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Fer's factorization as a symplectic integrator

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Summary. In this paper we analyze the main features of the so-called Fer expansion as a new method for integrating the ordinary differential equations derived from explicitly time-dependent Hamiltonian dynamical systems. This method is based on a factorization of the evolution operator as an infinite product of exponentials of Lie operators and thus exactly preserves the Poincaré integral invariants. Third and fourth-order expansions are considered and numerical results are presented for a quadratic Hamiltonian with various time-dependent frequencies. Comparison is done with other numerical integration schemes.

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1. Introduction

A number of techniques have been devised over the years for obtaining approximate solutions to the ordinary differential equations (ODE) corresponding to Hamiltonian dynamical systems. In particular, numerical integration methods for the solution of the initial-value problem have achieved high accuracy and efficiency. However, standard integration schemes – including the explicit Runge-Kutta class of algorithms – do not take into account important special features of the dynamics, such as the symplectic nature of the temporal evolution, which places severe restrictions on the global behaviour of the geometry of the dynamics.

Let us consider, for example, a Hamiltonian system with N degrees of freedom and a configuration manifold $\mathcal{Q}$. It is well known that on the cotangent

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bundle $T^*\mathcal{Q}$ (the phase space), with canonically conjugate coordinates $\boldsymbol{\xi} = (\xi_1, \ldots, \xi_{2N}) = (q_1, \ldots, q_N, p_1, \ldots, p_N)$, there exists a closed, non-degenerate, differential two-form

$$\omega^2 = \sum_{i=1}^{N} dp_i \wedge dq_i \tag{1}$$

such that $(T^*\mathcal{Q}, \omega^2)$ is a symplectic manifold [2]. The forms $\omega^2, (\omega^2)^2, \ldots, (\omega^2)^N$ are referred to as the Poincaré integral invariants and are preserved under the time evolution. When integrated over an arbitrary region of dimension $2k (1 \leq k \leq N)$, the $2k$-form ω^{2k} produces the invariant quantity

$$\int \ldots \int \sum_{i_1 < \ldots < i_k} dp_{i_1} \wedge \ldots \wedge dp_{i_k} \wedge dq_{i_1} \wedge \ldots \wedge dq_{i_k} \tag{2}$$

which is proportional to the sum of the oriented volumes of projections onto the coordinate spaces $(p_{i_1}, \ldots, p_{i_k}, q_{i_1}, \ldots, q_{i_k})$, where $1 \leq i_m \leq N$. In particular when $k = N$ we have Liouville's theorem on preservation of phase-space volume along the evolution. Generally, a transformation φ on the phase space preserving these symplectic invariants is called canonical or symplectic and its Jacobian matrix $\varphi'(\boldsymbol{\xi})$ has to satisfy [2]

$$\varphi'^{\mathrm{T}}(\boldsymbol{\xi}) J \varphi'(\boldsymbol{\xi}) = J \ , \tag{3}$$

where J is the matrix

$$J = \begin{pmatrix} 0 & I_N \\ -I_N & 0 \end{pmatrix} \tag{4}$$

with I_N the identity N-dimensional matrix.

Standard numerical integration techniques do not preserve symplectic invariants and thus they prove useful only in the investigation of short-time quantitative phenomena whereas long-time predictions about phase-space structures generally are more problematic [10].

Nevertheless, it is possible to devise numerical integration algorithms that approximate the time evolution transformation of the exact dynamics to any desired order in the time step and that are exactly symplectic [31, 16]. These are called symplectic integration algorithms (SIAs) and an increasing number of them have been constructed and used in the last years in many different contexts, such as Celestial Mechanics [37, 24, 19], hydrodynamics [10, 30] or Hamiltonian partial differential equations [27], just to quote a few examples. Their efficiency is compared with the standard fourth-order Runge-Kutta algorithm in the references [10, 5, 19, 28]. In particular, for autonomous Hamiltonian systems it has been shown that there is no secular change in the error of the total energy (which should be conserved exactly in the original flow) caused by the local truncation error. If the integrator is not symplectic, the error of the total energy grows secularly in general. The reason for this behaviour is that SIAs give the exact evolution of a

Hamiltonian system with a Hamiltonian function that is close to the Hamiltonian of interest to any desired order [10, 39]. This perturbed Hamiltonian can be explicitly constructed for symplectic Runge-Kutta, partitioned Runge-Kutta and Runge-Kutta-Nyström methods [20].

The research on symplectic integrators has proceeded along three different lines. The first one, ellaborated by Feng [14], makes use of generating functions to construct canonical transformations appropriate to carry out each integration step. This implicit SIA was later applied by Channell and Scovel [10]. The second way is related to the general class of Runge-Kutta methods. A subclass of s-stage implicit Runge-Kutta methods can be made symplectic with an appropriate election of the constants [32, 33]. As a result, the family of Gauss-Legendre Runge-Kutta methods are shown to be symplectic. The same is true for the family of Runge-Kutta-Nyström methods [4, 21] and for partitioned Runge-Kutta methods [21], which are especially suitable for separable Hamiltonian because then it is possible to obtain explicit symplectic integrators.

The third general scheme is to expand directly the evolution map as a product of explicitly computable time-dependent canonical transformations based on Lie algebraic techniques. This type of approach has been used by Yoshida [38] and Forest [17] for obtaining higher order explicit symplectic integrators in a simple way.

Symplectic integrators have a remarkable capacity for describing adequately the qualitative features of Hamiltonian systems, such as invariant sets and structures in phase space, even if the orbit is not followed with pointwise accuracy. Nevertheless, it is also possible to construct symplectic integrators with small truncation errors that are more efficient than conventional methods, even if one wants to compute an accurate numerical approximation to $\boldsymbol{\xi}(T)$ for a fixed final time T. An example of such a method can be found in the reference [4], where a explicit symplectic Runge-Kutta-Nyström method is constructed with a better performance than some standard variable-step codes.

In this paper we present the so-called classical Fer expansion [15, 7] as a possible explicit symplectic integrator for time-dependent Hamiltonian systems. When we apply this iterative procedure to an arbitrary Hamiltonian, we obtain a factorization of the time-evolution map as a product of exponentials of Lie operators. These kind of expansions have the advantage that the approximating systems are also Hamiltonian. A peculiarity of the Fer factorization is that each argument of the exponentials contains an infinity of orders in the expansion parameter, which could greatly favour its rate of convergence. Indeed, we will show that, at least for quadratic Hamiltonians, very few iterations are sufficient to achieve accurate results both for the orbits and conserved quantities. The analysis is performed by means of Lie transformations techniques [22, 11].

The paper is organized as follows: in Sect. 2 we review the necessary Lie algebraic tools and derive Fer's expansion for Hamiltonian systems. In Sect. 3 we apply the method to an one-dimensional quadratic Hamiltonian with various time-dependent frequencies and obtain analytic expressions for the successive approximants and the corresponding solutions. In Sect. 4 we present some nu-

merical experiments to show the performance of the method. In particular, we compare the third and fourth order Fer expansion with other numerical integration schemes, including symplectic ones, for some physically important examples, such as the Mathieu equation. Finally, Sect. 5 contains the conclusions.

2. Review of the Fer expansion

Let us consider the set $\mathscr{A}(T^*\mathcal{Q}, t)$ of all analytic real-valued time-dependent functions on the phase space $T^*\mathcal{Q}$. This set has the structure of an infinite-dimensional Lie algebra under the Poisson bracket composition law. Associated with each element $f(\boldsymbol{\xi}, t)$ of $\mathscr{A}(T^*\mathcal{Q}, t)$ there is a Lie operator which acts on general functions $g(\boldsymbol{\xi}, t)$. The Lie operator associated with the function f will be denoted by the L_f and it is defined by the rule

$$L_f g = [f, g] \tag{5}$$

where the square bracket stands for the Poisson bracket of the functions f and g. Note that L_f is nothing but the Lie derivative $-L_{X_f}$, where X_f is the vector field associated with f by means of the two-form ω^2, because [2, 36]

$$L_f g = [f, g] = -L_{X_f} g = \omega^2(X_f, X_g) \, . \tag{6}$$

On a bundle chart the operator L_f has the expression

$$L_f = \sum_{i=1}^{N} \frac{\partial f}{\partial q_i} \frac{\partial}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial}{\partial q_i} = \sum_{i,j=1}^{2N} \frac{\partial f}{\partial \xi_i} J_{ij} \frac{\partial}{\partial \xi_j} \tag{7}$$

where J_{ij} are the elements of the symplectic matrix of the Eq.(4). Thus L_f is a first-order linear partial-differential operator on $\mathscr{A}(T^*\mathcal{Q}, t)$, but it is important to realize that in general $L_f g$ is not a linear function on phase space. The set of Lie operators forms a Lie algebra under the commutator operation $\{L_f, L_g\} = L_f L_g - L_g L_f$. It can be proved that this commutator equals the Lie operator associated with the Poisson bracket of both functions, i.e., $\{L_f, L_g\} = L_{[f,g]}$.

It is possible to deal with power series in L_f. Of particular importance is the power series $\exp(L_f)$, called the Lie transformation associated with f. This is also a linear operator on $\mathscr{A}(T^*\mathcal{Q}, t)$ and its action on any function g is formally defined by

$$\exp(L_f) g = \sum_{n=0}^{\infty} \frac{1}{n!} (L_f)^n g = \sum_{n=0}^{\infty} \frac{1}{n!} \underbrace{[f, [f, \ldots, [f}_{n \text{ times}}, g] \ldots]] \, . \tag{8}$$

In particular, the transformation $\boldsymbol{\xi} \mapsto \boldsymbol{\xi}'$ given by

$$\xi_i'(\boldsymbol{\xi}, t) = \exp(L_f) \xi_i \, , \quad i = 1, \ldots, 2N \tag{9}$$

is symplectic [11].

Let $H(\xi, t)$ be an explicitly time-dependent Hamiltonian. It is well known that the time-evolution associated with H is a local canonical flow that preserves all the Poincaré integral invariants [36]. Let $\xi(\xi_0, t, t_0)$ denote the (in general nonlinear) mapping which gives the dynamic state at time t of a particle which was at ξ_0 at time t_0. We can identify a time-evolution operator $\mathscr{M}(t, t_0)$ with this canonical mapping according to the prescription

$$(\mathscr{M}(t, t_0)g)(\xi_0, t_0) = g(\xi(\xi_0, t, t_0), t) \,, \tag{10}$$

where $g \in \mathscr{A}(T^*\mathscr{Q}, t)$. In words, the action of the operator $\mathscr{M}$ is to evaluate the function g at the mapped point. In particular, we have

$$\mathscr{M}(t, t_0)\xi_i(t_0) = \xi_i(t) \,, \quad i = 1, \ldots, 2N \,. \tag{11}$$

The time derivative of $\mathscr{M}$ is defined in the usual way,

$$\frac{\partial \mathscr{M}}{\partial t} g = \lim_{\tau \to 0} \frac{\mathscr{M}(t + \tau, t_0)g - \mathscr{M}(t, t_0)g}{\tau} \tag{12}$$

and if g has no explicit time dependence, we obtain [6, 13, 16]

$$\frac{\partial}{\partial t}\mathscr{M}(t, t_0) = \mathscr{M}(t, t_0)L_{-H(\xi_0, t)} \,. \tag{13}$$

Solving Eq. (13) with the initial condition $\mathscr{M}(t_0, t_0) = \mathscr{T}$, where $\mathscr{T}$ denotes the identity map in phase space, is obviously equivalent to the resolution of the Hamilton equations of the motion.

When

$$\left[\int_{t_0}^{t} H(\xi_0, t')dt', H(\xi_0, t)\right] = 0$$

then

$$\mathscr{M}(t, t_0) = \exp(L_{A(\xi_0, t)}) \,, \quad A(\xi_0, t) = -\int_{t_0}^{t} H(\xi_0 t')dt' \,, \tag{14}$$

and this is the case if H is time-independent. In classical mechanics one can always drop out an explicit time dependence in the Hamiltonian by increasing the number of degrees of freedom. However this may complicate the algebraic structure of the problem. In particular, if $H(\xi, t)$ is a quadratic form, the dynamics expressed in the resultant $2(N + 1)$-dimensional phase space becomes in general nonlinear.

We can solve perturbatively Eq. (13) by means of the Neumann iterative procedure. Then one finds

$$\mathscr{M}(t, t_0) = \mathscr{T} + \sum_{n=1}^{\infty} \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n L_{-H(t_n)} \ldots L_{-H(t_2)} L_{-H(t_1)}, \tag{15}$$

where $H(t_i) \equiv H(\xi_0, t_i)$. An important drawback of this approach is that when expansion (15) is truncated, the corresponding approximation to the evolution operator does not preserve symplecticity.

Another possible scheme in order to find a formal solution of Eq. (13) is to express $\mathscr{M}$ as an infinite product of Lie transformations. As a first step we suppose that a solution can be written in the form

$$\mathscr{M}(t, t_0) = \mathscr{M}_1(t, t_0) \exp(L_{F_1}) , \tag{16}$$

where $F_1 = A(\xi_0, t)$. The map $\mathscr{M}_1$, is subject to the initial condition $\mathscr{M}_1(t_0, t_0) = \mathscr{T}$ and verifies equation [7]

$$\dot{\mathscr{M}}_1 \equiv \frac{\partial \mathscr{M}_1}{\partial t} = \mathscr{M}_1 L_{-H_1} , \tag{17}$$

with

$$H_1 \equiv H_1(\xi_0, t) = \sum_{k=1}^{\infty} \frac{k}{(k+1)!} (L_{F_1}^k H) . \tag{18}$$

Therefore the problem of determining $\mathscr{M}_1$ has in principle the same difficulties than that of $\mathscr{M}$. However it is worth noting that an expansion of the type (15) for $\mathscr{M}_1$ begins with a double integral, so we can expect that, at least for small values of t, the map $\mathscr{M}_1 - \mathscr{T}$ is closer to zero than $\mathscr{M} - \mathscr{T}$. What is more important, the above procedure for $\mathscr{M}$ can be repeated with $\mathscr{M}_1$ which leads to the following scheme:

$$\mathscr{M} = \mathscr{M}_n \exp(L_{F_n}) \ldots \exp(L_{F_2}) \exp(L_{F_1}) , \tag{19}$$

with $\mathscr{M}_n$ such that

$$\begin{aligned} &\dot{\mathscr{M}}_n = \mathscr{M}_n L_{-H_n} , \quad \mathscr{M}_n(t_0, t_0) = \mathscr{T} , \\ &H_0 \equiv H(\xi_0, t) , \quad H_n \equiv H_n(\xi_0, t) = \sum_{k=1}^{\infty} \frac{k}{(k+1)!} (L_{F_n}^k H_{n-1}) \\ &F_n(\xi, t, t_0) = - \int_{t_0}^{t} H_{n-1}(\xi_0, t') dt' , \quad n \geq 1 , \end{aligned} \tag{20}$$

that is called Fer's expansion for the classical evolution operator $\mathscr{M}$ [7]. In this way we can express the map $\mathscr{M}(t, t_0)$ as an infinite product of Lie transformations whose high order terms presumably are close to the identity $\mathscr{T}$. Now we suppose we replace H by εH, where $\varepsilon > 0$ is a small parameter. Then, as we can see in Eq. (19), F_n $(n \geq 2)$ contains an infinite number of powers of ε beginning with $\varepsilon^{2^{n-1}}$. When our Hamiltonian is of the form $H = H_0 + \varepsilon H_1$ this can always be done with the new Hamiltonian εH_1 in the so-called interaction picture [13].

When the functions involved in Eq. (19) belong to a solvable Lie subalgebra of $\mathscr{A}(T^*Q, t)$ then a finite product of Lie transforms is attained for the evolution map. Otherwise, we must truncate the infinite product of Eq. (19) for $\mathscr{M}$ in the nth term, $n = 1, 2, \ldots$. Obviously, this is accomplished by doing $\mathscr{M}_n = \mathscr{T}$. Thus we obtain an approximate expression for the evolution map in the form

$$\mathscr{M}(t, t_0) \simeq \exp(L_{F_n}) \ldots \exp(L_{F_2}) \exp(L_{F_1}) \tag{21}$$

with $F_i \equiv F_i(\boldsymbol{\xi}_0, t, t_0)$.

There are two comments to be considered concerning Eq. (21): first, this approximation is still symplectic in character and secondly, all the dependence of $\mathscr{M}$ in the parameter ε is included up to order ε^{2^n-1}. Thus, when the product of n Lie transformations of Eq. (21) is applied to the initial condition, we obtain a solution which is correct up to order ε^{2^n-1}, provided the action of the Lie transformations can be exactly evaluated. Such a property is called 'superconvergence' in the context of classical perturbation theory [23].

3. Application to quadratic Hamiltonians

In this section we apply the above deduced Fer expansion to a simple but non-trivial Hamiltonian. We consider a one-degree-of-freedom parametrically driven harmonic oscillator given by

$$H(q,p,t) = \frac{1}{2}[p^2 + \Omega^2(t)q^2] \tag{22}$$

where $\Omega^2(t)$ is a real-analytic function and whose corresponding equation of motion reads

$$\frac{d^2q}{dt^2} + \Omega^2(t)q = 0\ . \tag{23}$$

As it is well known, in general it is not possible to find an exact solution of Eq. (23) for an arbitrary function $\Omega(t)$. We can instead apply Fer's expansion and obtain an approximate solution for the corresponding initial value problem. This will enable us to appreciate the performance of the method by comparing with other analytical and numerical approximate schemes.

In appendix A we derive a recursive procedure for obtaining the functions F_i and their associated Lie operators $L_{F_i}, i \geq 1$, corresponding to the more general one degree of freedom linear Hamiltonian system $H(q,p,t) = A_0(t)p^2 + B_0(t)qp + C_0(t)q^2$. If we suppose that at the initial time t_0 the system is in $\boldsymbol{\xi}(t_0) \equiv (q(t_0), p(t_0)) = (q_0, p_0)$ we have for the Hamiltonian of Eq. (22)

$$\begin{aligned} F_i(q,p;t,t_0) &= -\alpha_i(t,t_0)p^2 - \beta_i(t,t_0)qp - \gamma_i(t,t_0)q^2 \\ L_{F_i} &= -\beta_i(p\partial_p - q\partial_q) - 2\gamma_i q\partial_p + 2\alpha_i p\partial_q \end{aligned}$$

with $i \geq 1$. In particular

$$\alpha_i = \frac{1}{2}(t - t_0)\ , \quad \beta_1 = 0\ , \quad \gamma_1 = \frac{1}{2}\int_{t_0}^{t} \Omega^2(t')dt' \tag{25}$$

and the expressions for $\alpha_i, \beta_i, \gamma_i, (i \geq 2)$, are given in Eq. (54) in terms of quadratures.

Eventually we need to know the action of the Lie transformations $\exp(L_{F_i})$ on the coordinates q, p. For the Hamiltonian (22) this can be exactly evaluated.

Indeed, the subalgebra of $\mathscr{A}(T^*\mathcal{Q}, t)$ involved in this case is $so(2,1)$, which is known to be non-solvable. A straightforward calculation shows that

$$\exp(L_{F_i})q = m_i^+ q + u_i^+ p \ , \quad \exp(L_{F_i})p = m_i^- p - u_i^- q \ , \tag{26}$$

where

$$m_i^\pm \equiv \cosh\eta_i \pm \frac{\beta_i}{\eta_i}\sinh\eta_i \ , \quad u_i^+ \equiv \frac{2\alpha_i}{\eta_i}\sinh\eta_i \ , \quad u_i^- \equiv \frac{2\gamma_i}{\eta_i}\sinh\eta_i \tag{27}$$

for $\eta_i = [\beta_i^2 - 4\alpha_i\gamma_i]^{1/2} \neq 0$. If $\eta_i = 0$ then $m_i^\pm = 1 \pm \beta_i$, $u_i^+ = 2\alpha_i$, $u_i^- = 2\gamma_i$.

From Eqs. (21, 24, 26) we can construct an approximation to the classical evolution operator $\mathscr{M}(t, t_0)$ and therefore an explicit approximate solution of the Eq. (23) to an arbitrary order in terms of quadratures. In particular, the third-order Fer expansion gives the solution in the following way:

$$\begin{aligned} q_{31} &= m_3^+ q_0 + u_3^+ p_0 & p_{31} &= m_3^- p_0 - u_3^- q_0 \\ q_{32} &= m_2^+ q_{31} + u_2^+ p_{31} & p_{32} &= m_2^- p_{31} - u_2^- q_{31} \\ q_3 &= m_1^+ q_{32} + u_1^+ p_{32} & p_3 &= m_1^- p_{32} - u_1^- q_{32} \end{aligned} \tag{28}$$

whereas the fourth-order solution is given by

$$\begin{aligned} q_{41} &= m_4^+ q_0 + u_4^+ p_0 & p_{41} &= m_4^- p_0 - u_4^- q_0 \\ q_{42} &= m_3^+ q_{41} + u_3^+ p_{41} & p_{42} &= m_3^- p_{41} - u_3^- q_{41} \\ q_{43} &= m_2^+ q_{42} + u_2^+ p_{42} & p_{43} &= m_2^- p_{42} - u_2^- q_{42} \\ q_4 &= m_1^+ q_{43} + u_1^+ p_{43} & p_4 &= m_1^- p_{43} - u_1^- q_{43} \end{aligned} \tag{29}$$

The quantities q_0 and p_0 are initial values and q_j, p_j, $j = 3, 4$ constitute the solution at time t. From Eq. (9) it is readily seen that the transformation from q_0, p_0 to q_{ij}, p_{ij} for all i, j is symplectic. Therefore the mappings

$$\begin{aligned} (q_0, p_0) &\mapsto (q_3, p_3) \\ (q_0, p_0) &\mapsto (q_4, p_4) \end{aligned}$$

are canonical.

Thus we obtain an approximate analytical solution $q(t)$, $p(t)$ to Eq. (23) that preserves symplecticity and that is the exact solution for a Hamiltonian system $\tilde{H}$ which is close in some sense to the original Hamiltonian of Eq. (22) [39]. As a matter of fact, it can be shown that the nth-order approximate expression given by Eq. (21) is nothing but the exact evolution map corresponding to the Hamiltonian

$$\tilde{H} = H - \mathrm{e}^{-L_{F_1}}\mathrm{e}^{-L_{F_2}}\ldots\mathrm{e}^{-L_{F_{n-1}}}\left(\sum_{k=1}^{\infty}\frac{(-1)^{k+1}}{(k+1)!}L_{F_n}^k H_{n-1}\right), \quad n > 1 \ , \tag{30}$$

the main properties of which will be the subject of future study [8].

On the other hand, Eqs. (28) and (29) can be seen from a computational point of view as the expressions of an explicit symplectic integrator. In fact, if

we consider q_0, p_0 as the solution in time t then Eqs. (28) and (29) provide the approximate solution in the time $t + h$, where h is the time step. Then we take this solution as the new initial condition and repeat the process. In this way we get a systematic procedure with all the characteristics of a symplectic integration scheme. This approach is expected to give good results because a high-order re-summation of the power series is considered in the expressions (28) and (29).

In the case of quadratic Hamiltonians it is not difficult to obtain an estimate of a quantity r such that with time intervals $(t - t_0) < r$ the factorization of Eq. (19) converges to the exact evolution map $\mathscr{M}(t, t_0)$. This means that $\mathscr{M}_n$ tends to the identity map $\mathscr{I}$ when n goes to infinity for $t \in [t_0, t_0 + r]$ [15]. In particular, for the Hamiltonian (22) this 'radius of convergence' r is given by the following equation

$$\mathrm{e}^{4k_0 r} - 4k_0 r - 1 = \frac{2k_0^2}{\Omega_{\max}^2}\zeta \ , \tag{31}$$

where $k_0 = \max\{\Omega_{\max}^2, 1\}$, $\Omega_{\max}^2$ is the maximum value of $\Omega^2(t)$ and ζ is the non-zero solution of the equation $\mathrm{e}^x = 2x + 1$, that is, $\zeta \sim 1.256431$.

If we denote $K_i(t) \geq 0$ a function with the property that $\|L_{F_{i+1}}\boldsymbol{\xi}\| \leq K_i(t)\|\boldsymbol{\xi}\|$, $i \geq 1$, then an estimate of the rate of convergence of the expansion (19) can be determined through that of the sequence $\{K_1, K_2, \ldots\}$. Indeed, it can be shown that

$$K_{n+1} \leq \frac{1}{4}\left[\mathrm{e}^{4K_n} - 4K_n - 1\right], \quad n \geq 1 \tag{32}$$

if $K_1 < \zeta/4$, so the convergence to zero is rather fast. In particular we can take

$$K_i(t) \equiv \sup\{|\beta_{i+1}(t)|,\ 2|\alpha_{i+1}(t)|,\ 2|\gamma_{i+1}(t)|\} \ . \tag{33}$$

In order to do practical calculations when Fer's factorization is applied as a SIA, we can choose a time step $h < r$. In this way our numerical approximate solution will converge to the exact one for each integration step. Moreover, we can estimate the rate of convergence by computing the numbers $K_i(t + h)$, $i = 1, 2 \ldots$ given by Eq. (33) and therefore an upper bound for the remainder.

Finally, it should be mentioned that the above analysis carried out for the Hamiltonian of Eq. (22) can be applied directly to the problem of integrating symmetric Riccati and Lyapunov matrix differential equations. In this case the positive definite character of the corresponding solutions is preserved [12].

4. Numerical results

In this section we consider the Hamiltonian of Eq. (22) with three particular functions $\Omega(t)$, chosen in order to embrace very different behaviours of the frequency and some cases of physical relevance. Our purpose is to show the performance of the Fer factorization as a symplectic integration algorithm. For

doing it, we will compare the third and fourth order of the expansion (Eqs. (28) and (29), respectively) with other numerical integration schemes. In particular we will consider:

a) the differential equation solver ODEX2 of Hairer and Wanner [21]. This scheme is based on the Gragg-Bulirsch-Stoer extrapolation algorithm [3, 35] and the Stoermer rule. It includes an automatic step size control and order selection;
b) the fourth order symplectic explicit Runge-Kutta-Nyström algorithm (SN4) given by Calvo and Sanz-Serna [4] for a Hamiltonian of the form

$$H(q,p) = T(p) + V(q) \ , \tag{34}$$

where q and p are canonical coordinates and $T(p) = 1/2 p^{\mathrm{T}} p$. This method is especially suitable for second-order Hamiltonian problems, and its performance is better than other explicit SIA;
c) the two-stage implicit Gauss-Legendre Runge-Kutta method (SRK4) given by [30] and [39], which is symplectic [32] and fourth-order accurate.

These two symplectic algorithms are described briefly in Appendix B. It is worth noting that, for the particular Hamiltonian of Eq. (22), SRK4 is also explicit, because analytic expressions for the auxiliary vectors $\mathbf{Y}_i$ of Eq. (61) can be obtained.

We are particularly interested in long time integration intervals, as it is in these conditions that the advantages of a better qualitative behaviour of the numerical scheme are more prominent. For short time intervals, local error considerations become more important in order to determine the performance of a given integration algorithm [4].

All the simulations have been run in a VAXstation 4000-90, the codes have been written in Fortran and the arithmetic is in double precision. In all the examples we have analyzed, a 4-points Gauss-Legendre formula [1] has been employed in order to evaluate numerically the quadratures of the Fer algorithm.

Example 1. As a first application we take

$$\Omega^2(t) = \frac{4a\cos 2t}{1 + a\cos 2t} \ , \tag{35}$$

with $0 < a < 1$. Clearly Ω^2 is a periodic function of t with period π. Equation (23) with Ω^2 given by Eq. (35) belongs to the special class of Hill equations for which an analytical solution can be found. In particular

$$q(t) = \frac{1 + a\cos 2t}{1 + a} \tag{36}$$

is a solution of the Eq. (23) with initial conditions $q_0 = 1$, $p_0 = 0$ at $t_0 = 0$ [9]. This fact can be used to check the pointwise accuracy of the integration methods over the time, as well as the long-term stability of the different numerical procedures, just by comparing the solution given by the approximate schemes with the exact result $q = 1$ at $t = 2n\pi$, $n = 1, 2, \ldots$.

In Fig. 1 we have plotted the quantity $\Delta q = \log_{10} |q_{\rm appr}(t_{\rm f}) - 1|$ for $a = 0.5$ and a final time $t_{\rm f}$ of 2000 periods as a function of the computational effort measured in CPU time (in seconds). Here $q_{\rm appr}(t_{\rm f})$ denotes the value of the coordinate at the time $t_{\rm f}$ obtained by means of the different numerical schemes and therefore Δq can be seen as an estimate of the final error introduced by them.

The points in the figure are obtained by:

a) the extrapolation method (ODEX2) with variable step size in each 2π-interval and tolerances for relative/absolute error test of 10^{-9}, 10^{-10}, 10^{-11}, 10^{-12} (squares joined by a solid line);
b) the implicit SRK4 symplectic integrator with timesteps $2\pi/1000$, $2\pi/1250$, $2\pi/1750$, $2\pi/2000$ (circles joined by a dash-dotted line);
c) the explicit SN4 with timesteps $2\pi/750$, $2\pi/1000$, $2\pi/1250$, $2\pi/1500$ (triangles joined by a dashed line);
d) the third-order Fer expansion (F3) with timesteps $h_1 = 2\pi/15$, $h_2 = 2\pi/25$, $h_3 = 2\pi/27$, $h_4 = 2\pi/30$ (plus signs joined by a square-dotted line). The estimate (31) for the radius of convergence is in this case $r \simeq 0.3412 (> h_i, i = 2, 3, 4)$.

Regarding Fig. 1 some comments are in order. First, SN4 provides a more accurate result than SRK4 with the same computational effort. This illustrates the well known fact that symplectic Runge-Kutta-Nyström methods are more appropriate than symplectic Runge-Kutta methods for the problem at hand. Secondly, the performance of F3 is even better than that of SN4. The reason for this behaviour is that F3 uses a step size about 50 times larger than that needed by SN4 and SRK4 for obtaining a similar accuracy, and this globally compensates the greater number of floating point operations per step required by the Fer procedure. On the other hand, the convergence of the expansion is guaranteed in each integration step, at least for h_2, h_3 and h_4. Finally, the performance of ODEX2 is superior for this example to the other integration algorithms we have tested.

Example 2. Next we consider the frequency given by

$$\Omega^2(t) = 1 + \frac{2\epsilon^2}{\cosh^2 \epsilon t} \ , \tag{37}$$

with $\epsilon > 0$. This example allows us to analyze adiabatic and sudden perturbations according to the value of the parameter ϵ. The solution of Eq. (23) is in this case

$$q(t) = \mathrm{Re}[A(\tanh \epsilon t + \mathrm{i}/\epsilon)\mathrm{e}^{-\mathrm{i}t}] \ , \tag{38}$$

where A is an arbitrary complex constant.

For the time-dependent harmonic oscillator with frequency (37) there is a constant of motion J of the form [25]

$$J(t) = J(t_0) = \frac{1}{2}[\rho^{-2} q^2 + (\rho p - \dot{\rho} q)^2] \ , \tag{39}$$

where ρ is given by [18]

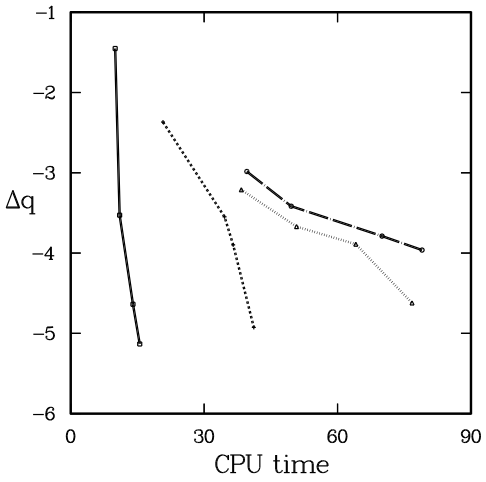

Fig. 1. Value of $\Delta q = \log_{10} |q_{\text{appr}}(t_f) - 1|$ at $t_f = 2000\pi$ vs. the CPU time of calculation (in seconds) for the Example 1 with $a = 0.5$. $q_{\text{appr}}(t)$ is computed by means of: ODEX2 with variable step size (solid line), SRK4 (dash-dotted line), SN4 (dashed line) and F3 (square-dotted line)

$$\rho(t) = \sqrt{\frac{1 + \epsilon^2 \, \tanh^2 \epsilon t}{1 + \epsilon^2}} \ , \tag{40}$$

and is a particular solution of the non-linear equation $\ddot{\rho} + \Omega^2(t)\rho - \rho^{-3} = 0$.

Now we can study the errors that the different integrators generate in the determination of the integral of motion (39). In particular, we choose $q_0 = p_0 = 1$ as initial conditions at the time t_0, then integrate the equations of the motion up to t_f with different symplectic schemes and finally compute the quantity

$$\Delta J \equiv \log_{10} \left| \frac{J(t_f) - J(t_0)}{J(t_0)} \right| \tag{41}$$

for various values of ϵ. We take $t_0 = -t_f = -20/\epsilon$, so that $\Omega(t_0) \simeq 1$ in all cases.

Figure 2 shows the function $\Delta J(\epsilon)$ defined by Eq. (41). Dash-dotted line is obtained by SRK4 with a step size $h = 0.009$, dashed line corresponds to SN4 with $h = 0.0125$ and square-dotted line is determined by means of F3 with $h = 0.3$. With this choice of timestep sizes the computational effort required by the different methods is similar. It has been shown [32] that the Gauss-Legendre Runge-Kutta methods conserve all quadratic first integrals of a given *autonomous* system. As we can see in Fig. 2, this is true for our time-dependent system (excluding round-off errors) only for very small values of the parameter ϵ. For $\epsilon > 0.9$ the error introduced by SRK4 is larger than that generated by SN4, although both of them follow the same pattern. On the other hand, the behaviour of $\Delta J(\epsilon)$ obtained by F3 is highly dependent on the value of ϵ considered. For $\epsilon < 0.05$ the results achieved by F3 and SRK4 are very similar and more accurate than those obtained by SN4. For $0.05 < \epsilon < 2$, the relative error in the

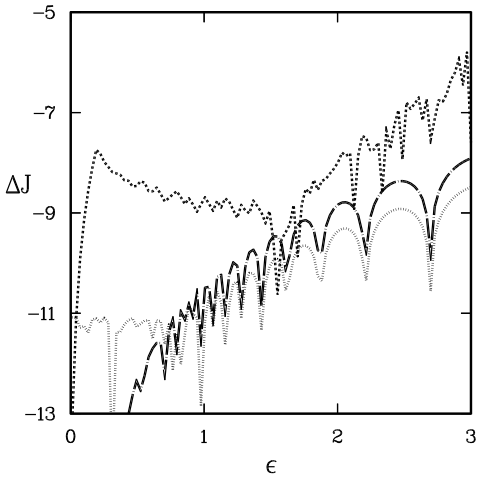

Fig. 2. Function $\Delta J(\epsilon)$ for the second example obtained by the symplectic integrators SRK4 with $h = 0.009$ (dash-dotted line), SN4 with $h = 0.0125$ (dashed line) and F3 with $h = 0.3$ (square-dotted line)

integral of the motion is stabilized about 10^{-8}, 10^{-9}, whereas for larger values of the parameter ϵ this error grows almost linearly with ϵ. This is so because for this value of ϵ the timestep size is too large in comparison with the width of the perturbation. If, on the other hand, we consider smaller values of h then we obtain more accurate results, but then, obviously, the computational effort increases. The same is true for the fourth order of the Fer expansion: we can obtain accurate results even with very large values of $\epsilon(\simeq 8)$, but the price to be paid is a dramatic increment in the CPU time. In any case, it is worth noticing that, for the whole range of the parameter ϵ analyzed, the quantity r, solution of Eq. (31), is smaller than the step size, so the convergence of the Fer expansion is not guaranteed at all. Nevertheless, for some values of ϵ, its performance is better than that of the other symplectic algorithms we have considered.

Concerning the standard extrapolation solver, ODEX2 with tolerance 10^{-10} achieves results that are very similar to that obtained by SN4, but with a CPU time that is about twice shorter.

Example 3. As a third and last example we take

$$\Omega^2(t) = \omega_0 - 2\epsilon \cos 2t \ , \tag{42}$$

with $\omega_0 > 0$, $\epsilon > 0$. This corresponds to the Mathieu equation, which has been studied widely for the last hundred years. As it is well known, the space of parameters (ω_0, ϵ) is divided into the so-called stable and unstable regions according to the nature of the solutions of the equation (23). More specifically, the point (ω_0, ϵ) belongs to the unstable region if there exists at least one solution which is unbounded with time, whereas it belongs to the stable region when the two linearly independent solutions are bounded. These bounded solutions

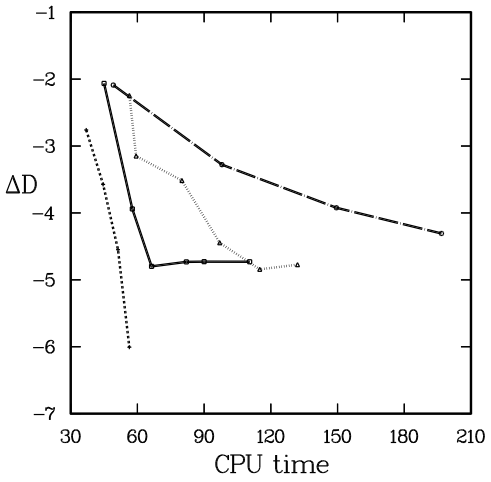

Fig. 3. Value of ΔD (Eq. (43)) at $t_f = 2000\pi$ vs. the CPU time (in seconds) when the Mathieu function $q(t) \equiv ce_{15}(t, 20)$ is considered. Curves are obtained by: ODEX2 with variable step size (solid line), SN4 (dash-dotted line), F3 (square-dotted line) and F4 (dashed line)

are doubly-periodic. The transition from stability to instability is shown by the existence of a periodic solution with period π or 2π [29]. This kind of solutions are expressed in terms of special functions (the so-called Mathieu functions), which must be obtained numerically or from the various published graphs and tables [1, 26]. In general, those functions are difficult to work with, not only analytically, but also numerically. Therefore it is useful to have both numerical algorithms for computing the solution and approximate analytic expressions for the Mathieu functions.

For this example we shall compute the quantity

$$\Delta D \equiv \log_{10} \|\mathbf{x}(t_f) - \mathbf{x}_{\text{appr}}(t_f)\| \tag{43}$$

at $t_f = 2000\pi$ by means of ODEX2, SN4, F3 and F4. Here, $\mathbf{x}(t) = (q(t), p(t))$, $q(t)$ is the particular Mathieu function whose value we want to approximate with the different numerical procedures $\|\cdot\|$ and denotes the Euclidean norm of $\mathbb{R}^2$.

i) Firstly we consider $q(t) = ce_{15}(t, \epsilon)$ with $\epsilon = 20$. As it is well known [1, 26], this is an even Mathieu function with exactly 15 zeros in any half-open interval of length π on the t-axis. It constitutes the solution of the Sturm-Liouville problem involving Eq. (23) and the boundary conditions $p(0) = \dot{q}(0) = q(\pi/2) = 0$ with period 2π. The characteristic value of ω_0 is $\omega_0 \equiv a_{15} \simeq 225.89515341$ and $q(0) \equiv ce_{15}(0, \epsilon = 20) \simeq 1.04708434$ [1]. With these tabulated values we can solve the initial value problem and compute ΔD at the final time t_f. Figure 3 shows ΔD against the CPU time obtained by:

a) ODEX2 with variable step size in each 2π-interval and tolerances 10^{-7}, 10^{-9}, 10^{-10}, 10^{-13} (squares joined by a solid line);

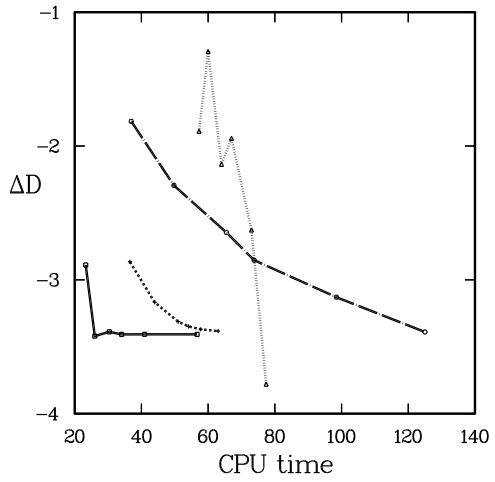

Fig. 4. Value of ΔD at $t_f = 2000\pi$ for the Mathieu function $q(t) \equiv se_{15}(t, 10)$. Curves are coded as in Fig. 3

b) SN4 with timesteps $2\pi/1000$, $2\pi/2000$, $2\pi/3000$, $2\pi/4000$ (circles joined by a dash-dotted line);
c) F3 with time steps $2\pi/50$, $2\pi/60$, $2\pi/70$, $2\pi/75$ (plus signs joined by a square-dotted line);
d) the fourth-order Fer expansion (F4) with time steps $2\pi/14$, $2\pi/15$, $2\pi/20$, $2\pi/25$, $2\pi/30$, $2\pi/35$ (triangles joined by a dashed line).

In this case the estimate (31) for the radius of convergence of the Fer expansion gives $r \simeq 0.00612$, much smaller than any of the step sizes tested. Nevertheless, the performance of the method (especially F3) is clearly better than that any other integration algorithm we have studied, including the extrapolation procedure ODEX2. Although convergence is not guaranteed, the fourth order of the expansion is more efficient than SN4 for the time interval we are considering. Its performance is also better than that of ODEX2 when high precision in the result is required.

ii) Now we take $q(t) = se_5(t, \epsilon)$, with $\epsilon = 10$. This is an odd 2π-periodic Mathieu function, solution of the boundary value problem given by Eq. (23) and the conditions $q(0) = \dot{q}(\pi/2) = 0$. The tabulated characteristic value of ω_0 is in this case $\omega_0 \equiv b_5 \simeq 26.76642636$ and $p(0) = \frac{d}{dt} se_5(t, 10)(t = 0) \simeq 3.4072268$. Figure 4 shows the quantity ΔD as a function of the CPU time when ΔD is calculated by means of ODEX2 (tolerances 10^{-9}, $10^{-10}, \ldots, 10^{-14}$), SN4 (timesteps $2\pi/750$, $2\pi/1000$, $2\pi/1250$, $2\pi/1500$, $2\pi/2000$, $2\pi/2500$), F3 (timesteps $2\pi/50$, $2\pi/60$, $2\pi/70$, $2, \pi/75$, $2\pi/80$, $2\pi/85$) and F4 (timesteps $2\pi/15$, $2\pi/16, \ldots, 2\pi/20$). The same code as in Fig. 3 has been used for points and lines.

The estimate of the radius of convergence of the Fer expansion is $r \simeq 0.0257$, about three times smaller than the minimum step size used by F3.

In this case the results obtained by F3 and ODEX2 practically coincide when high tolerances are considered in the ODEX2 algorithm, whereas, once again, F4 is the most performant integrator when high precision is required in the final result.

5. Conclusions

We have analyzed the main features of the Fer expansion as a method for obtaining an approximation to the evolution map in time-dependent Hamiltonian systems. When this systematic scheme is applied, $\mathscr{M}(t, t_0)$ is factorized as an infinite product of Lie transformations. This factorization is such that, after n iterations, all the dependence of $\mathscr{M}$ in the expansion parameter ε is ϵ^{2^n-1} included up to order.

In the simple but non-trivial case of a one-dimensional time-dependent harmonic oscillator, Eq. (22), we have constructed the Lie operators L_{F_i} of arbitrary order i and the third and fourth orders of the full expansion. Thus it is possible to have approximate analytical expressions for $q(t)$, $p(t)$ in terms of quadratures. They appear to converge to the true solution for an arbitrary frequency $\Omega(t)$, but with a finite radius of convergence. It is important to notice also that this approximation is symplectic, so we expect that it shall provide meaningful long-time predictions about phase-space main characteristics.

On the other hand, the above deduced approximate expressions for $q(t)$, $p(t)$, Eqs. (28) and (29), can be seen from a computational viewpoint as the successive steps of an explicit symplectic integration algorithm. We have analyzed its performance in some particular examples. Examples 1 and 3 have been chosen in order to study the long-term behaviour of the method, whereas with Example 2 we have tested the properties of conservation of the integrals of the motion. We have applied the third (F3) and fourth order (F4) Fer expansion to solve the initial value problem, and compared the corresponding results with those obtained by means of the explicit fourth order symplectic Runge-Kutta-Nyström SN4, the implicit SRK4 and by a ODE solver based on the extrapolation method (ODEX2). It has been shown that Fer expansion provides very accurate results both in the preservation of integrals of the motion and in the determination of the phase space trajectories with a reasonable computational effort.

Although the method, such as it has been considered here, can be applied in principle to any time-dependent Hamiltonian system, it is clear ihat severe restrictions must be imposed on the Hamiltonian function $H(\boldsymbol{\xi}, t)$ in order to get closed expressions for both the successive Lie operator L_{F_i} and the Lie transformations $\exp(L_{F_i})$. Nevertheless, for the important class of time-dependent linear Hamiltonian systems, as we have shown, its performance is clearly better than that of other standard methods when long time intervals are considered.

In summary, Fer's factorization, such as it is studied here, constitutes a new symplectic integrator especially well adapted to the study of general time-dependent systems with quadratic Hamiltonians. Its performance is comparable

to that of standard extrapolation algorithms with stringent tolerances for periodic problems and it is much better than that of other explicit and implicit symplectic integration methods. The degree of accuracy attained by Fer's expansion encourages to apply this scheme to more complex time-dependent Hamiltonian systems.

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A. Appendix

In this appendix we derive the expressions of the functions F_i and their associated Lie operators $L_{F_i} \geq 1$, corresponding to the more general one-dimensional quadratic Hamiltonian

$$H(q,p,t) = A_0(t)p^2 + B_0(t)qp + C_0(t)q^2 \ , \tag{44}$$

where $A_0(t)$, $B_0(t)$ and $C_0(t)$ are arbitrary functions of the time. For this Hamiltonian we get

$$\begin{aligned} F_1 &= -\alpha_1(t)p^2 - \beta_1(t)qp - \gamma_1(t)q^2 \\ L_{F_1} &= -\beta_1(t)(p\partial_p - q\partial_q) - 2\gamma_1(t)q\partial_p + 2\alpha_1(t)p\partial_q \end{aligned} \tag{45}$$

with

$$\alpha_1(t) = \int_{t_0}^{t} A_0(\tau)d\tau \ , \quad \beta_1(t) = \int_{t_0}^{t} B_0(\tau)d\tau \ , \quad \gamma_1(t) = \int_{t_0}^{t} C_0(\tau)d\tau \ . \tag{46}$$

In the case of the time-dependent harmonic oscillator, as it is obvious,

$$\alpha_1(t) = \frac{1}{2}(t - t_0) \ , \quad \beta_1(t) = 0 \ , \quad \gamma_1(t) = \frac{1}{2}\int_{t_0}^{t} \Omega^2(\tau)d\tau \ . \tag{47}$$

In general, suppose we know the i-th Fer's approximant ($i \geq 1$)

$$\begin{aligned} F_i &= -\alpha_i(t)p^2(t) - \beta_i(t)qp - \gamma_i(t)q^2 \\ L_{F_i} &= -\beta_i(t)(p\partial_p - q\partial_q) - 2\gamma_i(t)q\partial_p + 2\alpha_i(t)p\partial_q \ . \end{aligned} \tag{48}$$

Then, if we denote

$$\begin{aligned} f_{i1}(t) &= \frac{1}{2}(\beta_i^2 + \eta_i^2)A_{i-1} - \alpha_i\beta_i B_{i-1} + 2\alpha_i^2 C_{i-1} \ , \\ f_{i2}(t) &= -\beta_i A_{i-1} + \alpha_i B_{i-1} \\ f_{i3}(t) &= 2(\beta_i\gamma_i A_{i-1} - 2\alpha_i\gamma_i B_{i-1} + \alpha_i\beta_i C_{i-1}) \ , \\ f_{i4}(t) &= 2(-\gamma_i A_{i-1} + \alpha_i C_{i-1}) \\ f_{i5}(t) &= 2\gamma_i^2 A_{i-1} - \beta_i\gamma_i B_{i-1} + \frac{1}{2}(\beta_i^2 + \eta_i^2)C_{i-1} \ , \\ f_{i6}(t) &= -\gamma_i B_{i-1} + \beta_i C_{i-1} \ , \end{aligned} \tag{49}$$

with $\eta_i^2 = \beta_i^2 - 4\alpha_i\gamma_i$, we obtain for the i-th transformed Hamiltonian $H_i(q,p,t)$ the following compact expression

$$H_i(q,p,t) = A_i(t)p^2 + B_i(t)qp + C_i(t)q^2 \ , \tag{50}$$

where now

$$\begin{aligned}
A_i(t) &= \frac{-1}{2\eta_i^2}(f_{i2} - f_{i1})\cosh 2\eta_i - \frac{1}{2\eta_i}\left(\frac{1}{2\eta_i^2}f_{i1} - 2f_{i2}\right)\sinh 2\eta_i + \frac{1}{2\eta_i^2}f_{i2} \\
B_i(t) &= \frac{1}{\eta_i^2}(f_{i3} - \frac{1}{2}f_{i4})\cosh 2\eta_i + \frac{1}{\eta_i}(f_{i4} - \frac{1}{2\eta_i^2}f_{i3})\sinh 2\eta_i + \frac{1}{2\eta_i^2}f_{i4} \\
C_i(t) &= \frac{1}{2\eta_i^2}(2f_{i5} - f_{i6})\cosh 2\eta_i + \frac{1}{2\eta_i}(2f_{i6} - \frac{1}{\eta_i^2}f_{i5})\sinh 2\eta_i + \frac{1}{2\eta_i^2}f_{i6}
\end{aligned} \tag{51}$$

if $\eta_i \neq 0$, whereas

$$\begin{aligned}
A_i(t) &= \frac{4}{3}f_{i1} + f_{i2} \\
B_i(t) &= \frac{4}{3}f_{i3} + f_{i4} \\
C_i(t) &= \frac{4}{3}f_{i5} + f_{i6}
\end{aligned} \tag{52}$$

when $\eta_i = 0$. From Eq. (50) we obtain the expression of the $(i+1)$-th Fer's approximant in the form

$$\begin{aligned}
F_{i+1} &= -\alpha_{i+1}(t)p^2 - \beta_{i+1}(t)qp - \gamma_{i+1}(t)q^2 \\
L_{F_{i+1}} &= -\beta_{i+1}(t)(p\partial_p - q\partial_q) - 2\gamma_{i+1}(t)q\partial_p + 2\alpha_{i+1}(t)p\partial_q \ ,
\end{aligned} \tag{53}$$

with

$$\alpha_{i+1}(t) \int_{t_0}^{t} A_i(\tau)d\tau \ , \quad \beta_{i+1}(t) = \int_{t_0}^{t} B_i(\tau)d\tau \ , \quad \gamma_{i+1}(t) = \int_{t_0}^{t} C_i(\tau)d\tau \ . \tag{54}$$

We see that F_n is given only in terms of quadratures and, in this case, is just a quadratic form in the coordinate and momentum.

B. Appendix

i) Given a Hamiltonian

$$H(\mathbf{q},\mathbf{p},t) = T(\mathbf{p}) + V(\mathbf{q},t) \ , \tag{55}$$

with $\mathbf{q} = (q_1,\ldots,q_N)$, $\mathbf{p} = (p_1,\ldots,p_N)$ and $T(\mathbf{p}) = \frac{1}{2}\mathbf{p}^{\mathrm{T}}\mathbf{p}$, the corresponding equations of the motion can be written

$$\ddot{\mathbf{q}} = -\nabla V(\mathbf{q},t) \equiv \mathbf{f}(\mathbf{q},t) \ , \tag{56}$$

i.e., as a second-order system. For this problem, s-stage explicit Runge-Kutta-Nyström methods are given by [21]

$$\mathbf{Q}_i = \mathbf{q}_0 + c_i h \mathbf{p}_0 + h^2 \sum_{j<i} \bar{a}_{ij} \mathbf{k}'_j \ , \quad \mathbf{k}'_j = \mathbf{f}(\mathbf{Q}_j, t_0 + c_j h) \tag{57}$$

$$\mathbf{q}_1 = \mathbf{q}_0 + h\mathbf{p}_0 + h^2 \sum_{l=1}^{s} \bar{b}_l \mathbf{k}'_l \ , \quad \mathbf{p}_1 = \mathbf{p}_0 + h \sum_{l=1}^{s} b_l \mathbf{k}'_l \ ,$$

where h is a step size. As usual, the quantities $\mathbf{q}_0$ and $\mathbf{p}_0$ are initial values, whereas q_1 and p_1 are the numerical solution after a time h. These methods are symplectic if the following two conditions are satisfied:

$$\begin{aligned} \bar{b}_i &= b_i(1 - c_i) \ , \quad i = 1, \ldots, s \\ \bar{a}_{ij} &= b_j(c_i - c_j) \quad \text{for } i > j \ . \end{aligned} \tag{58}$$

We have FSAL (first same as last) methods when $c_1 = 0$, $c_s = 1$ and $\bar{a}_{sj} = \bar{b}_j$ for $1 \leq j \leq s - 1$. For this class of methods the last stage $\mathbf{Q}_s$ of the current step coincides with $\mathbf{q}_1$, which is the first stage of the next step. Therefore, a step of an FSAL s-stage method requires only $s - 1$ evaluations of the function $\mathbf{f}$.

Calvo and Sanz-Serna [4] derive a fourth-order, symplectic, FSAL Runge-Kutta-Nyström method whose coefficients are given by

$$\begin{aligned} c_1 &= 0, & b_1 &= 0.061758858135626325 \ , \\ c_2 &= 0.205177661542286386 \ , & b_2 &= 0.338978026553643355 \ , \\ c_3 &= 0.608198943146500973 \ , & b_3 &= 0.614791307175577566 \ , \\ c_4 &= 0.487278066807586965 \ , & b_4 &= -0.140548014659373380 \ , \\ c_5 &= 1 \ , & b_5 &= 0.125019822794526133 \ . \end{aligned} \tag{59}$$

It requires four functions evaluations per step, and its accuracy per step is comparable to that of standard non-symplectic Runge-Kutta-Nyström methods [4].

ii) A Runge-Kutta method for a general system of ODEs

$$\frac{d\mathbf{y}}{dt} = \mathbf{f}(\mathbf{y}, t) \ , \quad \mathbf{y} \in \mathbb{R}^d \tag{60}$$

is specified by an integer s (the number of stages) and constants a_{ij}, $(i \leq i, j \leq s)$, $b_i (1 \leq i \leq s)$. When $\mathbf{y}(t_n)$ is known, auxiliary vectors $\mathbf{Y}_i (1 \leq i \leq s)$ are defined through [34]

$$\mathbf{Y}_i = \mathbf{y}(t_n) + h \sum_{j=1}^{s} a_{ij} \mathbf{f}(\mathbf{Y}_j, t_n + c_j h) \tag{61}$$

with

$$c_i = \sum_{j=1}^{s} a_{ij} \ , \quad 1 \leq i \leq s \ .$$

Then one sets

$$\mathbf{y}(t_{n+1} \equiv t_n + h) = \mathbf{y}(t_n) + h \sum_{i=1}^{s} b_i \mathbf{f}(\mathbf{Y}_i, t_n + c_i h) \; . \tag{62}$$

When $a_{ij} = 0$ for $i \leq j$ the method is called explicit. Suppose now that (60) is Hamiltonian. For general Runge-Kutta methods, the map (62) is not symplectic. Nevertheless, if the $s \times s$ matrix with entries

$$M_{ij} = b_i a_{ij} + b_j a_{ji} - b_i b_j \quad (1 \leq i, j \leq s) \tag{63}$$

is identically zero then (62) constitutes a symplectic transformation [32]. As a particular case, we can consider the two-stage ($s = 2$) Gauss-Legendre Runge-Kutta method given by [30, 39]

$$\begin{aligned} (a_{ij}) &= \begin{pmatrix} \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} \\ \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} \end{pmatrix} \\ (b_i)^T &= \left(\tfrac{1}{2}, \tfrac{1}{2}\right) \; , \quad (c_i)^T = \left(\tfrac{1}{2} - \tfrac{1}{6}\sqrt{3}, \tfrac{1}{2} + \tfrac{1}{6}\sqrt{3}\right) \end{aligned} \tag{64}$$

which is implicit and fourth-order accurate.

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