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Symplectic integration using solvable maps

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Abstract. In this paper, a symplectic integration algorithm using solvable maps is investigated. Examples are studied in two and four dimensions. The method is shown to give good results.

1. Introduction

Suppose we are interested in the long-term stability of particles being transported through a non-integrable Hamiltonian system. As the system is assumed to be non-integrable, the stability of the system is usually studied using numerical integration. Conventional numerical integration techniques, however, do not preserve the symplectic nature of Hamiltonian systems [1] and can therefore give wrong results. Integration algorithms which explicitly preserve the symplectic nature are called symplectic integration methods [1].

Several symplectic integration methods have been discussed in the literature [1–17]. In this paper, we describe an alternate symplectic integration method using solvable maps. This differs from the earlier symplectic integration methods proposed by one of the authors [14, 17] as follows. There, symplectic integration was achieved using Cremona maps, for which the Taylor series expansion terminates after two terms when acting on phase space variables. In the present method, symplectic integration is achieved using solvable maps for which the Taylor series expansion can be summed up explicitly. This method was briefly dealt with earlier [18]. In this paper, we explore the method in detail.

2. Preliminaries

Let $z = (q_1, q_2, \ldots, q_n,\ p_1,\ p_2, \ldots, p_n)$ denote the $2n$-dimensional phase space variables. The Lie operator corresponding to a phase space function $f(z)$ is denoted by $:f(z):$. It acts on the space of phase space functions and its action is as shown below [19]:

$$:f(z):g(z) = [f(z), g(z)]. \tag{1}$$

Here $g(z)$ denotes another phase space function and $[f(z), g(z)]$ denotes the usual Poisson bracket of the functions $f(z)$ and $g(z)$. Further, the commutator of two Lie operators, here denoted by {, } satisfy the relation [19]

$$\{:f:, :g:\} =: [f, g]: . \tag{2}$$

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The exponential of a Lie operator is called a Lie transformation and is given as

$$\exp(:f(z):) = \sum_{n=0}^{\infty} \frac{:f(z):^n}{n!}. \tag{3}$$

The powers of $:f(z):$ are defined recursively by the relation

$$:f(z):^n g(z) =: f(z):^{n-1} [f(z), g(z)]$$

with

$$:f(z):^0 g(z) = g(z).$$

Also, the product of two Lie transformations is also a Lie transformation and can be combined using the Campbell–Baker–Hausdorff theorem [20]. In the present context it takes the form

$$\exp(:f:)\exp(:g:) = \exp(:h:) \tag{4}$$

with h given by the expression

$$h = f + g + (\tfrac{1}{2})[f, g] + (\tfrac{1}{12})[f, [f, g]] + (\tfrac{1}{12})[g, [g, f]] + \cdots. \tag{5}$$

The time evolution of a Hamiltonian system can be represented by a symplectic map $\mathcal{M}$ [19]. Symplectic maps are maps whose Jacobian matrix $M(z)$ satisfy the symplectic condition:

$$\tilde{M}(z) J M(z) = J \tag{6}$$

where $\tilde{M}$ is the transpose of M and J is the fundamental symplectic matrix defined as follows:

$$J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \tag{7}$$

where I is a $n \times n$ identity matrix. Matrices M that satisfy (6) are called symplectic matrices and the corresponding maps $\mathcal{M}$ symplectic maps.

Denoting the initial and final locations of the particle by z^i and z^f respectively, the evolution of a Hamiltonian system can be described as [19]:

$$z^f = \mathcal{M} z^i. \tag{8}$$

Using the Dragt–Finn factorization theorem [19], the symplectic map $\mathcal{M}$ can be factorized as

$$\mathcal{M} = \hat{M} e^{:f_3:} e^{:f_4:} \ldots e^{:f_m:} \ldots. \tag{9}$$

Here $:f_m:$ is the Lie operator corresponding to the homogeneous polynomial f_m (in z) of degree m. The f_m are uniquely determined by the factorization theorem. $\hat{M}$ denotes the Lie transformation corresponding to the Jacobian matrix M of the symplectic map $\mathcal{M}$.

As $\mathcal{M}$ involves an infinite number of Lie transformations, for any practical computations, we have to truncate $\mathcal{M}$ after a finite number of Lie transformations:

$$\mathcal{M} = \hat{M} e^{:f_3:} e^{:f_4:} \ldots e^{:f_m:}. \tag{10}$$

Each one of the Lie transformations in equation (9) can be shown to be a symplectic map and hence the map can be truncated at any order without losing symplecticity. However, while implementing the above as a numerical algorithm, we need to know the explicit action of each one of these exponential factors on the phase space coordinates. Since we cannot evaluate the infinite number of terms present in each Lie transformation, we need to evaluate the action of these transformations using some other method. The most straightforward method is to truncate the Taylor series expansion of each Lie transformation (cf equation (3)) after a finite number of terms. This, however, violates the symplectic condition. Although, this method is justifiable in short-term tracking, it does not work well in long-term tracking as the non-symplecticity can lead to spurious damping or even chaotic behaviour which is not present in the original system [17]. Such behaviour can obviously lead to wrong predictions regarding the long-term stability of the Hamiltonian system being studied. Therefore, we refactorize $\mathcal{M}$ in terms of simpler symplectic maps that can be evaluated both exactly and quickly. In this paper, this refactorization is achieved though the so-called 'solvable maps' [18].

3. Solvable map method

Solvable maps are generalizations of Cremona maps. The class of Cremona maps includes only those symplectic maps for which the Taylor series expansion terminates when acting on phase space coordinates. The class of solvable maps also includes those symplectic maps for which the Taylor series expansion can be summed up explicitly. One simple example of such a map is $\exp(:aq_1^{l+2} + bq_1^{l+1}p_1:)$. Its action on phase space variables can be given explicitly as follows (for $l \geqslant 1$):

$$q_1' = \exp(:aq_1^{l+2} + bq_1^{l+1}p_1:)q_1 = \frac{q_1}{(1 + lbq_1^l)^{\frac{1}{l}}} \tag{11}$$

$$p_1' = \exp(:aq_1^{l+2} + bq_1^{l+1}p_1:)p_1 = \frac{E - a(q_1')^{l+2}}{b(q_1')^{l+1}} \tag{12}$$

where

$$E = aq_1^{l+2} + bq_1^{l+1}p_1. \tag{13}$$

The basic idea behind the solvable map method is to represent each nonlinear factor $\exp(:f_m:)$ in (10) as a product of solvable maps. That is,

$$\exp(:f_m:) = \exp(:g_1)\exp(:g_2)\ldots\exp(:g_n) \qquad \text{for} \quad m \geqslant 3. \tag{14}$$

Since each solvable map can be evaluated explicitly, the symplectic condition is not violated if we refactorize $\mathcal{M}$ in terms of solvable maps.

3.1. One degree of freedom

For simplicity, we restrict ourselves to a general sixth-order symplectic map in one dimension

$$\mathcal{M}_6 = \hat{M}\exp(:f_3:)\ldots\exp(:f_6:) \tag{15}$$

where [19]

$$\begin{aligned}
f_3 &= a_1q_1^3 + a_2q_1^2p_1 + a_3q_1p_1^2 + a_4p_1^3 \\
f_4 &= a_5q_1^4 + a_6q_1^3p_1 + \cdots + a_9p_1^4 \\
f_5 &= a_{10}q_1^5 + a_{11}q_1^4p_1 + \cdots + a_{14}q_1p_1^4 + a_{15}p_1^5 \\
f_6 &= a_{16}q_1^6 + a_{17}q_1^5p_1 + \cdots + a_{21}q_1p_1^5 + a_{22}p_1^6.
\end{aligned} \tag{16}$$

It should be noted that there is an explicit algorithm [19] for determining M and the coefficients a_1 through a_{22} from the Hamiltonian system that we want to study.

We now refactorize the above symplectic map in terms of solvable maps:

$$\mathcal{M}_6 = \hat{M}\exp(:g_1:)\ldots\exp(:g_{12}:) \tag{17}$$

where

$$
\begin{aligned}
g_1 &= b_1 q_1^3 + b_2\, q_1^2\, p_1 & g_2 &= b_3\, q_1\, p_1^2 + b_4 p_1^3 \\
g_3 &= b_5 q_1^4 + b_6\, q_1^3\, p_1 & & \\
g_4 &= b_7\, q_1^2\, p_1^2 & g_5 &= b_8\, q_1\, p_1^3 + b_9 p_1^4 \\
g_6 &= b_{10} q_1^5 + b_{11}\, q_1^4\, p_1 & & \\
g_7 &= b_{12}\, q_1^3\, p_1^2 + b_{18}\, q_1^4\, p_1^2 & g_8 &= b_{13}\, q_1^2\, p_1^3 + b_{20}\, q_1^2\, p_1^4 \\
g_9 &= b_{14}\, q_1\, p_1^4 + b_{15} p_1^5 & & \\
g_{10} &= b_{16} q_1^6 + b_{17}\, q_1^5\, p_1 & g_{11} &= b_{19}\, q_1^3\, p_1^3 \\
g_{12} &= b_{21}\, q_1\, p_1^5 + b_{22} p_1^6. & &
\end{aligned}
\tag{18}
$$

Here the unknown coefficients b_1 through b_{22} occurring in the above equation are determined by comparing the original form of $\mathcal{M}_6$ with its refactorized form using CBH theorem (cf equation (4)) and ensuring that the terms match (up to order 6):

$$
\exp(:f_3:)\ldots\exp(:f_6:) = \exp(:g_1:)\ldots\exp(:g_{12}:) \text{ up to order 6.} \tag{19}
$$

This is easily accomplished and the expressions for the coefficients are given in appendix B. These coefficients parametrize the system under study and reduce to real numbers once the system is fixed.

We now consider two applications of the above method. The first example is to find the region of stability of the following simple symplectic map:

$$
\mathcal{M} = \hat{M} \exp[:(q_1 + p_1)^3:] \tag{20}
$$

where

$$
M = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{21}
$$

and $\theta = \frac{\pi}{3}$.

We chose this example since the exact action of the above map is known and hence the exact region of stability can also be determined. The action of $\exp[:(q_1 + p_1)^3:]$ on phase space variables can be given as follows:

$$
\begin{aligned}
q_1' &= q_1 - 3(q_1 + p_1)^2 \\
p_1' &= p_1 + 3(q_1 + p_1)^2.
\end{aligned}
\tag{22}
$$

The numerical results obtained using the fourth-order solvable map method and the exact results are shown in figure 1. This figure gives the phase space portraits for two initial conditions. We observe that there is excellent agreement between results obtained using solvable maps and the exact results. Further, the region of stability obtained using solvable maps agrees well with the exact region of stability. On the other hand, if we use the generating function method of symplectic integration as applied to maps [21], the region of stability is greatly overestimated. In this method, the map is stable even for the initial condition (10.0, 0.0) (see figure 2) whereas the exact map becomes unstable at (0.07, 0.0).

Next, we consider an application of the solvable map method to the nonlinear pendulum Hamiltonian. It has been shown [17] that nonsymplectic integration methods gives rise to spurious chaotic behaviour where there is none, even for this simple system. Such problems become accentuated when long-term integration is performed to study stability of more complicated Hamiltonian systems.

The nonlinear pendulum is described by the following Hamiltonian H:

$$
H(q_1, p_1) = \frac{p_1^2}{2} - \cos q_1 + 1. \tag{23}
$$

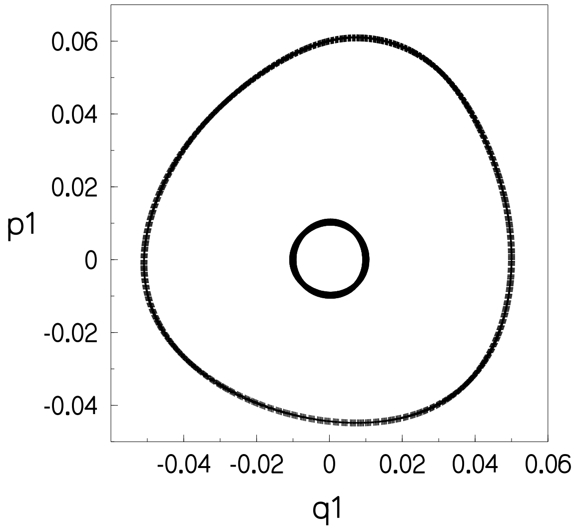

Figure 1. This figure shows the phase space plots for two initial conditions. The exact results are shown as a line and the solvable map results as crosses.

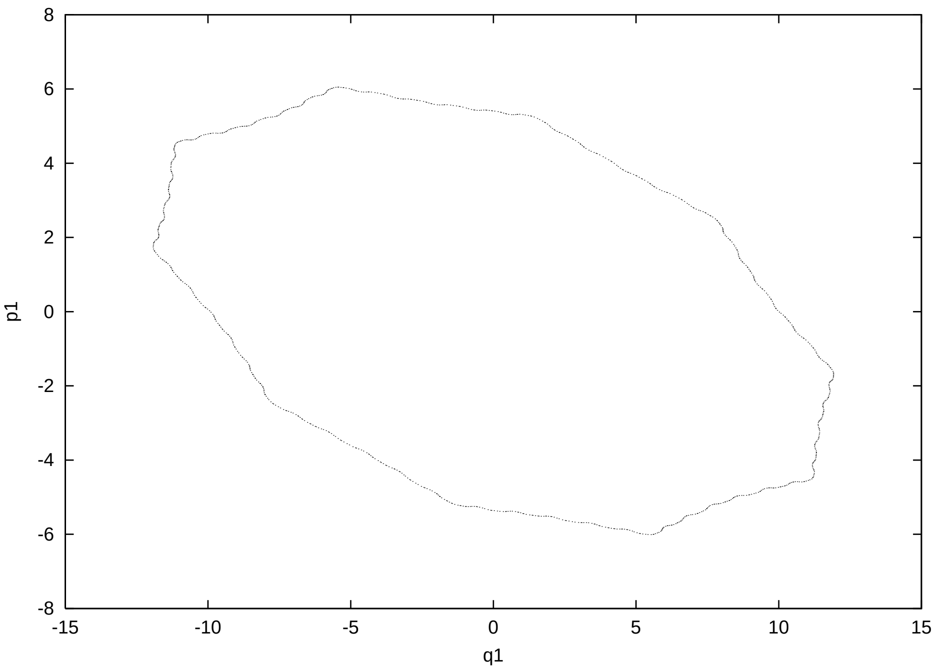

Figure 2. This figure shows the phase space plot for initial condition (10.0, 0.0) using the generating function method applied to maps.

To use the solvable map method we first need to represent this Hamiltonian in terms of a symplectic map $\mathcal{M}$. To order 6, this is given by [17]:

$$\mathcal{M} = \hat{M} e^{:f_4:} e^{:f_6:} \tag{24}$$

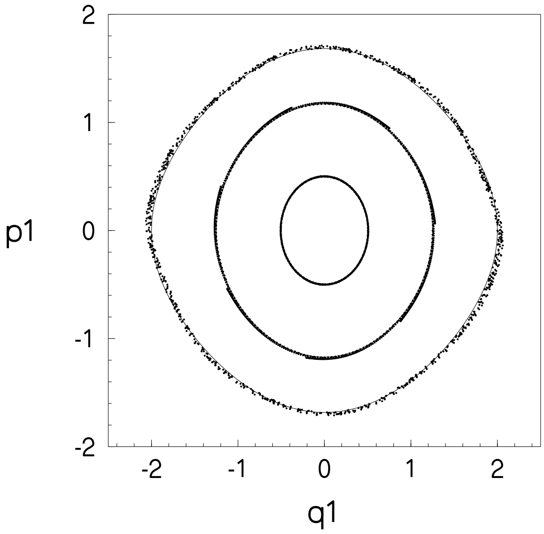

Figure 3. This figure shows the phase space plots for three initial conditions for the pendulum map. The exact results are shown as a line and the solvable map results as dots.

where (for unit time)

$$M = \begin{pmatrix} 0.5403 & 0.8415 \\ -0.8415 & 0.5403 \end{pmatrix} \tag{25}$$

and

$$\begin{aligned} f_4 = {} & 2.411 \times 10^{-2} q_1^4 - 3.812 \times 10^{-2} q_1^3 p_1 + 3.716 \times 10^{-2} q_1^2 p_1^2 \\ & -2.089 \times 10^{-2} q_1 p_1^3 + 5.168 \times 10^{-3} p_1^4 \\ f_6 = {} & 1.200 \times 10^{-4} q_1^6 - 1.026 \times 10^{-3} q_1^5 p_1 + 1.390 \times 10^{-3} q_1^4 p_1^2 - 6.657 \times 10^{-4} q_1^3 p_1^3 \\ & -8.008 \times 10^{-5} q_1^2 p_1^4 + 1.748 \times 10^{-4} q_1 p_1^5 - 4.963 \times 10^{-5} p_1^6. \end{aligned} \tag{26}$$

The polynomials f_3 and f_5 are zero. We factorize the above map in terms of solvable maps as given in equation (16). The results obtained by numerically integrating the map equation (24) using the solvable map method are shown in figure 3. A variety of initial conditions have been used and the results obtained agree very well with the exact results. In this case, the generating function method also gives excellent results.

3.2. Two degrees of freedom

In the two degrees of freedom case, a general Hamiltonian can be written in the form

$$H(z) = H_2(z) + H_3(z) + H_4(z) + \cdots \tag{27}$$

where $H_m(z)$ contains all terms of the form $q_1^a p_1^b q_2^c p_2^d$ with $a+b+c+d = m$. The total number of such terms in $H_m(z)$ is ${}^{3+m}C_m$ [14]. That is, we need this many independent coefficients to parametrize $H_m(z)$. Therefore, to parametrize the nonlinear part $H_3(z) + H_4(z)$ (truncated at the fourth order), we require 55 independent coefficients. Consequently, the nonlinear part of the corresponding fourth-order symplectic map $\mathcal{M}_4$ is also parametrized by 55 coefficients. These coefficients reduce to fixed real numbers once the Hamiltonian is fixed.

Let us now consider the Lie representation of a general fourth-order symplectic map in two degrees of freedom:

$$\mathcal{M}_4 = \hat{M} \exp(: f_3 :) \exp(: f_4 :) \tag{28}$$

where f_m is a mth-order homogeneous polynomial in z. As seen above, f_3 and f_4 can be parametrized by 55 coefficients. We denote them by a_1 through a_{55}. The representation in terms of solvable maps is given by

$$\mathcal{M}_4 = \hat{M}\exp(:g_1:)\ldots\exp(:g_{11}:) \tag{29}$$

where the g are as follows:

$$\begin{aligned}
g_1 &= b_{21}q_1^4 + q_1^3(b_1 + b_{23}q_2) + q_1^2(b_3q_2 + b_{28}q_2^2) + q_1(b_8q_2^2 + b_{37}q_2^3) \\
&\quad + p_1(b_{14}q_2^2 + b_{47}q_2^3) + q_1p_1(b_6q_2 + b_{34}q_2^2) \\
g_2 &= b_{41}p_1^4 + p_1^3(b_{11} + b_{43}p_2) + p_1^2(b_{13}p_2 + b_{46}p_2^2) + p_1(b_{16}p_2^2 + b_{50}p_2^3) \\
&\quad + q_1(b_{10}p_2^2 + b_{40}p_2^3) + q_1p_1(b_7p_2 + b_{36}p_2^2) \\
g_3 &= b_{51}q_2^4 + b_{17}q_2^3 + b_{44}p_1^2q_2^2 + q_2(b_{12}p_1^2 + b_{42}p_1^3) + q_2p_2(b_{15}p_1 + b_{45}p_1^2) \\
g_4 &= b_{55}p_2^4 + b_{20}p_2^3 + b_{30}q_1^2p_2^2 + p_2(b_4q_1^2 + b_{24}q_1^3) + q_2p_2(b_6q_1 + b_{29}q_1^2) \\
g_5 &= q_1^2p_1(b_2 + b_{26}q_2 + b_{27}p_2) \\
g_6 &= q_1p_1^2(b_5 + b_{32}q_2 + b_{33}p_2) \\
g_7 &= q_2^2p_2(b_{18} + b_{38}q_1 + b_{48}p_1) \\
g_8 &= q_2p_2^2(b_{19} + b_{39}q_2 + b_{49}p_2) \\
g_9 &= b_{22}q_1^3p_1 + b_{52}q_2^3p_2 \\
g_{10} &= b_{31}q_1p_1^3 + b_{54}q_2p_2^3 \\
g_{11} &= b_{25}q_1^2p_1^2 + b_{35}q_1p_1q_2p_2 + b_{53}q_2^2p_2^2.
\end{aligned} \tag{30}$$

Thus an arbitrary fourth-order symplectic map can be represented using a product of 12 solvable maps (including the linear map $\hat{M}$). The coefficients b_1 through b_{55} that occur in the above equation are obtained by comparing the original symplectic map with the refactorized symplectic map term by term using the Campbell–Baker–Hausdorff series (cf equation (4)). The expressions for the coefficients obtained by this procedure are given in appendix B. These 55 coefficients parametrize the solvable map representation just as the coefficients a_1 through a_{55} parametrize the original symplectic map. The coefficients b_i reduce to real numbers once the symplectic map is fixed. The solvable map factorization given above is not unique even after imposing the requirement that the number of solvable maps be a minimum. A numerical study of the various systems studied here using different possible factorizations indicates that all of them give very similar results.

We now illustrate the method using the following map for which exact results are known:

$$\mathcal{M} = \hat{M}\exp[:(q_1 + p_1 + q_2 + p_2)^3:] \tag{31}$$

where

$$M = \begin{pmatrix} \cos\theta & \sin\theta & 0 & 0 \\ -\sin\theta & \cos\theta & 0 & 0 \\ 0 & 0 & \cos\theta & \sin\theta \\ 0 & 0 & -\sin\theta & \cos\theta \end{pmatrix} \tag{32}$$

and $\theta = \frac{\pi}{3}$. Again, as in the previous examples, excellent agreement between solvable map results and the exact results are observed.

We have also applied the method to more complicated Hamiltonian systems like particle storage rings. We studied a static storage ring that is designed to store protons. The storage ring is composed entirely of dipoles, quadrupoles and drifts with the exception of two pairs of sextupoles. It is for such complicated Hamiltonian systems that the efficacy of our method is best revealed. Since there are many constituent elements (in storage rings like the Large Hadron Collider, there can be thousands of elements), numerical integration using Hamiltonians for each element is cumbersome and slow. On the other hand, a map-based approach where one represents the entire storage ring in terms of a single map is much faster [22]. When this is combined with our solvable map refactorization, one obtains a symplectic integration algorithm which is both fast and accurate. In the solvable map method, whether the system being studied is the simple map considered above or the complicated storage ring that we will now consider, the number of solvable maps required is at most 12 (it can be less if some of the g_i are zero). But in conventional integration methods, the running time for the algorithm increases with the increase in the number of constituent units of the system. Therefore, for such complex real-life systems, the solvable map method is much faster.

We studied a static storage ring represented by the following symplectic map:

$$\mathcal{M}_4 = \hat{M} \exp(: f_3 :) \exp(: f_4 :) \tag{33}$$

where [21]

$$\hat{M} = \begin{pmatrix} 0.371731 & 4.86128 & 0.0 & 0.0 \\ -0.307966 & -1.33728 & 0.0 & 0.0 \\ 0.0 & 0.0 & 0.548139 & 2.60973 \\ 0.0 & 0.0 & -0.110952 & 1.29610 \end{pmatrix} \tag{34}$$

and

$$\begin{aligned} f_3 = {} & -0.517141 q_1^3 - 4.87906 q_1^2 p_1 - 14.3568 q_1 p_1^2 - 0.574807 q_1 q_2^2 \\ & +2.15359 q_1 q_2 p_2 - 0.233856 q_1 p_2^2 - 10.0954 p_1^3 - 4.86770 p_1 q_2^2 \\ & +25.1785 p_1 q_2 p_2 - 24.9554 p_1 p_2^2 \end{aligned} \tag{35}$$

$$\begin{aligned} f_4 = {} & -1.12262 q_1^4 - 18.5081 q_1^3 p_1 - 116.575 q_1^2 p_1^2 + 0.365400 q_1^2 q_2^2 \\ & +2.98491 q_1^2 q_2 p_2 - 33.8546 q_1^2 p_2^2 - 305.622 q_1 p_1^3 - 1.43029 q_1 p_1 q_2^2 \\ & +32.7886 q_1 p_1 q_2 p_2 - 232.418 q_1 p_1 p_2^2 - 337.958 p_1^4 - 10.9181 q_2^2 p_1^2 \\ & +31.3454 q_2 p_1^2 p_2 - 320.703 p_1^2 p_2^2 - 0.710814 q_2^4 + 13.6088 q_2^3 p_2 \\ & -87.0309 q_2^2 p_2^2 + 229.570 q_2 p_2^3 - 247.209 p_2^4. \end{aligned} \tag{36}$$

The factorization of the above map in terms of the 11 solvable maps given in equation (30) is as follows:

$$\begin{aligned} g_1 &= -4.9074 q_1^4 - 0.5171 q_1^3 + 0.2010 q_1^2 q_2^2 - 0.5748 q_1 q_2^2 \\ &\quad -4.8677 p_1 q_2^2 + 39.023 q_1 p_1 q_2^2 \\ g_2 &= -120.5502 p_1^4 - 10.0954 p_1^3 - 769.9028 p_1^2 p_2^2 - 24.9554 p_1 p_2^2 \\ &\quad -0.2339 q_1 p_2^2 - 173.6485 q_1 p_1 p_2^2 \\ g_3 &= -0.7108 q_2^4 + 137.8813 p_1^2 q_2^2 + q_2 p_2 (25.1785 p_1 - 424.9587 p_1^2) \\ g_4 &= -247.2091 p_2^4 - 54.2869 q_1^2 p_2^2 + 27.5011 q_2 p_2 q_1^2 \\ g_5 &= -4.8791 q_1^2 p_1 \\ g_6 &= -14.3568 q_1 p_1^2 \\ g_9 &= -40.7815 q_1^3 p_1 + 15.6037 q_2^3 p_2 \\ g_{10} &= -157.8536 q_1 p_1^3 + 205.6419 q_2 p_2^3 \\ g_{11} &= -245.1402 q_1^2 p_1^2 - 90.106 q_1 p_1 q_2 p_2 - 66.5219 q_2^2 p_2^2. \end{aligned}$$

The polynomials g_7 and g_8 are zero. The q_1–p_1 phase plots for the system using our solvable map method are given in figure 4. From theoretical considerations, we would expect the phase space curves to approach a triangular shape due to the one-third resonance caused by the presence of sextupoles. Our numerical results using solvable maps (figure 4) agrees with the theoretical analysis.

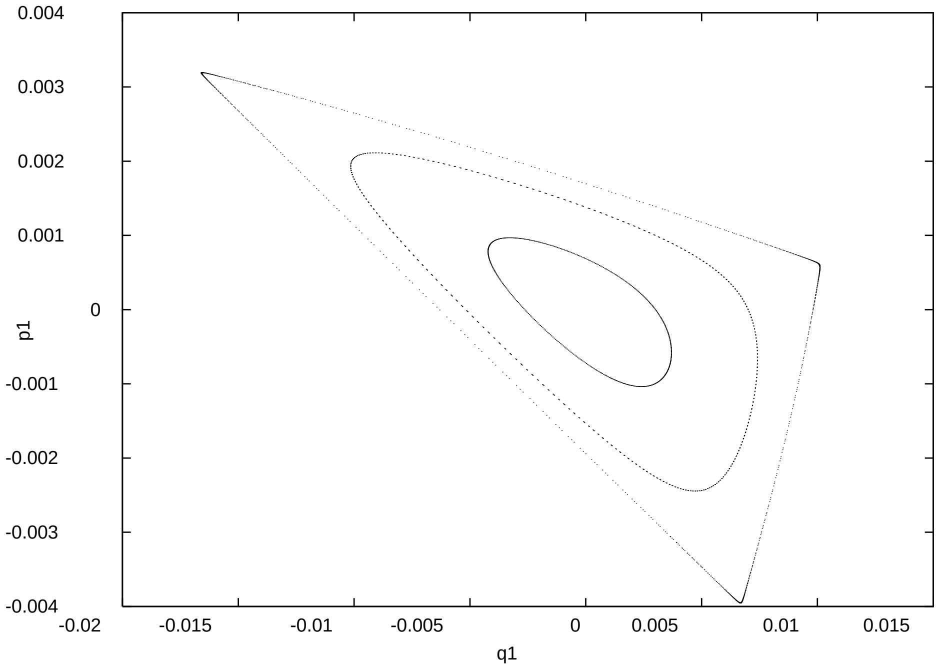

Figure 4. This figure shows the phase space plot for a storage ring using the solvable map method.

3.3. Error analysis

In our method, we first truncate the symplectic map to a given order and then refactorize it using a product of solvable maps. Both these stages give rise to errors. When we truncate the symplectic map $\mathcal{M}$ at the nth order, we obtain

$$\mathcal{M}_n = \hat{M}\exp(:f_3:)\exp(:f_4:)\ldots\exp(:f_n:). \tag{37}$$

The leading term that has been omitted is $\exp(:f_{n+1}:)$. From properties of Lie transformations and Lie operators [19], we have

$$\exp(:f_{n+1}:)z = z + [f_n + 1, z] + \cdots \tag{38}$$

where [,] denotes the usual Poisson bracket. Now, $[f_n + 1, z]$ gives terms of the form z^n [19]. Thus, error due to truncation of the symplectic map is of order z^n.

Next, we refactorize the truncated symplectic map $\mathcal{M}_n$ as a product of k solvable maps:

$$\mathcal{M}_n = \hat{M}\exp(:g_1:)\exp(:g_2:)\ldots\exp(:g_k:). \tag{39}$$

These solvable maps are obtained by first using the CBH series to combine the Lie transformations and then comparing with the original symplectic map. Both these maps are made to agree up to order n. Therefore, the leading error term is again of the form $\exp(:h_{n+1}:)$ giving rise to an error of order z^n.

4. Conclusions

We have studied a symplectic integration algorithm using solvable maps. It was shown to give good results in various examples. It provides a fast and accurate symplectic integration method for complicated Hamiltonian systems. Another advantage of this method is that it can be easily extended to higher dimensions since the computations involved are not that difficult when packages like Mathematica or Maple are used. The solvable map factorization for three degrees of freedom has already been carried out and involves 20 solvable maps.

Acknowledgments

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Appendix A

The expressions for b that occur in (18) are given as follows:

$$b_i = a_i \qquad \text{for} \quad i = 1, \ldots, 5 \quad \text{and} \quad i = 9$$
$$b_6 = a_6 - 3a_1a_3$$
$$b_7 = a_7 - \frac{9a_1a_4}{2} - 3\frac{a_2a_3}{2}$$
$$b_8 = a_8 - 3a_2a_4$$
$$b_{10} = a_{10} + 3a_1^2a_3$$
$$b_{11} = a_{11} + 9a_1^2a_4 + 2a_1a_2a_3$$
$$b_{12} = a_{12} - 10a_1a_3^2 + a_2^2a_3 + 12a_1a_2a_4$$
$$b_{13} = a_{13} - 2a_2a_3^2 + 5a_2^2a_4 - 24a_1a_3a_4$$
$$b_{14} = a_{14} - 18a_1a_4^2 - 4a_2a_3a_4$$
$$b_{15} = a_{15} - 6a_2a_4^2$$
$$b_{16} = a_{16} - \frac{27a_1^3a_4}{4} + 6a_1a_3a_5 + \frac{9a_1^2a_2a_3}{4}$$
$$b_{17} = a_{17} - 4a_5a_7 + \frac{45a_1^2a_3^2}{2} + 36a_1a_4a_5 - \frac{a_1a_2^2a_3}{2} + 12a_2a_3a_5 - \frac{27a_1^2a_2a_4}{2}$$
$$b_{18} = a_{18} - 6a_8a_5 - 2a_6a_7 - \frac{a_2^3a_3}{4} + \frac{3a_1a_2a_3^2}{2} + 18a_1a_4a_6 - \frac{57a_1a_2^2a_4}{4}$$
$$+6a_2a_3a_6 + 36a_2a_4a_5 + 54a_1^2a_3a_4$$
$$b_{19} = a_{19} - 4a_8a_6 - 8a_9a_5 - 15a_1a_3^3 + 81a_1^2a_4^2 + 3a_2^2a_3^2 - 5a_2^3a_4 + 24a_2a_4a_6$$
$$+18a_1a_2a_3a_4$$
$$b_{20} = a_{20} - 2a_8a_7 - 6a_9a_6 - \frac{3a_2a_3^3}{4} + 54a_1a_2a_4^2 - \frac{171a_1a_3^2a_4}{4} + 12a_2a_4a_7 + \frac{3a_2^2a_3a_4}{2}$$
$$b_{21} = a_{21} - 4a_9a_7 + \frac{45a_2^2a_4^2}{2} - \frac{81a_1a_3a_4^2}{2} - \frac{3a_2a_3^2a_4}{2}$$
$$b_{22} = a_{22} - \frac{81a_1a_4^3}{4} - 6a_9a_2a_4 + \frac{27a_2a_3a_4^2}{4}.$$

Appendix B

The expressions for b that occur in (29) are given as follows:

$$b_i = a_i \qquad \text{for} \quad i = 1, \ldots 20$$

$$b_{21} = \frac{-3a_1a_2}{2} - \frac{a_3a_4}{2} + a_{21}$$
$$b_{22} = -3a_1a_5 - \frac{a_4a_6}{2} - \frac{a_3a_7}{2} + a_{22}$$
$$b_{23} = -(a_2a_3) - a_4a_8 - \frac{a_3a_9}{2} + a_{23}$$
$$b_{24} = -(a_2a_4) - \frac{3a_1a_7}{2} - a_3a_{10} + a_{24}$$
$$b_{25} = \frac{-3a_2a_5}{2} - \frac{a_6a_7}{2} - \frac{9a_1a_{11}}{2} - \frac{a_4a_{12}}{2} - \frac{a_3a_{13}}{2} + a_{25}$$
$$b_{26} = -2a_3a_5 + \frac{a_2a_6}{2} - a_7a_8 - \frac{a_6a_9}{2} - 3a_1a_{12} - a_4a_{14} - \frac{a_3a_{15}}{2} + a_{26}$$
$$b_{27} = -2a_4a_5 + \frac{a_2a_7}{2} + \frac{a_7a_9}{2} - a_6a_{10} - 3a_1a_{13} - \frac{a_4a_{15}}{2} - a_3a_{16} + a_{27}$$
$$b_{28} = \frac{-(a_2a_8)}{2} - a_8a_9 - \frac{3a_4a_{17}}{2} - \frac{a_3a_{18}}{2} + a_{28}$$
$$b_{29} = a_4a_6 - a_3a_7 - \frac{a_2a_9}{2} - 2a_8a_{10} - \frac{3a_1a_{15}}{2} + a_4a_{18} - a_3a_{19} + a_{29}$$
$$b_{30} = a_4a_7 - \frac{a_2a_{10}}{2} + a_9a_{10} - \frac{3a_1a_{16}}{2} + \frac{a_4a_{19}}{2} - \frac{3a_3a_{20}}{2} + a_{30}$$
$$b_{31} = 3a_2a_{11} + \frac{a_7a_{12}}{2} - \frac{a_6a_{13}}{2} + a_{31}$$
$$b_{32} = \frac{-(a_5a_6)}{2} - 3a_3a_{11} + 2a_2a_{12} - \frac{a_9a_{12}}{2} - a_8a_{13} - a_7a_{14} - \frac{a_6a_{15}}{2} + a_{32}$$
$$b_{33} = \frac{-(a_5a_7)}{2} + 3a_4a_{11} + a_{10}a_{12} + 2a_2a_{13} + \frac{a_9a_{13}}{2} + \frac{a_7a_{15}}{2} - a_6a_{16} + a_{33}$$
$$b_{34} = -(a_5a_8) - 2a_3a_{12} + a_2a_{14} - a_9a_{14} - a_8a_{15} + \frac{3a_7a_{17}}{2} - \frac{a_6a_{18}}{2} + a_{34}$$
$$b_{35} = -(a_5a_9) + 2a_4a_{12} - 2a_3a_{13} - 2a_{10}a_{14} + a_2a_{15} - 2a_8a_{16} + a_7a_{18} - a_6a_{19} + a_{35}$$
$$b_{36} = -(a_5a_{10}) + 2a_4a_{13} + a_{10}a_{15} + a_2a_{16} + a_9a_{16} + \frac{a_7a_{19}}{2} - \frac{3a_6a_{20}}{2} + a_{36}$$
$$b_{37} = \frac{-3a_9a_{17}}{2} - a_8a_{18} + a_{37}$$
$$b_{38} = \frac{-(a_7a_8)}{2} + \frac{a_6a_9}{2} + a_4a_{14} - a_3a_{15} + 3a_{10}a_{17} + \frac{a_9a_{18}}{2} - 2a_8a_{19} + a_{38}$$
$$b_{39} = \frac{a_7a_9}{2} + \frac{a_6a_{10}}{2} + a_4a_{15} - a_3a_{16} + 2a_{10}a_{18} - \frac{a_9a_{19}}{2} - 3a_8a_{20} + a_{39}$$
$$b_{40} = a_4a_{16} + a_{10}a_{19} + a_{40}$$
$$b_{41} = \frac{3a_5a_{11}}{2} + \frac{a_{12}a_{13}}{2} + a_{41}$$
$$b_{42} = \frac{-3a_6a_{11}}{2} + a_5a_{12} - a_{13}a_{14} + a_{42}$$
$$b_{43} = a_5a_{13} + \frac{a_{13}a_{15}}{2} + a_{12}a_{16} + a_{43}$$
$$b_{44} = \frac{-3a_8a_{11}}{2} - a_6a_{12} + \frac{a_5a_{14}}{2} - a_{14}a_{15} + \frac{3a_{13}a_{17}}{2} - \frac{a_{12}a_{18}}{2} + a_{44}$$
$$b_{45} = \frac{3a_9a_{11}}{2} - a_7a_{12} - a_6a_{13} + \frac{a_5a_{15}}{2} - 2a_{14}a_{16} + a_{13}a_{18} - a_{12}a_{19} + a_{45}$$

$$b_{46} = \frac{a_5 a_{16}}{2} + a_{15}a_{16} + \frac{a_{13}a_{19}}{2} - \frac{3a_{12}a_{20}}{2} + a_{46}$$
$$b_{47} = -(a_8 a_{12}) - a_{14}a_{18} + a_{47}$$
$$b_{48} = a_9 a_{12} - a_8 a_{13} + \frac{a_7 a_{14}}{2} - \frac{a_6 a_{15}}{2} + 3a_{16}a_{17} + \frac{a_{15}a_{18}}{2} - 2a_{14}a_{19} + a_{48}$$
$$b_{49} = -(a_{10}a_{12}) + a_9 a_{13} - \frac{a_7 a_{15}}{2} - \frac{a_6 a_{16}}{2} + 2a_{16}a_{18} - \frac{a_{15}a_{19}}{2} - 3a_{14}a_{20} + a_{49}$$
$$b_{50} = a_{16}a_{19} - \frac{3a_{15}a_{20}}{2} + a_{50}$$
$$b_{51} = \frac{-3a_{17}a_{18}}{2} + a_{51}$$
$$b_{52} = \frac{a_9 a_{14}}{2} - \frac{a_8 a_{15}}{2} - 3a_{17}a_{19} + a_{52}$$
$$b_{53} = \frac{a_{10}a_{14}}{2} + \frac{a_9 a_{15}}{2} - \frac{a_8 a_{16}}{2} - \frac{3a_{18}a_{19}}{2} - \frac{9a_{17}a_{20}}{2} + a_{53}$$
$$b_{54} = \frac{-(a_{10}a_{15})}{2} + \frac{a_9 a_{16}}{2} + 3a_{18}a_{20} + a_{54}$$
$$b_{55} = \frac{3a_{19}a_{20}}{2} + a_{55}.$$

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