Symplectic maps for approximating polynomial Hamiltonian systems

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We study how to approximate polynomial Hamiltonian systems by composition of symplectic maps. Recently, a number of methods preserving the symplectic character have appeared. However, they are not completely satisfactory because, in general, they are computationally expensive, very difficult to obtain or their accuracy is relatively low. The efficiency of a numerical method depends on both its computational cost and its accuracy. Polynomial Hamiltonians are separable in exactly solvable parts, and this can be done in many different ways. Here we study how to find a separation for the Hamiltonian in a small number of cheaply computed terms. Since the proposed methods depend on some free parameters, we also indicate how to choose these parameters in order to improve the accuracy without increasing the computational cost.

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I. INTRODUCTION

Polynomial Hamiltonian systems appear frequently in accelerator physics [1–7] and it is important to build good integrators for numerical simulations. For the experiments in accelerator physics the particles are stored for a long time. During this time the particles give a huge number of turns around the storage ring, and it is very important to study the stability of the trajectories in order to avoid disappearance of too many of these particles in the walls of the ring.

Provided that the synchrotron radiation is neglected, the system can be considered as a Hamiltonian. Each part of the accelerator has associated a Hamiltonian and, by composition, it is possible to consider only one Hamiltonian for approximating a complete turn to the ring. If $z=(q,p)$ are the coordinates and momenta of a particle and z_0 are the initial conditions, we have, after one turn, $z(1)=\mathcal{M}_H z_0$, where $\mathcal{M}_H$ is the map associated to the Hamiltonian. Considering that the system is periodic, for N turns we have $z(N)=\mathcal{M}_H^N z_0$.

In general, it is not possible to find analytical expressions for $z(N)$, so numerical methods are required. Methods preserving the qualitative properties of the exact solution are essential in order to have a good picture of the stability regions. Therefore, we only consider *symplectic integrators*, that is, numerical methods that, when applied to a classical Hamiltonian system, preserve its symplectic character. The approach we propose belongs to this family of methods and it is usually referred to as *symplectification of maps* in the accelerator physics community.

One of the most important methods is the truncated Taylor map

$$z^{(T)}=\mathcal{M}_T z^0=R+\sum_{m=1}^{M_T}\sum_{i_1,\ldots,i_m} R_{i_1,\ldots,i_m} z^0_{i_1}\cdots z^0_{i_m}, \quad (1)$$

where $z^{(T)}$ is an approximation to $z(1)$, R is a vector, and z_i^0 is the ith component of z^0 (being $z^0\equiv z_0$). Here, M_T has to be high enough to preserve symplecticity up to a round-off error. In general, the dynamics of the system is mainly determined by the low order polynomials, $m=1,\ldots,M-1$ and the values $m=M,M+1,\ldots,M_T$ are introduced solely to preserve symplecticity up to round-off. Since the computational cost grows extraordinarily with m, it means that most of the work is done just to preserve symplecticity. For this reason, it seems logical to look directly for methods that exactly preserve symplecticity. It is well known that any transformation defined implicitly by a *mixed variable* canonical generator gives a symplectic map. Thus, in order to produce a symplectic map accurate up to order M, it is required that the map produced from the generating function agrees with it to that order. Unfortunately, the equations to solve are implicit and they have to be solved up to round-off to preserve symplecticity. If the generating function is cheap to compute (for example, a polynomial function) and a good starting point for the iteration algorithm is known, efficient methods can be obtained [8–12].

However, in general, explicit methods are faster and easier to implement, and in this paper we only consider explicit methods. Most of these algorithms are compositions of maps like

$$\textbf{do} \quad i=1,k_1$$
$$z^i=\mathcal{M}_i(z^{i-1}) \quad (2)$$
$$\textbf{enddo}$$

where $\mathcal{M}_i$ are symplectic maps such that $z^{k_1}=z(1)+r_M$, with r_M representing a polynomial of degree M and higher. There is a number of such methods [5,7,13] that are relatively simple but, the maps $\mathcal{M}_i$ usually involve the computation of roots and exponentials, k_1 can be relatively large, and the accuracy of the algorithms is frequently not very good. So, we are still paying a high price for preserving symplecticity.

A much cheaper but sophisticated approach was introduced by Irwin [14]. It can be considered as a particular case of Eq. (2), and looks like

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$$\begin{aligned}
&\textbf{do} \quad i=1,k_2\\
&\quad \overline{z^i}=R_i(\beta)z^{i-1}\\
&\quad q^i=\overline{q^i}\\
&\quad p^i=\overline{p^i}+G_i(q^i,\mathbf{b})\\
&\textbf{enddo}
\end{aligned} \tag{3}$$

where $\overline{z^i}=(\overline{q^i},\overline{p^i})$, R_i are symplectic linear transformations, $\beta=(\beta_1,\ldots,\beta_{j_{k_2}})$, $\mathbf{b}=(b_1,\ldots,b_{l_{k_2}})$ are parameters to be fixed, G_i are polynomial functions depending only on the coordinates, and are such that $z^{k_2}=(q^{k_2},p^{k_2})=z(1)+r_M$. This algorithm can be very cheap [usually with similar cost to the Taylor series map up to order M then, much cheaper to compute than Eq. (1) for $M<M_T$]. Irwin proposed to fix the values of β and to obtain $\mathbf{b}$ from a linear system of equation. He also proposed an optimization criterion in case we had more b_i variables than equations. Nevertheless, when this technique was implemented on some problems, its accuracy was rather poor, and it was abandoned. A deeper analysis, following Irwin's idea, for reducing the number of maps, k_2, was carried out in [15] using group properties for the linear maps but, as we mention later in more detail, the cost is not much reduced and still is not useful enough to make this technique competitive. However, Abell and Dragt [16,4] realized that the optimization of Eq. (3) should be done on the set of β coefficients. An impressive analysis was conducted and they found, for example, that in the two-dimensional phase space "*almost all sets are bad, good sets are rare, and very good sets are exceptional*." However, the complexity was so high that, even recently, some experts in symplectification of maps using generating functions [11] said that "*the approximation theory of that technique is difficult to manage, and the prospects of a practical advantage are still uncertain*." After the submission of the present paper, Ref. [17] appeared showing that, in spite of its complexity, it is still possible to find efficient methods for practical problems.

In [16,4], for given values of M and of the dimension of the phase space, sensitive vectors and Gram matrices were defined, and a set of β coefficients that maximized the minimum of their eigenvalues was sought. As the authors noticed, the results are very sensitive to β, and the optimal value is independent of the studied problem [16] [Chap. 16]. The sensitivity of the results with β seems logical because in a perturbation technique, such as this, the linear part gives the main contribution to the error, so small changes in the β coefficients can affect seriously the accuracy of the method. This indicates that, for most particular cases, the optimal method obtained will be a good one, but still not the optimal for each problem. Here, we propose a simple procedure to obtain the optimal solution for each particular problem.

In this paper we use kicks instead of the general linear transformation R_i (without loosing much generality), simplifying considerably the algorithm (3). For this particular case, we explicitly obtain the minimum value of k_2 in terms of the dimension of the phase space and M. Moreover, we reduce the number of β_i parameters just by introducing into the algorithm some simple and cheap (but not necessarily polynomial) maps. Then, instead of looking for optimal values for the β_i in a j_{k_2}-dimensional space, we will do it in a lower-dimensional space, reducing significantly the numerical search for their optimal values. In addition, we indicate how to introduce more terms (and more parameters) into the algorithm, in case a further optimization is desired. The whole procedure of optimization takes into account the coefficients of the Hamiltonian. The algorithm we propose looks like

$$\begin{aligned}
&\textbf{do} \quad i=1,k_3'\\
&\quad z^i=\mathcal{M}_i(z^{i-1})\\
&\textbf{enddo}\\
&\textbf{do} \quad i=k_3'+1,k_3\\
&\quad q^i=q^i+G_{i,1}(p^{i-1},\beta)\\
&\quad p^i=p^i+G_{i,2}(q^i,\mathbf{b})\\
&\textbf{enddo}
\end{aligned} \tag{4}$$

where $\mathcal{M}_i$ are some cheap symplectic maps (polynomials or quotient of polynomials), the $G_{i,1}$ are linear functions but, if desired, nonlinear terms can be included easily, and the $G_{i,2}$ are analogous to the G_i in Eq. (3). The b_i coefficients are the solution of linear systems, depending on the β_j and the coefficients of the particular problem considered. Finally, we indicate how to make numerical searches to find the optimal set of $\boldsymbol{\beta}$ for each particular problem. In order to illustrate the benefits of this proposed technique, we explicitly show how to implement it on simple examples.

II. MATHEMATICAL BACKGROUND

Let us denote by $z=(q,p)=(q_1,\ldots,q_n,p_1,\ldots,p_n)$ a vector in a $2n$-dimensional phase space, and $f(z)$, $g(z)$ two analytical functions. We denote the Poisson bracket of f and g by

$$\{f,g\}=\sum_{i,j}\frac{\partial f}{\partial z_i}J_{ij}\frac{\partial g}{\partial z_j} \quad \text{with} \quad J=\begin{pmatrix} 0 & I\\ -I & 0\end{pmatrix}. \tag{5}$$

Here I and 0 are the $n\times n$ identity and zero matrices, respectively. Following [1] we denote by $:f(z):$ the Lie operator associated to $f(z)$. It acts on a function $g(z)$ as

$$:f(z):g(z)=\{f(z),g(z)\}. \tag{6}$$

We define the Lie transformation associated to f by

$$e^{:f:}=\sum_{k=0}^{\infty}\frac{:f:^k}{k!}, \tag{7}$$

where $:f:^0 g = g$ and $:f:^k g = \{f,:f:^{k-1} g\}$. In order to make the paper self-contained, in the following we collect some properties of Lie operators and Lie transformations that are used later. We highly recommend Refs. [1,2] for more details and proofs.

Given an analytical function $g(z)$, an important property of Lie transformations is

$$e^{:f(z):} g(z) = g(e^{:f(z):} z), \tag{8}$$

where by $e^{:f(z):} z$ we must understand that the Lie transformation acts on each component of z. The relation

$$[:f:,:g:] \equiv :f::g: - :g::f: = :\{f,g\}: \tag{9}$$

indicates that the Lie algebra of functions, with the Poisson bracket as the product, is intimately related to the Lie algebra of Lie operators associated to functions, with the commutator as the product. Using the Baker-Campbell-Hausdorff (BCH) formula and Eq. (9), we have that

$$e^{:f:} e^{:g:} = e^{:h:}, \tag{10}$$

where

$$h = f + g + \tfrac{1}{2}\{f,g\} + \tfrac{1}{12}(\{f,\{f,g\}\} + \{g,\{g,f\}\}) + \cdots, \tag{11}$$

and the inverse of $e^{:f(z):}$ is $e^{-:f(z):}$. Another useful property is

$$e^{:f(z):} :g(z): e^{-:f(z):} = :e^{:f(z):} g(z): = :g(e^{:f(z):} z): \tag{12}$$

and then

$$e^{:f(z):} e^{:g(z):} e^{-:f(z):} = \exp[:g(e^{:f(z):} z):]. \tag{13}$$

For the particular cases $f(q)$ and $g(p)$, the Taylor series expansion of their associated Lie transformations (7) terminates when acting on (q,p),

$$e^{:f(q):} \begin{Bmatrix} q \\ p \end{Bmatrix} = \begin{Bmatrix} q \\ p + \nabla_q f(q) \end{Bmatrix}; \quad e^{:g(p):} \begin{Bmatrix} q \\ p \end{Bmatrix} = \begin{Bmatrix} q - \nabla_p g(p) \\ p \end{Bmatrix}. \tag{14}$$

Given a Hamiltonian function, $H(z):\mathbb{R}^{2n} \to \mathbb{R}$, the Hamilton equations are given by

$$\dot{z} = \{z, H(z)\} = -:H(z):z,$$

where the dot indicates derivative respect to t. The solution is

$$z_t = e^{-t:H(z_0):} z_0, \tag{15}$$

which can be considered as a change of coordinates from z_0 to z_t so, the Poisson bracket, $:H(z_0):z_0 = \{H(z_0), z_0\}$ [it has to be read as the Poisson bracket of $H(z_0)$ with each component of z_0] is well defined. If the Hamiltonian is time independent, then $H(z)$ is a constant of the motion because $(d/dt)H(z) = -\{H(z),H(z)\} = 0$, and then

$$z_t = e^{-t:H(z_0):} z_0 \quad \Rightarrow \quad z_0 = e^{t:H(z_t):} z_t, \tag{16}$$

since $H(z_t) = H(z_0)$. Finally, the action of a Lie transformation $e^{:f(z):} z$ can be considered as the time-1 flow of the Hamiltonian $H(z) = -f(z)$.

III. SPLITTING THE MAP IN SOLVABLE PARTS

Suppose $H(z)$ is the Hamiltonian containing all elements of the ring. In accelerator physics one is interested in the motion around the design orbit, so $\|z\|$ (for an unspecified norm) will be small. For this reason, it makes sense to write $H = \Sigma_i H_i$, where H_i are homogeneous polynomials of degree i, and to consider only terms up to a given order, say M,

$$H \sim \sum_{i=1}^{M} H_i. \tag{17}$$

Since H_1 and H_2 are exactly solvable, we can formally write

$$\exp(-:H:) = \exp(:f_1:)\exp(:f_2:)\mathcal{N} \tag{18}$$

with

$$\mathcal{N} = \exp\left(:\sum_{i>2} f_i:\right), \tag{19}$$

and where f_i are homogeneous polynomials of degree i. Usually it is only known the Taylor series expansion of $e^{-:H:} z_0$ up to order M, $\mathcal{T}_H^{(M)}(z_0)$, which, in general, does not preserve symplecticity. However, following [18] it is possible to write

$$e^{:g_1:} e^{:g_2:} \cdots e^{:g_M:} z_0 = \mathcal{T}_H^{(M)}(z_0) + r_M(z_0), \tag{20}$$

where r_M is a polynomial with terms of degree M and/or higher and the g_i are homogeneous polynomials of degree i. In the following, any letter with a subindex, i.e., g_k, will denote a generic and unspecified polynomial with terms of degree k or higher. We will indicate explicitly if the polynomial is homogeneous. Occurrences of the symbol g_k in different places do not necessarily refer to the same polynomial. Finally, from Eq. (20) and using the BCH formula, Eqs. (18) and (19) are easily obtained.

In this paper we are interested in approximating

$$e^{:f_3 + \cdots + f_M:} z, \tag{21}$$

but, this transformation usually cannot be solved analytically.

Given the homogeneous polynomial in a two-dimensional phase space

$$f_m = \sum_{i=0}^{m} a_i q^{m-i} p^i, \tag{22}$$

it is possible to write it as a sum of exactly solvable parts [5,7,19,20,13]. For example, each monomial $aq^n p^m$ is exactly solvable

$$\begin{Bmatrix} \overline{q} \\ \overline{p} \end{Bmatrix} = e^{a:q_0^n p_0^m:} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix} = \begin{Bmatrix} A^m q_0 \\ p_0 / A^n \end{Bmatrix} \tag{23}$$

with $A=[1+(n-m)aq_0^{n-1}p_0^{m-1}]^{1/(m-n)}$ if $m\neq n$. For $m=n$,

$$\begin{Bmatrix} \overline{q} \\ \overline{p} \end{Bmatrix} = e^{a:q_0^m p_0^m:} \begin{Bmatrix} q_0 \\ p_0 \end{Bmatrix} = \begin{Bmatrix} Eq_0 \\ p_0/E \end{Bmatrix}, \tag{24}$$

with $E=\exp(-amq_0^{m-1}p_0^{m-1})$. Observe that the evaluation of each map involves the computation of an exponential or a root [unless $n/(n-m)$ and $m/(n-m)$ were both integers]. Here $(\overline{q},\overline{p})$ are written in terms of a summable infinite series on (q_0,p_0). Notice also that Eq. (23) has singularities.

Another inconvenience is that, when considering the polynomial $f_3+\cdots+f_M$, the number of monomials increases considerably. However, the number of solvable terms can be reduced by grouping monomials that still have exact solution. The procedure is relatively simple, one has to find those Hamiltonians whose Hamilton equations

$$\dot{q}=\frac{\partial H}{\partial p}, \quad \dot{p}=-\frac{\partial H}{\partial q} \tag{25}$$

are exactly solvable. For example, in Eq. (24), if we take the Hamiltonian $H=-aq^m p^m$, the system to solve is

$$\dot{q}=-maq^m p^{m-1} \quad \Rightarrow \quad \dot{q}=-ma(q_0^{m-1}p_0^{m-1})q,$$

$$\dot{p}=maq^{m-1}p^m \quad \Rightarrow \quad \dot{p}=ma(q_0^{m-1}p_0^{m-1})p, \tag{26}$$

where we have considered the known fact that $H_0=-aq_0^m p_0^m$ is a constant of the motion so $qp=q_0p_0$, and integrating Eq. (26) from $t=0$ to 1, the solution (24) is obtained. Similarly, we can prove Eq. (23) (see [19]). On the other hand, if we consider $H=-(aq^m+bq^{m-1}p)$, $m>2$, we have [6]

$$\dot{q}=-bq^{m-1} \quad \Rightarrow \quad \overline{q}=q_0[1+(m-2)bq_0^{m-2}]^{1/(2-m)},$$

$$\dot{p}=amq^{m-1}+b(m-1)q^{m-2}p$$
$$\Rightarrow \quad \overline{p}=(H_0-a\overline{q}^m)/(b\overline{q}^{m-1}). \tag{27}$$

There are several works looking for different groups of monomials with exact solution, for splitting a polynomial in as few number of solvable terms as possible [6,7,13]. However, we must say that there is no unique way to separate a Hamiltonian in solvable parts, and in the following section we present a different way to split the Hamiltonian that usually gives more efficient methods. For higher-dimensional systems, it is interesting to remember the following properties.

(1) Given the $2r$-dimensional Hamiltonian

$$H=\prod_{i=1}^{r} H^{(i)}(q_i,p_i), \tag{28}$$

then each $H^{(i)}(q_i,p_i)$, $i=1,\ldots,r$ is a constant of the motion. In order to compute the flow for (q_s,p_s) the Hamiltonian $\alpha H^{(s)}(q_s,p_s)$ may be considered with $\alpha=\Pi_{i\neq s}H^{(i)}(q_i,p_i)$ being a constant.

(2) Given the $2r$-dimensional Hamiltonian

$$H=\sum_{i=1}^{r} H^{(i)}(q_i,p_i) \tag{29}$$

then each $H^{(i)}(q_i,p_i)$, $i=1,\ldots,r$ is a constant of the motion. In order to compute the flow for (q_s,p_s) only the Hamiltonian $H^{(s)}(q_s,p_s)$ has to be considered.

In many problems the Hamiltonian is separable in two parts, i.e., $H=A(p)+B(q)$ then, $e^{:\epsilon A+\epsilon B:}$ has to be approximated up to a given order in ϵ (usually the time step) where $e^{:\epsilon A:}$ and $e^{:\epsilon B:}$ are exactly solvable. In Refs. [21–28] the following approximations are proposed

$$e^{:\epsilon A+\epsilon B:}=\prod_{i=1}^{k} e^{:\epsilon a_i A:}e^{:\epsilon b_i B:}+O(\epsilon^{M+1}), \tag{30}$$

where k is fixed but sufficiently large, and the coefficients $\{a_i,b_i\}_{i=1}^k$ have to solve a system of nonlinear equations.

For some of these problems, other members of the Lie algebra generated by A and B are also solvable. This is the case when $A=p^2$, where $\{B(q),\{B(q),A(p)\}\}=C(q)$. Then, if the $e^{:\epsilon b_i B:}$ maps are replaced by the more general $\exp(:\epsilon b_i B+\epsilon^3 c_i C:)$ maps (with c_i constants to be determined), the resulting methods are, in general, more efficient [21,29,26]. We observe that an efficient way to build an integrator is to consider all maps that can be cheaply evaluated and to try to reproduce the original problem up to a given order by composition of these maps, and this is the procedure we propose in the following sections.

IV. USING CHEAP SOLVABLE MAPS

Let us consider the Hamiltonian $H=\frac{1}{2}(p^4+6p^2q^2+q^4)$. The fourth-order Taylor map, associated to the time-1 flow of H, is given by

$$q=q_0+2p_0(p_0^2+3q_0^2),$$

$$p=p_0-2q_0(q_0^2+3p_0^2),$$

which can be computed with eight multiplications and four additions. If we use the fourth-order factorization $e^{-:H:}\simeq e^{-:(1/2)p^4:}e^{-:(1/2)q^4:}e^{-:3p^2q^2:}$, the algorithm we obtain is

$$q_1=q_0+2p_0^3,$$

$$p_1=p_0-2q_1^3,$$

$$\alpha=\exp(6q_1p_1),$$

$$q=\alpha q_1,$$

$$p=p_1/\alpha,$$

which agrees with the Taylor map up to the fourth order. It requires ten multiplications, two additions and one exponential, being clearly more expensive. However, a different symplectification is given by

$$q_1 = q_0 + p_0,$$

$$p_1 = p_0 - q_1^3,$$

$$q_2 = q_1 - 2p_0,$$

$$p = p_1 - q_2^3,$$

$$q = q_2 + p,$$

which needs only five multiplications and five additions. The algorithm has been obtained using the approximation $e^{-:H:} \simeq e^{-:(1/2)p^2:} e^{-:(1/4)q^4:} e^{:p^2:} e^{-:(1/4)q^4:} e^{-:(1/2)p^2:}$. This can be seen as a symplectification of the truncated Taylor map by adding new polynomial terms to the series. This is a clear example showing that different symplectification techniques can produce algorithms with significantly different cost. In addition, we observe that it is possible to build a symplectification with similar cost to the Taylor map, or even cheaper.

Encouraged by the significant cost reduction that the method showed in examples like the above one, we studied how, given a general Hamiltonian, to build a factorization that preserves symplecticity and agrees with the Taylor series map up to a given order, having similar computational cost. We have seen from Eq. (14) that the computation of $e^{:f(q):}$ and $e^{:g(p):}$ is trivial. Therefore, we are interested in looking for integrators, which can be written as

$$\exp(:f_3 + \cdots + f_M:) = \prod_{i=1}^{k} e^{:Q^{(i)}(q):} e^{:P^{(i)}(p):} + O(R_{M+1}), \tag{31}$$

where $O(R_{M+1})$ contains operators associated to polynomials with terms of degree $M+1$ or higher and $Q^{(i)}(q)$, $P^{(i)}(p)$ are polynomial functions depending only on the coordinates and momenta, respectively.

Definition. A Cremona map is a symplectic map whose Taylor series expansion terminates.

Observe that

$$z_1 = \prod_{i=1}^{k} e^{:Q^{(i)}:} e^{:P^{(i)}:} z_0 = F(z_0) \tag{32}$$

is a polynomial function of z_0, and this approximation can be considered as a Cremona map [4,16,14].

In the following we show in a simple way that this kind of factorization is always possible, and we present how to obtain some of them. Obviously, the optimal integrator (the best choice for k and the polynomials $Q^{(i)}$ and $P^{(i)}$) depends on each particular problem. This is what happens in symplectic integrators for Eq. (30) where the best choice of k and the coefficients $\{a_i, b_i\}$ depend on the structure of A and B (if $\{B,\{B,\{B,A\}\}\}=0$, or if $\|B\| \ll \|A\|$, etc.) as well as the desired accuracy.

A. Two-dimensional system

For simplicity, we start with the two-dimensional system, $z=(q,p) \in \mathbb{R}^2$, and we consider the homogeneous polynomial of degree m, Eq. (22). We have the following theorem.

Theorem 1. Given $\beta_i \in \mathbb{R}$, $i=0,\ldots,m$, such that $\beta_i \neq \beta_j$, $i \neq j$ then we can write

$$\sum_{i=0}^{m} a_i q^{m-i} p^i = \sum_{j=0}^{m} b_j (q + \beta_j p)^m. \tag{33}$$

Proof. We prove the theorem by giving the solution for the coefficients b_j. We have

$$(q + \beta_j p)^m = \sum_{i=0}^{m} C_m^i \beta_j^i q^{m-i} p^i, \tag{34}$$

where $C_m^i := m!/i!(m-i)!$. Then, from Eq. (33) we have

$$a_i = \sum_{j=0}^{m} C_m^i \beta_j^i b_j, \quad i=0,\ldots,m, \tag{35}$$

which can be written in matrix form

$$\overbrace{\begin{pmatrix} C_m^0 & 0 & \cdots & 0 \\ 0 & C_m^1 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & \cdots & C_m^m \end{pmatrix}}^{C^{(m)}} \overbrace{\begin{pmatrix} 1 & \cdots & 1 \\ \beta_0 & \cdots & \beta_m \\ \vdots & & \vdots \\ \beta_0^m & \cdots & \beta_m^m \end{pmatrix}}^{V^{(m)}(\beta)} \begin{Bmatrix} b_0 \\ b_1 \\ \vdots \\ b_m \end{Bmatrix} = \begin{Bmatrix} a_0 \\ a_1 \\ \vdots \\ a_m \end{Bmatrix}. \tag{36}$$

Observe that $V^{(m)}(\beta)$ is a Vandermonde matrix having inverse provided that $\beta_i \neq \beta_j$ for $i \neq j$, as is the case. Then, the solution is given by

$$\begin{Bmatrix} b_0 \\ \vdots \\ b_m \end{Bmatrix} = (V^{(m)})^{-1} \begin{Bmatrix} a_0/C_m^0 \\ \vdots \\ a_m/C_m^m \end{Bmatrix}. \tag{37}$$

■

This theorem can be considered equivalent to the Theorem 5 given in [30], but here we give the explicit relation between the coefficients b_i and β_i, a_i. In [31] a similar separation was done where the β_j coefficients correspond to the Gaussian points and then the b_j can be written in terms of the Gaussian weights and Legendre polynomials of the β_j that minimize a given norm. However, for the purpose of this work, we prefer not to fix the values of the β_j coefficients at this point.

We can think of $\{q^{m-i}p^i\}_{i=0}^m$ and $\{(q+\beta_i p)^m\}_{i=0}^m$ as two different bases for homogeneous polynomials of degree m, and the linear relation (37) corresponds to a change of coordinates. For a general polynomial we have the following.

Corollary 1. Given a general polynomial of degree M in two dimensions and $\beta_i \in \mathbb{R}$, $i=0,\ldots,M$, such that $\beta_i \neq \beta_j$ for $i \neq j$ then we can write

$$\sum_{m=1}^{M} \sum_{i=0}^{m} a_i^{(m)} q^{m-i} p^i = \sum_{m=1}^{M} \left(\sum_{j=0}^{m} b_j^{(m)} (q+\beta_j p)^m \right) = \sum_{j=0}^{M} \left(\sum_{m=j}^{M} b_j^{(m)} (q+\beta_j p)^m \right) \tag{38}$$

with $b_0^{(0)} = 0$.

Theorem 2. The Lie transformation associated to the polynomial

$$\sum_{m=j}^{M} b_j^{(m)} (q+\beta_j p)^m \tag{39}$$

has a finite Taylor series expansion, being a Cremona map.

Proof. From Eq. (14) we have

$$e^{-\beta \frac{1}{2}:p^2:} q = q + \beta p, \tag{40}$$

and from Eq. (13) we have

$$\exp(-\beta\tfrac{1}{2}:p^2:)\exp(:bq^m:)\exp(\beta\tfrac{1}{2}:p^2:) = \exp[:b(e^{-\beta(1/2):p^2:}q)^m:] = \exp[:b(q+\beta p)^m:].$$

Similarly

$$\exp\left(-\beta_j \frac{1}{2}:p^2:\right)\exp\left(:\sum_{m=j}^{M} b_j^{(m)} q^m:\right)\exp\left(\beta_j \frac{1}{2}:p^2:\right) = \exp\left(:\sum_{m=j}^{M} b_j^{(m)} (q+\beta_j p)^m:\right). \tag{41}$$

Considering that the three exponentials on the left hand side of Eq. (41) are exactly solvable in a finite Taylor series expansion, then it is the whole map. ■

Using the result of Theorem 2 and Corollary 1 we have that the polynomial we are interested, $f_3+\cdots+f_M$, is separable in $M+1$ solvable parts.

Finally, we have the following theorem.

Theorem 3. Under conditions of Corollary 1 and given the polynomial

$$f_3 + \ldots + f_M = \sum_{m=3}^{M} \sum_{i=0}^{m} a_i^{(m)} q^{m-i} p^i, \tag{42}$$

it is possible to write

$$e^{:f_3+\ldots+f_M:} \simeq \prod_{j=0}^{M} \exp\left(:\sum_{m=j}^{M} d_j^{(m)} (q+\beta_j p)^m:\right) \tag{43}$$

$$= \prod_{j=0}^{M} \exp\left(:-\beta_j \frac{1}{2} p^2:\right) \exp\left(:\sum_{m=j}^{M} d_j^{(m)} q^m:\right) \times \exp\left(:\beta_j \frac{1}{2} p^2:\right)$$

$$= \exp\left(:-\beta_0 \frac{1}{2} p^2:\right) \prod_{j=0}^{M} \exp(:Q^{(j)}(q):) \times \exp[:P^{(j)}(p):], \tag{44}$$

where $Q^{(j)} = \sum_{m=j}^{M} d_j^{(m)} q^m$, $P^{(j)} = (\beta_j - \beta_{j+1})\frac{1}{2}p^2$, with $\beta_{M+1}=0$, $d_j^{(m)}=0$ for $m<3$ and $j>m$, and where $d_j^{(m)}$ are functions depending on $a_j^{(m)}$ and β_j.

Proof. Using the BCH formula, equating terms and proceeding order by order (starting with $m=3$) we get recursively (see [4,15] for more details on this kind of procedure) the coefficients $d_j^{(m)}$ in terms of the $a_j^{(m)}$'s and β_j's. ■

Example 4.1. Let us consider the following functions:

$$f_4 = \sum_{i=0}^{4} a_i^{(4)} q^{4-i} p^i, \quad f_6 = \sum_{i=0}^{6} a_i^{(6)} q^{6-i} p^i. \tag{45}$$

These functions appear, for example, when considering the Hamiltonian associated to the pendulum ($H = p^2/2 - \cos q$), after taking the factorization

$$e^{:H:} = \hat{M} e^{:f_4+f_6:} + O(R_8), \tag{46}$$

$\hat{M}$ being a linear transformation [32]. In the approximation to $e^{:f_4+f_6:}$ we compare the cost of the methods following the separation in groups of monomials and the new separation previously proposed. According to [13] it is possible to separate $f_3+\cdots+f_6$ in 12 terms. If $f_3=f_5=0$ only eight of them are different from 0, and we can write

$$e^{:f_4+f_6:} = \prod_{i=1}^{8} e^{:g^{(i)}:} + O(R_8), \tag{47}$$

where

$$g^{(1)}=c_1q^4+c_2q^3p,\quad g^{(4)}=c_6q^4p^2,\quad g^{(7)}=c_{10}q^3p^3,$$
$$g^{(2)}=c_3q^2p^2,\quad g^{(5)}=c_7q^2p^4,\quad g^{(8)}=c_{11}qp^5+c_{12}p^6,$$
$$g^{(3)}=c_4qp^3+c_5p^4,\quad g^{(6)}=c_8q^6+c_9q^5p.$$

The coefficients c_i can be evaluated in terms of the $a_i^{(n)}$ using the BCH formula and equating terms [13]. Observe that the evaluation of $g^{(1)}$, $g^{(3)}$, $g^{(6)}$, and $g^{(8)}$ involve the computation of a root and for $g^{(2)}$ and $g^{(7)}$ an exponential, being $g^{(4)}$ and $g^{(5)}$ the cheapest to compute. On the other hand, from Theorem 3 we have

$$\exp(:f_4+f_6:) \tag{48}$$
$$=\exp\left(-:\beta_0\frac{1}{2}p^2:\right)\prod_{i=0}^{6}\exp(:d_i^{(4)}q^4+d_i^{(6)}q^6:)$$
$$\times\exp\left[:(\beta_i-\beta_{i+1})\frac{1}{2}p^2:\right]+O(R_8)$$

with $\beta_7=0$ and $d_5^{(4)}=d_6^{(4)}=0$. Observe that the number of Lie transformations is very similar to Eq. (47) but now each one involves only few multiplications and additions. We have computed Eqs. (47) and (48) repeatedly on different initial conditions and values of $a_i^{(n)}$, and we found that Eq. (48) is approximately four times faster. In addition, the algorithm has still seven free parameters, $\beta_0,\ldots,\beta_6$, to improve the accuracy of the method.

V. GENERALIZATION TO MORE VARIABLES

Let us consider the system with six variables, $z=(q_1,q_2,q_3,p_1,p_2,p_3)$, where a homogeneous polynomial of degree m can be written as

$$f_m=\sum_{i^{(6)}=m}a_{i_1,\ldots,i_6}q_1^{i_1}p_1^{i_2}q_2^{i_3}p_2^{i_4}q_3^{i_5}p_3^{i_6}, \tag{49}$$

with $i^{(6)}=i_1+\cdots+i_6$, which contains C_{m+5}^m monomials. Grouping terms we can rewrite Eq. (49) in the form

$$f_m=\sum_{m^{(3)}=m}g_{m_1m_2m_3}, \tag{50}$$

with $m^{(3)}=m_1+m_2+m_3$ and

$$g_{m_1m_2m_3}=\sum_{i_1=0}^{m_1}\sum_{i_2=0}^{m_2}\sum_{i_3=0}^{m_3}a_{i_1i_2i_3}^{(m_1m_2m_3)}q_1^{m_1-i_1}p_1^{i_1}q_2^{m_2-i_2}$$
$$\times p_2^{i_2}q_3^{m_3-i_3}p_3^{i_3}, \tag{51}$$

with $a_{i_1i_2i_3}^{(m_1m_2m_3)}=a_{m_1-i_1,i_1,m_2-i_2,i_2,m_3-i_3,i_3}$. Each polynomial $g_{m_1m_2m_3}$ contains $R_{m_1m_2m_3}\equiv(m_1+1)(m_2+1)(m_3+1)$ monomials, and these monomials are the same that appear when expanding the product

$$(q_1+\beta_1p_1)^{m_1}(q_2+\beta_2p_2)^{m_2}(q_3+\beta_3p_3)^{m_3}$$
$$=\sum_{i_1=0}^{m_1}\sum_{i_2=0}^{m_2}\sum_{i_3=0}^{m_3}C_{m_1}^{i_1}C_{m_2}^{i_2}C_{m_3}^{i_3}\beta_1^{i_1}\beta_2^{i_2}\beta_3^{i_3}q_1^{m_1-i_1}$$
$$\times p_1^{i_1}q_2^{m_2-i_2}p_2^{i_2}q_3^{m_3-i_3}p_3^{i_3}. \tag{52}$$

There is a problem in the generalization of Theorem 1 to more variables. The matrices with elements $\beta_1^{i_1}\beta_2^{i_2}\beta_3^{i_3}$, for different values of β_1,β_2,β_3, are not necessarily Vandermonde matrices, and their inverse is not guaranteed. Keeping this in mind, we proceed as follows.

Let us denote $S^{(m)}=\max\{R_{m_1m_2m_3}:m_1+m_2+m_3=m\}$. We define the ceiling function $\mathrm{Ce}:\mathbb{R}\to\mathbb{Z}$ such that given a real number it rounds up to the next integer. Then, it is easy to prove that

$$S^{(m)}=\begin{cases}\left(\frac{m}{3}+1\right)^3 & \text{if}\quad \frac{m}{3}=\mathrm{Ce}\left(\frac{m}{3}\right),\\ \left(\frac{m+1}{3}+1\right)^2\left(\frac{m-2}{3}+1\right) & \text{if}\quad \frac{m+1}{3}=\mathrm{Ce}\left(\frac{m+1}{3}\right),\\ \left(\frac{m+2}{3}+1\right)\left(\frac{m-1}{3}+1\right)^2 & \text{if}\quad \frac{m+2}{3}=\mathrm{Ce}\left(\frac{m+2}{3}\right),\end{cases} \tag{53}$$

and in a four-dimensional space ($m_3=0$)

$$S^{(m)}=\begin{cases}\left(\frac{m}{2}+1\right)^2 & \text{if}\quad \frac{m}{2}=\mathrm{Ce}\left(\frac{m}{2}\right),\\ \left(\frac{m+1}{2}+1\right)\left(\frac{m-1}{2}+1\right) & \text{if}\quad \frac{m+1}{2}=\mathrm{Ce}\left(\frac{m+1}{2}\right).\end{cases} \tag{54}$$

Theorem 4. Given $\beta_j=(\beta_{j,1},\beta_{j,2},\beta_{j,3})\in\mathbb{R}^3, j=1,\ldots,S^{(m)}+r$, with $r\geqslant 0$ chosen such that the matrices $V^{(m_1m_2m_3)}$ with components

$$V_{u,s}^{(m_1m_2m_3)}=\beta_{j_s,1}^{i_1}\beta_{j_s,2}^{i_2}\beta_{j_s,3}^{i_3}, \tag{55}$$

with $u=(m_3+1)(m_2+1)i_1+(m_3+1)i_2+i_3+1$, $i_k=0,\ldots,m_k$, $k=1,2,3$, $m_1+m_2+m_3=m$, $s=1,\ldots,R_{m_1m_2m_3}$ are nonsingular for at least one subset $\{j_i\}_{i=1}^{R_{m_1m_2m_3}}$ of $\{1,2,\ldots,S^{(m)}+r\}$, then each polynomial $g_{m_1m_2m_3}$ in Eq. (50) can be written as

$$g_{m_1m_2m_3}=\sum_{s=1}^{R_{m_1m_2m_3}} b_{j_s}^{(m_1m_2m_3)}(q_1+\beta_{j_s,1}p_1)^{m_1}\times(q_2+\beta_{j_s,2}p_2)^{m_2}(q_3+\beta_{j_s,3}p_3)^{m_3} \tag{56}$$

for different subsets $\{j_i\}_{i=1}^{R_{m_1m_2m_3}}$.

Proof. Similarly to the proof of Theorem 1, there exist at least one subset $\{j_i\}_{i=1}^{R_{m_1m_2m_3}}$ of $\{1,2,\ldots,S^{(m)}+r\}$ such that the matrix with elements given in Eq. (55) is nonsingular. Then, after expanding Eq. (56) we see that

$$\begin{Bmatrix} b_{j_1}^{(m_1m_2m_3)} \\ \vdots \\ b_{j_{R_{m_1m_2m_3}}}^{(m_1m_2m_3)} \end{Bmatrix} = (V^{(m_1m_2m_3)})^{-1} \begin{Bmatrix} A_1^{(m_1m_2m_3)} \\ \vdots \\ A_{R_{m_1m_2m_3}}^{(m_1m_2m_3)} \end{Bmatrix} \tag{57}$$

with

$$A_{(m_3+1)(m_2+1)i_1+(m_3+1)i_2+i_3+1}^{(m_1m_2m_3)} = a_{m_1-i_1,i_1,m_2-i_2,i_2,m_3-i_3,i_3}/(C_{m_1}^{i_1}C_{m_2}^{i_2}C_{m_3}^{i_3}).$$

Here, $b^{(m_1m_2m_3)}\in\mathbb{R}^N$ with $N=S^{(m)}+r$ but, only the previous $R_{m_1m_2m_3}$ components of the vector are different from 0.

Corollary 2. It is possible to write

$$f_m=\sum_{s=1}^{S^{(m)}+r}\left(\sum_{m^{(3)}=m} b_s^{(m_1m_2m_3)}(q_1+\beta_{s,1}p_1)^{m_1}\times(q_2+\beta_{s,2}p_2)^{m_2}(q_3+\beta_{s,3}p_3)^{m_3}\right), \tag{58}$$

where one possible solution for the vectors $b^{(m_1m_2m_3)}\in\mathbb{R}^N$ can be obtained taking only the $R_{m_1m_2m_3}$ components of each vector different from 0 according to Theorem 4.

Theorem 5. The Lie transformation associated to the polynomial

$$\sum_{m^{(3)}=m} b_s^{(m_1m_2m_3)}(q_1+\beta_{s,1}p_1)^{m_1}(q_2+\beta_{s,2}p_2)^{m_2}\times(q_3+\beta_{s,3}p_3)^{m_3} \tag{59}$$

has a finite Taylor expansion, being a Cremona map.

Theorem 6. Under conditions of Theorem 4 and given a general polynomial $f_3+\cdots+f_M$ in the six-dimensional phase space, it is possible to write

$$e^{:f_3+\ldots+f_M:}\simeq e^{:P^{(0)}:}\prod_{j=1}^{S^{(m)}+r} e^{:Q^{(j)}:}e^{:P^{(j)}:} \tag{60}$$

with

$$Q^{(j)}=\sum_{m=3}^{M}\sum_{m^{(3)}=m} d_j^{(m_1m_2m_3)}q_1^{m_1}q_2^{m_2}q_3^{m_3}, \tag{61}$$

$$P^{(j)}=\frac{1}{2}\sum_{i=1}^{3}(\beta_{j,i}-\beta_{j+1,i})p_i^2, \quad j=0,\ldots,S^{(m)}+r,$$

with $Q^{(0)}=\beta_{0,i}=\beta_{S^{(m)}+r+1,i}=0$ and where the coefficients $d_j^{(m_1m_2m_3)}$ depend on the coefficients $a_{m_1-i_1,i_1,m_2-i_2,i_2,m_3-i_3,i_3}$ and $\beta_{j,i}$.

Using the notation $\mathbf{q}=(q_1,q_2,q_3)$, $\mathbf{p}=(p_1,p_2,p_3)$ and

$$\nabla_q Q^{(i)}=\left(\frac{\partial Q^{(i)}}{\partial q_1},\frac{\partial Q^{(i)}}{\partial q_2},\frac{\partial Q^{(i)}}{\partial q_3}\right),$$

$$\nabla_p P^{(i)}=\left(\frac{\partial P^{(i)}}{\partial p_1},\frac{\partial P^{(i)}}{\partial p_2},\frac{\partial P^{(i)}}{\partial p_3}\right),$$

the algorithm for computing Eq. (60) is given by

$$\mathbf{q}_1=\mathbf{q}_0-\nabla_p P^{(0)}(\mathbf{p}_0)$$

do $j=1,S^{(m)}+r$

$$\mathbf{p}_j=\mathbf{p}_{j-1}+\nabla_q Q^{(j)}(\mathbf{q}_j)$$

$$\mathbf{q}_{j+1}=\mathbf{q}_j-\nabla_p P^{(j)}(\mathbf{p}_j)$$

enddo

where $\mathbf{q}_0$ and $\mathbf{p}_0$ correspond to the initial conditions. Here, $\mathbf{q}_i$, $\mathbf{p}_i$ correspond to the value of the vectors at the intermediate stages. Considering that the Lie transformation acts on initial conditions, the computation has to be done from left to right.

Observe that each evaluation is very cheap, where many of the coefficients of $d_j^{(m_1m_2m_3)}$ can be taken identically 0. In general, if the polynomial $f_3+\cdots+f_M$ contains all monomials ($\Sigma_{m=3}^{M}C_{m+5}^{m}$), it is possible to consider the same number of coefficients $d_j^{(m_1m_2m_3)}$ different from 0.

A. Generalization of the linear transformations

In this paper we have considered as linear maps the Lie transformations associated to $\Sigma_j\beta_j\frac{1}{2}p_j^2$ but, more general transformations depending only on the momenta can be considered

$$P=\sum_{ij}\ \beta_{ij}p_ip_j+\sum_{ijk}\ \gamma_{ijk}p_ip_jp_k+\cdots, \tag{62}$$

where the $\gamma_{ijk},\ldots$ can easily be used for reducing the number of $d_j^{(m_1m_2m_3)}$ coefficients, or just to have more free parameters for optimizing the algorithm. Another possibility is to consider the most general linear transformation, $\Sigma_{i,j}S_{i,j}z_iz_j$, with S a symmetric matrix. In the two-dimensional phase space we have $K=a\frac{1}{2}p^2+bpq+c\frac{1}{2}q^2$, and

$$e^{-:K:}q=(Aq+Bp)=A\left(q+\frac{B}{A}p\right)=Ae^{-(B/2A):p^2:}q,$$

if $A\neq 0$, where $A=\cosh(\eta)+(b/\eta)\sinh(\eta)$,$B=(a/\eta)\sinh(\eta)$ and $\eta=\sqrt{b^2-ac}$. Then, with the exception of the trivial case $A=0$, to use the linear transformations depending only on p is equivalent to the most general linear transformation. However, this is not the case for higher dimensions since all q_i and p_i are mixed by the linear transformations. It increases considerably the number of parameters of the method at the price of a higher computational cost but, allows to write the algorithm with less that $S^{(m)}+r$ transformations [16,4,14,15]. However, the number of coefficients $d_j^{(m_1m_2m_3)}$ different from 0 is essentially the same. Since we will be interested in using these parameters for optimizing the algorithm, we think that to work with such a number of free parameters can increase the error of the method (instead of reducing it) unless an extremely delicate analysis is carried out. For this reason, we decided just to use the previous cheap and simple maps, depending only on the momenta.

For our scheme, the coefficients $\beta_{i,j}$ have to satisfy very few constraints and the coefficients $d_j^{(m_1m_2m_3)}$ are relatively easy to obtain. In addition, in most cases it is possible to take $r=0$. This is the case, for example, in the four dimensional space $(m_3=0)$. All matrices that have to be nonsingular, according to Theorem 4, are submatrices of a matrix with elements $\beta_{j,1}^{i_1}\beta_{j,2}^{i_2}$, $i_1=0,\ldots,m_1$,$i_2=0,\ldots,m_2$, $0\leqslant i_1+i_2\leqslant m$ which is of dimension $\mathbb{R}^{u\times u}$ with $u=\Sigma_{i=0}^{m}(i+1)=[(m+1)(m+2)]/2$. According to Eq. (54) we have that $u<2S^{(m)}$ and we can choose $2S^{(m)}$ values of $\beta_{j,1}$, $\beta_{j,2}$ such that all previous matrices are invertible. However, in the six-dimensional space we have that $u=\Sigma_{i=0}^{m}[(i+1)(i+2)]/2=[6+11m+6m^2+m^3]/6$, which is higher than $3S^{(m)}$ for $m>4$. However, as mentioned, this fact does not make the algorithm much more costly.

Example 5.1. In order to illustrate how to obtain one possible method in a high-dimensional system, we consider the example in four dimensions presented in [15] for a static storage ring represented by the symplectic map

$$\mathcal{M}_4=\hat{M}e^{:f_3:}e^{:f_4:}, \tag{63}$$

where $\hat{M}$ is a 4×4 symplectic matrix and f_3, f_4 can be written in the following form:

$$\begin{aligned}f_3=&a_{1,1}^{(3)}q_1^3+a_{1,2}^{(3)}q_1^2p_1+a_{1,3}^{(3)}q_1p_1^2+a_{1,4}^{(3)}p_1^3+a_{2,1}^{(3)}q_1q_2^2\\&+a_{2,2}^{(3)}q_1q_2p_2+a_{2,3}^{(3)}q_1p_2^2+a_{2,4}^{(3)}p_1q_2^2+a_{2,5}^{(3)}p_1q_2p_2\\&+a_{2,6}^{(3)}p_1p_2^2,\end{aligned}$$

$$\begin{aligned}f_4=&a_{1,1}^{(4)}q_1^4+a_{1,2}^{(4)}q_1^3p_1+a_{1,3}^{(4)}q_1^2p_1^2+a_{1,4}^{(4)}q_1p_1^3+a_{1,5}^{(4)}p_1^4\\&+a_{2,1}^{(4)}q_2^4+a_{2,2}^{(4)}q_2^3p_2+a_{2,3}^{(4)}q_2^2p_2^2+a_{2,4}^{(4)}q_2p_2^3+a_{2,5}^{(4)}p_2^4\\&+a_{3,1}^{(4)}q_1^2q_2^2+a_{3,2}^{(4)}q_1^2q_2p_2+a_{3,3}^{(4)}q_1^2p_2^2+a_{3,4}^{(4)}q_1p_1q_2^2\\&+a_{3,5}^{(4)}q_1p_1q_2p_2+a_{3,6}^{(4)}q_1p_1p_2^2+a_{3,7}^{(4)}p_1^2q_2^2+a_{3,8}^{(4)}p_1^2q_2p_2\\&+a_{3,9}^{(4)}p_1^2p_2^2.\end{aligned}$$

Observe that f_3 and f_4 only contain 29 from amongst the $C_6^3+C_7^4=54$ monomials. If we define $u_i^{(n)}=(q_1+\beta p_1)^{n-i}(q_2+\beta p_2)^i$ we observe that all monomials appearing in f_3, f_4 are the monomials contained in $u_0^{(3)}$, $u_2^{(3)}$, $u_0^{(4)}$, $u_2^{(4)}$, and $u_4^{(4)}$. Since $S^{(4)}=9$ and this number corresponds to the number of monomials in $u_2^{(4)}$ then we can take

$$e^{:f_3:}e^{:f_4:}=e^{:P^{(0)}(p):}\prod_{j=1}^{9}e^{:Q^{(j)}(q):}e^{:P^{(j)}(p):}+O(R_5) \tag{64}$$

with

$$Q^{(j)}=d_{1,j}^{(3)}q_1^3+d_{2,j}^{(3)}q_1q_2^2+d_{1,j}^{(4)}q_1^4+d_{2,j}^{(4)}q_2^4+d_{3,j}^{(4)}q_1^2q_2^2, \tag{65}$$

$$P^{(j)}=\tfrac{1}{2}(\beta_{j,1}-\beta_{j+1,1})p_1^2+\tfrac{1}{2}(\beta_{j,2}-\beta_{j+1,2})p_2^2,\quad j=0,\ldots,9,$$

and $Q^{(0)}=\beta_{0,1}=\beta_{0,2}=\beta_{10,1}=\beta_{10,2}=0$.

We can choose nine pairs $\beta_{j,1},\beta_{j,2}$, $j=1,\ldots,9$ such that all matrices originating from the previous products are nonsingular. We have $d^{(3)},d^{(4)}\in\mathbb{R}^9$ but, only $d_{3,j}^{(4)}$ has to have all components different from 0. However, if desired, we can take all components of the vectors different from 0 and an optimization procedure can be used. This reduces, in general, the absolute value of the coefficients $d_{j,k}^{(i)}$, producing a method with smaller errors [14,15]. In the following we show how to simplify even more the procedure for both choosing the $\beta_{i,j}$ and obtaining the coefficients $d_{i,j}^{(k)}$.

Finally, we must mention that the approximation to $\mathcal{M}_4$ using Eq. (64) is several times faster than using a factorization in monomials [5] or different groups of monomials [13,7].

VI. CHOOSING AN ALTERNATIVE BASIS

In the preceding sections we observed that the computational cost of a given splitting method is clearly dependent on how the Hamiltonian has been split. In the two-dimensional phase space we have considered two bases for writing an homogeneous polynomial of degree m,

$$f_m=\sum_{i=0}^{m}\ \alpha_i^{(1,2)}\mathcal{P}_{m,i}^{(1,2)} \tag{66}$$

with $\mathcal{P}^{(1)}_{m,i}=q^{m-i}p^i$ and $\mathcal{P}^{(2)}_{m,i}=(q+\beta_i p)^m$, $i=0,\ldots,m$. The drawback of using $\mathcal{P}^{(1)}_{m,i}$ is that the Lie transformations associated to some elements of the basis are relatively costly. The problem of using $\mathcal{P}^{(2)}_{m,i}$ could be that, for large m, many β_i are necessary. This may be uncomfortable to work with, specially when a higher-dimensional space is considered, and when looking for a good set of values for these β_i.

On the other hand, the Lie transformation associated to some elements of $\mathcal{P}^{(1)}_{m,i}$ are very cheap to compute. Suppose that $\mathcal{P}^{(1)}_{m,i}$, $i=0,\ldots,r$ are the cheap terms, then we can consider the new basis $\{\mathcal{P}^{(3)}_{m,i}\}^m_{i=0}=\{\mathcal{P}^{(1)}_{m,0},\ldots,\mathcal{P}^{(1)}_{m,r},\mathcal{P}^{(2)}_{m,r+1},\ldots,\mathcal{P}^{(2)}_{m,m}\}$ where all terms are cheap to compute and a smaller number of β_i are necessary.

Example 6.1. In f_6 we have $\{\mathcal{P}^{(1)}_{6,i}\}^6_{i=0}=\{q^6,q^5p,q^4p^2,q^3p^3,q^2p^4,qp^5,p^6\}$ but, the Lie transformations associated to q^6, q^4p^2, q^2p^4, and p^6 only involve multiplications and additions. Then, an interesting basis could be $\{\mathcal{P}^{(3)}_{6,i}\}^6_{i=0}=\{q^6,q^4p^2,q^2p^4,p^6,(q+\beta_1p)^6,(q+\beta_2p)^6,(q+\beta_3p)^6\}$. If f_4 also appears in the Hamiltonian, the natural choice for the basis would be $\{\mathcal{P}^{(3)}_{4,i}\}^4_{i=0}=\{q^4,p^4,(q+\beta_1p)^4,(q+\beta_2p)^4,(q+\beta_3p)^4\}$, which allows to group them with the elements of $\mathcal{P}^{(3)}_{6,i}$ without needing additional Lie transformations. Finally, $e^{:f_4+f_6:}$ can be written as the product of seven simple Lie transformations. Observe that this is not a Cremona map since the terms q^4p^2 and q^2p^4 are now present. These terms have a singularity and one has to decide if it is or it is not worth to use them for a given problem.

Example 6.2. The polynomial f_3+f_4 in the four-dimensional phase space has 55 independent monomials, and 28 among them can be grouped in four cheaply and exactly solvable polynomials,

$$g_1=\sum_{i=1}^{3} b_i q_1^{3-i}q_2^i+\sum_{i=0}^{4} b_{4+i}q_1^{4-i}q_2^i,$$

$$g_3=\sum_{i=1}^{3} p_1^i(b_{15+2i}q_2^{3-i}+b_{16+2i}q_2^{4-i}),$$

$$g_2=\sum_{i=1}^{3} b_{8+i}p_1^{3-i}p_2^i+\sum_{i=0}^{4} b_{12+i}p_1^{4-i}p_2^i,$$

$$g_4=\sum_{i=1}^{3} q_1^i(b_{21+2i}p_2^{3-i}+b_{22+2i}p_2^{4-i}).$$

The polynomials $u^{(n)}_i=(q_1+\beta p_1)^{n-i}(q_2+\beta p_2)^i$ contain $(n-i+1)(i+1)$ different monomials. Then, among all $u^{(n)}_i$, we have to consider more carefully $u^{(4)}_1$, $u^{(4)}_2$, and $u^{(4)}_3$, since they have 8, 9 and 8 different monomials, respectively. But, observe that each g_i contains an element of $u^{(4)}_1$, $u^{(4)}_2$, and $u^{(4)}_3$ so, only five more terms are necessary to reproduce all monomials, and this can be achieved with

$$e^{:f_3+f_4:}=\left(\prod_{i=1}^{4} e^{:g_i:}\right)e^{:P^{(0)}(p):}\prod_{i=1}^{5} e^{:Q^{(i)}(q):}e^{:P^{(i)}(p):}+O(R_5). \tag{67}$$

We can choose five pairs $\beta_{j,1},\beta_{j,2}$, $j=1,\ldots,5$ such that all matrices originating from the previous products are nonsingular, and we have to invert matrices of dimension 5×5 or smaller. We have now $d^{(3)},d^{(4)}\in\mathbb{R}^5$, having most of them several components identically 0.

VII. OPTIMIZING THE ALGORITHMS

In previous sections we only considered the computational cost of the algorithms. It is possible to use the free parameters β_i in order to slightly reduce the number of maps in the factorization at the extraordinary price of needing to solve very complicated nonlinear systems of equations. On the other hand, to consider algorithms with free parameters for optimization purposes usually produces more efficient methods [28]. Then, we can use these β_i in order to get (without increasing the cost) more accurate results. From Theorem 3 we have, in the two-dimensional phase space,

$$\exp(:f_3+\cdots+f_M:)=\left[e^{:-\beta_0(1/2)p^2:}\prod_{i=0}^{M} e^{:Q^{(i)}(q):}e^{:P^{(i)}(p):}\right]\times e^{:R_{M+1}:}+O(R_{M+2}), \tag{68}$$

where R_{M+1} is a homogeneous polynomial of degree $M+1$, containing the leading error terms

$$R_{M+1}=\sum_{i=0}^{M+1}\alpha_i q^{M+1-i}p^i \tag{69}$$

and α_i, $i=0,\ldots,M+1$, depend on the coefficients β_i, $i=0,\ldots,M$ we have chosen, and the coefficients of the problem. If we define the error of a method by $E_1\equiv(\Sigma_i\alpha_i^2)^{1/2}$, then we can look for the coefficients β_i that minimize E_1. Since E_1 also depends on the coefficients $a^{(m)}_i$, the optimal choice for the β_i will depend on each particular problem. A simpler procedure to choose the best set of coefficients β_i is to consider that $F(z)=f_3+\cdots+f_M$ is a constant of the motion. Then, we can take a number of different initial conditions in the region of interest. For each initial condition z_0, we evaluate the relative error $|[F(z_1)-F(z_0)]/F(z_0)|$, where z_1 is the one map approximation, and finally we take its average value, say $E_2(\beta)$. Next, we have to repeat the same process for different values of $\beta=(\beta_0,\ldots,\beta_M)$ and to look for the value that minimizes $E_2(\beta)$. In general, $E_1(\beta)$ and $E_2(\beta)$ have their minimum very close to each other, and it is enough to compute only E_2 since it is easier to do it. Observe that E_1, $E_2:\mathbb{R}^{M+1}\to\mathbb{R}$ are positive definite functions, and their minimums can be obtained numerically in a relatively easy way. If the problem is simple enough, we can take random values for the β_i, to compute E_1 and/or E_2, and to make a finer search around the best results. Alternatively, we can choose a randomized approach as initial guess, and to apply a combination of Powell's hybrid method (NAG routine C05NBF) and the optimization routine E04JYF. In case the routine does not converge to a local minimum, a new random value can be used for a new search [28]. Several local minimums can be found, and one has to choose the optimal one.

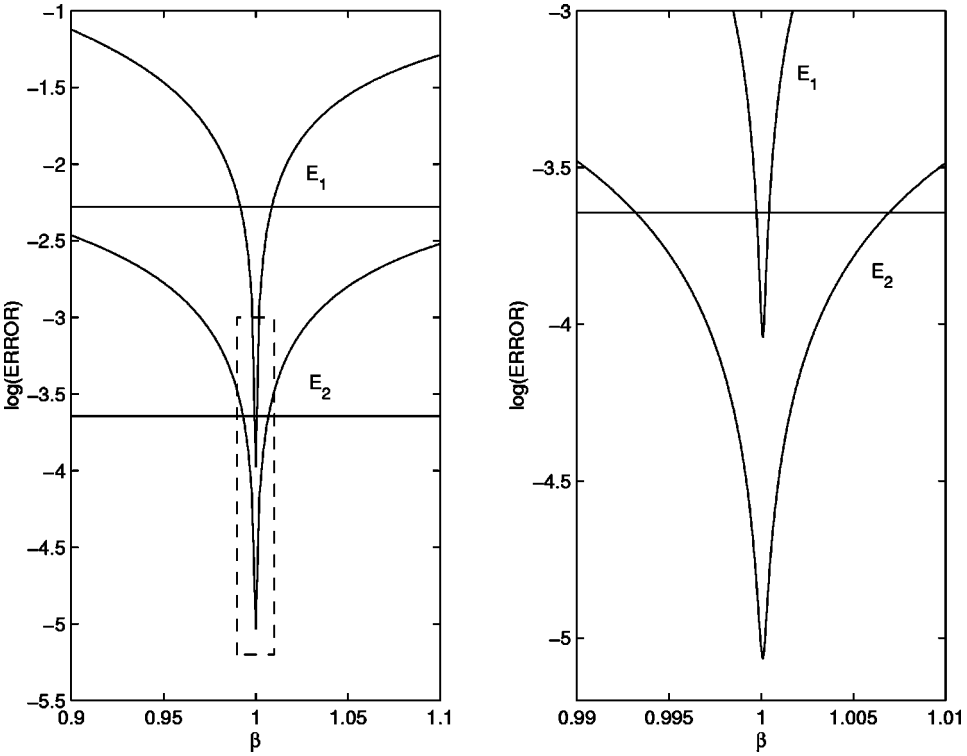

FIG. 1. Error of the method (70) for $(\beta_1,\beta_2,\beta_3)=(-1.030,0.217,-1.022)\beta$. E_1 measures the Euclidean norm of the coefficients at the leading error term and E_2 measures the average relative error in the Hamiltonian. The horizontal lines correspond to the errors obtained with Eq. (71).

Example 7.1. Let us consider f_4 from Eq. (45) with [32]

$$(a_0^{(4)},\ldots,a_4^{(4)})=10^{-2}\times(2.411,-3.812,3.716,-2.089,0.5168)$$

and the basis $\{q^4,p^4,(q+\beta_1 p)^4,(q+\beta_2 p)^4,(q+\beta_3 p)^4\}$. We consider the approximation

$$e^{:f_4:}\simeq e^{:d_1 q^4:}e^{:d_2 p^4:}\prod_{i=1}^{3}\exp(:d_{i+2}(q+\beta_i p)^4:). \quad (70)$$

We took 100 different initial conditions in the region $q_0,p_0\in(-1/2,1/2)$ and measured the values of $E_1(\beta)$ and $E_2(\beta)$ for a large number of different values of $\beta_1,\beta_2,\beta_3\in(-2,2)$. Numerical experiments indicated that most local minimums of E_1 and E_2 nearly coincide, as expected. In particular, an interesting local minimum for both was found at $\beta_{op}=(\beta_1,\beta_2,\beta_3)\simeq(-0.897,-0.239,-1.033)$. However, if we slightly change our problem, for example replacing $a_1^{(4)}$ by $a_1^{(4)}/10$, we observe that β_{op} is no longer optimal so, a new search has to be done, and the optimal value we found is $\beta_{op}\simeq(-1.030,0.217,-1.022)$. In order to illustrate how the error depends on the choice of the β_i, in Fig. 1 we present, for this last case, the results obtained for $E_1(\beta)$ and $E_2(\beta)$ along the uniparametric family $(\beta_1,\beta_2,\beta_3)=(-1.030\beta,0.217\beta,-1.022\beta)$ with $\beta\in(0.9,1.1)$, which approximately cross through the minimum at $\beta=1$. Observe that the minimum is very narrow. This is in agreement with the comments on [4] where only very few values of the parameters in the Cremona maps had small error coefficients. For comparison, we have computed

$$e^{:f_4:}=e^{:g^{(1)}:}e^{:g^{(2)}:}e^{:g^{(3)}:} \quad (71)$$

with $g^{(1)}=c_1q^4+c_2q^3p$, $g^{(2)}=c_3q^2p^2$, and $g^{(3)}=c_4qp^3+c_5p^4$. In Fig. 1 we show in horizontal lines the values of E_1 and E_2 obtained. We found that the computational cost of Eq. (71) is approximately three times more expensive and still it gives an error more than one order of magnitude higher than Eq. (70) for β_{op}. Very similar results are obtained for the original problem with the previous value of β_{op}.

Notice that the error at the minimum decreases by several orders of magnitude, and it is very sensitive to the value of β. In addition, at the minimum we see that $\beta_1\approx\beta_3$, and this fact makes the corresponding Vandermonde matrix nearly singular, and the coefficients b_i can take large values. We think it is important to better understand this point in order to locate the minimums, especially when we are working in a higher-dimensional space, were many $\beta_{i,j}$ coefficients are involved.

In Refs. [16,4] a factorization similar to Eq. (60) is considered but, replacing the $e^{:P^{(j)}:}$ factors by more general linear symplectic transformations $\mathcal{L}_j$. From the relation between this set of linear transformations (acting on a normalized basis of polynomials depending only on coordinates) and another basis for general polynomials (composed by normalized monomials) they build the named *sensitive vectors*. From these vectors they build the corresponding *Gram matrix*, whose eigenvalues indicate how good is the choice of the set of $\mathcal{L}_j$. For instance, if we choose the basis $\{(q+\beta_i p)^4\}_{i=0}^4$, the sensitive vectors are $\sigma^r=(\sigma_0^r,\ldots,\sigma_4^r)$, $r=0,\ldots,4$, with $\sigma_j^r=(C_4^r)^{1/2}\beta_j^r$, and the

components of the Gram matrix are $\Gamma_{rs}=\frac{1}{5}\Sigma_{j=0}^{4}\sigma_j^r\sigma_j^s$, being closely related to the Vandermonde matrix.

In our context, this analysis would be equivalent, in some sense, to the study of the eigenvalues of the matrices $V^{(m_1m_2m_3)}$ for maximizing the minimum eigenvalue, in order to get relatively small values for the coefficients $b_j^{(m_1m_2m_3)}$. One expects that, after the composition of the exponentials, the error will remain relatively small. On the other hand, we observed that the optimal choice for the linear transformations also depends on each particular problem (on the coefficients $a_{i_1,\ldots}$). However, this analysis for the eigenvalues of $V^{(m_1m_2m_3)}$ can give a good starting point for the numerical search of the β coefficients, and this could be the subject of a future work.

VIII. CONCLUSIONS

In this paper we have studied different symplectic map approximations for polynomial Hamiltonian systems. In general, one has to separate the Hamiltonian in solvable parts. Next, one has to compute each part and finally, to compose the results in order to have an approximation to the original Hamiltonian. However, the Hamiltonian can be separated in many different ways. The efficiency of a method depends on its computational cost and its accuracy. But, it depends on how H is separated. We have analyzed this aspect in the paper and presented methods (most of them are Cremona maps) with the following properties.

(1) They are cheap to compute. The cost, in general, is very similar to the corresponding Taylor map up to the same order.

(2) There is a systematic and easy procedure for building the methods.

(3) They have a number of free parameters for optimizing the methods, and this can be done very easily.

The numerical experiments clearly confirm the efficiency of the new methods versus other schemes, although this is ultimately dependent on each particular problem.

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