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Splitting Methods for Non-autonomous Hamiltonian Equations

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We present an algorithm for numerically integrating non-autonomous Hamiltonian differential equations. Special attention is paid to the separable case and, in particular, a new fourth-order splitting method is presented which in a certain measure is optimal. In combination with a new way of handling non-autonomous problems, the schemes we present are based on Magnus expansions and they show very promising results when applied to Hamiltonian ODEs and PDEs.

Key Words: non-linear time-dependent differential equations; initial value problems; numerical methods; free Lie algebra; Magnus expansion; symplectic.

1. INTRODUCTION

Geometric integration (GI) of differential equations has been a research area spinning off many useful results in the past decade. The focus of GI is the construction of numerical methods that retain algebraic and differential algebraic structures. By doing so in a natural way it leads to improved numerical accuracy. Maybe most importantly, structures that are stable under perturbations lend themselves to backward error analysis results which can be used to predict and analyse error growth of numerical methods [27]. Hamiltonian systems whose phase spaces possess a symplectic structure are maybe the most important of such systems. Special symplectic integrators retaining this structure have been constructed, and the most successful integrators of this type are *splitting methods*. Since the pioneering papers of Ruth [26], Candy and Rozmus [8], Suzuki [28], and Yoshida [30], a large number of methods have appeared [17, 19, 27]. This new family of methods have been successfully applied in celestial mechanics [29], plasma simulations [9], quantum mechanics [13, 16], etc. Essentially, the methods work by splitting the vector field defining the differential equation into a sum whose terms are exactly integrable, and they are thus of quite a general nature.

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In this paper we present new numerical methods for solving nonlinear differential equations

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t), \qquad \mathbf{x}_0 = \mathbf{x}(t_0) \in \mathbb{R}^n, \tag{1}$$

with $\mathbf{f} \in \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$ (henceforth, $t_0 = 0$). In the linear case, $\mathbf{f}(\mathbf{x}, t) = A(t)\mathbf{x}$, the Magnus expansion [21] represents the solution as an exponential, $\mathbf{x}(t) = \exp(\Omega(t))\mathbf{x}(0)$. This expansion has been successfully used for obtaining efficient numerical methods [5, 14, 22] both because it preserves the structure of the exact solution and because of the special treatment of the time-dependent part. In the nonlinear case, the time-dependent part of $\mathbf{f}(\mathbf{x}, t)$ plays an important role in many problems. In this case it is important to have numerical methods which can take special care of the time-dependent part while preserving the qualitative properties of the exact solution. The simplest and most used trick for avoiding the time-dependent functions is to consider t as a new coordinate, x_t, thus increasing the dimension of the phase space, whereupon one solves the transformed equation

$$\frac{d\mathbf{y}}{dt} = \mathbf{F}(\mathbf{y}), \tag{2}$$

with a standard algorithm, where $\mathbf{y} = (\mathbf{x}, x_t)$ and $\mathbf{F}(\mathbf{y}) = (\mathbf{f}(\mathbf{y}), 1)$. In many cases this transformation is not very efficient for numerically solving the problem. Examples of problems where this could be the case are as follows:

- If the explicit time dependency of $\mathbf{f}$ has a relatively short time scale, then the main contribution to the error will originate from it. By explicitly handling the time dependency specialised quadratures, or even exact integrals, can be applied.
- If the time-dependent functions appearing in $\mathbf{f}$ are expensive to evaluate, the methods for solving (2) will in general be expensive since they do not attempt to minimise the number of time evaluations.
- There are many numerical methods which are especially efficient for solving (1) if $\mathbf{f}$ is time independent and has some special structure. In (2) the time dependency is eliminated, but the structure of the equation can be destroyed, and one has to resort to more general and less efficient methods. This is the case, for example, if one considers the Hamiltonian $H(\mathbf{q}, \mathbf{p}, t) = \mathbf{p}^T M(t)\mathbf{p} + V(\mathbf{q}, t)$. Runge–Kutta–Nyström (RKN) methods for Hamiltonians with quadratic kinetic energy cannot be used after the introduction of the new coordinates associated to the time and its momentum, as we will see later in more detail.

To avoid these problems, we present numerical methods based on the Magnus series. Over one time step, h, the Magnus approximation can be considered a time-averaging method, where as an example the standard averaging of (1) gives

$$\frac{d\hat{\mathbf{x}}}{dt} = \hat{\mathbf{f}}(\hat{\mathbf{x}}), \qquad \mathbf{x}(0) = \mathbf{x}(0),$$

with $\hat{\mathbf{f}}(\hat{\mathbf{x}}) = \frac{1}{h}\int_0^h \mathbf{f}(\hat{\mathbf{x}}, s)\, ds$. This is an approximation that in turn leads to a second-order approximation to the solution $\hat{\mathbf{x}}(h) = \mathbf{x}(h) + O(h^3)$. As we will see, this corresponds to truncating the Magnus series after the first term.

This paper contains two main parts:

1. First, we generalise the Magnus expansion to non-linear systems. In general, methods which are direct applications of the Magnus expansion are difficult to implement or are very expensive to run. Motivated by these facts we show how to write this exponential as a product of exponentials, which are much easier to compute. In particular, we present two fourth-order factorisations of the Magnus expansion.

2. Frequently the vector field takes the form $\mathbf{f} = \mathbf{f}_A + \mathbf{f}_B$, with $\mathbf{f}_A$ and $\mathbf{f}_B$ exactly solvable. In this case, usually each term in the Magnus factorisation will correspond to the flow associated to a sum of two exactly solvable vector fields. Thus, it is interesting to implement the Magnus factorisation with fourth-order splitting methods, such as

$$\exp(h(X+Y)) = \prod_{i=1}^{m} \exp(ha_i X)\exp(hb_i Y) + O(h^5), \tag{3}$$

where X and Y are two operators which do not commute. This family of methods are usually referred to as partitioned Runge–Kutta (PRK) methods [27]. To get an efficient implementation, we made a search for good fourth-order splitting methods and found a novel splitting method optimised for the second-order problem $\frac{d^2\mathbf{x}}{dt^2} = \mathbf{g}(\mathbf{x}, t)$. This method also showed very favourable performance for other structures on the vector fields $\mathbf{f}_A$ and $\mathbf{f}_B$.

This paper is organised as follows. Section 2 contains a short review of the Magnus series for linear systems and how it can be used to construct numerical methods for such systems. Next, we take the formalism of linear systems a step further and use the Magnus series as a representation of the solution of non-linear non-autonomous ODEs. Section 3 introduces a factorisation of the Magnus series derived from the Baker–Campbell–Hausdorff formula, which removes the otherwise cumbersome commutators. We prove that the new methods are time symmetric and present an error analysis. To implement the new methods when the vector field is separable into two solvable parts, Section 4 introduces splitting methods for nonautonomous separable systems. That section also summarises the known fourth-order methods from the literature. In addition, a new method that has been specially optimised is presented. Section 5 contains a set of numerical experiments showing the efficacy of the proposed schemes versus other well-known symplectic integrators found in the literature.

2. MAGNUS SERIES FOR NON-AUTONOMOUS SYSTEMS

2.1. Linear Systems

Let us start with the linear systems

$$\frac{d\mathbf{x}}{dt} = A(t)\mathbf{x}, \qquad \mathbf{x}(0) = \mathbf{x}_0, \tag{4}$$

with $A(t) \in \mathbb{R}^{n\times n}$. One popular perturbative method for solving (4), while preserving the qualitative properties of the exact solution, can be obtained through the Magnus expansion [21]. Magnus assumed that the solution can be written in the form

$$\mathbf{x}(t) = \exp(\Omega(t))\mathbf{x}_0, \tag{5}$$

with $\Omega = \sum_{i=1}^{\infty} \Omega_i$. The first two terms are given by

$$\Omega_1(t) = \int_0^t A(s_1)\, ds_1, \qquad \Omega_2(t) - \frac{1}{2}\int_0^t ds_1 \int_0^{s_1} ds_2 [A(s_1), A(s_2)], \tag{6}$$

with $[A, B] = AB - BA$. The Magnus expansion has been used mainly in quantum mechanics as an analytical approximation to the solution (see [2] and references therein) because it preserves the unitarity of the propagator (if A is skew-Hermitian). Recently, it has been used as a basis for efficient numerical integrators [5, 14, 22] because the approximate solution is restricted to the same space as the exact flow, retaining the geometric properties of the exact solutions. Provided that $A(t)$ is a bounded matrix, the series is absolutely convergent for a sufficiently small t [2, 23] and accurate approximations can be expected for such t; even a moderate number of terms give very accurate approximations. In this case, the Magnus series is a good candidate for constructing numerical methods. The main problem with the series is the evaluation of multidimensional intergrals. It is, however, possible to evaluate all multidimensional integrals using standard unidimensional quadratures derived from collocation principles [14]. For example, using a Gauss–Legendre quadrature with n points (n evaluations of $A(t)$ per step), it is possible to obtain a numerical method of order $2n$ in the time step. In order to improve the efficiency and to simplify the methods, the Magnus series is written in terms of unidimensional integrals so that the application of quadrature becomes even more transparent [5].

Let us denote by $Z^{(i)}(h)$, $i = 0, 1$, the unidimensional integrals associated with $Z(t)$,

$$Z^{(0)}(h) = \int_0^h Z(s)\, ds, \qquad Z^{(1)}(h) = \frac{1}{h}\int_{-h/2}^{h/2} s Z(s + h/2)\, ds, \tag{7}$$

where $Z(t)$ is a function, a vector, or a matrix, depending on the circumstance. The integrals can be approximated using a numerical quadrature to obtain a computational algorithm. Let us, as an example, consider the fourth-order Gaussian quadrature for solving (7); then

$$Z^{(0)} = \frac{h}{2}(Z_1 + Z_2) + O(h^5), \qquad Z^{(1)} = \frac{\sqrt{3}h}{12}(Z_2 - Z_1) + O(h^5), \tag{8}$$

where $Z_i = Z(c_i h)$, $i = 1, 2$, and $c_{1,2} = 1/2 \mp \sqrt{3}/6$.

When the system is integrated over one time step h, two fourth-order approximations to $\Omega(h)$ are given by

$$\Omega(h) = \Omega_1(h) + \Omega_2(h) + O(h^5) \tag{9}$$

$$= A^{(0)} + \left[A^{(1)}, A^{(0)}\right] + O(h^5). \tag{10}$$

Higher order methods in terms of unidimensional integrals or Gaussian quadratures can be found in [5, 22].

2.2. Nonlinear Systems

First, we consider the autonomous system

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}), \qquad \mathbf{x}_0 = \mathbf{x}(0) \tag{11}$$

and denote its flow by $\mathbf{x}(t) = \Phi_{\mathbf{f}}^t \mathbf{x}_0$. Given a smooth function $\psi : \mathbb{R}^n \to \mathbb{R}$, the derivative in the direction of $\mathbf{f}$ is a new function, whose value at $\mathbf{x}_0$ is

$$\begin{aligned}(L_{\mathbf{f}}\psi)(\mathbf{x}_0) &= \left.\frac{d}{dt}\right|_{t=0} \psi\left(\Phi_{\mathbf{f}}^t \mathbf{x}\right) \\ &= f_1(\mathbf{x})\frac{\partial \psi}{\partial x_1} + \cdots + f_n(\mathbf{x})\frac{\partial \psi}{\partial x_n}\bigg|_{\mathbf{x}=\mathbf{x}_0},\end{aligned} \tag{12}$$

with $\mathbf{x} = (x_1, \ldots, x_n)$ and $\mathbf{f} = (f_1, \ldots, f_n)$ (see [1, Chap. 8] for more details). We can then write the differential operator $L_{\mathbf{f}}$ as

$$L_{\mathbf{f}} = \sum_{i=1}^{n} f_i \frac{\partial}{\partial x_i}. \tag{13}$$

$L_{\mathbf{f}}$ is usually called the Lie derivative (or operator)[1] associated with $\mathbf{f}$. Given two functions ψ_1 and ψ_2, it is easy to prove the properties

$$L_{\mathbf{f}}(\alpha_1\psi_1 + \alpha_2\psi_2) = \alpha_1 L_{\mathbf{f}}\psi_1 + \alpha_2 L_{\mathbf{f}}\psi_2, \qquad \alpha_1, \alpha_3 \in \mathbb{R}, \tag{14}$$

$$L_{\mathbf{f}}(\psi_1\psi_2) = \psi_1 L_{\mathbf{f}}\psi_2, +\psi_2 L_{\mathbf{f}}\psi_1, \tag{15}$$

and by induction we can prove Leibniz's formula

$$L_{\mathbf{f}}^k(\psi_1\psi_2) = \sum_{i=0}^{k} \binom{k}{i} \left(L_{\mathbf{f}}^i\psi_1\right)\left(L_{\mathbf{f}}^{\mathrm{k}-i}\psi_2\right), \tag{16}$$

with $L_{\mathbf{f}}^i\psi = L_{\mathbf{f}}(L_{\mathbf{f}}^{i-1}\psi)$ and $L_{\mathbf{f}}^0\psi = \psi$, justifying the name Lie derivative. In addition, given vector fields $\mathbf{f}$ and $\mathbf{g}$,

$$\begin{aligned}\alpha_1 L_{\mathbf{f}} + \alpha_2 L_{\mathbf{g}} &= L_{\alpha_1\mathbf{f}+\alpha_2\mathbf{g}}, \\ [L_{\mathbf{f}}, L_{\mathbf{g}}] &= L_{\mathbf{f}}L_{\mathbf{g}} - L_{\mathbf{g}}L_{\mathbf{f}} = L_{\mathbf{h}},\end{aligned} \tag{17}$$

where $\mathbf{h}$ is another vector field corresponding to the Lie bracket of the vector fields, $\mathbf{h} = (\mathbf{f}, \mathbf{g})$, whose components are

$$h_i = (\mathbf{f}, \mathbf{g})_i = L_{\mathbf{f}}g_i - L_{\mathbf{g}}f_i = \sum_{j=1}^{n}\left(f_j\frac{\partial g_i}{\partial x_j} - g_j\frac{\partial f_i}{\partial x_j}\right). \tag{18}$$

Using Lie derivatives, we can write (11) as

$$\frac{d\mathbf{x}}{dt} = L_{\mathbf{f}(\mathbf{x})}\mathbf{x}, \tag{19}$$

[1] Some authors refer to $L_{\mathbf{f}}$ as the Liouville operator, after the transformation of nonlinear ODEs to a linear PDE carrying the same name.

where $L_{\mathbf{f}}$ acts on each component of $\mathbf{x}$ (remembering that $L_{\mathbf{f}}$ acts on functions). With this notation in place, the flow can formally be written as

$$\Phi_{\mathbf{f}}^t \mathbf{x} = \exp(tL_{\mathbf{f}})\mathbf{x} = \left(\sum_{k=0}^{\infty} \frac{t^k}{k!} L_{\mathbf{f}}^k \right) \mathbf{x}, \tag{20}$$

where $\exp(tL_{\mathbf{f}})$ is the Lie transform associated with $\mathbf{f}$. Again $\exp(tL_{\mathbf{f}})$ acts on each component of $\mathbf{x}$. Given an analytic function ψ and taking into account (14) and (16), it is easy to prove the following important property for Lie transforms:

$$\exp(tL_{\mathbf{f}})\psi(\mathbf{x}) = \psi(\exp(tL_{\mathbf{f}})\mathbf{x}). \tag{21}$$

Therefore, the composition of two flows can be rewritten in terms of Lie transforms as

$$\Phi_{\mathbf{f}}^t \Phi_{\mathbf{g}}^s \psi(\mathbf{x}) = \psi(\exp(sL_{\mathbf{g}}) \exp(tL_{\mathbf{f}})\mathbf{x}). \tag{22}$$

Observe that the order of the Lie transforms has been reversed so that the calculations have to be done from left to right. A Lie transform can be considered as a transform of coordinates from $\mathbf{x}_0$ to $\mathbf{x}_t = \exp(tL_{\mathbf{f}(\mathbf{x}_0)})\mathbf{x}_0$. One can see that $\exp(tL_{\mathbf{f}(\mathbf{x}_0)})$ similarly to $L_{\mathbf{f}(\mathbf{x}_0)}$, operates on functions of $\mathbf{x}_0$. It propagates forward in time according to the vector field $\mathbf{f}(\mathbf{x}_0)$ [12]. This point of view has been central in accelerator physics and optics, mainly since the paper of Dragt [11], where the notation: $\mathbf{f}:$ is used for the Lie derivative $L_{\mathbf{f}}$. Similarly, in Hamiltonian perturbation theory, such representations of coordinate transforms have been very fruitful.

Let us consider now the non-autonomous equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t). \tag{23}$$

The flow $\mathbf{x}(t) = \Phi_{\mathbf{f}}^t \mathbf{x}_0$ can locally be considered a Lie transform acting on initial conditions, so property (21) is valid for $\Phi_{\mathbf{f}}^t$. Thus $\mathbf{f}(\mathbf{x}, t) = \mathbf{f}(\Phi_{\mathbf{f}}^t \mathbf{x}_0, t) = \Phi_{\mathbf{f}}^t \mathbf{f}(\mathbf{x}_0, t)$ and Eq. (23) can be written as

$$\frac{d}{dt} \Phi_{\mathbf{f}}^t \mathbf{x}_0 = \Phi_{\mathbf{f}}^t L_{\mathbf{f}(\mathbf{x}_0,t)} \mathbf{x}_0; \tag{24}$$

thus,

$$\frac{d}{dt} \Phi_{\mathbf{f}}^t = \Phi_{\mathbf{f}}^t L_{\mathbf{f}(\mathbf{x}_0,t)}. \tag{25}$$

Now, Magnus's expansion can be used to obtain an approximate solution for $\Phi_{\mathbf{f}}^t$. If we consider $\Phi_{\mathbf{f}}^t = \exp(L_{\mathbf{w}(\mathbf{x}_0,t)})$, with $\mathbf{w} = \sum_i \mathbf{w}_i$, we obtain for the first two terms (taking into account (17) and that the position of $L_{\mathbf{f}}$ is on the right side)

$$\mathbf{w}_1(\mathbf{x}_0, t) = \int_0^t \mathbf{f}(\mathbf{x}_0, s)\, ds, \qquad \mathbf{w}_2(\mathbf{x}_0, t) = -\frac{1}{2} \int_0^t ds_1 \int_0^{s_1} ds_2 (\mathbf{f}(\mathbf{x}_0, s_1), \mathbf{f}(\mathbf{x}_0, s_2)). \tag{26}$$

Observe that the sign of $\mathbf{w}_2$ is changed when compared with Ω_2 in (6). Thus, for a time step $t = h$ we have

THEOREM 2.1. *Given* $\mathbf{w}_1, \mathbf{w}_2, \mathbf{f}^{(0)}$, *and* $\mathbf{f}^{(1)}$ *defined according to* (26) *and* (7) *and for a time step* $t = h$, *the following are fourth-order approximations to the exact solution of* (25):

$$\Phi_{\mathbf{f}}^h = \exp(L_{\mathbf{w}}) = \exp\left(L_{\mathbf{w}_1+\mathbf{w}_2}\right) + O(h^5) \tag{27}$$

$$= \exp\left(L_{\mathbf{f}^{(0)}+(\mathbf{f}^{(0)},\mathbf{f}^{(1)})}\right) + O(h^5). \tag{28}$$

Proof. This is similar to the proof in [2, 14]. Let us consider the Taylor expansion in t of $\mathbf{f}(\mathbf{x}_0, t)$,

$$\mathbf{f}(\mathbf{x}_0, t) = \mathbf{f}_0 + t\mathbf{f}_1 + t^2\mathbf{f}_2 + t^3\mathbf{f}_3 + \cdots, \tag{29}$$

with

$$\mathbf{f}_i = \frac{1}{i!}\frac{\partial^i}{\partial t^i}\mathbf{f}(\mathbf{x}, t)\bigg|_{t=0,\mathbf{x}=\mathbf{x}_0}.$$

Substituting the expansion into the integrals, with a little of algebra, and taking into account that the expressions are time symmetric, we find that $\mathbf{w}_{2i} = O(h^{2i+1})$ and $\mathbf{w}_{2i+1} = O(h^{2i+3})$, $i > 0$, so $\mathbf{w} = \mathbf{w}_1 + \mathbf{w}_2 + O(h^5)$. In a similar way we find that $\mathbf{f}^{(0)} + (\mathbf{f}^{(0)}, \mathbf{f}^{(1)}) = \mathbf{w}_1 + \mathbf{w}_2 + O(h^5)$. ■

It is important to bear in mind that a time step h of the exact flow $\Phi_{\mathbf{f}}^h$ is written as the time-1 flow of the vector field $\mathbf{w}(\mathbf{x}_0, h)$.

2.2.1. *Hamiltonian Systems*

Many important differential equations are Hamiltonian and deserve special attention, emphasising the qualitative properties of such systems. Even though the general treatment above is still valid, we now present the Hamiltonian version of the same results for the convenience of the reader. Given the Hamiltonian function $H(\mathbf{q}, \mathbf{p}, t) : \mathbb{R}^{2l} \times \mathbb{R} \to \mathbb{R}$, where $\mathbf{q}, \mathbf{p} \in \mathbb{R}^l$ are the coordinates and momenta of the system, the Hamiltonian equations are

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H}{\partial \mathbf{p}}, \qquad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{q}}. \tag{30}$$

By introducing the notation $\mathbf{x} = (\mathbf{q}, \mathbf{p}) = (q_1, \ldots, q_l, p_1, \ldots, p_l)$, (30) can be simplified to

$$\frac{d\mathbf{x}}{dt} = L_{H(\mathbf{x},t)}\mathbf{x}, \tag{31}$$

where L_H is the Lie derivative associated with the function H,

$$L_H = \sum_{i=1}^{l}\left(\frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i}\right) = \sum_{i,j=1}^{l}\frac{\partial H}{\partial x_i}J_{i,j}\frac{\partial}{\partial x_j}, \tag{32}$$

with $J = \left(\begin{smallmatrix} 0 & -I \\ I & 0 \end{smallmatrix}\right)$ and I is the $l \times l$ identity matrix. This Lie derivative is a particular case of $L_{\mathbf{f}}$ when $\mathbf{f} = -J\frac{\partial H}{\partial \mathbf{x}}$, and all previous results are valid. It is interesting to mention that given two functions H and G

$$[L_H, L_G] = L_K,$$

where $K = \{H, G\} = L_G H$ is the Lie Poisson bracket of functions on phase space $\mathbb{R}^{2l}$.

The Magnus approximations (27) and (28) now take the form

$$\Phi_H^h = \exp(L_W) = \exp\left(L_{W_1+W_2}\right) + O(h^5) \tag{33}$$

$$= \exp\left(L_{H^{(0)}+\{H^{(0)},H^{(1)}\}}\right) + O(h^5), \tag{34}$$

where

$$\begin{aligned} W_1(\mathbf{x}_0, h) &= \int_0^h H(\mathbf{x}_0, s)\, ds, \\ W_2(\mathbf{x}_0, h) &= -\frac{1}{2}\int_0^h ds_1 \int_0^{s_1} ds_2 \{H(\mathbf{x}_0, s_1), H(\mathbf{x}_0, s_2)\}. \end{aligned} \tag{35}$$

The Magnus expansion as an analytical approximation for Hamiltonian systems was first presented in [24]. To illustrate how the Magnus approximation can be used, let us consider the Hamiltonian

$$H(\mathbf{q}, \mathbf{p}, t) = T(\mathbf{p}, t) + V(\mathbf{q}, t), \tag{36}$$

which is separable into two easily solvable parts. If we integrate this system for a time step h using (34), then

$$H^{(i)} = T^{(i)}(\mathbf{p}) + V^{(i)}(\mathbf{q}),$$

and the integration for a time step h is equivalent to solving the autonomous Hamiltonian

$$\hat{H}(\mathbf{q}, \mathbf{p}) = T^{(0)}(\mathbf{p}) + V^{(0)}(\mathbf{q}) + \left\{T^{(0)}(\mathbf{p}), V^{(1)}(\mathbf{q})\right\} + \left\{V^{(0)}(\mathbf{q}), T^{(1)}(\mathbf{p})\right\}$$

for a time step $t = 1$. The main problem in numerically solving this system using, for example, symplectic integrators is that, in general, the Hamiltonian is no longer separable into easily solvable parts.

Another possibility for solving (36) is to rewrite the Hamiltonian as an autonomous system with two new coordinates and momenta,

$$\tilde{H} = \left(T\left(\mathbf{p}, q_1^t\right) + p_2^t\right) + \left(V\left(\mathbf{q}, q_2^t\right) + p_1^t\right) = \tilde{H}_1 + \tilde{H}_2, \tag{37}$$

which is separable into two solvable parts, so that the splitting or PRK method (3) can be used. Then one step of the method becomes

$$(\mathbf{q}_h, \mathbf{p}_h) = \prod_{i=1}^{m} \exp(h a_i \mathcal{H}_1(\mathbf{p}_0, \beta_i h)) \exp(h b_i \mathcal{H}_2(\mathbf{q}_0, \alpha_i h))(\mathbf{q}_0, \mathbf{p}_0), \tag{38}$$

where $\alpha_i = \sum_{j=1}^{i} a_j$, $\beta_i = \sum_{j=0}^{i-1} b_j$, with $b_0 = 0$ and $\mathcal{H}_1 = L_{\tilde{H}_1}$, $\mathcal{H}_2 = L_{\tilde{H}_2}$. This method is very easy to use, but unless special attention is paid to the implementation the performance can be reduced.

- The method requires m evaluations of the time-dependent functions in T and V. As we will see later, the most efficient fourth-order methods have $m \geq 5$. On the other hand, using Magnus and the Gaussian quadrature only two evaluations are necessary. At the same time, if T and V share the same time-dependent functions, only two evaluations are necessary for Magnus versus $2m$ using (38).
- It is important to keep in mind that if T is quadratic in momenta, e.g., $T = \mathbf{p}^T M(t)\mathbf{p}$, with $M \in \mathbb{R}^{l\times l}$, it is not possible to use RKN methods when splitting the Hamiltonian as in (37), and thus a less efficient PRK method has to be used.

As we can see, both techniques (Magnus and splitting) have advantages and disadvantages. In the next section, we will show how to construct new numerical methods which share the advantages of the previous techniques, i.e., are easy to use and efficiently manage the time-dependent part.

3. FACTORING THE MAGNUS SERIES

Let us assume that $\exp(\alpha_1 L_{\mathbf{f}^{(0)}} + \alpha_2 L_{\mathbf{f}^{(1)}})$ is easy to evaluate analytically or numerically. This is the case, for example, for the Hamiltonian (36) where the previous $\alpha_1\mathbf{f}^{(0)} + \alpha_2\mathbf{f}^{(1)}$ term would be associated to the Hamiltonian

$$\begin{aligned}\hat{H}(\mathbf{q},\mathbf{p}) &= \alpha_1\big(T^{(0)}(\mathbf{p}) + V^{(0)}(\mathbf{q})\big) + \alpha_2\big(T^{(1)}(\mathbf{p}) + V^{(1)}(\mathbf{q})\big)\\ &= \big(\alpha_1 T^{(0)}(\mathbf{p}) + \alpha_2 T^{(1)}(\mathbf{p})\big) + \big(\alpha_1 V^{(0)}(\mathbf{q}) + \alpha_2 V^{(1)}(\mathbf{q})\big)\\ &= \hat{T}(\mathbf{p}) + \hat{V}(\mathbf{q}),\end{aligned} \tag{39}$$

where a splitting method can be applied.

THEOREM 3.1. *Given $A^{(0)}$, $A^{(1)}$, $\mathbf{f}^{(0)}$, and $\mathbf{f}^{(1)}$ defined according to* (7) *and a time step $t = h$, the following are fourth-order approximations to the exact solutions of* (4) *and* (25),

$$\Phi_A^h = \exp(\Omega(h)) \tag{40}$$

$$= \exp\left(\frac{1}{2}A^{(0)} + 2A^{(1)}\right)\exp\left(\frac{1}{2}A^{(0)} - 2A^{(1)}\right) + O(h^5) \tag{41}$$

$$= \exp\big(A^{(1)}\big)\exp\big(A^{(0)}\big)\exp\big(-A^{(1)}\big) + O(h^5), \tag{42}$$

$$\Phi_{\mathbf{f}}^h = \exp\big(L_{\mathbf{w}(h)}\big) = \exp\Big(L_{\frac{1}{2}\mathbf{f}^{(0)} - 2\mathbf{f}^{(1)}}\Big)\exp\Big(L_{\frac{1}{2}\mathbf{f}^{(0)} + 2\mathbf{f}^{(1)}}\Big) + O(h^5) \tag{43}$$

$$= \exp\big(-L_{\mathbf{f}^{(1)}}\big)\exp\big(L_{\mathbf{f}^{(0)}}\big)\exp\big(L_{\mathbf{f}^{(1)}}\big) + O(h^5), \tag{44}$$

where $\mathbf{f}^{(i)} = \mathbf{f}^{(i)}(\mathbf{x}_0, h),\ i = 0, 1$.

Proof. From the definitions (7) we observe that $Z^{(0)}(h) = O(h)$ and $Z^{(1)}(h) = O(h^2)$. Then, using the BCH formulas

$$\exp(X)\exp(Y) = \exp\left(X + Y + \frac{1}{2}[X,Y] + \frac{1}{12}([X,[X,Y]] + [Y,[Y,X]]) + \cdots\right),$$

$$\exp(X)\exp(Y)\exp(-X) = \exp\left(Y + [X,Y] + \frac{1}{2}[X,[X,Y]] + \cdots\right),$$

we see that (41) and (42) agree with (10), and (43) and (44) agree with (28) up to order h^4, respectively. ■

3.1. Time Symmetry

Next, we study if the new methods preserve time symmetry.

DEFINITION. A one-step method, $\mathbf{x}_h = \Theta(t_0 + h, t_0, \mathbf{x}_0)$, is time symmetric if it satisfies $\mathbf{x}_0 = \Theta(t_f - h, t_f, \mathbf{x}_h)$ with $t_f = t_0 + h$.

In other words, if we integrate an ODE numerically over one step, h, followed by an integration of the same ODE backwards in time using the same method but with time step $-h$, we recover the initial condition. If we use the short notation $\Theta(h)$ for the method, then Θ is time symmetric if

$$\Theta^{-1}(h) = \Theta(-h). \tag{45}$$

Time symmetry is an important qualitative property of the exact solution, and sometimes it is interesting to preserve it in numerical approximations. This has been shown in case for ODEs with periodic solutions and small perturbations of such. Numerical experiments show that time symmetry can be a geometric quality on an equal footing with symplecticity for Hamiltonian ODE systems. For the methods presented in Theorem 3.1 we have the following theorem.

THEOREM 3.2. *The fourth-order approximations* (41)–(44) *preserve time symmetry.*

Proof. From definition (7) and rewriting $Z^{(0)}(h) = \int_{-h/2}^{h/2} Z(s + h/2)\, ds$, we have $Z^{(0)}(-h) = -Z^{(0)}(h)$, $Z^{(1)}(-h) = Z^{(1)}(h)$, which is the symmetry for $A^{(i)}(h)$ and $\mathbf{f}^{(i)}(\mathbf{x}_0, h)$, $i = 0, 1$. Considering (41), we have

$$\begin{aligned}\Theta(-h) &\equiv \exp\left(\frac{1}{2}A^{(0)}(-h) + 2A^{(1)}(-h)\right)\exp\left(\frac{1}{2}A^{(0)}(-h) - 2A^{(1)}(-h)\right)\\ &= \exp\left(-\frac{1}{2}A^{(0)}(h) + 2A^{(1)}(h)\right)\exp\left(-\frac{1}{2}A^{(0)}(h) - 2A^{(1)}(h)\right) \equiv \Theta^{-1}(h);\end{aligned}$$

hence it is time symmetric. A similar proof holds for (42). However, for the nonlinear case it is not so straightforward. If we consider (43), then

$$\begin{aligned}\mathbf{x}_h &= \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h) - 2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h) + 2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\mathbf{x}_0\\ &= \Psi_1(\mathbf{x}_0),\end{aligned} \tag{46}$$

and we have to prove that, using the same method on $\mathbf{x}_h$ with a time step $-h$, we recover the initial condition $\mathbf{x}_0$:

$$\begin{aligned}&\Theta(t_f - h, t_f, \mathbf{x}_h)\\ &\quad\equiv \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,-h) - 2\mathbf{f}^{(1)}(\mathbf{x}_h,-h)}\right)\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,-h) + 2\mathbf{f}^{(1)}(\mathbf{x}_h,-h)}\right)\mathbf{x}_h\\ &\quad= \exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,h) + 2\mathbf{f}^{(1)}(\mathbf{x}_h,h)}\right)\exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_h,h) - 2\mathbf{f}^{(1)}(\mathbf{x}_h,h)}\right)\mathbf{x}_h\\ &\quad= \Psi_2(\mathbf{x}_h).\end{aligned}$$

Taking into account how Lie transforms act and using (46), we have

$$\begin{aligned}
&\Theta(t_f - h, t_f, x_h) = \Psi_2(\mathbf{x}_h)\\
&\quad = \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)-2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)+2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\Psi_2(\mathbf{x}_0)\\
&\quad = \exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)-2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\exp\left(L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)+2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\\
&\qquad \times \exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)+2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\exp\left(-L_{\frac{1}{2}\mathbf{f}^{(0)}(\mathbf{x}_0,h)-2\mathbf{f}^{(1)}(\mathbf{x}_0,h)}\right)\mathbf{x}_0 = \mathbf{x}_0,
\end{aligned}$$

as we wanted to prove. A similar proof can be used for (44). ■

3.2. Error Estimation

The fourth-order methods (27), (28), (43), and (44) give different approximations to the exact solution,[2] and it is interesting to know how the errors depend on $\mathbf{f}$ and its derivatives. In this section we will give the leading error for each method. The exact solution is given formally by $\mathbf{x}(h) = \exp(L_{\mathbf{w}(\mathbf{x}_0,h)})\mathbf{x}_0$. Considering the Taylor expansion (29), evaluating the integrals, and using the BCH formula in (43) and (44), we can write all approximations as $\tilde{\mathbf{x}}(h) = \exp(L_{\tilde{\mathbf{w}}(h)})\mathbf{x}_0$, where $\tilde{\mathbf{w}}$ is a vector depending on the $\mathbf{f}_i$'s and their Lie brackets. Considering that $\tilde{\mathbf{w}} = \mathbf{w} + O(h^5)$, it follows that the local error is given by

$$\begin{aligned}
\mathbf{x}(h) - \tilde{\mathbf{x}}(h) &= \left(\exp\left(L_{\mathbf{w}(\mathbf{x}_0,h)}\right) - \exp\left(L_{\tilde{\mathbf{w}}(\mathbf{x}_0,h)}\right)\right)\mathbf{x}_0\\
&= L_{\mathbf{w}(\mathbf{x}_0,h)-\tilde{\mathbf{w}}(\mathbf{x}_0,h)}\mathbf{x}_0 + O(h^6)\\
&= (\mathbf{w} - \tilde{\mathbf{w}})(\mathbf{x}_0) + O(h^6),
\end{aligned} \tag{47}$$

so the leading error term is given by the vector $\mathbf{w} - \tilde{\mathbf{w}}$ evaluated at initial conditions, which is of order $O(h^5)$. After a few simple algebraic operations, all approximations take the form

$$\mathbf{w} - \tilde{\mathbf{w}} = h^5(\alpha_1(\mathbf{f}_1, \mathbf{f}_2) + \alpha_2(\mathbf{f}_0, (\mathbf{f}_0, \mathbf{f}_2)) + \alpha_3(\mathbf{f}_1, (\mathbf{f}_0, \mathbf{f}_1)) + \alpha_4(\mathbf{f}_0, (\mathbf{f}_0, (\mathbf{f}_0, \mathbf{f}_1)))) + O(h^6), \tag{48}$$

where the values of $\alpha_1, \alpha_2, \alpha_3$, and α_4 for each method are given in Table I. If a numerical quadrature is used for evaluating the integrals, then more terms will appear in the leading error term, depending on the quadrature used.

TABLE I
Coefficients of the Leading Error Term (48) for M4 (Eq. (27)), M4I (Eq. (28)), 2EX (Eq. (43)), and 3EX (Eq. (44))

	α_1	α_2	α_3	α_4
M4	0	$\frac{1}{360}$	$-\frac{1}{240}$	$-\frac{1}{720}$
M4I	$\frac{1}{360}$	$\frac{1}{360}$	$-\frac{1}{240}$	$-\frac{1}{720}$
2EX	$\frac{1}{360}$	$\frac{1}{360}$	$\frac{1}{2160}$	$-\frac{1}{2880}$
3EX	$\frac{1}{360}$	$\frac{1}{360}$	$-\frac{1}{1440}$	$-\frac{1}{720}$

[2] But if, e.g., $(\mathbf{f}(\mathbf{x}, t_1), \mathbf{f}(\mathbf{x}, t_2)) = 0$, $\forall t_1, t_2$, then all methods give the exact solution.

It is important to remember that the efficiency of a method depends not only on its error but also on its computational cost. For the methods considered, the computational cost is highly dependent on the problem.

4. SEPARABLE SYSTEMS

Frequently, Eq. (1) is separable into two parts, $\mathbf{f}(\mathbf{x}, t) = \mathbf{f}_A(\mathbf{x}, t) + \mathbf{f}_B(\mathbf{x}, t)$, such that

$$\frac{d\mathbf{x}}{dt} = \alpha_1 \mathbf{f}_A^{(0)}(\mathbf{x}) + \alpha_2 \mathbf{f}_A^{(1)}(\mathbf{x}), \qquad \frac{d\mathbf{x}}{dt} = \beta_1 \mathbf{f}_B^{(0)}(\mathbf{x}) + \beta_2 \mathbf{f}_B^{(1)}(\mathbf{x}) \tag{49}$$

are exactly solvable (or at least easy to evaluate up to the desired order). Thus, each exponential in the Magnus factorisations (43) and (44) is the sum of exactly solvable terms, and standard splitting (PRK or RKN) methods can be used.

Considering that the new methods based on Magnus series are of fourth order, we are interested in splitting methods such as (3), of this order of accuracy. In the literature we find a number of methods, many especially tailored for particular structures of X and Y. To avoid the use of different methods for each problem, we will present a new fourth-order method which works more efficiently for the important case of quadratic kinetic energy ("RKN" problems) than any other method we found in the literature. In addition, it will work as efficiently as the best PRK method we know for the most general case of X and Y and will be competitive for other structures assumed on X and Y.

We have

$$\prod_{i=1}^{m} \exp(h a_i X) \exp(h b_i Y) = \exp(h(X+Y)) + h^5 R + O(h^6), \tag{50}$$

where R constitutes the main error terms. Such a method is completely determined by the vectors $\mathbf{a} = (a_1, \ldots, a_m)$ and $\mathbf{b} = (b_1, \ldots, b_m)$ and can be considered a PRK method.

Let us study the general case where no special structure is assumed on X and Y (the FLA [free Lie algebra] case). Let $L(X, Y)$ denote the algebra whose elements are X, Y, and all elements obtained through the vector space operations of addition and multiplication by scalars together with the commutator. The subset $L_5(X, Y)$ of commutators with five operators can be represented by the six-dimensional basis

$$\begin{aligned} E_{5,1} &= [X,[X,[X,[X,Y]]]], & E_{5,6} &= [Y,[Y,[Y,[Y,X]]]], \\ E_{5,2} &= [Y,[X,[X,[X,Y]]]], & E_{5,5} &= [X,[Y,[Y,[Y,X]]]], \\ E_{5,3} &= [X,[X,[Y,[Y,X]]]], & E_{5,4} &= [Y,[Y,[X,[X,Y]]]]; \end{aligned}$$

thus we can write $R = \sum_{i=1}^{6} r_i E_{5,i}$. It is usual to define the leading error coefficient of (50) as the Euclidian norm of the vector $\mathbf{r} = (r_1, \ldots, r_6)$; i.e., $\mathcal{E} = \sqrt{\sum_i r_i^2}$. Then, to compare the efficiency of different methods, one has to consider its cost per step. In (50), m is usually proportional to the cost of one step, but not always. For example, the second-order leapfrog method $\exp(\frac{h}{2}A)\exp(B)\exp(\frac{h}{2}A)$ would correspond to $m = 2$ with $\mathbf{a} = (1/2, 1/2)$ and $\mathbf{b} = (1, 0)$, but since $b_2 = 0$ the last "A-exponential" can be concatenated with the first one in the next step. Thus, effectively the cost per step is lowered by one function evaluation. This is also the case of all symmetric compositions. In such cases, we will assume that the

cost is proportional to $m-1$ instead of m. This property is usually referred to as first same as last (or just FSAL). With these assumptions the standard definition for the effective error is $E_f = \mu \mathcal{E}^{1/4}$, where $\mu = m$ or $\mu = m-1$ accordingly. This is a measure of the accuracy as $h \to 0$ for nonstiff problems. We will take the method with the smaller effective error as the most efficient method. It is important to note that the adjoint composition of (50) (obtained through reversing the order of the exponentials) has exactly the same order and error, and therefore we need not consider those cases here.

In the following we consider different structures for X and Y, and for each case we look for the most efficient splitting method.

1. **RKN**. This corresponds to the special case in which $[Y,[Y,[Y,X]]] = 0$. Considering that now $E_{5,5} = E_{5,6} = 0$, a complete description of the leading error term is given by the vector $\mathbf{r} = (r_1, \ldots, r_4)$. In this case X and Y are qualitatively different and cannot be interchanged. For example, if in (50) we take $a_1 = 0$ we will find methods with different E_f values than when we consider $b_m = 0$. In [27] a nonsymmetric composition with $m = 5$ and $a_1 = 0$ is presented, whose effective error constant is $E_f = 0.476$. With $m = 4$ a method with $E_f = 0.509$ has been found [17]. Symmetric compositions with $b_m = 0$ can also be found in [18] for $m = 5$ and $m = 6$ with $E_f = 0.634$ and $E_f = 0.527$, respectively. We found no other symmetric compositions with $a_1 = 0$, and hence a search for methods with $m = 5$ and $m = 6$ was initiated. In the first case no improved methods were found, while for $m = 6$ a new method with $E_f = 0.360$ was discovered; let us denote this method as S^*. S^* is the most efficient method known to us of this type and it is given by the coefficients

$$\mathbf{a} = (0, a_2, a_3, a_4, a_3, a_2), \qquad \mathbf{b} = (b_1, b_2, b_3, b_3, b_2, b_1), \tag{51}$$

with

$$\begin{aligned} &a_2 = 0.254, \quad a_3 = -0.032290201410934288448, \quad a_4 = 1 - 2(a_2 + a_3), \\ &b_1 = 0.084, \quad b_2 = 0.682281125946589406371, \qquad b_3 = \frac{1}{2} - (b_1 + b_2). \end{aligned} \tag{52}$$

The error coefficients of the method are given by

$$\mathbf{r} = 10^{-5} \times (-0.82, 2.13, -0.65, -1.28, 23.07, 9.95), \tag{53}$$

and $E_f = (m-1)(\sqrt{r_1^2 + \cdots + r_4^2})^{1/4} = 0.360$.

Observe that for this type of problem Y commutes with $[Y,[Y,X]]$ and for many other problems both operators represent exactly solvable ODEs. It is therefore also interesting to consider not only exponentials of X and Y but instead of the Y's, $C_{b_i,c_i} = b_i Y + h^2 c_i [Y,[Y,X]]$ (called a modified potential). If the commutator is not very expensive to evaluate, such methods can possibly lead to very efficient schemes, and one scheme of this type is presented in [15]:

$$\mathbf{a} = \left(0, \frac{1}{2}, \frac{1}{2}\right), \qquad \mathbf{b} = \left(\frac{1}{6}, \frac{2}{3}, \frac{1}{6}\right), \qquad \mathbf{c} = \left(0, -\frac{1}{72}, 0\right). \tag{54}$$

The effective error of the method is $E_f = \mu_m \mathcal{E}^{1/4} = \mu_m 0.164$, where μ_m will depend on the cost of the modified potentials. It is usual to take into consideration the cost as a number

in the interval $\mu_m \in (\mu, \mu + \pi)$, where π is the number of modified potentials appearing in the scheme. With this criterion we find $E_f \in (0.327, 0.491)$, and in practice it does not improve the previous method by much. We have analysed the uni-parametric family of solutions in the case $c_1 = c_3 \neq 0$, obtaining a minimum very close to $c_1 = c_3 = 0$, with $E_f = \mu_m 0.156$. This improvement is too small to compensate for the presence of extra modified potentials. The case $b_3 = c_3 = 0$ gave two solutions, but these solutions also had a bigger error constant.

2. **Free Lie Algebra (FLA)**. This corresponds to the general case where no simplification in the algebra is possible. In this case, it seems preferable to consider only symmetric compositions where X and Y are interchangeable. The Ruth–Yoshida method with $m = 4$ given in [30] has $E_f = 1.335$. For $m = 5$ and $m = 6$ we found two methods with $E_f = 0.708$ and $E_f = 0.623$, respectively [17]. The RKN scheme S^*, being symmetric, turns out to be by a stroke of luck a fourth-order method also for this case with $E_f = 0.630$. This is, essentially, as efficient as the best method and has the additional property of being much better in the RKN case; so we conclude this paragraph by recommending scheme S^*.

3. **RKN2**. This corresponds to the case $[Y, [Y, [Y, X]]] = [X, [X, [X, Y]]] = 0$. We will take $\mathbf{r} = (r_3, r_4)$ in the definition of the error, because $E_{5,1} = E_{5,2} = E_{5,5} = E_{5,6} = 0$. Observe that now X and Y can be considered qualitatively equivalent, and they are interchangeable. Several families of nonsymmetric methods where the coefficients of (50) satisfy the relation $b_{m+1-i} = a_i,\ i = 1, \ldots, m$, are presented in [13]. This symmetry imposes that $r_3 = r_4$, which is a useful property in some cases. For example, in [6] these schemes were applied to a particular representation of the Schrödinger equation where unitarity was not exactly preserved (as was the case for other symplectic integrators) but was retained at higher order than the order of the method because $r_3 = r_4$. The most efficient fourth-order methods of [13], denoted by $(m = 4, n = 4)$ and $(m = 6, n = 4)$, have $E_f = 0.342$ and $E_f = 0.322$, respectively. On the other hand, S^* has $E_f = 0.308$ for this problem and is also here a good candidate for a numerical algorithm.

4. **Near-Integrable (NI)**. This is the case in which $\|Y\| \ll \|X\|$ for some norm. It is therefore natural to optimise the accuracy with this priori information; hence one can consider a smaller number of order conditions when constructing the method. It is now the case that $\|E_{5,i}\| \ll \|E_{5,1}\|,\ i = 2, \ldots, 6$, and an efficient method will be the one that minimises the coefficient of $E_{5,1}$. For this problem, it is difficult to define a useful effective error because one has to consider h as well as the size of $\|Y\|$ in the measure. Again, X and Y are qualitatively different and the number of possible methods is higher. For example, in [18] we found two symmetric second-order methods (taking $m = 3$ and $a_1 = 0$ or $b_3 = 0$) which work in practice as fourth-order methods for many problems. One of them is given by (54), taking $c_2 = 0$. Even more efficient symmetric fourth-order methods are presented in [18], cancelling the coefficients of $E_{5,1}$, $[X, E_{5,1}]$, $[X, [X, E_{5,1}]]$, and $[X, [X, [X, E_{5,1}]]]$, and the most efficient corresponds to the "(8, 4) *BAB*" method. The error coefficients of this method are $\mathbf{r} = 10^{-5} \times (0, 1.08, -44.79, \ldots)$, where the coefficients of $E_{5,2}$ and $E_{5,3}$ (containing two B operators) give the main contribution to the overall error. From these coefficients and comparing with the coefficient of $E_{5,1}$ in (53), -0.82×10^{-5}, we can see that, unless $\|Y\| \lessapprox \|X\|/50$, the method S^* will be more efficient (the coefficient of $[X, [X, E_{5,1}]]$ in S^* is also very small). If $\|B\|$ was even smaller it would be sufficient to use the second-order method (54) with $c_2 = 0$ because the main contribution to the error would come from the Magnus approximation.

In conclusion, we have presented a new method which works very efficiently under many assumptions on the vector fields. It is at least as accurate as some methods designed for special vector fields. In our opinion, for most of the problems, it is highly recommended to use only the new method.

One class of very efficient methods includes those based on processing techniques [3, 4, 20]. However, in this section we have considered only non-processed methods because we are dealing with a time-dependent problem (X and Y change at each step) and because each step is approximated by two or three different exponentials. The processing technique would be efficient for our problem only if the evaluation of each exponential in (43) and (44) was split into a relatively large number of substeps, which is the case only for extremely slowly varying vector fields.

5. NUMERICAL EXAMPLES

In this section we present numerical experiments that highlight the efficiency of the proposed schemes. First, we study the performance of the new splitting method S^* applied to several different separable autonomous Hamiltonians, in each of which there exist specially tailored schemes with which we compare our method. Next, we apply the factored Magnus series to non-autonomous systems to produce autonomous approximations which in turn are solved using the new splitting scheme S^*. Finally, we study how the new methods perform for oscillatory vector fields with different time scales for the frequency of the time-dependent function.

5.1. Autonomous Systems

In the following, we test S^* on four different systems of the types, separable (FLA), quadratic kinetic energy (RKN), quadratic Hamiltonian (RKN2), and near-integrable (NI). We will compare S^* with the most efficient schemes in each case accordingly. In particular, we will consider the following methods:

- FLA: The most efficient fourth-order symmetric method given in [19], denoted by S_{FLA}(triangles joined by lines).
- RKN: The most efficient fourth-order symmetric method given in [19], denoted by S_{RKN} (squares joined by lines).
- RKN2: The $(m = 4, n = 4)$ scheme presented in [13], denoted by S_{RKN2} (asterisks joined by lines).
- NI: The scheme $(8, 4) - BAB$ presented in [18], denoted by S_{NI} (diamonds joined by lines).
- The new scheme S^* (circles joined by broken lines).
- The well-known symmetric fourth-order method of Ruth–Yoshida [30] (crosses joined by lines). This is used as a reference method, because it is the best known and has been used in many papers.

We consider four autonomous Hamiltonian systems and use the average error in energy as a measure of accuracy. The interval of integration is not of great importance since the average error in energy is always bounded by constants for all methods and problems studied.

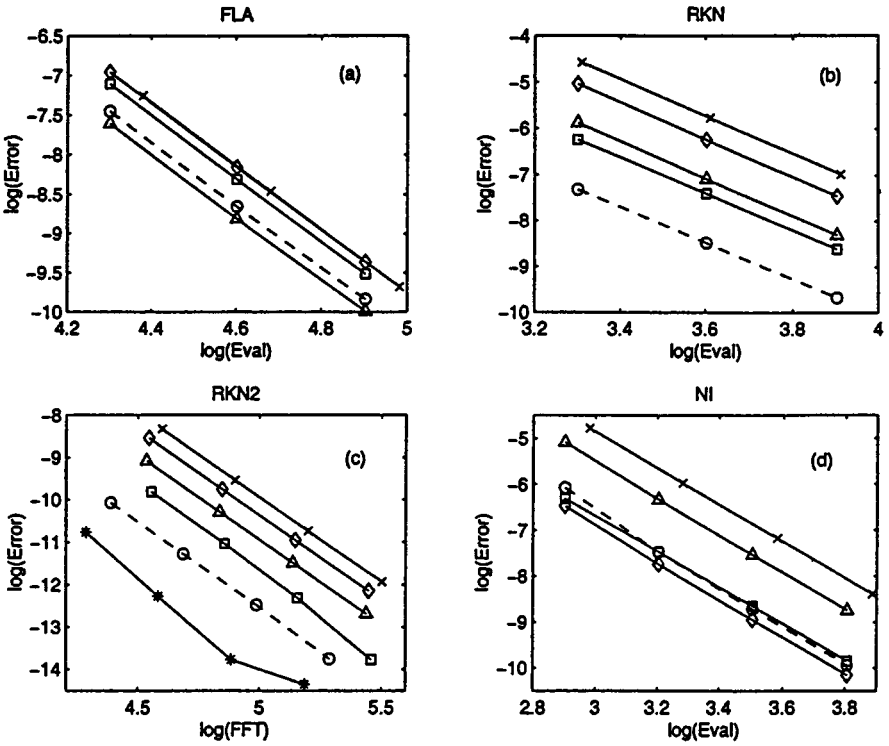

FIG. 1. Average relative errors in energy vs number of evaluations for the Hamiltonians suitable for FLA (a), RKN (b), RKN2 (c) and NI (d).

(a) FLA. The Hamiltonian considered is

$$H = \frac{1}{2}(p^2 + q^2) + \frac{1}{2}p^2q^2, \tag{55}$$

which is separable into two exactly solvable parts with no possible simplification in the algebra. The initial conditions used are $(q, p) = (2, 0)$, and we integrated the system along the interval $t \in [0, 20 \cdot 2\pi]$. Taking into account that all symmetric methods considered are also fourth-order methods for FLA problems, in Fig. 1a we present the average error in energy versus the number of function evaluations for different time steps. The numerical experiment agrees very well with the theoretical result from the effective error analysis.

(b) RKN. The simple Hamiltonian associated with the pendulum will be used as a system suitable for RKN methods,

$$H = \frac{1}{2}p^2 - \cos(q). \tag{56}$$

The initial conditions used are $(q, p) = (0, 1)$, and we integrated the system along the interval $t \in [0, 20 \cdot 2\pi]$. In Fig. 1b we give the average error in energy versus the number of function evaluations for several time steps. In this case, the new method clearly shows its superiority. Observe that it is approximately three orders of magnitude more accurate than the Ruth–Yoshida method at the same computational cost, while it is one order of magnitude more accurate than the previously most efficient method, S_{RKN}.

(c) RKN2. The simplest Hamiltonian suitable for RKN2 methods is the harmonic oscillator $H = p^2/2 + q^2/2$. But, to better understand the interest in RKN2 methods, we will study a less trivial system. Let us consider the Schrödinger equation with the Morse potential

$$i\frac{d}{dt}\psi(x,t) = \left(-\frac{1}{2\mu}\frac{\partial^2}{\partial x^2} + D(1-e^{-\alpha x})^2\right)\psi(x,t), \qquad \psi(x,0) = \psi_0(x), \quad (57)$$

with parameters $\mu = 1745$ a.u., $D = 0.2251$ a.u., and $\alpha = 1.1741$ a.u., corresponding to the HF molecule. As initial conditions we will take the ground state, whose energy is $E_0 = w_0/2 - w_0^2/(16D)$, where $w_0 = \alpha\sqrt{2D/\mu}$, and we will integrate along the interval $t \in [0, 20 \cdot 2\pi/w_0]$. We assume that the system is defined in the interval $x \in [-0.8, 4.32]$, and we split this interval into $N = 64$ parts of length $\Delta x = 0.08$. Next we consider $c_n = \psi(x_n, t)$ where $x_n = x_0 + n\Delta x$, $n = 1, \ldots, N$, thus obtaining the finite-dimensional linear equation

$$i\frac{d\mathbf{c}}{dt} = \mathbf{H}\mathbf{c}, \qquad \mathbf{c}(0) = \mathbf{c}_0, \quad (58)$$

where $\mathbf{c} = (c_1, \ldots, c_N)^T \in \mathbb{C}^N$ and $\mathbf{H} = \mathbf{T} + \mathbf{V} \in \mathbb{C}^{N\times N}$. Here $\mathbf{V}$ is a diagonal matrix associated with the potential and with diagonal values $V(x_i)$, $i = 1, \ldots, N$, and $\mathbf{T}$ is a full matrix associated with the kinetic energy. Fast Fourier transforms (FFT), $\mathbf{F}$, give a way of evaluating $\mathbf{Tc} = \mathbf{F^{-1}D_T F c}$, where $\mathbf{D_T}$ is diagonal and $\mathbf{Fc}$ and $\mathbf{F}^{-1}\mathbf{c}$ can be evaluated using only $O(N\log(N))$ operations. If we define the real vectors $\mathbf{q} = \mathrm{Re}\ \mathbf{c}$ and $\mathbf{p} = \mathrm{Im}\ \mathbf{c}$, then solving (58) is equivalent to solving

$$\frac{d}{dt}\begin{Bmatrix}\mathbf{q}\\ \mathbf{p}\end{Bmatrix} = \begin{pmatrix}0 & \mathbf{H}\\ -\mathbf{H} & 0\end{pmatrix}\begin{Bmatrix}\mathbf{q}\\ \mathbf{p}\end{Bmatrix}, \quad (59)$$

which can be considered as the system associated with the N-dimensional Hamiltonian $\mathcal{H} = \frac{1}{2}\mathbf{p}^T\mathbf{H}\mathbf{p} + \frac{1}{2}\mathbf{q}^T\mathbf{H}\mathbf{q}$. Evaluating the exponential of (59) is prohibitively expensive, and one has to look for alternative techniques. Since in this case the Hamiltonian is separable into two solvable parts, the exponentiation can be done with RKN2 methods.

In Fig. 1c, we present the relative average error in energy versus the number of FFTs for different time steps. The biggest time step taken corresponds to the stability limit of each method. Observe the advantage of S^* versus the other methods not especially designed for RKN2 problems. The good performance of the specially tailored RKN2 method can be explained from the fact that the solutions of (58) and (59) evolve through a unitary and an orthogonal transform, respectively. The splitting methods used preserve symplecticity but not orthogonality for this problem. However, this particular RKN2 method preserves unitarity to fifth order, as can be seen from the slope of its curve. This method has been used in [6] in a time-dependent problem. Finally, we have to say that the RKN2 method works this efficiently only if one uses the error in energy as a measure of accuracy, while the error in position still behaves as predicted by the effective error analysis.

(d) NI. As a Hamiltonian suitable for NI methods we will consider the one used by Hénon-Heiles,

$$H = \frac{1}{2}(p_x^2 + p_y^2 + x^2 + y^2) + \left(x^2 y - \frac{1}{3}y^3\right). \quad (60)$$

TABLE II
Effective Error of the Methods Used in the Numerical Examples

	$E_{f,\mathrm{FLA}}$	$E_{f,\mathrm{RKN}}$	$E_{f,\mathrm{RKN2}}$	$10^5\mathcal{E}_{\mathrm{NI}}$
FLA	0.623	0.618	0.573	$12.7+15.6\epsilon$
RKN	0.727	0.527	0.454	$1.00+12.2\epsilon$
RKN2	—	—	0.342	—
NI	0.812	0.799	0.799	$0.00+44.8\epsilon$
S^*	0.630	0.360	0.308	$0.82+2.22\epsilon$
Ruth-Roshida	1.335	1.231	1.216	$60.7+483\epsilon$

Note. $E_{f,\Lambda}=\mu\mathcal{E}_\Lambda$, with $\Lambda=$ FLA, RKN, RKN2, or NI, $\mu=m$ for RKN2 and $\mu=m-1$ for the others. In NI methods we use a different definition for the error $\mathcal{E}_{\mathrm{NI}}=(\mu/5)^4\,(|r_1|+\epsilon\sqrt{r_2^2+r_3^2})$ ($\epsilon\approx\|B\|/\|A\|$).

We will study the evolution near the origin with initial conditions $x=y=p_x=p_y=1/100$, where the cubic term can be considered as a small perturbation. In Fig. 1d, we give the average relative error in energy versus the number of evaluations. S_{NI} is the most efficient, but S_{RKN} and S^* have very similar performance since in both cases r_1 is very small.

To better compare the results obtained in the numerical examples with the results theoretically expected, we have collected the effective error of the various methods in Table II.

Before this section concludes, it is important to note that for time-dependent Hamiltonians of the form $H=X(t)+Y(t)$, the nature of the system might change as time evolves between the classes Separable, RKN-type, RKN2-type, and Near-integrable. Thus the new splitting method presented is a very natural candidate, which is nearly optimal for all these cases.

Motivated by the above results, a deep search for symmetric fourth- and sixth-order metods for FLA and RKN was started, and very efficient methods were obtained [7]. In the search for fourth-order methods, taking both symmetric compositions and $m=7$, we improved the efficiency slightly for FLA and RKN methods separately, but not both together.

5.2. Non-autonomous Systems

In this section we will consider some Hamiltonians systems which are separable like (36). The new schemes (43) and (44) take the form

$$\Theta_H^h=\exp(\mathcal{T}_1+\mathcal{V}_1)\exp(\mathcal{T}_2+\mathcal{V}_2)+O(h^5) \tag{61}$$

$$=\exp\big(-\mathcal{T}^{(1)}-\mathcal{V}^{(1)}\big)\exp\big(\mathcal{T}^{(0)}+\mathcal{V}^{(0)}\big)\exp\big(\mathcal{T}^{(1)}+\mathcal{V}^{(1)}\big)+O(h^5), \tag{62}$$

where $\mathcal{T}_{1,2}=L_{\frac{1}{2}T^{(0)}\mp 2T^{(1)}}$, $\mathcal{V}_{1,2}=L_{\frac{1}{2}V^{(0)}\mp 2V^{(1)}}$, $\mathcal{T}^{(i)}=L_{T^{(i)}}$, $\mathcal{V}^{(i)}=L_{V^{(i)}}$, $i=0,1$. If we use the new splitting method, S^*, for each exponential in (61), we obtain

$$\Theta_H^h=\exp(b_1\mathcal{V}_1)\exp(a_2\mathcal{T}_1)\exp(b_2\mathcal{V}_1)\cdots\exp(a_2\mathcal{T}_1)\exp(b_2\big(\mathcal{V}_1+\mathcal{V}_2)\exp(a_1\mathcal{T}_2)$$
$$\cdots\exp(b_2\mathcal{V}_2)\exp(a_2\mathcal{T}_2)\exp(b_1\mathcal{V}_2)+O(h^5). \tag{63}$$

If we consider that the last exponential $\exp(b_1\mathcal{V}_2)$ can be concatenated with the first exponential $\exp(b_1\mathcal{V}_1)$ of the next step, then the method requires 10 evaluations of $\exp(\mathcal{T})$ and $\exp(\mathcal{V})$. Similarly, the scheme (62) requires 15 evaluations of each exponential. However, if the kinetic energy is time-independent, then $\mathcal{T}^{(1)}=0$ and the scheme S^* applied to (62)

gives

$$\Theta_H^h = \exp\big(b_1\mathcal{V}^{(0)} - \mathcal{V}^{(1)}\big)\exp\big(a_2\mathcal{T}^{(0)}\big)\exp\big(b_2\mathcal{V}^{(0)}\big) \cdots \exp\big(b_2\mathcal{V}^{(0)}\big)\exp\big(a_2\mathcal{T}^{(0)}\big)\exp\big(b_1\mathcal{V}^{(0)} + \mathcal{V}^{(1)}\big) + O(h^5), \tag{64}$$

and one step requires only five evaluations of $\exp(\mathcal{T})$ and $\exp(\mathcal{V})$.

EXAMPLE 1 (LINEARLY FORCED POTENTIAL). Let us consider a Hamiltonian with a linearly forced potential:

$$H(\mathbf{q}, \mathbf{p}, t) = \frac{1}{2}\mathbf{p}^T\mathbf{p} + V(\mathbf{q}) + f(t)\mathbf{q}. \tag{65}$$

Considering that

$$\{H(\mathbf{q}, \mathbf{p}, t_1), H(\mathbf{q}, \mathbf{p}, t_2)\} = (f(t_1) - f(t_2))\mathbf{p},$$

it is easy to check that (27), (28), and (44) are equivalent, so we will only consider (43) and (44). As a simple example, we take the forced pendulum,

$$H = \frac{1}{2}p^2 - \cos(q) - F\cos(wt)q, \tag{66}$$

with F and w constants. This Hamiltonian is one of the most popular non-linear systems appearing in textbooks because of its simplicity and its richness in qualitative properties.

At this point, we are only interested in the error introduced by the approximations (43) and (44), so each of the exponentials will be evaluated up to machine accuracy (with the help of splitting methods). The integrals will be evaluated both analytically and numerically using the fourth-order Gaussian quadrature previously mentioned. We take $F = 1/10$, $w = 2$ and initial conditions $(q, p) = (0, 1)$ and use measure the average error in (q, p) along the interval $t \in [0, 5000 \cdot 2\pi]$, using the same time step $h = \pi/20$ for all methods.

Figure 2a shows the results when the integrals are evaluated analytically: 2EX and 3EX refer to (43) and (44), respectively. As a reference, we show the results obtained using the standard fourth-order Runge–Kutta method. Observe that the error of the RK4 method grows faster since it is not symplectic. Other non-symplectic methods such as standard multistep algorithms have the same qualitative behaviour, so they are not considered in this paper. We then approximate the integrals using the fourth-order Gaussian quadrature as in (8) (2EXq and 3EXq). Figure 2b shows the results obtained. We also present the results obtained, for the same time step, when using the S_{RKN} and S^* methods directly without using Magnus. Note the improvement in accuracy for 2EX when using quadratures.

It is important to remember that the efficiency of a method also depends on its computational cost. This point will be considered in the following examples.

EXAMPLE 2. Let us consider the Hamiltonian studied in [8],

$$H(q, p, t) = \frac{1}{2}p^2 + \frac{1}{2}q^2 + \varepsilon\sum_{i=1}^{k}\cos(q - \omega_i t), \tag{67}$$

which describes the motion of a charged particle in a constant magnetic field perturbed by k electrostatic plane waves (propagting along the direction of the motion), each with the same wavenumber and amplitude, but with different temporal frequencies ω_i. This Hamiltonian

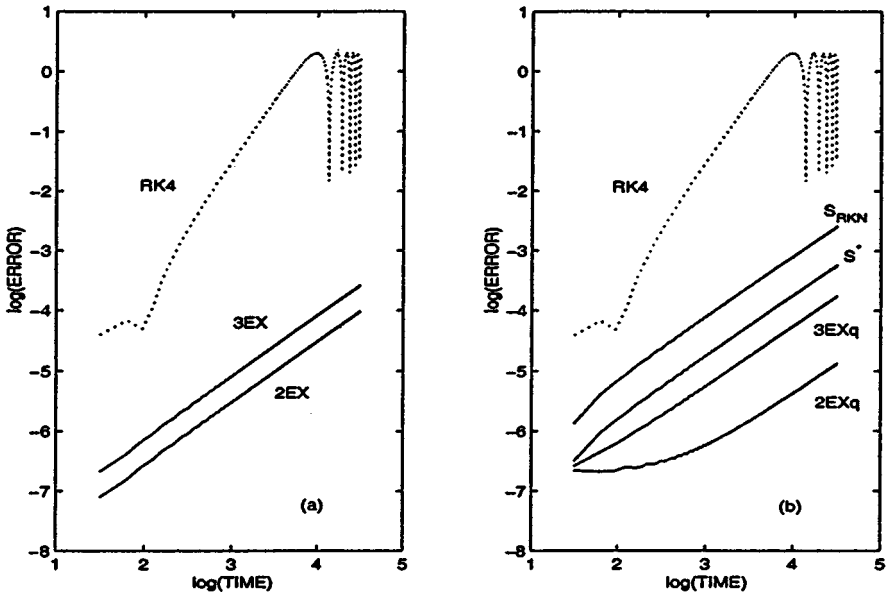

FIG. 2. Average errors in position vs time for the forced pendulum (66).

can be written as

$$H(q,\,p,\,t) = \frac{1}{2}p^2 + \frac{1}{2}q^2 + \varepsilon\cos(q)g_1(t) + \varepsilon\sin(q)g_2(t), \tag{68}$$

with $g_1(t) = \sum_{i=1}^{k}\cos(w_k t)$, $g_2(t) = \sum_{i=1}^{k}\sin(w_i t)$. Observe that, for moderate values of k, the cost of evaluating one step using a given method will be, essentially, proportional to the number of evaluations of $g_1(t)$ and $g_2(t)$, because it is the most costly part of the Hamiltonian.

We take as initial conditions $q_0 = 0$, $p_0 = 11.2075$, and we choose $\omega_i = i\omega_0$, with $\omega_0 = 1/10$ and $k = 10$. Figure 3 show the Poincaré mappings obtained by plotting points at discrete times $t_j = 2\pi j/w_0$, with 1000 plotted points. For $\varepsilon = 0.25$ we see a closed trajectory and for $\varepsilon = 1.25$ we find five closed and very narrow trajectories.

The kinetic energy is time-independent and quadratic in momentum, so it is possible to use RKN methods. We will compare the RKN methods S_{RKN} and S^* (five evaluations of g_1 and g_2 per step) versus the schemes based on Magnus, (43) and (44), also implemented with S^* according to (63) and (64). The integrals are approximated using the mentioned Gaussian quadrature (the quadrature gives, essentially, the same result as the analytical solution).

Let us denote by $(q_k,\,p_k) = (q(t_k),\,p(t_k))$ the points at the Poincaré map. Given a method and a time step $h = 2\pi/N$ with N an integer, we obtain a set of points $(\tilde{q}_k,\,\tilde{p}_k)$, and we define $\delta = \max\{|q_k - \tilde{q}_k| + |p_k - \tilde{p}_k| : k = 1, \ldots, 100\}$. For each method we choose the minimum value of N such that $\delta < 10^{-3}$, and for this value of N we measure the CPU time in seconds. Table III shows the results obtained, where the superiority of the methods based on Magnus is clear, 2EXq being the most efficient.

EXAMPLE 3. Let us consider the equation

$$\ddot{\mathbf{q}} = A\dot{\mathbf{q}} + \mathbf{f}(\mathbf{q}, t), \qquad \mathbf{q}_0 = \mathbf{q}(t_0) \in \mathbb{R}^l, \tag{69}$$

with $A^T = A \in \mathbb{R}^{l\times l}$, $\mathbf{f}(\mathbf{q}, t) = -\frac{\partial}{\partial \mathbf{q}}V(\mathbf{q}, t)$, and where the dots indicate derivatives respect

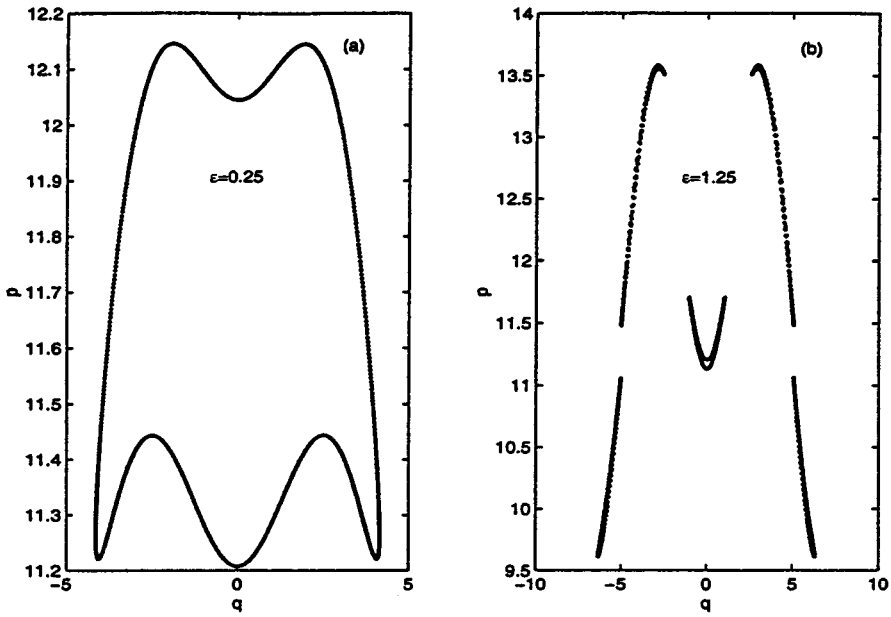

FIG. 3. Poincaré map of a single trajectory of (68). Initial conditions are $(q_0, p_0) = (0, 11.2075)$, $k = 10$, $w_0 = 1/10$ and (a) $\epsilon = 0.25$ and (b) $\epsilon = 1.25$.

to t. Then for $l = 1$, this system can be obtained from the Hamiltonian

$$H = \frac{1}{2}\mathbf{p}^T M(t)\mathbf{p} + M^{-1}(t)V(\mathbf{q}, t), \tag{70}$$

with $\dot{M} = AM$ so that $M = \exp(tA)$ and where $\mathbf{p} = M^{-1}\ \dot{\mathbf{q}}$ and has the form (36). For $l > 1$ we can consider the system

$$\dot{\mathbf{q}} = M(t)\mathbf{p}$$
$$\dot{\mathbf{p}} = M(t)^{-1}\frac{\partial}{\partial \mathbf{q}}V(\mathbf{q}, t).$$

A general PRK method applied to (37) requires m evaluations of $M(t)$ and another m evaluations of $M^{-1}(t)$ at different points. On the other hand a Magnus-based method requires only two evaluations $M(t)$ and $M^{-1}(t)$ at the same points (if using, e.g., the fourth-order Gaussian quadrature).

TABLE III
Minimum Value of N Such That $\delta < 10^{-3}$

	$\varepsilon = 0.25$		$\varepsilon = 1.25$	
	CPU (S)	N	CPU (S)	N
2EXq	4.00	38	7.70	74
3EXq	4.90	58	10.6	121
S^*	8.50	38	15.6	71
S_{RKN}	10.7	48	14.8	68
RK4	12.0	152	26.5	331

Note. The Time Step is $h = 2\pi/N$.

These considerations are very important because, in most of the cases, the cost of the method will be essentially the cost of the evaluations of $M(t)$ and $M^{-1}(t)$.

If the matrix A is time-dependent, then $M(t)$ will be the solution of the equation $\dot{M} = A(t)M$, which can be solved numerically using the Magnus expansion for linear systems.

A system of coupled Duffing oscillators is a particular case of (69). Examples of two-dimensional coupled systems can be found in [25]. For simplicity, we consider the one-dimensional case

$$\ddot{q} = \epsilon\dot{q} + q - q^3 + \delta\cos(wt), \tag{71}$$

with $\epsilon = 10^{-4}$, $\delta = 10^{-3}$, $\omega = 1/2$, and initial conditions $p(0) = 0.0$ and $q(0) = 1.75$. For solving its Hamiltonian system, we will consider the following:

1. The new factored Magnus method (43), denoted by 2EXq, where the integrals are approximated using the Gaussian quadrature, implemented with the new optimised RKN method S^*.
2. The optimal fourth-order PRK method, S_{FLA}, applied to (70) using the splitting (37). This would correspond to the solution of (1) using the transformation (2) and having the inefficiency mentioned in the third point.
3. The Ruth–Yoshida fourth-order PRK method. It is used only as a reference because it is a well-known method and has been frequently used.
4. The classical RK method of order 4, RK4. It is used only as a reference.

The time step chosen is normalised so that the computational cost in terms of execution time is the same for all schemes (on the machines we used). Figure 4 clearly shows

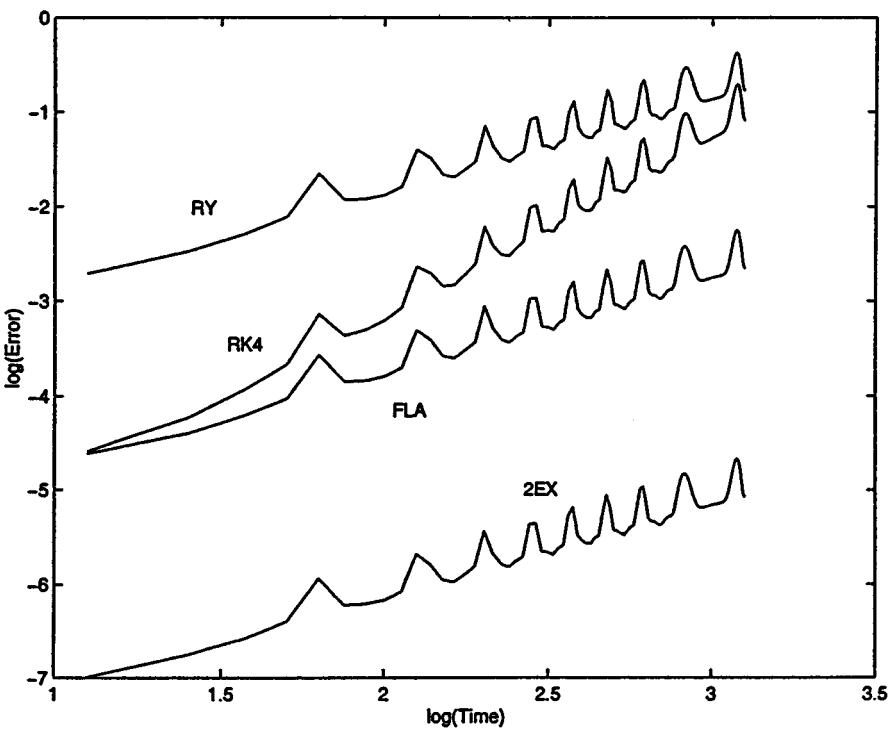

FIG. 4. Relative errors in position vs time at the same computational cost.

the advantage of handling the time dependency explicitly when solving nonautonomous problems. The computational saving in this problem comes from reducing the number of function evaluations in addition to allowing a specialised RKN method to be applied. The plot shows clearly that the Ruth–Yoshida method has effective error orders of magnitude larger than the most optimised methods, while S_{FLA} gives an error approximately two and a half orders of magnitude larger than the Magnus-based splitting method. For reference the number of time-dependent function evaluations for the Magnus-based method, S_{FLA}, Ruth–Yoshida, and Runge–Kutta is for this example 2, 5, 3, and 2 per step, respectively.

This system has chaotic evolution for the parameters and initial conditions chosen, but the small value of ϵ makes the system close to integrable and the chaotic effect very small. This explains the linear error growth observed in the experiment along the interval studied.

5.3. Performance for Different Time Scales

In this paper we have presented new numerical methods derived from the Magnus series. The error of these methods will come from the Magnus series truncation and from the particular factorisation considered, and it is ultimately dependent on the smoothness in the variable t of the vector field $\mathbf{f}(\mathbf{x}, t)$. To have a better idea about the performance of the new methods in problems with different time scales, we will consider again the forced pendulum

$$H = \frac{1}{2}p^2 - \cos(q) - F\cos(\omega t)q, \tag{72}$$

with $F = 1/10$, initial conditions $(q, p) = (0, 1)$, and we wil study the error of the methods for $\omega \in [1/10, 100]$ and $t \in [0, 100 \cdot 2\pi]$.

Considering that all methods are of the same order and qualitatively the same error growth, for each value of w we will look for the number of evaluations required to reach a given accuracy. The various methods are all implemented with Gaussian quadrature for integrals using the new splitting method. We will also consider the symmetric RKN method S_{RKN} for comparison.

In Fig. 5 we give the number of evaluations against w at fixed accuracy 10^{-8} in (q, p). Figure 5a shows the number of evaluations of the potential plus the number of time-dependent functions evaluations, a number which is for this example proportional to the CPU time because the cost of the derivative of the potential $(\sin(q))$ is similar to one evaluation of the time-dependent function $(\cos(wt))$.

In Fig. 5b we present the same computation but the cost is given as the number of time-dependent function evaluations. This picture would be representative of problems where the time-dependent part was the most expensive, as is the case of the two previous autonomous systems. The scheme (44) is superior only if evoluation of the potential is expensive and when values of ω are around the resonance, but its performance deteriorates as $\omega \to \infty$. If the time-dependent part is expensive, or the frequency is particularly high or low compared to the natural frequency of the autonomous systems ($F = 0$), then (43) with two exponentials is always the best scheme. In the region $\omega \in [0, 1/2]$ the Magnus approximation is very accurate (in the limit $\omega \to 0$ the system would be autonomous) and the error comes only from the splitting method used. Thus, if the evaluation of the potential is cheaper than evaluating the time-dependent part, it is more efficient to use high-order splitting methods or to split the time step and to use the fourth-order splitting method repeatedly.

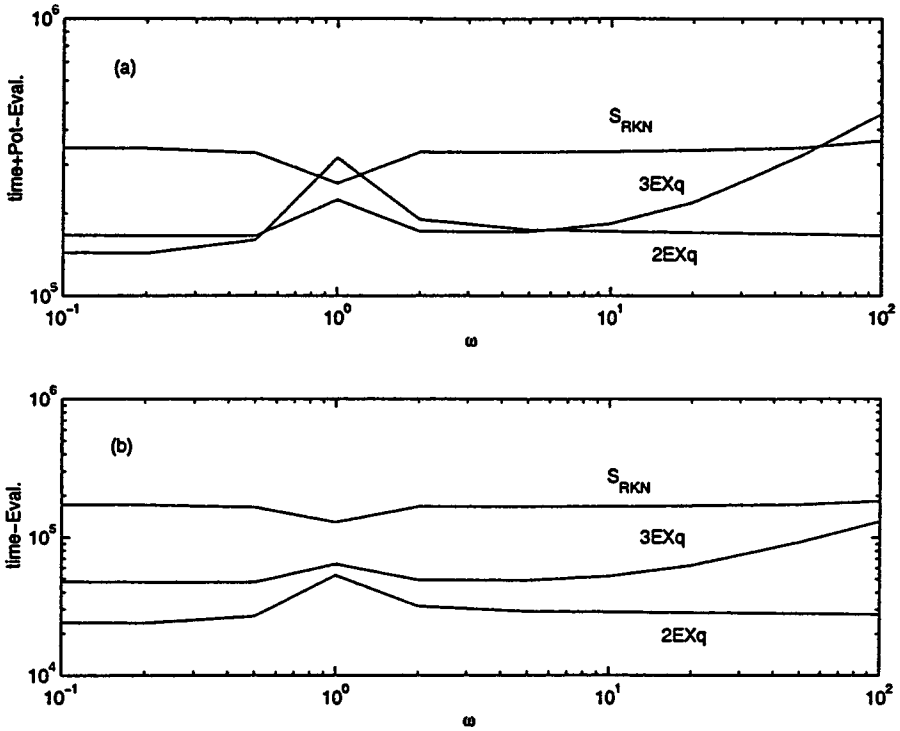

FIG. 5. Number of evaluations vs w for the forced pendulum (72) for the new methods based on Magnus (2EXq, 3EXq) and a standard symplectic integrator (S_{RKN}): (a) number of evaluations of the potential plus the time dependent evaluations (equivalent to the CPU time for this particular problem); (b) number of time dependent evaluations.

Observe that according to Fig. 5b, 2EXq is approximately seven times faster (for most of the frequencies) than the standard symplectic S_{RKN} in case the time-dependent part is the most expensive to evaluate.

6. CONCLUSIONS

We have presented new numerical integration schemes for ordinary differential equations which evolve on the same solution manifold as the exact solution. These methods are based on Magnus expansions and can be considered *geometric integrators*, retaining many of the qualitative properties of the exact solution. To avoid the presence of the troublesome commutators we factor the fourth-order Magnus series as a product of two and three simple exponentials. Such an approach seems to be attractive for separable Hamiltonian systems, where the otherwise present commutators would render the Hamiltonian non separable.

To implement these schemes in an optimal way, we also presented a new fourth-order symmetric splitting method. This method works more efficiently than other fourth-order methods we found in the literature for RKN problems. At the same time, it works nearly as efficiently as the best methods especially designed for general separable problems, linear problems, and near integrable problems.

The numerical experiments show the high performance of the new methods, in particular when the time-dependent part of the system is expensive to evaluate. The high accuracy

obtained comes both from the efficient management of the time-dependent functions, using the averaging technique, and from the efficiency of the new splitting method.

The good results obtained encouraged us to look for higher order splitting methods [7] as well as more sophisticated schemes for different types of problems. New methods for evaluating operator exponentials when splitting methods cannot be used or are expensive constitute an important part of the approach presented in this paper, and we hope to return to this topic at a later point.

Sixth-order methods based on factored Magnus series have also been studied by the authors. They require only three evaluations of the time-dependent functions (if a sixth-order Gaussian quadrature is used), but a minimum of five exponentials are necessary. Furthermore, good sixth-order spliting methods require at least 10 stages [7]; so if each exponential in the Magnus factorisation is implemented with one of these methods, each step will involve such a large number of evaluations that they will probably becomes on competitive versus other methods. For this reason, they have not been studied in the same detail as the fourth-order methods and are not presented in this paper.

A very interesting application of the idea presented in this paper is the geometric integration of stochastically perturbed Hamiltonian systems. For such systems the non-autonomous terms are exchanged with random terms [10]. Making sure the appropriate calculus was applied, we were able to construct low-order symplectic methods for such systems. Preliminary numerical experiments showed that these methods give results which are qualitatively closer to the true solutions, retaining, e.g., certain invariant measures compared to traditional schemes for stochastic ODES.

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