

# Explicit symplectic RKN methods for perturbed non-autonomous oscillators: Splitting, extended and exponentially fitting methods

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## ARTICLE INFO

### Article history:

Received 19 November 2014

Received in revised form

18 February 2015

Accepted 12 March 2015

Available online 20 March 2015

### Keywords:

Perturbed non-autonomous oscillatory systems

Splitting methods

Extended RKN methods

Exponentially fitted RKN methods

## ABSTRACT

We consider the numerical integration of perturbed non-autonomous oscillatory systems using high order methods. The autonomous case has been efficiently integrated using explicit and symplectic Runge–Kutta–Nyström (RKN) methods like extended RKN methods, exponentially fitting RKN methods and splitting methods for perturbed systems. Recently, it has been shown that explicit and symplectic extended RKN methods and exponentially fitting RKN methods are equivalent (Wu et al., 2012) and in this work we show that these methods are also equivalent to splitting methods for perturbed oscillators. We provide a constructive proof which at the same time allows us to build for the first time new explicit and symplectic extended RKN methods for the non-autonomous problem (for multidimensional time dependent frequencies). The new methods obtained, while built from splitting methods, are different in the treatment of the time-dependent terms and can be superior in some cases. We build some new methods and show their performance on numerical examples.

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## 1. Introduction

We consider the numerical integration of perturbed non-autonomous systems of oscillators with explicitly time-dependent frequencies

$$q'' + \Omega^2(t)q = \varepsilon f(t, q), \quad (1)$$

where  $q \in \mathbb{R}^d$ ,  $|\varepsilon| \ll 1$ ,  $\Omega^2(t)$  is a smooth symmetric positive semi-definite matrix, and  $f(t, q) = -\nabla V(t, q)$ , being  $V$  a scalar function. We show how to build new symplectic extended Runge–Kutta–Nyström (RKN) methods for the numerical integration of this problem. To this purpose, we first consider the numerical integration of the autonomous problem

$$q'' + \Omega^2 q = \varepsilon f(q), \quad (2)$$

which is equivalent to compute the evolution for a classical Hamiltonian system with Hamiltonian function

$$H(q, p) = \frac{1}{2}p^T p + \frac{1}{2}q^T \Omega^2 q + \varepsilon V(q) = H_0(q, p) + \varepsilon V(q), \quad (3)$$

where  $q, p$  are the coordinates and associated momenta (for this problem  $p = q'$ ), and the Hamilton equations are given by

$$z' = J \nabla H, \quad (4)$$

where  $z = (q, p)$  and  $J$  is the skew-symmetric symplectic matrix.

The numerical integration of perturbed oscillators with constant frequencies has been studied by many researchers during the last decades and a number of methods have been proposed. On one hand very stable methods have been developed to allow for large time steps and few evaluation of the (usually computationally expensive) non-linear perturbation force (typically low order methods are considered) e.g., Gautschi's and Deuffhard's trigonometric methods [1–3], the impulse method [4], the mollified impulse method [5], or generalizations of the previous ones (see [6] and references therein). On the other hand, high order methods to reach high accuracy have also been proposed, being this the problem to be considered in this work.<sup>1</sup> Some classes of methods built for this goal are explicit symplectic extended Runge–Kutta–Nyström (ERKN) methods or explicit symplectic exponentially fitting RKN (EFRKN) methods. They have been deeply analyzed for Hamiltonian systems and a number of methods for different problems have been published (see [7–14] and references therein). In [11] it is shown that ERKN are equivalent to EFRKN, but these methods correspond to different ideas and derivation. The ERKN integrators are proposed based on the variation of constants formula while

<sup>1</sup> This class of methods are frequently used for long time integrations with a constant time step. For relatively large time steps, some resonances between the frequency of the system and the time step can occur and, in spite relatively highly accurate results can be obtained with some very large time steps, one should use small enough time steps, i.e. high accuracies, to avoid the resonances.

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the EFRKN methods are derived by applying the exponential fitting techniques to the multidimensional modified RKN methods.

Closely related to the previous methods are the splitting methods (SMs) for solving general first order perturbed differential equations of the form

$$x' = A(x) + \varepsilon B(x). \quad (5)$$

SMs correspond to a composition of the maps associated to the exact (or approximate) solutions of the equations<sup>2</sup>:

$$x' = A(x), \quad x' = \varepsilon B(x). \quad (6)$$

If  $\Phi_h^A, \Phi_h^B$  denote the  $h$ -flows associated to the solution of each equation, an approximation to the exact flow,  $\Phi_h$ , can be obtained with an  $s$ -stage composition [15–20]

$$\Phi_h^{(p_1, \dots, p_k)} = \Phi_{a_{s+1}h}^A \circ \Phi_{b_sh}^B \circ \Phi_{a_sh}^A \circ \dots \circ \Phi_{b_1h}^B \circ \Phi_{a_1h}^A \quad (7)$$

where we make use of the FSAL property (the last map is reused in the first map of the following step). This split allows to build methods where the error depends on the small parameter,  $\varepsilon$ , as follows:

$$\Phi_h - \Phi_h^{(s_1, \dots, s_k)} = \mathcal{O}(\varepsilon h^{s_1+1} + \dots + \varepsilon^k h^{s_k+1}),$$

where  $k$  is chosen such that  $s_i \geq s_{i+1}$ ,  $i = 1, \dots, k-1$ , and we say the method has generalized order  $(s_1, \dots, s_k)$ . If  $\Phi_h^A, \Phi_h^B$  are symplectic maps, the composition is, by construction, symplectic and if each map is time-symmetric, a palindromic composition preserves this symmetry.

In this work we show that (explicit and symplectic) extended RKN methods, exponentially fitting RKN methods and splitting RKN methods, when applied to the numerical solution of (2), are equivalent to each other. Their main difference for this application remains in the derivation and in some cases in the computational cost since the flow of the algorithms for exponentially fitting and extended methods (which are equivalent for this problem) is different to the one for splitting methods. In addition, while the order conditions are, obviously, equivalent, the analysis for the dominant error terms which allow to build efficient methods differ considerably. In addition, SM are well suited methods to be improved with the use of modified potentials (force-gradient methods) or with the use of pre- and post-processors which allow to considerably improve the performance of the methods at marginal extra cost [17].

We make use of this relation to show how to build new explicit and symplectic ERKN for the non-autonomous problem (1) with global error of order

$$\mathcal{O}(h^{s_0} + \varepsilon h^{s_1} + \varepsilon^2 h^{s_2} + \dots) \quad (8)$$

and we say the method has generalized order  $(s_0; s_1, \dots, s_k)$ , i.e. in the limit when  $\varepsilon \rightarrow 0$  this is a method of order  $s_0$  for the non-autonomous oscillator. These new methods are built from splitting methods applied to (1) but their implementation does not correspond to a standard splitting method due to a different treatment of the time-dependent part so, the computational cost and accuracy can differ and we show that in some cases the new methods can be superior to standard splitting methods.

In Section 2 we present the explicit and symplectic ERKN and EFRKN methods. Section 3 introduces splitting methods for perturbed autonomous oscillators and we explicitly show that some low order ERKN methods are equivalent to properly chosen splitting methods. This equivalence is shown to be valid in general in Section 4 using a constructive proof. In Section 5 we build new explicit and symplectic ERKN methods for the non-autonomous problem following the previous constructive proof and in Section 6 we illustrate in some numerical examples the performance of the new methods. Section 7 gives the conclusions and indicates some interesting future work.

## 2. Explicit symplectic extended RKN (ERKN) methods

An  $s$ -stage explicit ERKN method for solving (2) is a one step method given by (with  $q'_i = p_i$ ):

$$Q_i = \phi_0(c_i v) q_0 + c_i h \phi_1(c_i v) p_0 + \varepsilon h^2 \sum_{j=1}^s a_{ij} f(Q_j), \quad i = 1, \dots, s, \quad (9)$$

$$q_1 = \phi_0(v) q_0 + h \phi_1(v) p_0 + \varepsilon h^2 \sum_{i=1}^s \bar{b}_i f(Q_i), \quad (10)$$

$$p_1 = -h\Omega^2 \phi_1(v) q_0 + \phi_0(v) p_0 + \varepsilon h \sum_{i=1}^s b_i f(Q_i), \quad (11)$$

where  $v = h\Omega$ ,  $c_i$  are the nodes and  $a_{ij}, \bar{b}_i, b_i$  are matrix valued functions of  $v$  with  $a_{ij} = 0$ ,  $j \geq i$ , and the  $\phi$ -functions are defined by

$$\phi_0(v) = \cos(v), \quad \phi_1(v) = \frac{\sin(v)}{v}.$$

The symplecticity conditions are given by [8,21]:

$$a_{ji} = b_i(c_j - c_i) \frac{\phi_1((c_j - c_i)v)}{\phi_0((1 - c_i)v)}, \quad j > i = 1, \dots, s-1, \quad (12)$$

$$\bar{b}_i = b_i(1 - c_i) \frac{\phi_1((1 - c_i)v)}{\phi_0((1 - c_i)v)}, \quad i = 1, \dots, s, \quad (13)$$

for  $b_i \neq 0$ ,  $i = 1, \dots, s$ . If  $c_i = 1 - c_{s+1-i}$ ,  $b_i = b_{s+1-i}$  then the scheme is time-symmetric. For example, a one-stage second order symmetric and symplectic method is given by

$$\begin{aligned} Q_1 &= \phi_0\left(\frac{1}{2}v\right) q_0 + \frac{h}{2} \phi_1\left(\frac{1}{2}v\right) p_0, \\ q_1 &= \phi_0(v) q_0 + h \phi_1(v) p_0 + \varepsilon \frac{h^2}{2} \phi_1\left(\frac{1}{2}v\right) f(Q_1), \\ p_1 &= -h\Omega^2 \phi_1(v) q_0 + \phi_0(v) p_0 + \varepsilon h \phi_0\left(\frac{1}{2}v\right) f(Q_1), \end{aligned} \quad (14)$$

which corresponds to  $s = 1$ ,  $c_1 = \frac{1}{2}$  and the choice  $b_1 = \phi_0(\frac{1}{2}v)$ . We refer to this method as the ERKN2a method, but other choices for  $b_1$  are also valid as far as  $b_1 = 1 + \mathcal{O}(h^2)$  (for example, in [8] it was taken  $b_1 = \phi_1(v)$  for a scalar problem).

Another one-stage second order symmetric and symplectic method (taking into account the FSAL property) is given by

$$\begin{aligned} Q_1 &= q_0, \\ Q_2 &= \phi_0(v) q_0 + h \phi_1(v) p_0 + \varepsilon \frac{h^2}{2} \phi_1(v) f(Q_1), \\ q_1 &= \phi_0(v) q_0 + h \phi_1(v) p_0 + \varepsilon \frac{h^2}{2} \phi_1(v) f(Q_1), \\ p_1 &= -h\Omega^2 \phi_1(v) q_0 + \phi_0(v) p_0 + \varepsilon \frac{h}{2} (\phi_0(v) f(Q_1) + f(Q_2)), \end{aligned} \quad (15)$$

which corresponds to  $s = 2$ ,  $c_1 = 0$ ,  $c_2 = 1$ ,  $b_1 = \frac{1}{2} \phi_0(v)$ ,  $b_2 = \frac{1}{2}$ . Notice that since  $q_1 = Q_2$ , in the following step this will correspond to the value of  $Q_1$  so, one can reuse  $f(Q_2)$  as  $f(Q_1)$  in the following step (FSAL property), and this method is considered in practice as a one step method. We refer to this method as the ERKN2b method, but other choices for  $b_1, b_2$  can also be considered, e.g. in [8] it was taken  $b_1 = \phi_1(v) - (1 - \phi_0(v))/v^2$ ,  $b_2 = (1 - \phi_0(v))/v^2$  (for a scalar problem).

<sup>2</sup> The vector fields  $A(x)$  and  $B(x)$  can also be originated from a semidiscretization of a PDE.

We also present the two-stage method obtained in [11] (referred as the SMEFMKN2s2 method) which shows a high performance in practice

$$\begin{aligned} Q_1 &= \phi_0(c_1\nu)q_0 + c_1h\phi_1(c_1\nu)p_0 \\ Q_2 &= \phi_0(c_2\nu)q_0 + c_2h\phi_1(c_2\nu)p_0 \\ &\quad + \varepsilon \frac{h^2}{2} (c_2 - c_1)\phi_1((c_2 - c_1)\nu)f(Q_1) \\ q_1 &= \phi_0(\nu)q_0 + h\phi_1(\nu)p_0 \\ &\quad + \varepsilon \frac{h^2}{2} (c_2\phi_1(c_2\nu)f(Q_1) + c_1\phi_1(c_1\nu)f(Q_2)) \\ p_1 &= -h\Omega^2\phi_1(\nu)q_0 + \phi_0(\nu)p_0 \\ &\quad + \varepsilon \frac{h}{2} (\phi_0(c_2\nu)f(Q_1) + \phi_0(c_1\nu)f(Q_2)), \end{aligned} \quad (16)$$

with  $c_1 = \frac{3-\sqrt{3}}{6}$ ,  $c_2 = \frac{3+\sqrt{3}}{6}$ . This method has global error of order  $\mathcal{O}(\varepsilon h^4 + \varepsilon^2 h^2)$  and, as we will show, this method is equivalent to the very simple two stage ABA splitting method of generalized order (4,2) obtained by McLachlan in [19].

### 2.1. Exponentially fitting RKN methods

Exponentially fitting methods for the numerical integration of differential equations are methods build with the goal to exactly solve the problem when the solution takes the form

$$q(t) = \sum_{i=1}^l w_i(t) \exp(\mu_i t) \quad (17)$$

where  $w_i$  are polynomial functions. The first step is, obviously, to estimate the values of the frequencies [22–24].

However, when applied to Eq. (2) the goal is to build methods which exactly solve the unperturbed problem

$$q'' + \Omega^2 q = 0. \quad (18)$$

Since  $\Omega^2$  is a positive definite matrix, then  $\mu_i = i\sigma_i$  where  $\sigma_i$  are the real eigenvalues of  $\Omega$  and the degree of the polynomials  $w_i$  depend on the multiplicity of the eigenvalues. If the functions  $\phi_0(\nu)$ ,  $\phi_1(\nu)$  are exactly evaluated or accurately approximated, the values of  $\sigma_i$  and their multiplicities are not necessary to be known in advance. Following [11], these methods are referred as multidimensional exponentially fitted modified RKN methods, and the explicit and symplectic ones are written as

$$Q_i = C_i q_0 + D_i h p_0 + \varepsilon h^2 \sum_{j=1}^s a_{ij} f(Q_j), \quad i = 1, \dots, s \quad (19)$$

$$q_1 = C q_0 + D h p_0 + \varepsilon h^2 \sum_{i=1}^s \bar{b}_i f(Q_i), \quad (20)$$

$$h p_1 = F q_0 + E h p_0 + \varepsilon h^2 \sum_{i=1}^s b_i f(Q_i), \quad (21)$$

where  $C, D, C_i, D_i, E, F, b_i, \bar{b}_i$ ,  $i = 1, \dots, s$  and  $a_{ij}$ ,  $i, j = 1, \dots, s$  are matrix-valued functions of  $\nu$ . In [11] it is shown that these methods are equivalent to the previous symplectic explicit extended RKN methods.

### 3. Splitting methods for perturbed problems

If we write Eq. (2) as a first order system of equations (with  $q' = p$ )

$$\begin{aligned} \frac{d}{dt} \begin{pmatrix} q \\ p \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -\Omega^2 & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} + \varepsilon \begin{pmatrix} 0 \\ f(q) \end{pmatrix} \\ &= A(q, p) + \varepsilon B(q) \end{aligned} \quad (22)$$

then splitting methods for perturbed systems can be applied. The  $h$ -flow associated to each map is given by

$$\begin{aligned} \Phi_h^A : \begin{pmatrix} q_1 \\ p_1 \end{pmatrix} &= \begin{pmatrix} \cos(\nu)q_0 + \Omega^{-1} \sin(\nu)p_0 \\ -\Omega \sin(\nu)q_0 + \cos(\nu)p_0 \end{pmatrix}, \\ \Phi_h^B : \begin{pmatrix} q_1 \\ p_1 \end{pmatrix} &= \begin{pmatrix} q_0 \\ p_0 + \varepsilon h f(q_0) \end{pmatrix}. \end{aligned} \quad (23)$$

Splitting methods for perturbed systems given by a composition like (7) have been successfully used for the numerical integration of problems in celestial mechanics [25–27], quantum mechanics [28, 29] and parabolic PDEs using complex coefficients [30], as well as for the numerical integration of problems with explicitly time-dependent frequency,  $\Omega(t)$ , [28–32].

Notice that Eq. (22) corresponds to the Hamilton equations (4) with Hamiltonian function (3). If  $\{H_0(q, p), V(q)\}$  denotes the Poisson bracket then, since  $H_0$  is quadratic in momenta, it is easy to check that  $\{V, \{H_0, V\}\} = \tilde{V}(q)$  is a function depending only on coordinates and then  $\{V, \{V, \{H_0, V\}\}\} = 0$ , which simplifies the Lie algebra associated to this problem. Then, highly efficient splitting RKN methods can be obtained [33] (see also [16,6,19] and references therein). However, for this perturbed problem it is more advantageous to consider that the system is split into a dominant part and a perturbation and to build methods tailored for this structure (which can also take into account the fact that  $\{V, \{V, \{H_0, V\}\}\} = 0$ ) [15,19].

The splitting method (7) applies as follows (using the previous notation and taking  $b_{s+1} = 0$ )

$$\begin{aligned} Q_0 &= q_0, \quad P_0 = p_0 \\ \text{for } i &= 1 : s + 1 \\ Q_i &= \phi_0(a_i\nu)Q_{i-1} + a_i h \phi_1(a_i\nu)P_{i-1} \\ \bar{P}_i &= -a_i h \Omega^2 \phi_1(a_i\nu)Q_{i-1} + \phi_0(a_i\nu)P_{i-1}, \\ P_i &= \bar{P}_i + \varepsilon b_i h f(Q_i) \end{aligned} \quad (24)$$

end

$$q_1 = Q_{s+1}, \quad p_1 = P_{s+1}.$$

Let us now consider the following one-stage second order ABA composition method, referred as the impulse method or Strang splitting method for perturbed systems

$$\Phi_h^{(2,2)} = \Phi_{\frac{1}{2}h}^A \circ \Phi_{b_1 h}^B \circ \Phi_{\frac{1}{2}h}^A, \quad (25)$$

whose error is of order  $\mathcal{O}(\varepsilon h^3 + \varepsilon^2 h^3)$ , i.e. of generalized order (2, 2). For consistency, one should impose  $b_1 = 1$ , but since the method is of second order and the leading error is of order  $\mathcal{O}(\varepsilon h^2)$ , one could take  $b_1 = 1 + \mathcal{O}(h^2)$  which allows for some freedom. The scheme is given by the following algorithm (half rotation–kick–half rotation)

$$\begin{aligned} Q_1 &= \phi_0\left(\frac{1}{2}\nu\right)q_0 + \frac{h}{2}\phi_1\left(\frac{1}{2}\nu\right)p_0 \\ P_1 &= -\frac{h}{2}\Omega^2\phi_1\left(\frac{1}{2}\nu\right)q_0 + \phi_0\left(\frac{1}{2}\nu\right)p_0, \\ Q_2 &= Q_1 \\ P_2 &= P_1 + \varepsilon b_1 h f(Q_1) \\ q_1 &= \phi_0\left(\frac{1}{2}\nu\right)Q_2 + \frac{h}{2}\phi_1\left(\frac{1}{2}\nu\right)P_2 \\ p_1 &= -\frac{h}{2}\Omega^2\phi_1\left(\frac{1}{2}\nu\right)Q_2 + \phi_0\left(\frac{1}{2}\nu\right)P_2. \end{aligned} \quad (26)$$

It is easy to check that this map,  $(q_1, p_1) = \Phi_h^{(2,2)}(q_0, p_0)$ , is equivalent to the composition of the flow associated to the Hamiltonian

$$\varepsilon V \left( \phi_0 \left( \frac{1}{2} \nu \right) q + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p \right) \quad (27)$$

followed by a rotation. The Hamilton equations for the Hamiltonian (27) are (taking into account that  $\phi_i(\nu)^T = \phi_i(\nu)$  since  $\Omega$  is a symmetric matrix)

$$\begin{aligned} q' &= \frac{\partial \varepsilon V}{\partial p} = -\varepsilon \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) f \left( \phi_0 \left( \frac{1}{2} \nu \right) q + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p \right) \\ p' &= -\frac{\partial \varepsilon V}{\partial q} = \varepsilon \phi_0 \left( \frac{1}{2} \nu \right) f \left( \phi_0 \left( \frac{1}{2} \nu \right) q + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p \right) \end{aligned}$$

where  $V(\phi_0(\frac{1}{2}\nu)q + \frac{h}{2}\phi_1(\frac{1}{2}\nu)p)$  is a constant of motion, as well as the force  $f$  so, its flow for one step of length  $hb$  is given by a shift

$$\begin{aligned} Q &= q_0 - \varepsilon b \frac{h^2}{2} \phi_1 \left( \frac{1}{2} \nu \right) f \left( \phi_0 \left( \frac{1}{2} \nu \right) q_0 + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p_0 \right) \\ P &= p_0 + \varepsilon b h \phi_0 \left( \frac{1}{2} \nu \right) f \left( \phi_0 \left( \frac{1}{2} \nu \right) q_0 + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p_0 \right). \end{aligned}$$

If we consider a time step of length  $b_1 h$  of this map followed by a rotation originated from the  $h$ -flow of the harmonic oscillator, i.e.

$$\begin{aligned} Q &= q_0 - \varepsilon b_1 \frac{h^2}{2} \phi_1 \left( \frac{1}{2} \nu \right) f \left( \phi_0 \left( \frac{1}{2} \nu \right) q_0 + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p_0 \right) \\ P &= p_0 + \varepsilon b_1 h \phi_0 \left( \frac{1}{2} \nu \right) f \left( \phi_0 \left( \frac{1}{2} \nu \right) q_0 + \frac{h}{2} \phi_1 \left( \frac{1}{2} \nu \right) p_0 \right), \\ q_1 &= \phi_0(\nu)Q + h\phi_1(\nu)P \\ p_1 &= -h\Omega^2 \phi_1(\nu)Q + \phi_0(\nu)P, \end{aligned} \quad (28)$$

we can easily check that the scheme (28) is equivalent to (26) as well as to (14) so, the one-stage ABA splitting method is equivalent to the EKR2a method.

In a similar way, the scheme given by the BAB composition

$$\Phi_h^{(2,2)} = \Phi_{b_1 h}^B \circ \Phi_h^A \circ \Phi_{b_1 h}^B \quad (29)$$

(where we can take  $b_1 = \frac{1}{2} + \mathcal{O}(h^2)$ ) corresponds to the following algorithm:

$$\begin{aligned} Q_1 &= q_0 \\ P_1 &= p_0 + \varepsilon b_1 h f(q_0) \\ Q_2 &= \phi_0(\nu)Q_1 + h\phi_1(\nu)P_1 \\ P_2 &= -h\Omega^2 \phi_1(\nu)Q_1 + \phi_0(\nu)P_1 \\ q_1 &= Q_2 \\ p_1 &= P_2 + \varepsilon b_1 h f(Q_2), \end{aligned} \quad (30)$$

or in short

$$\begin{aligned} P_1 &= p_0 + \varepsilon b_1 h f(q_0) \\ q_1 &= \phi_0(\nu)q_0 + h\phi_1(\nu)P_1 \\ P_2 &= -h\Omega^2 \phi_1(\nu)q_0 + \phi_0(\nu)P_1 \\ p_1 &= P_2 + \varepsilon b_1 h f(q_1). \end{aligned} \quad (31)$$

This algorithm is equivalent to a composition of the following maps: first by the  $(b_1 h)$ -flow originated from the Hamiltonian  $\varepsilon V(q)$  followed by the  $(b_1 h)$ -flow for the Hamiltonian,  $\varepsilon V(\phi_0(\nu)q + h\phi_1(\nu)p)$ , and finally by applying a rotation of length  $h$ , i.e.

$$\begin{aligned} Q_1 &= q_0 \\ P_1 &= p_0 + \varepsilon b_1 h f(q_0) \end{aligned}$$

$$\begin{aligned} Q_2 &= Q_1 - \varepsilon b_1 h^2 \phi_1(\nu) f(\phi_0(\nu)Q_1 + h\phi_1(\nu)P_1) \\ P_2 &= P_1 + \varepsilon b_1 h \phi_0(\nu) f(\phi_0(\nu)Q_1 + h\phi_1(\nu)P_1) \\ q_1 &= \phi_0(\nu)Q_2 + h\phi_1(\nu)P_2 \\ p_1 &= -h\Omega^2 \phi_1(\nu)Q_2 + \phi_0(\nu)P_2. \end{aligned} \quad (32)$$

Again, we can easily check that the scheme (32) is equivalent to (31) as well as to (15) so, this BAB splitting method is equivalent to the EKR2b method.

Let us now consider the splitting method of generalized order (4,2)

$$\Phi_h^{(4,2)} = \Phi_{a_3 h}^A \circ \Phi_{b_2 h}^B \circ \Phi_{a_2 h}^A \circ \Phi_{b_1 h}^B \circ \Phi_{a_1 h}^A \quad (33)$$

with coefficients [19]:  $a_1 = a_3 = \frac{3-\sqrt{3}}{6}$ ,  $a_2 = \frac{1}{\sqrt{3}}$ ,  $b_1 = b_2 = \frac{1}{2}$ . These coefficients are the solution of very simple order conditions (see [15] to find the order conditions up to relatively high orders):  $a_1 = a_3$ ,  $b_1 = b_2$  (to preserve time-symmetry) and

$$a_1 + a_2 + a_3 = 1, \quad b_1 + b_2 = 1, \quad b_1 a_1^2 + b_2 (a_1 + a_2)^2 = \frac{1}{3}.$$

In the same way as previously, it is very simple to check that this method is equivalent to the two-stage ERKN method (SMEFM-RKN2s2) given in (16).

#### 4. Equivalence between the families of methods

In this section we show that the explicit and symplectic ERKN methods given by (9)–(11) are equivalent to the splitting methods (24) where the real valued numbers  $c_i$  from (9)–(11) and  $a_i$  from (24) are related by

$$c_i = \sum_{j=1}^i a_j \quad (34)$$

and the coefficients  $a_{ij}$ ,  $\bar{b}_i$ ,  $b_i$  in (9)–(11) (which depend only on the coefficients  $b_i$  through the symplectic conditions) can be originated from an appropriate choice of the coefficients  $b_i$  in (24). Then the coefficients of ERKN (and EFRKN) methods can also be used for numerically solving more general problems. To understand the close relation between these families of methods can be of great interest since they are originated with different idea and derivation, and it can be used to build new methods.

Taking into account basic results from the Lie algebra for classical mechanics, we prove the following result:

**Theorem 1.** *An  $s$ -stage explicit symplectic ERKN method for solving Eq. (2) given by the scheme (9)–(11) corresponds to a splitting symplectic method given by the scheme (24) where  $c_i = \sum_{j=1}^i a_j$  and for an appropriate choice of the coefficients  $b_i$ .*

**Proof.** We present a constructive proof and to this purpose we found convenient to use Lie algebra techniques. For convenience of the reader not familiar with Lie algebraic techniques, in the following we briefly collect the results needed for the proof.

**Preliminaries on the Lie algebraic structure of classical mechanics.** We review some basic properties on the Lie algebraic structure of classical mechanics for Hamiltonian systems [34,35].

- Given two scalar functions,  $f(q, p), g(q, p) : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ , the Poisson bracket is defined as

$$\{f, g\} = \sum_{i=1}^d \left( \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right) = (\nabla f)^T J (\nabla g) \equiv -L_{f,g}$$

where  $L_f \equiv -(\nabla f)^T J \nabla$  is the Lie operator associated to the function  $f$  (the negative sign is introduced to simplify the presentation).



- The Hamilton equations can be written as:  $q' = L_H q$ ,  $p' = L_H p$  and the solution can formally be written as follows:

$$(q(t), p(t)) = e^{tL_H}(q, p) \Big|_{(q,p)=(q_0,p_0)} \\ = (e^{tL_H} q, e^{tL_H} p) \Big|_{(q,p)=(q_0,p_0)}. \quad (35)$$

Given a scalar function,  $g(q, p)$ , the Lie transform is defined as

$$e^{tL_H} g = \sum_{k=0}^{\infty} \frac{t^k}{k!} L_H^k g, \quad \text{where } L_H^0 g = g, \quad L_H^k g = L_H^{k-1}(L_H g),$$

and, if  $g$  is an analytic function (using the Leibnitz' rule for the derivation of a product of functions) we have that

$$e^{tL_H} g(q, p) = g(e^{tL_H} q, e^{tL_H} p). \quad (36)$$

The right-hand side of (35) has to be seen as particular cases for the choices of the functions  $f = H$ ,  $g(q, p) = q$  and  $g(q, p) = p$ . In short, we can write it as a change of coordinates from  $(q_0, p_0)$  to  $(q(t), p(t))$  given by a symplectic transformation

$$(q(t), p(t)) = (e^{tL_H(q_0, p_0)} q_0, e^{tL_H(q_0, p_0)} p_0).$$

- Given  $f(q, p)$ ,  $g(q, p)$  then

$$e^{L_H} L_H e^{-L_H} = L_{\bar{g}}, \quad e^{L_H} e^{L_H} e^{-L_H} = e^{L_{\bar{g}}}, \quad (37)$$

where  $\bar{g} = e^{L_H} g$ . In particular, we will make use of the following property:

$$e^{c_i h L_{H_0}} e^{b_i h L_{\varepsilon V(q)}} e^{-c_i h L_{H_0}} = e^{b_i h L_{\varepsilon V(\bar{q})}}, \quad (38)$$

where  $\bar{q} = \alpha_i q + \beta_i p$  and  $\alpha_i = \phi_0(c_i v)$ ,  $\beta_i = c_i h \phi_1(c_i v)$ .

- If we denote by  $\Phi_h^{f_i}(q, p) \equiv e^{hL_{f_i}(q, p)}$ ,  $i = 1, 2$  then

$$e^{hL_{f_1}} e^{hL_{f_2}}(q, p) = e^{hL_{f_1}} \Phi_h^{f_2}(q, p) = \Phi_h^{f_2}(e^{hL_{f_1}} q, e^{hL_{f_1}} p) \\ = \Phi_h^{f_2} \circ \Phi_h^{f_1}(q, p)$$

i.e. the order in which the maps act is the reverse to the order on which the Lie transforms are written.

- The  $h$ -flow associated to the Hamiltonian  $H = \varepsilon V(\alpha q + \beta p)$  is

$$(q_1, p_1) = e^{h\varepsilon L_V(\bar{q})}(q_0, p_0) \\ = (q_0 - h\varepsilon\beta f(\bar{q}), p_0 + h\varepsilon\alpha f(\bar{q})) \quad (39)$$

with  $\bar{q} = \alpha q_0 + \beta p_0$  (where  $f = -\nabla V$ ).

- The composition of the  $(hb_i)$ -flows associated to the Hamiltonians,  $V_i = V(\alpha_i q_0 + \beta_i p_0)$ ,  $i = 1, 2$ , is

$$\bar{q} = e^{hb_1 \varepsilon L_{V_1}} e^{hb_2 \varepsilon L_{V_2}} q_0 \\ = e^{\varepsilon hb_1 L_{V_1}} (q_0 - \varepsilon hb_2 \beta_2 f(\alpha_2 q_0 + \beta_2 p_0)) \\ = q_0 - \varepsilon hb_1 \beta_1 f(\alpha_1 q_0 + \beta_1 p_0) - \varepsilon hb_2 \beta_2 f(\hat{Q})$$

where

$$\hat{Q} = \alpha_2 e^{\varepsilon hb_1 L_{V_1}} q_0 + \beta_2 e^{\varepsilon hb_1 L_{V_1}} p_0 \\ = \alpha_2 (q_0 - \varepsilon hb_1 \beta_1 f(\alpha_1 q_0 + \beta_1 p_0)) \\ + \beta_2 (p_0 + \varepsilon hb_1 \alpha_1 f(\alpha_1 q_0 + \beta_1 p_0)) \\ = \alpha_2 q_0 + \beta_2 p_0 + \varepsilon hb_1 (-\alpha_2 \beta_1 + \beta_2 \alpha_1) \\ \times f(\alpha_1 q_0 + \beta_1 p_0)$$

and similarly we have

$$\bar{p} = e^{hb_1 \varepsilon L_{V_1}} e^{hb_2 \varepsilon L_{V_2}} p_0 \\ = e^{\varepsilon hb_1 L_{V_1}} (p_0 + \varepsilon hb_2 \beta_2 f(\alpha_2 q_0 + \beta_2 p_0)) \\ = p_0 + \varepsilon hb_1 \beta_1 f(\alpha_1 q_0 + \beta_1 p_0) + \varepsilon hb_2 \beta_2 f(\hat{Q}).$$

If  $\alpha_i = \phi_0(c_i v)$ ,  $\beta_i = h c_i \phi_1(c_i v)$ ,  $i = 1, 2$  then we have that

$$-\alpha_2 \beta_1 + \beta_2 \alpha_1 = h(c_2 - c_1) \phi_1((c_2 - c_1)v),$$

and  $\bar{q}, \bar{p}$  can be computed as follows:

$$Q_1 = \phi_0(c_1 v) q_0 + h c_1 \phi_1(c_1 v) p_0 \\ Q_2 = \phi_0(c_2 v) q_0 + h c_2 \phi_1(c_2 v) p_0 \\ + \varepsilon h b_1 (c_2 - c_1) \phi_1((c_2 - c_1)v) f(Q_1) \quad (40)$$

$$\bar{q} = q_0 - \varepsilon h^2 (b_1 c_1 \phi_1(c_1 v) f(Q_1) + b_2 c_2 \phi_1(c_2 v) f(Q_2))$$

$$\bar{p} = p_0 + \varepsilon h (b_1 \phi_0(c_1 v) f(Q_1) + b_2 \phi_0(c_2 v) f(Q_2)).$$

It is easy to extend this result to the composition of  $s$  maps as follows:

$$Q_1 = \alpha_1 q_0 + \beta_1 p_0 \\ Q_2 = \alpha_2 q_0 + \beta_2 p_0 + h \varepsilon (\bar{a}_{21} f(Q_1)) \\ \vdots \\ Q_s = \alpha_s q_0 + \beta_s p_0 + h \varepsilon (\bar{a}_{s1} f(Q_1) + \dots \\ + \bar{a}_{s,s-1} f(Q_{s-1})) \quad (41)$$

$$\bar{q} = q_0 - h \varepsilon (\delta_1 f(Q_1) + \dots + \delta_s f(Q_s))$$

$$\bar{p} = p_0 + h \varepsilon (\gamma_1 f(Q_1) + \dots + \gamma_s f(Q_s))$$

and  $\bar{a}_{ij}$ ,  $\delta_i$ ,  $\gamma_i$  (that must satisfy the symplectic conditions since by construction the scheme is symplectic) can be easily obtained from  $\alpha_i$ ,  $\beta_i$ ,  $b_i$ .

We are now ready to present the proof. Let us write the splitting method (7) in terms of a product of Lie transforms taking into account they appear in the reverse order to the composition of maps  $e^{h a_1 L_{H_0}} e^{h b_1 \varepsilon L_V} \dots e^{h a_s L_{H_0}} e^{h b_s \varepsilon L_V} e^{h a_{s+1} L_{H_0}}$ .

Let us include the identity map,  $e^{-h c_i L_{H_0}} e^{h c_i L_{H_0}}$ , after each Lie transform,  $e^{h b_i \varepsilon L_V}$ , so we have (notice that from (34)  $a_1 = c_1$ ,  $a_j = c_j - c_{j-1}$ ,  $j = 2, \dots, s$ )

$$(e^{h c_1 L_{H_0}} e^{h b_1 \varepsilon L_V} e^{-h c_1 L_{H_0}}) \dots (e^{h c_s L_{H_0}} e^{h b_s \varepsilon L_V} e^{-h c_s L_{H_0}}) e^{h L_{H_0}}$$

where  $c_{s+1} = \sum_{j=1}^{s+1} a_j = 1$ , and using the properties of Lie transforms (36)–(38) we have

$$\left( \prod_{i=1}^s \exp(h b_i \varepsilon L_V(\alpha_i q_0 + \beta_i p_0)) \right) \exp(h L_{H_0}),$$

where  $\alpha_i = \phi_0(c_i v)$ ,  $\beta_i = c_i h \phi_1(c_i v)$ . Let us write the map in a column vector form to easily see the vector components

$$\begin{pmatrix} q_1 \\ p_1 \end{pmatrix} = \left( \prod_{i=1}^s e^{h b_i \varepsilon L_V(\alpha_i q_0 + \beta_i p_0)} \right) e^{h L_{H_0}} \begin{pmatrix} q_0 \\ p_0 \end{pmatrix} \\ = \left( \prod_{i=1}^s e^{h b_i \varepsilon L_V(\alpha_i q_0 + \beta_i p_0)} \right) \begin{pmatrix} \phi_0(v) q_0 + h \phi_1(v) p_0 \\ -h \Omega^2 \phi_1(v) q_0 + \phi_0(v) p_0 \end{pmatrix} \\ = \begin{pmatrix} \phi_0(v) \bar{q} + h \phi_1(v) \bar{p} \\ -h \Omega^2 \phi_1(v) \bar{q} + \phi_0(v) \bar{p} \end{pmatrix} \quad (42)$$

and where  $\bar{q}, \bar{p}$  are given by (41) which obviously corresponds to the scheme (9)–(11) for appropriate choices of the parameters in the splitting method.

The symplectic conditions make the coefficients of the explicit and symplectic ERKN methods to uniquely depend on the  $s$  coefficients  $b_i$  (or another set of  $s$  independent coefficients) which are uniquely determined from the  $s$  independent coefficients  $b_i$  from the splitting composition and the result is proven in both ways. ■

Some advantages of splitting methods is that their performance can be easily improved using modified potentials (force-gradient methods) or using the processing technique as well as can be generalized to be used to solve problems with time-dependent frequencies. On the other hand, this constructive proof allows us to build new ERKN methods. In particular we present some new ERKN methods for perturbed oscillators with time-dependent frequencies which have some advantages versus similar splitting methods.

## 5. Methods for time-dependent frequencies

This constructive proof allows us to build new explicit and symplectic ERKN methods for the non-autonomous case (1). These methods are obtained from a splitting method following a similar procedure to the previous proof, but in an extended phase space. However, the final methods will not be equivalent to standard splitting methods so, they correspond to new methods, and the performance of the splitting and ERKN methods can differ depending on the problem.

Let us now consider the non-autonomous problem (1) or, equivalently,

$$\begin{aligned} \frac{d}{dt} \begin{pmatrix} q \\ p \end{pmatrix} &= \begin{pmatrix} 0 & 1 \\ -\Omega^2(t) & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix} + \varepsilon \begin{pmatrix} 0 \\ f(t, q) \end{pmatrix} \\ &= A(t, q, p) + \varepsilon B(t, q). \end{aligned} \quad (43)$$

Next, we take the time as a new variable,  $t = q_t$ , and the system is split as follows [29,32], so we have the equivalent system

$$\begin{aligned} \frac{d}{dt} \begin{pmatrix} q \\ p \\ q_t \end{pmatrix} &= \begin{pmatrix} 0 & 1 & 0 \\ -\Omega^2(q_t) & 0 & 0 \\ 0 & 0 & 1/q_t \end{pmatrix} \begin{pmatrix} q \\ p \\ q_t \end{pmatrix} + \varepsilon \begin{pmatrix} 0 \\ f(q_t, q) \\ 0 \end{pmatrix} \\ &= A(q_t, q, p) + \varepsilon B(q_t, q). \end{aligned} \quad (44)$$

To solve the evolution for the autonomous (non-linear) system  $A(q_t, q, p)$  along a time interval,  $t \in [t_\alpha, t_\beta]$ , is equivalent to solve the non-autonomous linear system

$$\frac{d}{dt} \begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\Omega^2(t) & 0 \end{pmatrix} \begin{pmatrix} q \\ p \end{pmatrix}, \quad (45)$$

for the same time interval, and we denote by  $\Phi^A(t_\beta, t_\alpha)$  the corresponding exact map.<sup>3</sup> The evolution for  $B(q_t, q)$  is trivial since  $q_t$  and  $q$  are frozen ( $q_t$  is frozen at the last instant reached by the map  $\Phi^A(t_\beta, t_\alpha)$ ). For example, the ABA composition (25) of generalized order (2, 2) has the following associated method for the non-autonomous case which retains the same generalized order (2, 2) for the time interval  $t \in [t_n, t_n + h]$

$$\begin{aligned} \Phi_h^{(2,2)} &= \Phi^A(t_n + h, t_n + h/2) \circ \Phi_{b_1h}^B(t_n + h/2) \\ &\quad \circ \Phi^A(t_n + h/2, t_n) \end{aligned} \quad (46)$$

where  $\Phi_{b_1h}^B(t_n + h/2)$  denotes the map in which the time is frozen at  $t = t_n + h/2$ .

If we denote

$$\Phi^A(t_\beta, t_\alpha) = \begin{pmatrix} A(t_\beta, t_\alpha) & B(t_\beta, t_\alpha) \\ -C(t_\beta, t_\alpha) & D(t_\beta, t_\alpha) \end{pmatrix}, \quad (47)$$

the method (46) corresponds to the following scheme (for simplicity we take  $t_n = 0$ ):

$$\begin{aligned} Q_1 &= A(h/2, 0)q_0 + B(h/2, 0)p_0 \\ P_1 &= -C(h/2, 0)q_0 + D(h/2, 0)p_0 \\ P_2 &= P_1 + \varepsilon b_1 h f(h/2, Q_1) \\ q_1 &= A(h, h/2)Q_1 + B(h, h/2)P_2 \\ p_1 &= -C(h, h/2)Q_1 + D(h, h/2)P_2. \end{aligned} \quad (48)$$

Taking into account the property

$$\Phi^A(h, h/2) \circ \Phi^A(h/2, 0) = \Phi^A(h, 0), \quad (49)$$

i.e.

$$\begin{aligned} &\begin{pmatrix} A(h, h/2) & B(h, h/2) \\ -C(h, h/2) & D(h, h/2) \end{pmatrix} \begin{pmatrix} A(h/2, 0) & B(h/2, 0) \\ -C(h/2, 0) & D(h/2, 0) \end{pmatrix} \\ &= \begin{pmatrix} A(h, 0) & B(h, 0) \\ -C(h, 0) & D(h, 0) \end{pmatrix} \end{aligned}$$

we can write (46) as follows:

$$\begin{aligned} \Phi_h^{(2,2)} &= \Phi^A(h, 0) \circ (\Phi^A(h/2, 0))^{-1} \circ \Phi_{b_1h}^B(h/2) \\ &\quad \circ \Phi^A(h/2, 0) \end{aligned} \quad (50)$$

which, after few operations, corresponds to the following ERKN method:

$$\begin{aligned} Q_1 &= A(h/2, 0)q_0 + B(h/2, 0)p_0, \\ q_1 &= A(h, 0)q_0 + B(h, 0)p_0 + \varepsilon h b_1 B(h, h/2)f(h/2, Q_1), \\ p_1 &= -C(h, 0)q_0 + D(h, 0)p_0 + \varepsilon h b_1 D(h, h/2)f(h/2, Q_1). \end{aligned} \quad (51)$$

Obviously, the maps  $\Phi^A$  cannot be written in a closed form and they have to be replaced by numerical schemes. Notice that property (49) is no longer satisfied by the numerical schemes. If we denote by  $\Phi_{s_0}^A$  a numerical method of order  $s_0$  then

$$\Phi_{s_0}^A(h, h/2) \circ \Phi_{s_0}^A(h/2, 0) \neq \Phi_{s_0}^A(h, 0). \quad (52)$$

If we replace  $\Phi^A$  by  $\Phi_{s_0}^A$ , then the method obtained has generalized order  $(s_0; 2, 2)$  according to (8). The ERKN and splitting methods are no longer equivalent because the scheme (48) uses  $\Phi_{s_0}^A(h/2, 0)$  and  $\Phi_{s_0}^A(h, h/2)$  while the scheme (51) uses in addition  $\Phi_{s_0}^A(h, 0)$ . The computational cost can differ as well as the magnitude of the dominant error terms. On the other hand, the evaluations used to compute  $\Phi_{s_0}^A(h/2, 0)$  and  $\Phi_{s_0}^A(h, h/2)$  can be reused to approximate  $\Phi^A(h, 0)$  at a higher order in  $h$  or at higher accuracy and can improve the performance of the scheme at no significant extra cost.

For example, suppose we use a Magnus integrator to approximate a linear time-dependent oscillator given by

$$x' = M(t)x, \quad x(0) = x_0.$$

A method of order  $p$  for the interval  $t \in [0, h]$  is given by  $x(h) \simeq \exp(\Omega^{[p]}(h, 0))x(0)$  where  $\Omega^{[p]}$  is an element of the Lie algebra of  $M_i \equiv M(c_i h)$  evaluated on a quadrature rule (of order  $p$  or higher), i.e. a linear combination of  $M_i$  and nested commutators between them.

For example, a second order method which uses the trapezoidal rule corresponds to

$$\Omega^{[2]}(h, 0) = \frac{h}{2} (M_1 + M_2) = h \begin{pmatrix} 0 & 1 \\ -\bar{\Omega}^2 & 0 \end{pmatrix}$$

<sup>3</sup> Since the exact flow of the non-autonomous problem is, in general, not known, we will ultimately replace their flows by numerical integrators.

where  $c_1 = 0$ ,  $c_2 = 1$ ,  $\bar{\Omega}^2 = \frac{1}{2}(\Omega_1^2 + \Omega_2^2)$  and  $\Omega_i^2 = \Omega^2(c_i h)$ . We can use this second order method as the maps  $\Phi_2^A(h/2, 0)$  and  $\Phi_2^A(h, h/2)$ , i.e.

$$\begin{aligned}\Phi_2^A(h/2, 0) &= e^{\Omega^{[2]}(h/2, 0)} = \exp \frac{h}{2} \begin{pmatrix} 0 & 1 \\ -\bar{\Omega}_1^2 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \phi_0 \left( \frac{1}{2} v_1 \right) & \frac{h}{2} \phi_1 \left( \frac{1}{2} v_1 \right) \\ -\frac{h}{2} \bar{\Omega}_1^2 \phi_1 \left( \frac{1}{2} v_1 \right) & \phi_0 \left( \frac{1}{2} v_1 \right) \end{pmatrix} \\ \Phi_2^A(h, h/2) &= e^{\Omega^{[2]}(h, h/2)} = \exp \frac{h}{2} \begin{pmatrix} 0 & 1 \\ -\bar{\Omega}_2^2 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \phi_0 \left( \frac{1}{2} v_2 \right) & \frac{h}{2} \phi_1 \left( \frac{1}{2} v_2 \right) \\ -\frac{h}{2} \bar{\Omega}_2^2 \phi_1 \left( \frac{1}{2} v_2 \right) & \phi_0 \left( \frac{1}{2} v_2 \right) \end{pmatrix}\end{aligned}$$

where

$$2\bar{\Omega}_1^2 = \Omega^2(0) + \Omega^2\left(\frac{h}{2}\right), \quad 2\bar{\Omega}_2^2 = \Omega^2\left(\frac{h}{2}\right) + \Omega^2(h)$$

being symmetric and positive semidefinite matrices and  $v_i = h\bar{\Omega}_i$ ,  $i = 1, 2$ . This way we obtain a method of generalized order  $(2; 2, 2)$ .

In the algorithm (51) we can replace  $\Phi^A(h, 0)$  by  $\Phi_2^A(h, 0) := \Phi_2^A(h, h/2) \circ \Phi_2^A(h/2, 0)$  which is also a second order method. However, when computing  $\Phi_2^A(h/2, 0)$  and  $\Phi_2^A(h, h/2)$  we have used enough evaluations of  $\Omega^2(t)$  to obtain a fourth-order Magnus integrator. A fourth-order method using Newton–Côte quadrature ( $c_1 = 0$ ,  $c_2 = 1/2$ ,  $c_3 = 1$ ) for the interval  $t \in [0, h]$  is given by

$$\begin{aligned}\Omega^{[4]}(h, 0) &= \frac{h}{6} (M_1 + 4M_2 + M_3) + \frac{h^2}{12} (M_3M_1 - M_1M_3) \\ &= h \begin{pmatrix} \alpha & 1 \\ -\beta & -\alpha \end{pmatrix}\end{aligned}$$

where  $M_k = M(kh)$  and  $\alpha = \frac{h}{12}(\Omega_3^2 - \Omega_1^2)$ ,  $\beta = \frac{h}{6}(\Omega_1^2 + 4\Omega_2^2 + \Omega_3^2)$ . Even more accurate results can be obtained with the same evaluations of  $\Omega^2(t)$  if we consider the two exponential fourth-order commutator-free Magnus integrator for this quadrature rule [36] given by

$$\begin{aligned}\Phi_4^A(h, 0) &= \exp \frac{h}{2} \begin{pmatrix} 0 & 1 \\ -\frac{1}{6}(-\Omega_1^2 + 4\Omega_2^2 + 3\Omega_3^2) & 0 \end{pmatrix} \\ &\quad \times \exp \frac{h}{2} \begin{pmatrix} 0 & 1 \\ -\frac{1}{6}(3\Omega_1^2 + 4\Omega_2^2 - \Omega_3^2) & 0 \end{pmatrix}.\end{aligned}\quad (53)$$

Since the maps  $\Phi_2^A(h/2, 0)$  and  $\Phi_2^A(h, h/2)$  in the algorithm are multiplied by a factor  $h\varepsilon$ , this new scheme would be of generalized order  $(4; 2, 2)$ . This new method could provide more accurate results in spite of the symmetry of the whole method is broken.

The splitting method (48) corresponds to the following scheme:

$$\begin{aligned}Q_1 &= \phi_0 \left( \frac{1}{2} v_1 \right) q_0 + \frac{h}{2} \phi_1 \left( \frac{1}{2} v_1 \right) p_0 \\ P_1 &= -\frac{h}{2} \bar{\Omega}_1^2 \phi_1(v_1) q_0 + \phi_0 \left( \frac{1}{2} v_1 \right) p_0 \\ P_2 &= P_1 + \varepsilon b_1 h f(h/2, Q_1) \\ q_1 &= \phi_0 \left( \frac{1}{2} v_2 \right) Q_1 + \frac{h}{2} \phi_1 \left( \frac{1}{2} v_2 \right) P_2 \\ p_1 &= -\frac{h}{2} \bar{\Omega}_2^2 \phi_1 \left( \frac{1}{2} v_2 \right) Q_1 + \phi_0 \left( \frac{1}{2} v_2 \right) P_2\end{aligned}\quad (54)$$

while the ERKN method is given by

$$\begin{aligned}Q_1 &= \phi_0 \left( \frac{1}{2} v_1 \right) q_0 + \frac{h}{2} \phi_1 \left( \frac{1}{2} v_1 \right) p_0 \\ q_1 &= A(h, 0) q_0 + B(h, 0) p_0 + \varepsilon \frac{h^2}{2} \phi_1 \left( \frac{1}{2} v_2 \right) f(h/2, Q_1) \\ p_1 &= -C(h, 0) q_0 + D(h, 0) p_0 + \varepsilon h \phi_0 \left( \frac{1}{2} v_2 \right) f(h/2, Q_1),\end{aligned}\quad (55)$$

where for  $A(h, 0)$ ,  $B(h, 0)$ ,  $C(h, 0)$ ,  $D(h, 0)$  we propose to take the commutator-free method (53), i.e.

$$\begin{pmatrix} A(h, 0) & B(h, 0) \\ -C(h, 0) & D(h, 0) \end{pmatrix} = \Phi_4^A(h, 0)$$

which is a method of generalized order  $(4; 2, 2)$  without new evaluations of  $\Omega^2(t)$ .

**High order ERKN methods.** Given the  $s$ -stage splitting method (24) its generalization to the non-autonomous case is

$$\begin{aligned}Q_0 &= q_0, \quad P_0 = q_0 \\ \text{for } i &= 1 : s + 1 \\ Q_i &= A_{s_0}(c_i h, c_{i-1} h) Q_{i-1} + B_{s_0}(c_i h, c_{i-1} h) P_{i-1} \\ \bar{P}_i &= -C_{s_0}(c_i h, c_{i-1} h) Q_{i-1} + D_{s_0}(c_i h, c_{i-1} h) P_{i-1} \\ P_i &= \bar{P}_i + \varepsilon b_i h f(c_i h Q_i)\end{aligned}\quad (56)$$

**end**

$$q_1 = Q_{s+1}, \quad p_1 = P_{s+1}$$

which requires the numerical integrators  $\Phi_{s_0}^A(c_i h, c_{i-1} h)$ ,  $i = 1, \dots, s$ , while the generalization to the non-autonomous case for the explicit symplectic ERKN methods is given by the scheme

$$\begin{aligned}Q_i &= A_{s_0}(c_i h, 0) q_0 + B_{s_0}(c_i h, 0) p_0 \\ &\quad + \varepsilon h^2 \sum_{j=1}^s a_{ij} f(c_j h, Q_j), \quad i = 1, \dots, s \\ q_1 &= A_{s_0}(h, 0) q_0 + B_{s_0}(h, 0) p_0 + \varepsilon h^2 \sum_{i=1}^s \bar{b}_i f(c_i h, Q_i), \\ p_1 &= -C_{s_0}(h, 0) Q_0 + D_{s_0}(h, 0) p_0 + \varepsilon h \sum_{i=1}^s b_i f(c_i h, Q_i),\end{aligned}\quad (57)$$

which requires in addition to consider numerical integrators to approximate the maps  $\Phi^A(c_i h, 0)$ ,  $i = 1, \dots, s + 1$ .

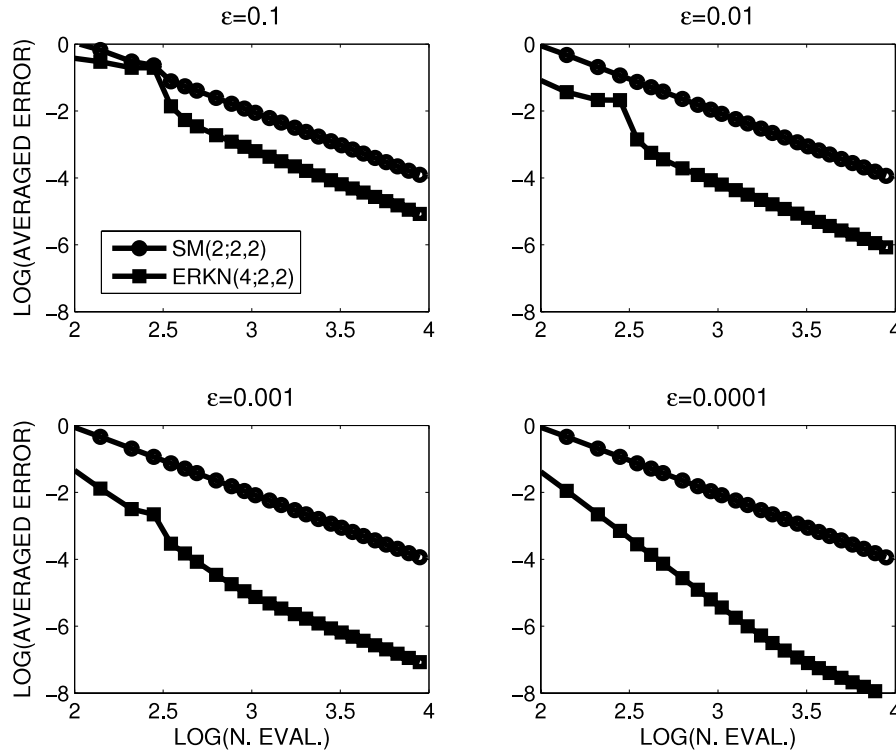
The proof is similar to the autonomous case if we consider the extended Hamiltonian taking the time as a new coordinate,  $q_t = t$ , its associated momenta,  $p_t = -H$ , and the split

$$\begin{aligned}H(q_t, q, p_t, p) &= \left( \frac{1}{2} p^T p + \frac{1}{2} q^T \Omega(q_t) q + p_t \right) + \varepsilon V(q_t, q) \\ &= H_0(q_t, q, p_t, p) + \varepsilon V(q_t, q).\end{aligned}$$

It is important to remark that, contrarily to the autonomous case, the ERKN and splitting schemes are no longer equivalent when numerical methods are used to approximate the flow associated to the non-autonomous linear part.

## 6. Numerical example

We consider a simple numerical example to illustrate that the new explicit symplectic ERKN methods that we have obtained show the expected order of accuracy. We compare the splitting method (54) of generalized order  $(2; 2, 2)$  with the ERKN method (55) of generalized order  $(4; 2, 2)$ .



**Fig. 1.** Averaged error along the time integration versus the number of force evaluations for the schemes (54) with  $b_1 = 1$  (SM(2; 2, 2)) and (55) where the fourth-order CF Magnus integrator is used for  $\Phi_4^A(h, 0)$  (ERKN(4; 2, 2)).

**Example.** Let us consider the Hamiltonian

$$H(q, p, t) = \frac{1}{2}p^2 + \frac{1}{2}f(t)q^2 + \varepsilon \sum_{j=1}^k \cos(q - \omega_j t) \quad (58)$$

where  $q, p \in \mathbb{R}$ , which describes the motion of a charged particle in a magnetic field perturbed by  $k$  electrostatic plane waves, each with the same wavenumber and amplitude, but with different temporal frequencies  $\omega_j$ . We set  $f(t) = 1 + g(t)$  (the case  $g = 0$  is analyzed in [37]). We take  $f(t) = 1 + \frac{1}{2} \cos(\frac{3}{2}t)$ , for the choices  $\varepsilon = 10^{-i}$ ,  $i = 1, 2, 3, 4$ . We take the remaining parameters and initial conditions as given in [37]:  $q_0 = 0$ ,  $p_0 = 11.2075$ ,  $\omega_j = j\omega_0$ ,  $\omega_0 = 7$ ,  $k = 3$ . We integrate the system along the interval  $t \in [0, 20\pi]$  and measure the exact solution numerically (using an accurate numerical method and taking a sufficiently small time step) at the following instants:  $t_n = n \frac{2\pi}{7}$ ,  $n = 1, 2, \dots, 70$ . In order to analyze the performance of the numerical methods, we choose a time step given by  $h_m = \frac{2\pi}{7m}$ , with  $m \in \mathbb{N}$ , and we compare the obtained approximation with the exact solution to compute the averaged two-norm error. Fig. 1 shows the results obtained where we clearly observe the benefit from the use of a high order method to compute the flow for the non-autonomous oscillator. The generalized order (4; 2, 2) is clearly manifest: the slope of the curves behaves as second order for  $h \rightarrow 0$ , as third order when  $\varepsilon = \mathcal{O}(h)$  and as fourth-order for  $\varepsilon \rightarrow 0$ . It is important to remark that this higher accuracy is reached at essentially no extra cost.

On the other hand, the techniques used to build splitting methods provide us with simpler tools to obtain methods at very high generalized order [15] and to incorporate force-gradient and the processing technique on non-autonomous equations (see [32] and references therein) being an interesting subject to be considered in the future.

## 7. Conclusions

We have considered the numerical integration of perturbed non-autonomous oscillatory systems using tailored explicit and symplectic Runge–Kutta–Nyström methods. In particular we have considered the following explicit and symplectic RKN methods: extended RKN methods, exponentially fitting RKN methods and splitting RKN methods for perturbed systems. It is known that explicit and symplectic extended and exponentially fitting RKN methods are equivalent and we have shown that these methods are also equivalent to splitting methods for perturbed oscillators. We have provided a constructive proof making use of basic properties for the Lie algebraic structure of the underlined Hamiltonian system. This constructive proof allowed us to build for the first time new explicit and symplectic extended RKN methods for the non-autonomous problem (for multidimensional time dependent frequencies). Several low order methods are explicitly obtained and it has been indicated how higher order methods can be obtained. The new methods, while obtained from splitting methods, are different and show to be superior in some cases. An efficient numerical integrator for the linear non-autonomous oscillator allows to improve the performance of the methods considerably, and this has been illustrated on some numerical examples. Finally, since splitting methods for perturbed systems have been successfully used for the numerical integration of problems in celestial mechanics, quantum mechanics and parabolic PDEs, this equivalence between these classes of methods showed that ERKN and EFRKN methods can also be used for numerically solving these more general problems, and it would be of great interest to study their performance on more general problems.

## Acknowledgment

The author acknowledges the Ministerio de Economía y Competitividad (Spain) for financial support through the coordinated project MTM2013-46553-C3-3-P.



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