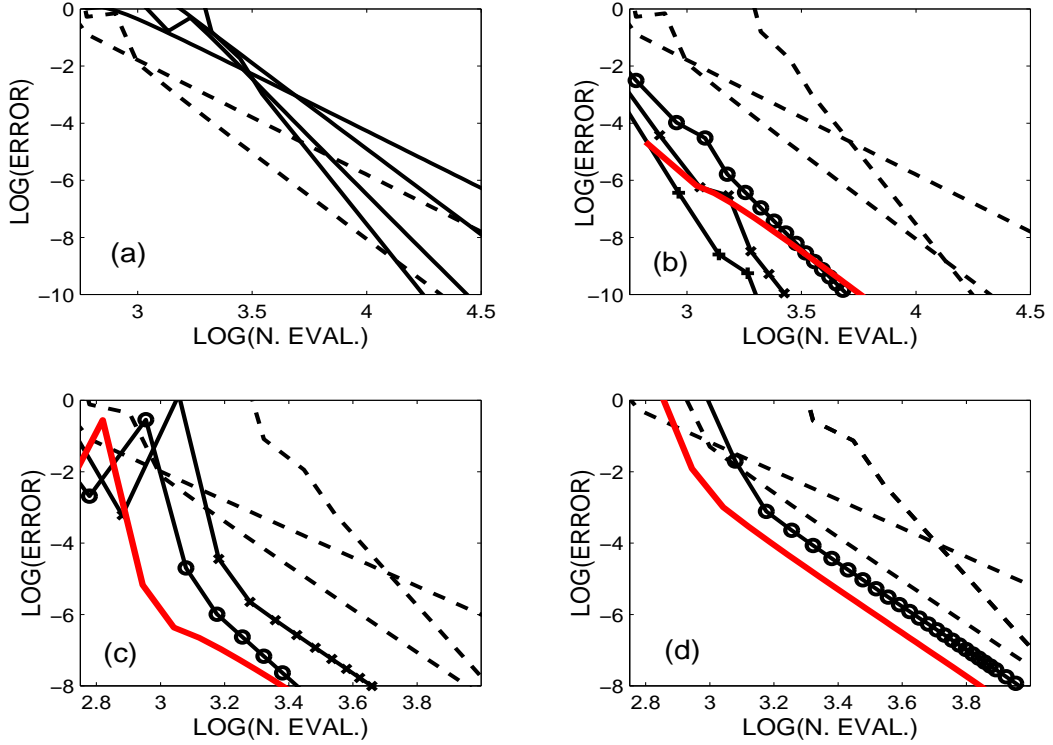


Figure 1: Average error versus number of force evaluations in the numerical integration of (39) with initial conditions $q(0) = 1.75$, $p(0) = 0$. For the autonomous case ($\epsilon = \delta = 0$) we consider: (a) standard methods for the separable system (37), $BM_4$ and $BM_6$ (dashed lines) and $S_4^{(2)}$, $S_6^{(2)}$, $S_8^{(2)}$, $S_{10}^{(2)}$ (solid lines), and (b) $BM_4$, $BM_6$, $S_{10}^{(2)}$ (dashed lines) versus $SGM_8$ (lines with circles), $SGM_{10}$ (lines with $\times$), $SGM_{12}$ (lines with $+$) and $S_6$ (thick solid lines). For the non-autonomous case we take $\delta = \omega = 1/2$ with: (c) $\epsilon = 2 \cdot 10^{-5}$; and (d) $\epsilon = 2 \cdot 10^{-2}$.

(ii) As a second perturbed harmonic oscillator we choose the Mathieu equation, $q'' + (\omega^2 + \epsilon \cos(t))q = 0$, with $q \in \mathbb{R}$. We take the same initial conditions and period of integration as before and compare the relative error for $\epsilon = 1/4$ with $\omega = 2$ and $\omega = 5$. In the last case, the system corresponds to a highly oscil-

latory system with a relatively small time-dependent perturbation as frequently occurs after semidiscretising many PDEs. The results obtained are shown in Figure 2, where the same coding as before has been used for the curves.
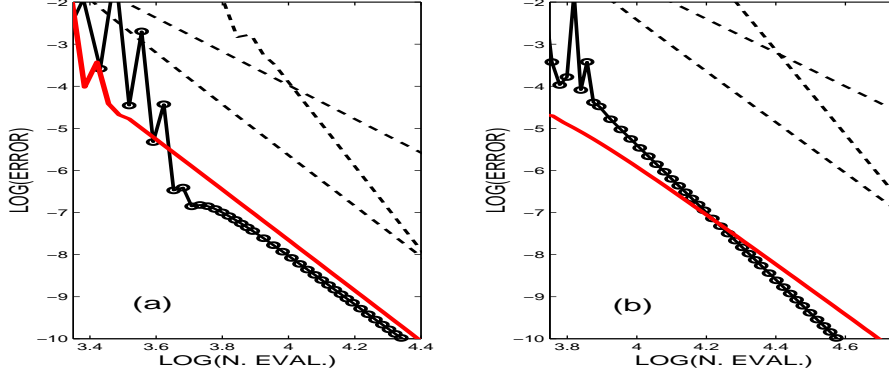


Figure 2: Same as Fig. 1 but for the Mathieu equation $q'' + (\omega^2 + \epsilon \cos(t))q = 0$ with $\epsilon = 1/4$ and (a) $\omega = 2$, (b) $\omega = 5$.

**The Schrödinger equation**. To illustrate the interest of the new integrators proposed here, we consider now (as a less trivial example) the Walker-Preston model of a diatomic molecule in a strong laser field [20]. This system is described by the one-dimensional Schrödinger equation (in units where $\hbar = 1$)

$$i\frac{\partial}{\partial t}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + V(x) + f(t)x\right)\psi(x,t), \tag{40}$$

with $\psi(x,0) = \psi_0(x)$. Here $V(x) = D\left(1 - e^{-\alpha x}\right)^2$ is the Morse potential and $f(t)x = A\cos(\omega t)x$ accounts for the laser field. This problem is used as a test bench for the numerical methods presented in [8] and [18] and we take the same values for the parameters as those authors: $\mu = 1745$ *a.u.*, $D = 0.2251$ *a.u.* and $\alpha = 1.1741$ *a.u.* (corresponding to the HF molecule), $A = 0.011025$ *a.u.* and laser frequency $w = 0.01787$. We assume that the system is defined in the interval $x \in [-0.8, 4.32]$, which is split into $N = 64$ parts of length $\Delta x = 0.08$, and impose periodic boundary conditions.

After space discretization, eq. (40) leads to the complex linear equation

$$u' = H(t)u, \tag{41}$$

with $u \in \mathbb{C}^N$ and $u_k(t) = \psi(x_k,t)(\Delta x)^{1/2}$. Here $x_k = x_0 + (k-1)\Delta x$ and $H(t) = T + \hat{V}(t)$ is an Hermitian matrix (real and symmetric). If we split $u = x + iy$, the $N$-dimensional linear complex system (41) can be written as

$$x' = H(t)y, \qquad y' = -H(t)x, \tag{42}$$

which corresponds to (1) with $M(t) = N(t) = H(t)$ and appropriate dimensions. As initial conditions we take the ground state of the Morse potential, $\phi(x) = \sigma \exp\big(-(\gamma - 1/2)\alpha\,x\big) \exp\big(-\gamma \mathrm{e}^{-\alpha x}\big)$, with $\gamma = 2D/w_0$, $w_0 = \alpha\sqrt{2D/\mu}$ and $\sigma$ is a normalizing constant.

To check accuracy, we consider the instantaneous mean energy of the diatomic molecule, $E(t) = u^T(t)H(t)u(t)$, for the time range $t \in [0, 100\tau]$ with $\tau = 2\pi/\omega$. As usual, the exact solution is accurately approximated using a sufficiently small time step. We measure the averaged relative error in $E(t)$ evaluated at $t = \tau, 2\tau, \ldots, 100\tau$. The algorithm requires to compute repeatedly products $Hx$ and $Hy$. Here $\hat{V}(t)$ is a diagonal matrix with elements $\hat{V}_{jj} = V(x_j) + f(t)x_j$, and $Tx, Ty$ can be efficiently computed using FFTs [2, 7]. Notice also that in (11) we now have

$$M_i = h\sum_{j=1}^{k} \rho_{ij} H(t + c_j h) = ha_i^{(1)}T + ha_i^{(1)}V + hX\sum_{j=1}^{k}\rho_{ij}f(t + c_j h) \qquad (43)$$

when $H(t)$ plays the role of $M(t)$ and

$$N_i = h\sum_{j=1}^{k} \sigma_{ij} H(t + c_j h) = hb_i^{(1)}T + hb_i^{(1)}V + hX\sum_{j=1}^{k}\sigma_{ij}f(t + c_j h) \qquad (44)$$

when $H(t)$ plays the role of $N(t)$. Here $X$ is a diagonal matrix with diagonal elements $X_{jj} = x_j$. Observe that the products $H_i x$ and $H_i y$ only require one FFT and its inverse and thus an $m$-stage method requires $4m$ FFTs per step. In [18] a fourth-order method for the system (42) is considered (the system was previously converted into an autonomous system as shown in (37)), showing a clear improvement with respect to the second order Magnus integrator (combined with a third order splitting scheme) given in [8]. The results achieved by the fourth-order BM$_4$ are very similar to those obtained by the scheme considered in [18] (with slightly better stability limit). Figure 3 shows the efficiency plots for the methods. The largest time step (i.e. the smaller number of FFTs) corresponds to the stability limit of the method (an overflow appears if the time step is slightly increased). The superiority of the new splitting methods (and especially, of the scheme S$_6$) is manifest both with respect to efficiency and the stability limit.

## 5    Conclusions and outlook

There exists in the literature a large number of excellent splitting methods for numerically integrating partitioned linear systems. Nevertheless, most of these methods cannot be used when there is an explicit time dependency in the equations, since the usual strategy of treating the time variable as an additional coordinate often modifies the special structure of the system.

In this paper we have presented a procedure for adapting efficient splitting schemes when the system is explicitly time-dependent by considering the
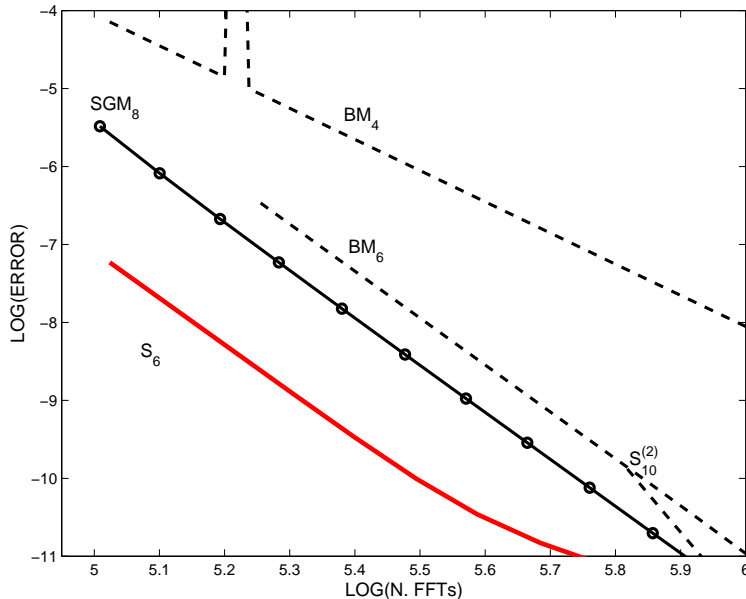
Figure 3: Average relative error in $E(t)$ versus the number of FFTs for the one-dimensional Schrödinger equation (40) written in the form (42) after space discretization.

formal solution obtained with the Magnus expansion. In particular, from the symmetrized version of the methods designed in [7] we have built a new family of sixth-order integrators for the problem defined by equation (1). The new schemes are shown to be more efficient than previous families of algorithms in all cases analysed here. In any case, we should remark that their accuracy decreases in comparison with the original schemes applied to autonomous problems. This motivates the search of new and more powerful integration methods for time independent partitioned linear systems, a problem currently under investigation. In fact, the scheme $S_6$ presented in this paper may be considered as a first step in that approach, whose ultimate goal is to construct splitting methods showing a high efficiency both in autonomous and non-autonomous linear equations of the form (1). This family of algorithms could be extremely useful in the numerical integration of such kind of problems.

## Acknowledgements

grateful to Prof. Qin Sheng for inviting them to contribute to this special issue and for his endless patience during the submission process of our paper.

# A    Appendix

In this appendix, for the convenience of the reader, we collect the explicit expressions of the polynomials $\lambda_{i_1 \cdots i_l}$, $\mu_{i_1 \cdots i_l}$ appearing in (28).

Introducing

$$s_j^{(n)} = \sum_{l=1}^{j} a_l^{(n)}, \qquad u_j^{(n)} = \sum_{l=j}^{m} b_l^{(n)}, \qquad n = 1, \ldots, 5,$$

the consistency conditions are simply $s_m^{(1)} = u_{m+1}^{(1)} = 1$. Taking into account these equalities, one has

$$\lambda_3 = s_m^{(3)}, \qquad \lambda_5 = s_m^{(5)}, \qquad \lambda_{21} = \sum_{j=1}^{m} a_j^{(2)} u_j^{(1)},$$

$$\lambda_{23} = \sum_{j=1}^{m} a_j^{(2)} u_j^{(3)}, \qquad \lambda_{41} = \sum_{j=1}^{m} a_j^{(4)} u_j^{(1)},$$

$$\lambda_{131} = -\frac{1}{12} \sum_{j=1}^{m} b_j^{(3)} ((-1 + 2s_j^{(1)})^2 + 2s_j^{(1)}(s_j^{(1)} - 1)),$$

$$\lambda_{113} = \frac{1}{2} \sum_{j=1}^{m} b_j^{(1)} s_j^{(3)} (1 - 2s_j^{(1)}), \qquad \lambda_{122} = \frac{1}{2} \sum_{j=1}^{m} b_j^{(2)} s_j^{(2)} (1 - 2s_j^{(1)}),$$

$$\lambda_{212} = -\frac{1}{2} \sum_{j=1}^{m} b_j^{(1)} (s_j^{(2)})^2,$$

$$\lambda_{1112} = -\frac{1}{6} \sum_{l=1}^{m} (a_l^{(1)})^2 u_l^{(2)} - \frac{1}{6} \sum_{l=1}^{m-1} a_l^{(1)} \sum_{j=l+1}^{m} a_j^{(1)} (-1 - 3u_l^{(1)}$$
$$+ 3u_j^{(1)})(u_l^{(2)} + u_j^{(2)}),$$

$$\lambda_{1121} = -\frac{1}{12} \sum_{l=2}^{m} (a_l^{(1)})^2 u_l^{(2)} - \frac{1}{6} \sum_{l=1}^{m-1} a_l^{(1)} \sum_{j=l+1}^{m} a_j^{(1)} (2u_l^{(1)} u_l^{(2)} -$$
$$u_l^{(2)} u_j^{(1)} - 3u_l^{(1)} u_j^{(2)} - u_l^{(2)} + 2u_j^{(2)}),$$

and the expressions for $\mu_{i_1 \cdots i_l}$ are obtained from the corresponding $\lambda_{i_1 \cdots i_l}$ by interchanging the roles of $a_i^{(n)}$ and $b_i^{(n)}$.

# References

[1] S. Blanes and F. Casas, Splitting methods for non-autonomous separable dynamical systems, *J. Phys. A: Math. Gen.* **39** (2006), pp. 5405-5423.

15

[2] S. Blanes, F. Casas, and A. Murua, Symplectic splitting operator methods tailored for the time-dependent Schrödinger equation, *J. Chem. Phys.*, **124** (2006), 234105.

[3] S. Blanes, F. Casas, and A. Murua, On the linear stability of splitting methods, (2006). Submitted

[4] S. Blanes, F. Casas, and A. Murua, work in progress.

[5] S. Blanes, F. Casas and J. Ros, Improved high order integrators based on Magnus expansion, *BIT* **40** (2000), pp. 434-450.

[6] S. Blanes and P.C. Moan, Practical symplectic partitioned Runge–Kutta and Runge–Kutta–Nyström methods, *J. Comp. Appl. Math.* **142** (2002), pp. 313-330.

[7] S. Gray and D.E. Manolopoulos, Symplectic integrators tailored to the time-dependent Schrödinger equation, *J. Chem. Phys.* **104** (1996), pp. 7099-7112.

[8] S. Gray and J.M. Verosky, Classical Hamiltonian structures in wave packet dynamics, *J. Chem. Phys.* **100** (1994), pp. 5011–5022.

[9] E. Hairer, C. Lubich, and G. Wanner, *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations* (2nd edition), Springer Series in Computational Mathematics **31**, Springer-Verlag, (2006).

[10] A. Iserles, H.Z. Munthe-Kaas, S.P. Nørsett and A. Zanna, Lie group methods, *Acta Numerica* **9** (2000), pp. 215-365.

[11] A. Iserles and S.P. Nørsett, On the solution of linear differential equations in Lie groups, *Philosophical Trans. Royal Soc.* A **357** (1999), pp. 983-1019.

[12] B. Leimkuhler and S. Reich, *Simulating Hamiltonian Dynamics*, Cambridge University Press, Cambridge (2004).

[13] W. Magnus, On the exponential solution of differential equations for a linear operator, *Commun. Pure Appl. Math.* **7** (1954), pp. 649-673.

[14] R.I. McLachlan and R. Quispel, Splitting methods, *Acta Numerica* **11** (2002), pp. 341-434.

[15] R.I. McLachlan and R.G.W. Quispel, Geometric integrators for ODEs, *J. Phys. A: Math. Gen.*, **39** (2006), pp. 5251–5285.

[16] R. Rieben, D. White, and G. Rodrigue, High-order symplectic integration methods for finite element solutions to time dependent Maxwell equations, *IEEE Trans. Antennas Propagat.* **52** (2004), pp. 2190–2195.

[17] J.M. Sanz-Serna and M.P. Calvo, *Numerical Hamiltonian Problems*, Chapman & Hall, London (1994).

[18] J.M. Sanz-Serna and A. Portillo, Classical numerical integrators for wavepacket dynamics, *J. Chem. Phys.* **104** (1996), pp. 2349-2355.

[19] M. Sophronious and G. Spaletta, Derivation of symmetric composition constants for symmetric integrators, *Optimization Methods Software*, **20** (2005), 597–613

[20] R.B. Walker and K. Preston, Quantum versus classical dynamics in treatment of multiple photon excitation of anharmonic-oscillator, *J. Chem. Phys.* **67** (1977), pp. 2017-2028.

[21] H. Yoshida, Construction of higher order symplectic integrators, *Phys. Lett. A* **150** (1990), pp. 262-268.