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Symplectic Integrators for Polynomial Hamiltonians with Applications to Accelerator Physics

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Abstract

We show how to build efficient symplectic integrators for polynomial Hamiltonian systems. The efficiency of a numerical method depends both on its computational cost as well as on its accuracy. Polynomial Hamiltonians are separable in exactly solvable parts in many different ways, and we will study how to find a separation for the Hamiltonian in a few number of cheap terms. The new methods will depend on some free parameters and we will also indicate how to choose these parameters in order to improve the accuracy without increasing the computational cost.

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1 Introduction

In this paper we study how to obtain new efficient symplectic integrators for polynomial Hamiltonian systems. This class of systems appear frequently in accelerator physics [4, 5, 6, 8, 11, 17, 21] and it is important to have good integrators. 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 that too many of these particles disappear in the walls of the ring.

Provided the sincrotron radiation is neglected, the system can be considered as 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 is the initial condition we will 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 will have $z(N)=\mathcal{M}_H^N z_0$.

In general, it is not possible to obtain 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 and we will only consider symplectic integrators. At the same time we are interested in numerical methods as cheap as possible to compute which at the same time had a good accuracy. In general, for each problem (or Hamiltonian) it is necessary to make a complicated analysis in order to obtain an efficient method. However, in this paper we will show how to obtain, in an easy way, cheap symplectic integrators which are very efficient in most of the cases.

2 Mathematical Background

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

$$\{f,g\}=\sum_{i,j}\frac{\partial f}{\partial z_i}J_{ij}\frac{\partial g}{\partial z_j} \qquad with \qquad J=\begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}. \tag{1}$$

Here I and 0 are the $n\times n$ identity and zero matrices, respectively. Following [4] we will denote by $:f(z):$ the Lie operator associated to $f(z)$. It acts on a function, $g(z)$, as

$$:f(z):g(z)=\{f(z),g(z)\}. \tag{2}$$

We define the Lie transformation associated to f by

$$e^{:f:}=\sum_{k=0}^{\infty}\frac{:f:^k}{k!}, \tag{3}$$

where

$$:f:^0 g=g, \qquad :f:^k g=\{f\,,:f:^{k-1}g\}. \tag{4}$$

In order to make the paper self consistent, in the following we collect some properties of Lie operators and Lie transformations which we will use later. We highly recommend refs. [4, 5] for more details and proofs.

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

$$e^{:f(z):}g(z) = g(e^{:f(z):}z). \tag{5}$$

Considering that

$$[:f:,:g:] \;\equiv :f::g: - :g::f: = :\{f,g\}:, \tag{6}$$

we see that the Lie algebra of functions, with the Poisson bracken 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 (6), we have that

$$e^{:f:}e^{:g:} = e^{:h:}, \tag{7}$$

where

$$h = f + g + \frac{1}{2}\{f,g\} + \frac{1}{12}\left(\{f,\{f,g\}\} + \{g,\{g,f\}\}\right) + \dots \tag{8}$$

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

$$e^{:f(z):} : g(z) : e^{-:f(z):} = \, : e^{:f(z):}g(z) : \, = \, : g(e^{:f(z):}z) : \tag{9}$$

and then

$$\exp\left(:f(z):\right)\exp\left(:g(z):\right)\exp\left(-:f(z):\right) = \exp\left(:g(e^{:f(z):}z):\right). \tag{10}$$

For the particular cases $f(q)$ and $g(p)$, the Taylor expansion of their associated Lie transformations (3) terminates when acting on (q,p)

$$e^{:f(q):}\left\{\begin{array}{c} q \\ p \end{array}\right\} = \left\{\begin{array}{c} q \\ p + \nabla_q f(q) \end{array}\right\}; \quad e^{:g(p):}\left\{\begin{array}{c} q \\ p \end{array}\right\} = \left\{\begin{array}{c} q - \nabla_p g(p) \\ p \end{array}\right\}. \tag{11}$$

Given a Hamiltonian function, $H(z) \in \mathbb{R}$, the Hamilton equations are given by

$$\begin{aligned} \dot{z} &= \{z\,,\, H(z)\} \\ &= -:H(z):z, \end{aligned} \tag{12}$$

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

$$z_t = e^{-t:H(z_0):}z_0, \tag{13}$$

which can be considered as a change of coordinates from z_0 to z_t, and then the Poisson bracket, $: H(z_0) : z_0 = \{H(z_0), z_0\}$, is well defined. If the Hamiltonian is time-independent then $H(z)$ is a constant of the movement since $\frac{d}{dt}H(z) = -\{H(z), H(z)\} = 0$, and then

$$z_t = e^{-t:H(z_0):}z_0 \quad \Rightarrow \quad z_0 = e^{t:H(z_t):}z_t, \tag{14}$$

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 $H(z) = -f(z)$.

3 Splitting the map in solvable parts

Let us consider that $H(z)$ 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 has sense to consider $H = \sum_i H_i$ where H_i are homogeneous polynomials of degree i, and to consider only terms up to a given order, say M

$$H \sim \sum_{i=1}^{M} H_i. \tag{15}$$

Considering that H_1 and H_2 are exactly solvable we can formally write

$$\exp\left(- : H :\right) = \exp\left(: f_1 :\right)\, \exp\left(: f_2 :\right)\, \mathcal{N} \tag{16}$$

with

$$\mathcal{N} = \exp\left(: \sum_{i>2} f_i :\right), \tag{17}$$

and where f_i are homogeneous polynomials of degree i. Usually it is only known the Taylor 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 [7] it is possible to write

$$e^{:g_1:}\, e^{:g_2:} \dots e^{:g_M:} z_0 = \mathcal{T}_H^{(M)}(z_0) + r_{M+1}(z_0) \tag{18}$$

where r_{M+1} is a polynomial with terms of degree $M+1$ or higher and the g_is are homogeneous polynomial 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. Ocurrences of the symbol g_k in different places do not necessarily refer to the same polynomial. Finally, from (18) and using the BCH formula, (16) and (17) are easily obtained.

In this paper we are interested in approximating

$$e^{:f_3+\ldots+f_M:}z, \tag{19}$$

but, this transformation usually has not explicit solution.

Given the homogeneous polynomial in a two dimensional space

$$f_m = \sum_{i=0}^{m} a_i\, q^{m-i} p^i, \tag{20}$$

it is possible to write it as a sum of exactly solvable parts [14, 11, 21, 22, 18]. For example, each monomial $aq^n p^m$ is exactly solvable:

$$\left\{ \begin{array}{c} \bar{q} \\ \bar{p} \end{array} \right\} = e^{a:q_0^n p_0^m:} \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\} = \left\{ \begin{array}{c} A^m q_0 \\ p_0/A^n \end{array} \right\} \tag{21}$$

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

$$\left\{ \begin{array}{c} \bar{q} \\ \bar{p} \end{array} \right\} = e^{a:q_0^m p_0^m:} \left\{ \begin{array}{c} q_0 \\ p_0 \end{array} \right\} = \left\{ \begin{array}{c} Eq_0 \\ p_0/E \end{array} \right\} \tag{22}$$

with $E = \exp(-amq_0^{m-1}p_0^{m-1})$. Observe that the evaluation of each transformation involves the computation of an exponential or a root (unless $n/(n-m)$ and $m/(n-m)$ were both integers). Here $(\bar{q}, \bar{p})$ are written in terms of a summable infinite series on (q_0, p_0). Observe that (21) has singularities.

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

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q} \tag{23}$$

are exactly solvable. For example, in (22), if we take the Hamiltonian $H = -aq^m p^m$, the system to solve is

$$\left. \begin{array}{c} \dot{q} = -maq^m p^{m-1} \\ \dot{p} = maq^{m-1}p^m \end{array} \right\} \quad \Rightarrow \quad \left\{ \begin{array}{c} \dot{q} = -ma(q_0^{m-1}p_0^{m-1})q \\ \dot{p} = ma(q_0^{m-1}p_0^{m-1})p \end{array} \right. \tag{24}$$

where we have considered the known fact that $H_0 = -aq_0^m p_0^m$ is a constant of the movement so $qp = q_0 p_0$ and integrating (24) from $t = 0$ to 1, the solution (22) is obtained. Similarly we can obtain the solution for (21) (see [14]). On the other hand, if we consider $H = -(aq^m + bq^{m-1}p)$, $m > 2$, we have [17]

$$\left.\begin{array}{l} \dot{q} = -bq^{m-1} \\ \dot{p} = amq^{m-1} + b(m-1)q^{m-2}p \end{array}\right\} \Rightarrow \left\{ \begin{array}{l} \bar{q} = q_0[1 + (m-2)bq_0^{m-2}]^{\frac{1}{2-m}} \\ \bar{p} = (H_0 - a\bar{q}^m) \,/\, \left(b\bar{q}^{m-1}\right). \end{array}\right. \tag{25}$$

There are several works looking for different groups of monomials with exact solution in order to write a polynomial in as few number of solvable terms as possible [17, 21, 18]. However, we must say that there is not a unique way to separate a Hamiltonian in solvable parts, and in the next section we will present a different way to split the Hamiltonian which usually gives more efficient methods. For higher dymensional systems, it is interesting to remember the following properties:

1. Given the $2r$-dimensional Hamiltonian

$$H = \prod_{i=1}^{r} H^{(i)}(q_i, p_i), \tag{26}$$

then each $H^{(i)}(q_i, p_i)$, $\; i = 1, \ldots, r$ is a constants of the movement. For computing the flow for (q_s, p_s) one can consider the Hamiltonian $\alpha H^{(s)}(q_s, p_s)$ with $\alpha = \prod_{i \neq s} H^{(i)}(q_i, p_i)$ being a constant.

2. Given the $2r$-dimensional Hamiltonian

$$H = \sum_{i=1}^{r} H^{(i)}(q_i, p_i) \tag{27}$$

then each $H^{(i)}(q_i, p_i)$, $\; i = 1, \ldots, r$ is a constants of the movement. For computing the flow for (q_s, p_s) one can consider only the Hamiltonian $H^{(s)}(q_s, p_s)$.

On the other hand, in many problems the Hamiltonian is separable in two parts, i.e. $H = A(p) + B(q)$, and one has to approximate $e^{:\epsilon A + \epsilon B:}$ up to a given order in ϵ (usually the time step) where $e^{:\epsilon A:}$ and $e^{:\epsilon B:}$ are exactly solvable. Then, one can consider [19, 10, 23, 24, 20, 2, 3]

$$e^{:\epsilon A + \epsilon B:} = \prod_{i=1}^{k} e^{:\epsilon a_i A:}\, e^{:\epsilon b_i B:} + O(\epsilon^{M+1}), \tag{28}$$

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.

Some times, other terms of the Lie algebra generated by A and B are also solvable. This is the case when $A = p^2$, where $\{B(q), \{B(q), A(p)\}\} = C(q)$ and we can substitute the $e^{:\epsilon b_i B:}$ terms by the more general $e^{:\epsilon b_i B + \epsilon^3 c_i C:}$ terms (with c_i a constant to be determined), giving more efficient methods [19, 13, 2]. We observe that an efficient way to build an integrator is to consider all elements which can be cheaply evaluated and to try to reproduce the original problem up to a given order by composition of these elements.

4 Using cheap solvable parts

We have seen from (11) that the computation of $e^{:f(q):}$ and $e^{:g(p):}$ are trivial. Based in this fact, in this paper we are interested in looking for integrators which can be written as

$$e^{:f_3+\ldots+f_M:} = \prod_{i=1}^{k} e^{:Q^{(i)}(q):}\, e^{:P^{(i)}(p):} + O(R_{M+1}), \tag{29}$$

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

$$z_1 = \prod_{i=1}^{k} e^{:Q^{(i)}:}\, e^{:P^{(i)}:}\, z_0 = F(z_0) \tag{30}$$

is a polynomial function of z_0, and then this approximation can be considered as a Cremona map [1, 8, 12].

In the following we will prove in a simple way that this factorization is always possible and we will present an easy way to obtain some possible compositions. Obviously, the optimal integrator (the best choice for k and the polynomials $Q^{(i)}$ and $P^{(i)}$) will depend on each particular problem. This is what happens in symplectic integrators for (28) where the best choice of k and the coefficients $\{a_i,\ b_i\}$ will 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.

4.1 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 (20). We have:

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

$$\sum_{i=0}^{m} a_i \, q^{m-i} p^i = \sum_{j=0}^{m} b_j (q + \beta_j p)^m. \tag{31}$$

PROOF: We will prove the Theorem by giving the solution for the coefficients b_j. We have that

$$(q + \beta_j p)^m = \sum_{i=0}^{m} C_m^i \beta_j^i q^{m-i} p^i, \tag{32}$$

where $C_m^i := \dfrac{m!}{i!(m-i)!}$. Then, from (31) we have

$$a_i = \sum_{j=0}^{m} C_m^i \beta_j^i b_j, \qquad i = 0, \ldots, m, \tag{33}$$

which can be written in matrix form

$$\overbrace{\begin{pmatrix} C_m^0 & 0 & \ldots & 0 \\ 0 & C_m^1 & & \vdots \\ \vdots & & \ddots & \vdots \\ 0 & \ldots & \ldots & C_m^m \end{pmatrix}}^{C^{(m)}} \overbrace{\begin{pmatrix} 1 & \ldots & 1 \\ \beta_0 & \ldots & \beta_m \\ \vdots & & \vdots \\ \beta_0^m & \ldots & \beta_m^m \end{pmatrix}}^{V^{(m)}(\beta)} \left\{ \begin{array}{c} b_0 \\ b_1 \\ \vdots \\ b_m \end{array} \right\} = \left\{ \begin{array}{c} a_0 \\ a_1 \\ \vdots \\ a_m \end{array} \right\}. \tag{34}$$

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

$$\left\{ \begin{array}{c} b_0 \\ \vdots \\ b_m \end{array} \right\} = \left(V^{(m)} \right)^{-1} \left\{ \begin{array}{c} a_0 / C_m^0 \\ \vdots \\ a_m / C_m^m \end{array} \right\}. \qquad \square \tag{35}$$

This Theorem can be considered equivalent to the Theorem 5 given in [9], but here we give the explicit relation between the coefficients b_i and β_i, a_i. We can think on $\{q^{m-i} p^i\}_{i=0}^m$, and $\{(q + \beta_i p)^m\}_{i=0}^m$ as two different basis for homogeneous polynomials of degree m, and the linear relation (35) corresponds to a change of coordinates. For a general polynomial we have:

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

$$\begin{aligned} \sum_{m=1}^{M} \sum_{i=0}^{m} a_i^{(m)}\, q^{m-i} p^i &= \sum_{m=1}^{M} \left(\sum_{j=0}^{m} b_j^{(m)} (q + \beta_j p)^m \right) \\ &= \sum_{j=0}^{M} \left(\sum_{m=j}^{M} b_j^{(m)} (q + \beta_j p)^m \right). \end{aligned} \tag{36}$$

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

Theorem 2: The Lie transformation associated to the polynomial

$$\sum_{m=j}^{M} b_j^{(m)} (q + \beta_j p)^m \tag{37}$$

has a finite Taylor expansion, being a Cremona map.

PROOF: From (11) we see that

$$e^{-\beta \frac{1}{2} :p^2:} q = q + \beta p, \tag{38}$$

and from (10) we have

$$\begin{aligned} \exp\left(-\beta \frac{1}{2} : p^2 :\right) \exp\left(: b q^m :\right) \exp\left(\beta \frac{1}{2} : p^2 :\right) &= \exp\left(: b \left(e^{-\beta \frac{1}{2} :p^2:} q\right)^m :\right) \\ &= \exp\left(: b (q + \beta p)^m :\right). \end{aligned}$$

Similarly

$$\begin{aligned} &\exp\left(-\beta_j \frac{1}{2} : p^2 :\right) \exp\left(: \sum_{m=j}^{M} b_j^{(m)} q^m :\right) \exp\left(\beta_j \frac{1}{2} : p^2 :\right) \\ &= \exp\left(: \sum_{m=j}^{M} b_j^{(m)} (q + \beta_j p)^m :\right). \end{aligned} \tag{39}$$

Considering that the three exponentials on the left hand side of (39) are exactly solvable in a finite Taylor expansion, then it is the whole map. □

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

Finally, we have:

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

$$f_3+\ldots+f_M=\sum_{m=3}^{M}\sum_{i=0}^{m}a_i^{(m)}q^{m-i}p^i \tag{40}$$

it is possible to write

$$e^{:f_3+\ldots+f_M:}\simeq \exp\left(:-\beta_0\frac{1}{2}p^2:\right)\prod_{j=0}^{M}\exp\left(:Q^{(j)}(q):\right)\,\exp\left(:P^{(j)}(p):\right), \tag{41}$$

where

$$\begin{aligned} Q^{(j)} &= \sum_{m=j}^{M} d_j^{(m)}q^m, \qquad (42)\\ P^{(j)} &= (\beta_j-\beta_{j+1})\frac{1}{2}p^2, \qquad j=0,\ldots,M, \qquad \beta_{M+1}=0 \end{aligned}$$

with $d_j^{(m)}=0$ for $m<3$ and $j>m$, and where $d_j^{(m)}$ are functions depending on $a_j^{(m)}$ and β_j.

Proof: From (41), (42) we have that

$$\begin{aligned} & e^{:-\beta_0\frac{1}{2}p^2:}\prod_{j=0}^{M}e^{:Q^{(j)}:}\,e^{:P^{(j)}:}\\ &= \prod_{j=0}^{M}\exp\left(:-\beta_j\frac{1}{2}p^2:\right)\,\exp\left(:\sum_{m=j}^{M}d_j^{(m)}q^m:\right)\,\exp\left(:\beta_j\frac{1}{2}p^2:\right)\\ &= \prod_{j=0}^{M}\exp\left(:\sum_{m=j}^{M}d_j^{(m)}(q+\beta_j p)^m:\right)=\prod_{j=0}^{M}e^{:g^{(j)}:}. \end{aligned} \tag{43}$$

Using the BCH formula, equating terms and proceeding order by order (starting with $m=3$) we get recursively (see [8, 15] for more details on the 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

$$f_4=\sum_{i=0}^{4}a_i^{(4)}q^{4-i}p^i, \qquad f_6=\sum_{i=0}^{6}a_i^{(6)}q^{6-i}p^i. \tag{44}$$

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

$$e^{:H:} = \hat{M} e^{:f_4+f_6:} + R_8, \tag{45}$$

being $\hat{M}$ a linear transformation [16]. In the approximation to $e^{:f_4:+f_6:}$ we will compare the cost of the methods following the separation in groups of monomials and the new separation proposed previously. According to [18] it is possible to approximate $e^{:f_3:+\ldots+f_6:}$ by 12 terms. If $f_3 = f_5 = 0$ only 8 of them are different from 0, and we can write

$$e^{:f_4+f_6:} = \prod_{i=1}^{8} e^{:g^{(i)}:} + R_8, \tag{46}$$

where

$$\begin{array}{lll} g^{(1)} = c_1 q^4 + c_2 q^3 p & g^{(4)} = c_6 q^4 p^2 & g^{(7)} = c_{10} q^3 p^3 \\ g^{(2)} = c_3 q^2 p^2 & g^{(5)} = c_7 q^2 p^4 & g^{(8)} = c_{11} q p^5 + c_{12} p^6 \\ g^{(3)} = c_4 q p^3 + c_5 p^4 & g^{(6)} = c_8 q^6 + c_9 q^5 p. & \end{array}$$

The coefficients c_i can be evaluated in terms of the $a_i^{(n)}$ using the BCH formula and equating terms [18]. 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. On the other hand, from Theorem 3 we have

$$\begin{aligned} &\exp\left(: f_4 + f_6 :\right) = \\ &\exp\left(- : \beta_0 \frac{1}{2} p^2 :\right) \prod_{i=0}^{6} \exp\left(: d_i^{(4)} q^4 + d_i^{(6)} q^6 :\right) \exp\left(: (\beta_i - \beta_{i+1}) \frac{1}{2} p^2 :\right) + R_8 \end{aligned} \tag{47}$$

with $\beta_7 = 0$ and $d_5^{(4)} = d_6^{(4)} = 0$. Observe that the number of Lie transformations is very similar to (46) but now each one involves only a few multiplications and additions. We have computed (46) and (47) repeatedly on different initial conditions and values of $a_i^{(n)}$, and we found that (47) is approximately four times cheaper. In addition, the algorithm has still seven free parameters, $\beta_0, \ldots, \beta_6$, for improving the accuracy of the method, as we will see later in more detail.

5 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 an homogeneous polynomial of degree m can be written as

$$f_m = \sum_{i^{(6)}=m} a_{i_1,\ldots,i_6}\, q_1^{i_1}\, p_1^{i_2}\, q_2^{i_3}\, p_2^{i_4}\, q_3^{i_5}\, p_3^{i_6}, \tag{48}$$

with $i^{(6)} = i_1 + \ldots + i_6$, which contains C^m_{m+5} monomials. Grouping terms we can rewrite (48) in the form

$$f_m = \sum_{m^{(3)}=m} g_{m_1 m_2 m_3} \tag{49}$$

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

$$g_{m_1 m_2 m_3} = \sum_{i_1=0}^{m_1} \sum_{i_2=0}^{m_2} \sum_{i_3=0}^{m_3} a^{(m_1 m_2 m_3)}_{i_1 i_2 i_3}\, q_1^{m_1-i_1}\, p_1^{i_1}\, q_2^{m_2-i_2}\, p_2^{i_2}\, q_3^{m_3-i_3}\, p_3^{i_3}, \tag{50}$$

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

$$\begin{aligned} & (q_1 + \beta_1 p_1)^{m_1} (q_2 + \beta_2 p_2)^{m_2} (q_3 + \beta_3 p_3)^{m_3} \\ = & \sum_{i_1=0}^{m_1} \sum_{i_2=0}^{m_2} \sum_{i_3=0}^{m_3} C^{i_1}_{m_1} C^{i_2}_{m_2} C^{i_3}_{m_3}\, \beta_1^{i_1} \beta_2^{i_2} \beta_3^{i_3}\, q_1^{m_1-i_1}\, p_1^{i_1}\, q_2^{m_2-i_2}\, p_2^{i_2}\, q_3^{m_3-i_3}\, p_3^{i_3}. \end{aligned} \tag{51}$$

There is a problem in the generalisation 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 $\beta_1, \beta_2, \beta_3$ are not necessarily Vandermonde matrices, and the invertivility is not guaranteed. Keeping this in mind, we proceed as follow:

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

$$S^{(m)} = \begin{cases} \left(\frac{m}{3} + 1\right)^3 & if \quad \frac{m}{3} = Ce(\frac{m}{3}) \\ \left(\frac{m+1}{3} + 1\right)^2 \left(\frac{m-2}{3} + 1\right) & if \quad \frac{m+1}{3} = Ce(\frac{m+1}{3}) \\ \left(\frac{m+2}{3} + 1\right) \left(\frac{m-1}{3} + 1\right)^2 & if \quad \frac{m+2}{3} = Ce(\frac{m+2}{3}), \end{cases} \tag{52}$$

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

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

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 $r \geq 0$ chosen such that the matrices $V^{(m_1 m_2 m_3)}$ with components

$$V_{u,s}^{(m_1 m_2 m_3)} = \beta_{j_s,1}^{i_1} \beta_{j_s,2}^{i_2} \beta_{j_s,3}^{i_3}, \tag{54}$$

with $u = (m_3+1)(m_2+1)i_1 + (m_3+1)i_2 + i_3 + 1$, $i_1 = 0, \ldots, m_1$, $i_2 = 0, \ldots, m_2$, $i_3 = 0, \ldots, m_3$, $m_1 + m_2 + m_3 = m$, $s = 1, \ldots, R_{m_1 m_2 m_3}$ are nonsingular for at least one subset $\{j_i\}_{i=1}^{R_{m_1 m_2 m_3}}$ of $\{1, 2, \ldots, S^{(m)} + r\}$, then each polynomial $g_{m_1 m_2 m_3}$ in (49) can be written as

$$g_{m_1 m_2 m_3} = \sum_{s=1}^{R_{m_1 m_2 m_3}} b_{j_s}^{(m_1 m_2 m_3)} (q_1 + \beta_{j_s,1} p_1)^{m_1} (q_2 + \beta_{j_s,2} p_2)^{m_2} (q_3 + \beta_{j_s,3} p_3)^{m_3} \tag{55}$$

for different subsets $\{j_i\}_{i=1}^{R_{m_1 m_2 m_3}}$.

Proof: Simlarly to the proof of Theorem 1 we have that there exist at least one subset $\{j_i\}_{i=1}^{R_{m_1 m_2 m_3}}$ of $\{1, 2, \ldots, S^{(m)} + r\}$ such that the matrix with elements given in (54) is nonsingular. Then, after expanding (55) we see that

$$\left\{ \begin{array}{c} b_{j_1}^{(m_1 m_2 m_3)} \\ \vdots \\ b_{j_{R_{m_1 m_2 m_3}}}^{(m_1 m_2 m_3)} \end{array} \right\} = \left(V^{(m_1 m_2 m_3)} \right)^{-1} \left\{ \begin{array}{c} A_1^{(m_1 m_2 m_3)} \\ \vdots \\ A_{R_{m_1 m_2 m_3}}^{(m_1 m_2 m_3)} \end{array} \right\} \tag{56}$$

with

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

Here, $b^{(m_1 m_2 m_3)} \in \mathbb{R}^N$ with $N = S^{(m)} + r$ but, only the previous $R_{m_1 m_2 m_3}$ components of the vector are different from 0.

Corollary 2: It is possible to write

$$f_m = \sum_{s=1}^{S^{(m)}+r} \left(\sum_{m^{(3)}=m} b_s^{(m_1 m_2 m_3)} (q_1 + \beta_{s,1} p_1)^{m_1} (q_2 + \beta_{s,2} p_2)^{m_2} (q_3 + \beta_{s,3} p_3)^{m_3} \right) \tag{57}$$

where one possible solution for the vectors $b^{(m_1 m_2 m_3)} \in \mathbb{R}^N$ can be obtained taking different from 0 only $R_{m_1 m_2 m_3}$ components of each vector according to Theorem 4.

Theorem 5: The Lie transformation associated to the polynomial

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

has a finite Taylor expansion, being a Cremona map.

Theorem 6: Under conditions of Theorem 4 and given a general polynomial $f_3 + \ldots + f_M$ in the six dimensional space then, it is possible to write

$$e^{:f_3+\ldots+f_M:} \simeq e^{:P^{(0)}:} \prod_{j=1}^{S^{(m)}+r} e^{:Q^{(j)}:} e^{:P^{(j)}:}, \tag{59}$$

with

$$\begin{aligned} Q^{(j)} &= \sum_{m=3}^{M} \sum_{m^{(3)}=m} d_j^{(m_1 m_2 m_3)} q_1^{m_1} q_2^{m_2} q_3^{m_3}, \qquad (60) \\ P^{(j)} &= \frac{1}{2}\sum_{i=1}^{3} (\beta_{j,i} - \beta_{j+1,i}) p_i^2, \qquad j = 0, \ldots, S^{(m)} + r, \end{aligned}$$

with $Q^{(0)} = \beta_{0,i} = \beta_{S^{(m)}+r+1,i} = 0$ and where the coefficients $d_j^{(m_1 m_2 m_3)}$ 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

$$\nabla_q Q^{(i)} = \left(\frac{\partial Q^{(i)}}{\partial q_1}, \frac{\partial Q^{(i)}}{\partial q_2}, \frac{\partial Q^{(i)}}{\partial q_3} \right), \quad \nabla_p P^{(i)} = \left(\frac{\partial P^{(i)}}{\partial p_1}, \frac{\partial P^{(i)}}{\partial p_2}, \frac{\partial P^{(i)}}{\partial p_3} \right),$$

the algorithm for computing (59) is given in Table 1, 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 act on initial conditions, the computation has to be done from left to right.

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

Table 1: Algorithm for computing the map (59).

Observe that each evaluation is very cheap and that many of the coefficients of $d_j^{(m_1 m_2 m_3)}$ can be taken identically 0. In general, if the polynomial $f_3+\ldots+f_M$ contains all monomials ($\sum_{m=3}^{M} C_{m+5}^{m}$), it is possible to consider the same number of coefficients $d_j^{(m_1m_2m_3)}$ which are different from 0. The main difference with other Cremona maps [1, 8, 12, 15] is that instead of $\nabla_p P^{(j)}$ they consider a more general linear symplectic transformation acting on $(q_1, q_2, q_3, p_1, p_2, p_3)$. This allows to write the algorithm with less that $S^{(m)}+r$ transformations. But, the number of coefficients $d_j^{(m_1m_2m_3)}$ different from 0 is essentially the same, the computational cost is very similar and the complexity for building a particular method is considerably higher.

For the scheme we propose, the coefficeints $\beta_{i,j}$ have to satisfy very few constrains and the coefficients $d_j^{(m_1m_2m_3)}$ are relatively easy to obtain. In addition, in most of the cases it is possible to take $r=0$. This is the case, for example, in the four dimensional space ($m_3=0$). All matrices which have to be non singular according to Theorem 4 are submatrices of a matrix with elements $\beta_{j,1}^{i_1}\beta_{j,2}^{i_2}$, $i_1=0,\ldots,m_1, i_2=0,\ldots,m_2$, $0\leq i_1+i_2\leq m$ which is of dimension $\mathbb{R}^{u\times u}$ with $u=\sum_{i=0}^{m}(i+1)=\frac{(m+1)(m+2)}{2}$. According to (53) 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 $u=\sum_{i=0}^{m}\frac{(i+1)(i+2)}{2}$ which is higher that $3S^{(m)}$ for $m>4$. But, as mentioned, this fact does not make the algorithm much more costly.

Example 5.1. In order to illustrate how to obtain a 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

$$\mathcal{M}_4 = \hat{M} e^{:f_3:}\, e^{:f_4:} \tag{61}$$

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

$$\begin{aligned}
f_3 &= a_{1,1}^{(3)}q_1^3 + a_{1,2}^{(3)}q_1^2p_1 + a_{1,3}^{(3)}q_1p_1^2 + a_{1,4}^{(3)}p_1^3 \\
&\quad + a_{2,1}^{(3)}q_1q_2^2 + a_{2,2}^{(3)}q_1q_2p_2 + a_{2,3}^{(3)}q_1p_2^2 + a_{2,4}^{(3)}p_1q_2^2 + a_{2,5}^{(3)}p_1q_2p_2 + a_{2,6}^{(3)}p_1p_2^2, \\
f_4 &= a_{1,1}^{(4)}q_1^4 + a_{1,2}^{(4)}q_1^3p_1 + a_{1,3}^{(4)}q_1^2p_1^2 + a_{1,4}^{(4)}q_1p_1^3 + a_{1,5}^{(4)}p_1^4 \\
&\quad + a_{2,1}^{(4)}q_2^4 + a_{2,2}^{(4)}q_2^3p_2 + a_{2,3}^{(4)}q_2^2p_2^2 + a_{2,4}^{(4)}q_2p_2^3 + a_{2,5}^{(4)}p_2^4 \\
&\quad + a_{3,1}^{(4)}q_1^2q_2^2 + a_{3,2}^{(4)}q_1^2q_2p_2 + a_{3,3}^{(4)}q_1^2p_2^2 + a_{3,4}^{(4)}q_1p_1q_2^2 + a_{3,5}^{(4)}q_1p_1q_2p_2 + a_{3,6}^{(4)}q_1p_1p_2^2 \\
&\quad + a_{3,7}^{(4)}p_1^2q_2^2 + a_{3,8}^{(4)}p_1^2q_2p_2 + a_{3,9}^{(4)}p_1^2p_2^2.
\end{aligned}$$

Observe that f_3, f_4 only contains 29 of the 54 ($C_6^3+C_7^4$) 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 of $u_2^{(4)}$ then it is possible to write

$$e^{:f_3:}e^{:f_4:}=e^{:P^{(0)}(p):}\prod_{j=1}^{9}e^{:Q^{(j)}(q):}\,e^{:P^{(j)}(p):}+O(R_5), \tag{62}$$

with

$$\begin{aligned} Q^{(j)} &= d_{1,j}^{(3)}q_1^3+d_{2,j}^{(3)}q_1q_2^2+d_{1,j}^{(4)}q_1^4+d_{2,j}^{(4)}q_2^4+d_{3,j}^{(4)}q_1^2q_2^2, \qquad (63)\\ P^{(j)} &= \frac{1}{2}(\beta_{j,1}-\beta_{j+1,1})p_1^2+\frac{1}{2}(\beta_{j,2}-\beta_{j+1,2})p_2^2, \qquad j=0,\ldots,9, \end{aligned}$$

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

It is possible to choose nine pairs $\beta_{j,1},\beta_{j,2},\ j=1,\ldots,9$ such that all matrices originated from the previous products are non singular. 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 a complicated optimization procedure [15] can be used.

In the following we will show how to simplify even more the procedure for both choosing the $\beta_{i,j}$s and obtaining the coefficients $d_{i,j}^{(k)}$.

Finally, we must mention that the approximation of $\mathcal{M}_4$ using (62) is several times cheaper than using a factorisation in monomials [11] or different groups of monomials [18, 21].

6 To choose alternative basis

In the previous 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 space we have considered two basis for writing an homogeneous polynomial of degree m

$$f_m=\sum_{i=0}^{m}\alpha_i^{(1,2)}\mathcal{P}_{m,i}^{(1,2)} \tag{64}$$

with $\mathcal{P}_{m,i}^{(1)}=q^{m-i}p^i$ and $\mathcal{P}_{m,i}^{(2)}=(q+\beta_ip)^m,\quad i=0,\ldots,m$. The trouble of using $\mathcal{P}_{m,i}^{(1)}$ is that the Lie transformations associated to some elements of the basis are relatively costly. The problem of using $\mathcal{P}_{m,i}^{(2)}$ could be that, for large m, many β_i are necessary, and this could be uncomfortable to work with, specially when a higher dimension space is considered.

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

Example 6.1. In f_6 we have $\{\mathcal{P}_{6,i}^{(1)}\}_{i=0}^{6}=\{q^6,q^5p,q^4p^2,q^3p^3,q^2p^4,qp^5,p^6\}$ but, the Lie transformation associated to q^6,q^4p^2,q^2p^4 and p^6 only involve multiplications, divisions and additions. Then, an interesting basis could be $\{\mathcal{P}_{6,i}^{(3)}\}_{i=0}^{6}=\{q^6,q^4p^2,q^2p^4,p^6,(q+\beta_1p)^6,(q+\beta_2p)^6,(q+\beta_3p)^6\}$. If f_4 also appears in the Hamiltonian, the natural choice for the basis would be $\{\mathcal{P}_{4,i}^{(3)}\}_{i=0}^{4}=\{q^4,p^4,(q+\beta_1p)^4,(q+\beta_2p)^4,(q+\beta_3p)^4\}$, which allows to group them with the elements of $\mathcal{P}_{6,i}^{(3)}$ 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 worth or it is not to use them for a given problem.

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

$$\begin{aligned}
g_1&=\sum_{i=1}^{3}b_iq_1^{3-i}q_2^i+\sum_{i=0}^{4}b_{4+i}q_1^{4-i}q_2^i, &\qquad g_3&=\sum_{i=1}^{3}p_1^i(b_{15+2i}q_2^{3-i}+b_{16+2i}q_2^{4-i})\\
g_2&=\sum_{i=1}^{3}b_{8+i}p_1^{3-i}p_2^i+\sum_{i=0}^{4}b_{12+i}p_1^{4-i}p_2^i, & g_4&=\sum_{i=1}^{3}q_1^i(b_{21+2i}p_2^{3-i}+b_{22+2i}p_2^{4-i}).
\end{aligned}$$

The polynomials $u_i^{(n)}=(q_1+\beta p_1)^{n-i}(q_2+\beta p_2)^i$, contain $(n-i+1)(i+1)$ different monomials. Then, among all $u_i^{(n)}$, we have to consider more carefully $u_1^{(4)}$, $u_2^{(4)}$ and $u_3^{(4)}$, since they have 8, 9 and 8 different monomials, respectively. But, observe that each g_i contains an element of $u_1^{(4)}$, $u_2^{(4)}$ and $u_3^{(4)}$ so, only five more terms are necessary to reproduce all monomials, and this can be achieved with

$$e^{:f_3+f_4:}=\left(\prod_{i=1}^{4}e^{:g_i:}\right)e^{:P^{(0)}(p):}\prod_{i=1}^{5}e^{:Q^{(i)}(q):}e^{:P^{(i)}(p):}+O(R_5). \qquad (65)$$

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

7 Optimizing the Algorithms

In previous sections we have been concerned only in the computational cost of the algorithms. It could be possible to use the free parameters β_is in order to reduce slightly more the number of terms in the factorization at the extraordinary price of having to solve very complicate nonlinear systems of equations. On the other hand, to have algorithms with free parameters for optimization purposes usually produces more efficient methods [3]. Then, we can use these β_is in order to get (without increasing the cost) more accurate results. From Theorem 3 we have, in a two dimensional space

$$e^{:f_3+\ldots+f_M:} = \left[e^{:-\beta_0 \frac{1}{2} p^2:} \prod_{i=0}^{M} e^{:Q^{(i)}(q):} e^{:P^{(i)}(p):} \right] e^{:R_{M+1}:} + O(R_{M+2}), \tag{66}$$

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

$$R_{M+1} = \sum_{i=0}^{M+1} \alpha_i q^{M+1-i} p^i \tag{67}$$

and $\alpha_i, \quad i = 0, \ldots, M+1$ depend on the coefficients $\beta_i, \quad i = 0, \ldots, M$ we have chosen. If we define the error of a method by: $E_1 \equiv \left(\sum_i |\alpha_i|^2 \right)^{1/2}$ then we can look for the coefficients β_i which minimize E_1. Observe that E_1 also depends on the coefficients $a_i^{(m)}$, and the optimal choice for the β_is will depend on each particular problem. A simpler form to choose the best set of coefficients β_i is to consider that $F(z) = f_3 + \ldots + f_M$ is a constant of the movement. Then, we can take a number of different initial conditions in the region of interest. For each initial condition, z_0, evaluate the relative error $|(F(z_1) - F(z_0))/F(z_0)|$ where z_1 is the one map approximation, and finally to 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 which minimizes $E_2(\beta)$. In general, we will have that $E_1(\beta)$ and $E_2(\beta)$ have their minimum very close to each other, and it will be enough to compute only E_2 since it is very easy to do it.

Example 7.1. Let us consider f_4 from (44) with [16]

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

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

$$\exp(:f_4:) = e^{:d_1 q^4:}\, e^{:d_2 p^4:} \prod_{i=1}^{3} e^{:d_{i+2}(q+\beta_i p)^4:}. \tag{68}$$

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 $\beta_1, \beta_2, \beta_3 \in (-2, 2)$. As expected, we found that the minimum of E_1 and E_2 nearly coincide. In order to show this and to illustrate how the error depends on the choice of the β_i, in Fig. 1 we present 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 $\beta \in (1/2, 3/2)$, which approximately cross through the minimum at $\beta = 1$. Observe that the minimum is very narrow. This is in agreement with the comments on [8] where only very few values of the parameters in the Cremona maps had small error coefficients. For comparison, we have computed

$$\exp(:f_4:) = e^{:g^{(1)}:}\, e^{:g^{(2)}:}\, e^{:g^{(3)}:} \tag{69}$$

with $g^{(1)} = c_1 q^4 + c_2 q^3 p$, $g^{(2)} = c_3 q^2 p^2$ and $g^{(3)} = c_4 q p^3 + c_5 p^4$. In Fig. 1 we show in horizontal lines the values of E_1 and E_2 obtained. We found that the computational cost of (69) is approximately three times more expensive and still it gives an error more that one order of magnitude higher than (68) for the choice $(\beta_1, \beta_2, \beta_3) = (-1.030, 0.217, -1.022)$ which stays near the minimum we found.

Observe that the error at the minimum decreases by several orders of magnitude, and it is very sensible 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 dimension space, were many $\beta_{i,j}$s coefficients are involved.

8 Conclusions

In this paper we have studied different symplectic integrators 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 coposse the results in ordre to have an approximation to the original Hamiltonian.

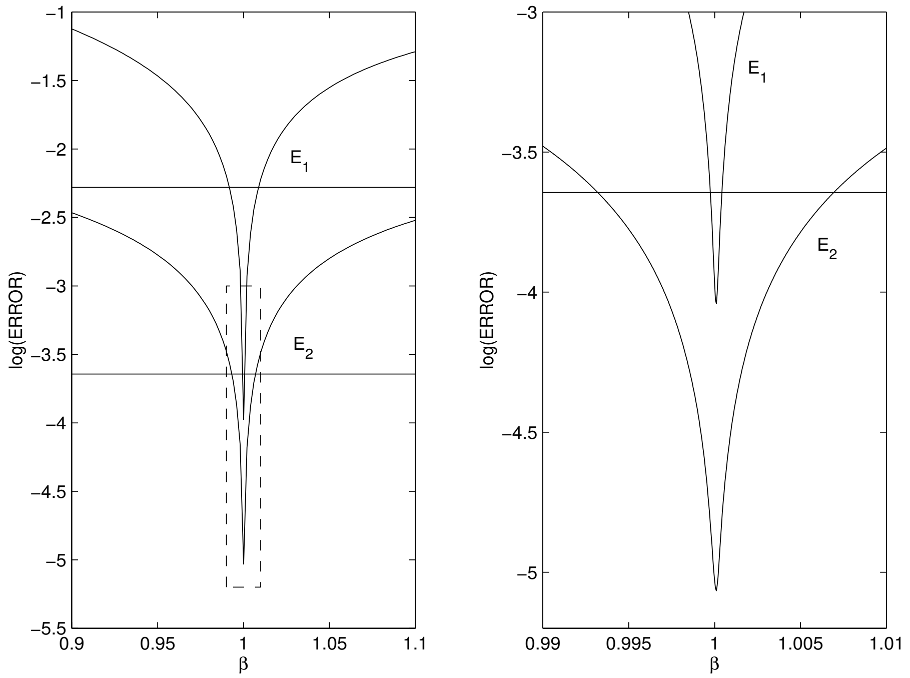

Figure 1: Error of the method (68) for $(\beta_1, \beta_2, \beta_3) = (-1.030, 0.217, -1.022)\beta$. E_1 measures the Euclidean norm of the coefficients at the leading error term and E_2 measures the average relative error in the Hamiltonian. The horizontal lines corespond to the errors obtained with (69).

However, the Hamiltonian can be separated in many different ways. The efficiency of a mehtod depends on its computational cost and its accuracy. But, this depends on how H is separated. We have analysed this aspect in the paper and presented new methods (most of them are Cremona maps) with the following properties:

1. They are cheap to compute.
2. There is a systematic and easy procedure for building the methods.
3. They have a number of free parameters for optimizing the mehtods, 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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