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# Symplectic integration of nonlinear Hamiltonian systems

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**Abstract.** There exist several standard numerical methods for integrating ordinary differential equations. However, if one is interested in integration of Hamiltonian systems, these methods can lead to wrong results. This is due to the fact that these methods do not explicitly preserve the so-called 'symplectic condition' (that needs to be satisfied for Hamiltonian systems) at every integration step. In this paper, we look at various methods for integration that preserve the symplectic condition.

**Keywords.** Symplectic integration; hamiltonian systems.

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## 1. Introduction

In this paper, we consider numerical integration methods for Hamiltonian systems. In particular, we would be interested in long-term integration of these systems. In these cases, it is important to preserve the Hamiltonian nature of the system at every integration step. Otherwise, one can get spurious damping or even chaotic behaviour which is not present in the original system. Such behaviour can obviously lead to wrong predictions regarding the long-term stability of the Hamiltonian system being studied.

In this paper, we look at various integration methods that overcome the above problem [1–20]. Such integration methods go by the name of symplectic integrators. In § 2, we introduce the basic concepts. In § 3, we consider the generating function methods for symplectic integration. Section 4 is devoted to symplectic Runge–Kutta (RK) and Runge–Kutta–Nystrom (RKN) methods. Section 5 introduces the Lie algebraic methods for integrating Hamiltonian systems. A better formulation of the generating function methods in this language is given. The jolt map factorization method for symplectic integration is also considered in some detail. Finally, integration using solvable maps is discussed. The concluding remarks can be found in § 6.

## 2. Basic concepts

Consider the following set of $2n$ first order differential equations:

$$\frac{dq}{dt} = \frac{\partial H(q,p)}{\partial p}, \quad \frac{dp}{dt} = -\frac{\partial H(q,p)}{\partial q}, \tag{2.1}$$

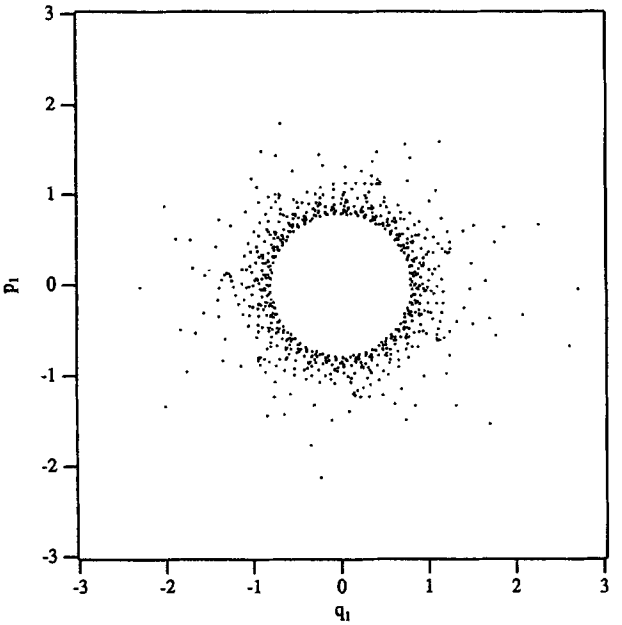


**Figure 1.** Numerical integration results using a non-symplectic fourth-order Taylor series map for the anharmonic oscillator. The initial condition used is $(q_1(0), p_1(0)) = (0.8, 0.0)$.

where $q, p \in R^n$. The initial conditions are given by $q(t_0) = q_0$ and $p(t_0) = p_0$. The above system of differential equations defines a Hamiltonian system where the Hamiltonian function $H$ is a function of the variables $q_i$, $p_i$ $(i = 1, 2, \ldots, n)$. The variables $q_i$ and $p_i$ constitute the phase space of the Hamiltonian system. Typically, $q_i$'s are the (generalized) coordinates and $p_i$'s the (generalized) momenta of the system.

Consider the Poisson bracket [,] of two phase space functions $f(q,p)$ and $g(q,p)$ defined as

$$[f(q,p), g(q,p)] = \sum_{i=1}^{n} \left[ \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right]. \tag{2.2}$$

Hamiltonian systems possess the remarkable property that they preserve the fundamental Poisson bracket $[q_i, p_j]$, that is

$$[q_i(t), p_j(t)] = [q_i(0), p_j(0)], \quad \forall\, i, j. \tag{2.3}$$

Equivalently, Hamiltonian systems preserve the symplectic 2-form $dp \wedge dq$. This condition is called the symplectic condition.

In general $H$ is a complicated function of $q$'s and $p$'s. Consequently, the resultant equations of motion [cf. eq. (2.1)] are nonlinear ordinary differential equations. Generically, such systems of nonlinear equations do not admit an analytic solution, that is, the system is non-integrable. Hence, one is forced to integrate these sets of ordinary differential equations numerically. There exist several standard methods for

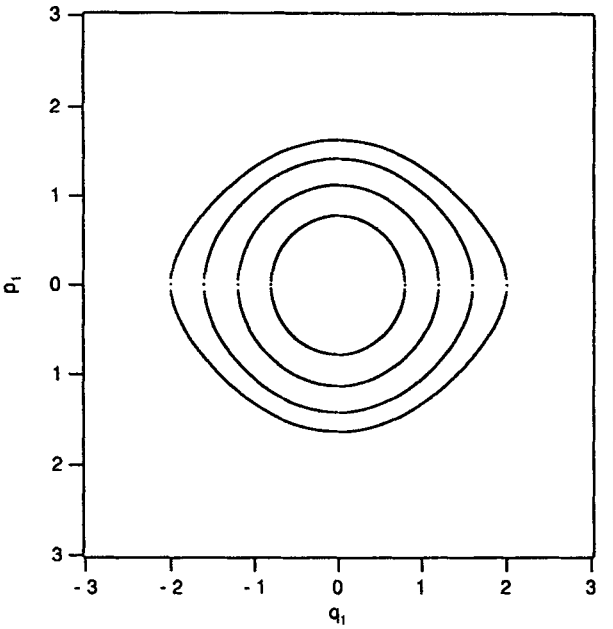


**Figure 2.** Numerical integration results using the exact symplectic map for the anharmonic oscillator. The initial conditions used are $(q_1(0), p_1(0)) = (0.8, 0.0)$, $(1.2, 0.0)$, $(1.6, 0.0)$, and $(2.0, 0.0)$.

numerical integration of a system of first order ordinary differential equations. However, these are general purpose methods and are not geared explicitly towards Hamiltonian systems. In particular, they do not preserve the symplectic condition at every step. For short-term integration this does not lead to much problems. For long-term integration, these non-symplectic methods can be a disaster. Since the symplectic condition is not preserved, even the qualitative nature of the solutions obtained by these methods can be very different from that of the exact solution. For example, one can get spurious damping or chaos where there is none. This can lead to wrong deductions regarding the long-term stability of the Hamiltonian system in question.

An example of how things can go wrong is shown in figure 1. This figure gives the result of integrating the nonlinear Hamiltonian system defined by the following Hamiltonian using a non-symplectic method

$$H = \frac{q_1^2 + p_1^2}{2} - \frac{q_1^4}{24}. \tag{2.4}$$

Looking at the figure, one might conclude that chaotic behaviour is present in the system. However, the exact solution of the system exhibited in figure 2 shows that this is not true. One way to avoid such a situation while using non-symplectic methods is to reduce the step size so that the symplectic violation is very small at each step. However, the computational cost of such a procedure for long-term numerical integration would be prohibitive. Therefore, one is lead to look for integration schemes which explicitly preserve the symplectic condition at every step. Such schemes are called symplectic integration methods and we look at some of them in the following sections.

## 3. Generating function methods

Symplectic integration methods were first discovered by DeVogelaere [1]. However, these results were not widely known. In 1983, Ruth [2] independently discovered symplectic integration methods using canonical generating functions.

The basic idea behind this method is as follows. For simplicity, let us consider a Hamiltonian given by the special form

$$H(q,p) = A(p) + V(q). \tag{3.1}$$

Ideally, we would like to make a canonical transformation such that the new Hamiltonian $H'$ in the new variables is identically zero. However, this is not practical. Hence, we attempt to make $H'$ zero up to a given order $t^k$ [2, 3]

$$H'(q',p',t) = O(t^{k+1}), \tag{3.2}$$

where $q'$ and $p'$ are the new variables after the canonical transformation. Using the equations of motion [cf. eq. (2.1)], we get

$$q'(t) = q_0 + O(t^{k+1}), \quad p'(t) = p_0 + O(t^{k+1}). \tag{3.3}$$

Thus, the motion is simple in the new coordinates. Once this is accomplished, we can invert the canonical transformation to get the motion in the original variables (accurate to order $k$). Therefore we get a map from $q(0), p(0)$ to $q(t), p(t)$ (again accurate to order $k$). Now we can repeat the process to go from $q(t), p(t)$ to $q(2t), p(2t)$ and so on. Thus, we have an integration algorithm (of order $k$) for the Hamiltonian system which allows us to step forward in time starting from the intitial conditions. Of course, we will typically take the time step $t$ at every stage to be small so that the error generated (which is of order $t^{k+1}$) is small. Since canonical transformations explicitly preserve the symplectic condition, we in fact have a symplectic integrator of order $k$.

We did not specify above how the canonical transformation is to be performed. This is done using the generating function method [21]. We use a generating function of the new coordinates and the old momenta [2, 3]

$$F_3(q',p,t) = -q' \cdot p + G(q',p,t). \tag{3.4}$$

Now we derive a simple symplectic integration method using the technique described above. Let the generating function be specified by [2]

$$G = -H(q',p)t = -[A(p) + V(q')]t. \tag{3.5}$$

Using the canonical transformation equations appropriate for this generating function [21] we get

$$\begin{aligned} p_i' &= p_i + \frac{\partial V(q')}{\partial q_i'} t, \\ q_i &= q_i' + \frac{\partial A(p)}{\partial p_i} t. \end{aligned} \tag{3.6}$$

Note that the momentum equation would in general be an implicit equation in $p$ which has to be inverted to obtain $p$ as a function of $p'$. This can be done explicitly only for

Hamiltonians having a simple form. In general, one has to solve the equation numerically to obtain $p$ as a function of $p'$. This complication is the greatest drawback of the generating function method. In our case, because of the special form of our Hamiltonian, we can easily invert the momentum equation. Then, we can write the new Hamiltonian in terms of $q'$ and $p'$ as follows [2]:

$$H' \sim t \sum_{i=1}^{n} \frac{\partial V(q')}{\partial q_i'} \frac{\partial A(p')}{\partial p_i'} + O(t^2). \tag{3.7}$$

Consequently, one gets

$$q' = q_0 + O(t^2), \quad p' = p_0 + O(t^2). \tag{3.8}$$

Thus, we have succeeded in obtaining a symplectic integration method of order 1 for our simple Hamiltonian.

Following the same procedure, one can in principle get symplectic integration methods of higher order. However, it is not easy to obtain the necessary canonical transformations. In general, one uses a series of transformations to attain the final goal. For example, for the special Hamiltonian given in (3.1), a fourth order symplectic integration method is given by the following equations [3]

$$p_i^{(l+1)} = p_i^{(l)} - c_l t \frac{\partial V}{\partial q_i^{(l)}}, \quad q_i^{(l+1)} = q_i^{(l)} - d_l t \frac{\partial A}{\partial p_i^{(l+1)}}; \quad l = 0, 1, 2, 3, 4. \tag{3.9}$$

Here the index $l$ labels successive canonical transformations. Moreover, $q^{(0)} = q_0$ and $p^{(0)} = p_0$ (the initial conditions). The unknown coefficients $c_l$, $d_l$ are determined by the condition that the new Hamiltonian in terms of the final canonical variables is zero upto order $t^4$. One possible solution is given below [3, 5]:

$$c_1 = c_4 = a + \tfrac{1}{2}, \; c_2 = c_3 = -a, \; d_1 = d_3 = 2a + 1, \; d_2 = -4a - 1, \; d_4 = 0, \tag{3.10}$$

where $a = 0.1756\ldots$.

The necessary canonical transformations become more and more difficult to solve for as one goes to higher orders. Further, for complicated Hamiltonians the inversion of the momenta equations becomes impossible analytically. One has to invert them numerically (typically using Newton–Raphson method) with its attendent convergence problems. Also, this slows down the integration algorithm considerably. We shall see that these problems are solved by using Lie algebraic methods.

## 4. Symplectic RK and RKN methods

In this section, we discuss Runge–Kutta and Runge–Kutta–Nystrom methods that are explicitly symplectic [14–20]. We start with the set of $2n$ first-order differential equations for a Hamiltonian system [cf. eq. (2.1)] which we reformulate as follows:

$$\frac{\mathrm{d}z}{\mathrm{d}t} = f(z), \quad z(t_0) = z_0,$$

where $z = (q,p)$ is a $2n$-vector and $f$ is a vector function specified by the right hand side of (2.1).

An $s$-stage Runge–Kutta method to integrate the above system of differential equations is given by [20]

$$Z_i = z_n + h\sum_{j=1}^{s} a_{ij} f(Z_j), \quad i = 1,2,\ldots,s, \tag{4.1}$$

$$z_{n+1} = z_n + h\sum_{j=1}^{s} b_j f(Z_j). \tag{4.2}$$

Here $h$ is the step size and $z_n$, $z_{n+1}$ are the values of phase space variables at the end of the $n$th and $(n+1)$th integration steps respectively. The coefficients $a_{ij}$ and $b_j$ have specific values depending on the RK method under consideration. The RK method is said to be explicit [20] if $a_{ij}$ vanishes for $i \leq j$. In this case, the vectors $Z_j$ can be solved recursively without having to solve any implicit equations. The method is called diagonally implicit if $a_{ij}$ vanishes for $i < j$ and implicit otherwise. It can be shown [17] that only implicit RK methods can be symplectic. These are symplectic if the following condition is satisfied [17]:

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i,j = 1,2,\ldots,s.$$

An example of a two-stage implicit RK method which is symplectic is specified by

$$a_{11} = a_{22} = \frac{1}{4}, \quad a_{12} = \frac{1}{4} - \frac{\sqrt{3}}{6}, \quad a_{21} = \frac{1}{4} + \frac{\sqrt{3}}{6}, \quad b_1 = b_2 = \frac{1}{2}. \tag{4.3}$$

This can be shown to be a symplectic integrator of order 4. In fact, this is one member of a family of symplectic RK methods which go by the name of Gauss–Legendre methods [20]. However, these are computationally costly methods. Iserles[16] has derived more efficient symplectic RK methods.

Next, we consider Runge–Kutta–Nystrom (RKN) methods. For simplicity, we restrict ourselves to Hamiltonians of the form $H = p^2/2 + V(q)$. The equations of motion for such Hamiltonians can be written as

$$\frac{\mathrm{d}^2 q}{\mathrm{d}t^2} = f(q),$$

where $f$ is the gradient of $-V$. The above system can be solved by an $s$-stage RKN method [20]

$$Q_i = q_n + hc_i p_n + h^2 \sum_{i=1}^{s} a_{ij} f(Q_j), \quad j = 1,2,\ldots,s, \tag{4.4}$$

$$p_{n+1} = p_n + h\sum_{j=1}^{s} b_j f(Q_j), \tag{4.5}$$

$$q_{n+1} = q_n + hp_n + h^2 \sum_{j=1}^{s} \bar{b}_j f(Q_j). \tag{4.6}$$

This method is symplectic if the following conditions are satisfied [15,18]

$$\bar{b}_i - b_i + b_i c_i = 0, \quad i = 1, 2, \ldots, s, \tag{4.7}$$

$$b_i a_{ij} - b_j a_{ji} - b_i \bar{b}_j + b_j \bar{b}_i = 0, \quad i = 1, 2, \ldots, j-1; \quad j = 2, 3, \ldots, s. \tag{4.8}$$

Unlike RK methods, explicit RKN methods can also be symplectic.

The simplest symplectic one-stage RKN method is the Stormer–Verlet method of order 2 specified by

$$a_{11} = 0, \quad c_1 = 0.5, \quad b_1 = 0.5, \quad \bar{b}_1 = 1.$$

The above method is used extensively in molecular dynamics simulations. Higher order symplectic RKN methods have been derived. The highest order method currently available is the explicit 13-stage method of order 8 obtained by Calvo and Sanz–Serna [19]. Symplectic RKN methods have also been obtained using collocation and perturbed collocation techniques [20].

## 5. Lie algebraic methods

One of the approaches to symplectic integration is the use of Lie algebraic methods [3, 5, 7–13]. Before going into the details we need to consider some mathematical preliminaries. The common denominator in all these approaches is the representation of Hamiltonian systems by symplectic maps [22] which are then iterated to obtain the time evolution of the system.

We start by defining certain mathematical objects. For simplicity, we restrict ourselves to three degree-of-freedom systems. Let us denote the collection of six phase-space variables $q_i$, $p_i$ $(i = 1, 2, 3)$ by the symbol $z$:

$$z = (q_1, p_1, q_2, p_2, q_3, p_3). \tag{5.1}$$

The Lie operator corresponding to a phase-space function $f(z)$ is denoted by: $f(z)$:. It is defined by its action on a phase-space function $g(z)$ as shown below

$$:f(z):g(z) = [f(z), g(z)]. \tag{5.2}$$

Here $[f(z), g(z)]$ denotes the usual Poisson bracket of the functions $f(z)$ and $g(z)$ [cf. eq. (2.2)]. Next, we define the exponential of a Lie operator. It is called a Lie transformation and is given by

$$e^{:f(z):} = \sum_{n=0}^{\infty} \frac{:f(z):^n}{n!}. \tag{5.3}$$

Powers of $:f(z):$ that appear in the above equation are defined recursively by the relation

$$:f(z):^n g(z) = :f(z):^{n-1}[f(z), g(z)], \tag{5.4}$$

with

$$:f(z):^0 g(z) = g(z). \tag{5.5}$$

For further details regarding Lie operators and Lie transformations, see [22].

The time evolution of the Hamiltonian system can be represented by a symplectic map $\mathcal{M}$ [22] as follows:

$$\frac{d\mathcal{M}}{dt} = \mathcal{M}: -H(z_0):. \tag{5.6}$$

Symplectic maps are maps whose Jacobian matrices $M(z)$ satisfy the following symplectic condition

$$\widetilde{M(z)}JM(z) = J, \tag{5.7}$$

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

$$J = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix}. \tag{5.8}$$

Matrices $M$ satisfying (5.7) are called symplectic matrices and the corresponding maps $\mathcal{M}$ symplectic maps. Symplectic maps explicitly preserve the symplectic condition. It can be shown [22] that the set of all $\mathcal{M}$'s forms an infinite dimensional Lie group of symplectic maps. On the other hand, the set of all real $6 \times 6$ symplectic matrices forms the finite dimensional real symplectic group $Sp(6, R)$.

The above map $\mathcal{M}$ gives the final state $z^{(1)}$ of a particle after one time step as a function of its initial state $z^{(0)}$:

$$z^{(1)} = \mathcal{M}z^{(0)}. \tag{5.9}$$

To obtain the state of a particle after $N$ time steps, one has to merely iterate the above mapping $N$ times i.e.

$$z^{(N)} = \mathcal{M}^N z^{(0)}. \tag{5.10}$$

Thus, we have obtained an integrator that is symplectic (since $\mathcal{M}$ preserves symplecticity). Moreover, we have the values of phase space variables after one time step as explicit functions of the initial values.

### 5.1 *Generating function methods*

We reformulate the generating function method using Lie algebraic techniques [3]. For a time-independent Hamiltonian, (5.6) can be solved formally to give

$$\mathcal{M}(t) = \exp(: -tH(z_0):). \tag{5.11}$$

If one could solve this explicitly, one would get a symplectic integrator valid to arbitrary order since symplectic maps explicitly preserve the symplectic condition. However, unless the Hamiltonian is integrable, one can not evaluate the Lie transformation on the right hand side. On the other hand, for special Hamiltonians, it may be possible to split

the Hamiltonian as follows:

$$\begin{aligned} H &= H_1 + H_2, \\ \mathcal{N}_i(t) &\equiv \exp(:-tH_i:) \quad i = 1,2, \end{aligned} \tag{5.12}$$

where the symplectic map $\mathcal{N}_i$ can be evaluated exactly (or up to order $t^k$, the order of the symplectic integration method that we wish to derive). The above restriction is a drawback of this method (equivalent to the invertibilty of momenta equation in § 3). We will overcome this restriction in the next subsection.

Under the assumption that $H$ can be split as above, one can construct symplectic integration methods as follows. Consider

$$\mathcal{N}(t) = \mathcal{N}_1(t)\mathcal{N}_2(t). \tag{5.13}$$

Since each symplectic map $\mathcal{N}_i$ is a canonical transformation [22], $\mathcal{N}$ is a product of two canonical transformations. Therefore, this is just a reformulation of the generating function method considered in § 3. Using the group-theoretical Campbell–Baker–Hausdorff (CBH) formula [23], one obtains

$$\mathcal{N}(t) = \mathcal{N}_1(t)\mathcal{N}_2(t) = \exp(:-tH_1 - tH_2 - t^2[H_1, H_2]/2 + \cdots:). \tag{5.14}$$

Using eq. (5.12), we get

$$\mathcal{N}(t) = \mathcal{M}(t) + O(t^2). \tag{5.15}$$

Thus, $\mathcal{N}(t)$ is a symplectic first-order approximation to $\mathcal{M}(t)$ and consequently, we get $z(t)$ as a function of $z(0)$ accurate to order $t$. In other words, we have succeeded in obtaining a first-order symplectic integrator. If we apply this to the $H$ given in (3.1) with $H_1 = A(p)$ and $H_2 = V(q)$, we get back (3.6). This again demonstrates the equivalence of this method with the generating function method described in § 3.

To obtain a fourth-order symplectic integrator, we start with the relation [3]

$$\mathcal{N}(t) = \mathrm{e}^A \mathrm{e}^B \mathrm{e}^{\alpha A} \mathrm{e}^{\beta B} \mathrm{e}^{\alpha A} \mathrm{e}^B \mathrm{e}^A,$$

where

$$2(1+\alpha)A = :-tH_1:, \quad (2+\beta) = :-tH_2:.$$

If

$$\alpha = 1 - 2^{1/3}, \quad \beta = \frac{4\alpha^2 - 4\alpha - 2}{(\alpha+1)^2},$$

we get [3]

$$\mathcal{N}(t) = \mathcal{M}(t) + O(t^5).$$

This is of course a symplectic integrator of order 4. This is actually the same integrator that we discussed in § 3 in a different form.

The above method was further generalized by Yoshida [7] to obtain symplectic integrators of arbitrary even orders for Hamiltonians of the form given in (3.1).

### 5.2 *Symplectic completion of symplectic jets*

In this approach [8–10, 12, 13], symplecticity is achieved by refactorizing the truncated symplectic map using the so-called 'jolt maps'.

We start by factorizing the symplectic map $\mathcal{M}$ [cf. eq. (5.6)] representing the Hamiltonian system using the Dragt–Finn factorization theorem [22, 24] from Lie perturbation theory:

$$\mathcal{M} = \hat{M} e^{:f_3:} e^{:f_4:} \cdots e^{:f_n:} \cdots . \tag{5.16}$$

Here $\hat{M}$ gives the linear part of the map and hence has an equivalent representation in terms of the Jacobian matrix $M(0)$ of the map $\mathcal{M}$ at the origin [22]:

$$\hat{M} z_i = M_{ij} z_j = (Mz)_i. \tag{5.17}$$

Thus, $\hat{M}$ is said to be the Lie transformation corresponding to the $6 \times 6$ matrix $M$ belonging to $Sp(6, R)$. The infinite product of Lie transformations $\exp(:f_n:)$ $(n = 3, 4, \ldots)$ in (5.16) represents the nonlinear part of $\mathcal{M}$. Here $f_n(z)$ denotes a homogeneous polynomial (in $z$) of degree $n$ uniquely determined by the factorization theorem.

One can not use $\mathcal{M}$ in the form given in (5.16) for numerical computations since it involves an infinite number of Lie transformations. Using the perturbation theory approach, we therefore truncate $\mathcal{M}$ as follows:

$$\mathcal{M} \approx \hat{M} e^{:f_3:} e^{:f_4:} \cdots e^{:f_P:}. \tag{5.18}$$

However, each exponential $e^{:f_n:}$ in $\mathcal{M}$ still contains an infinite number of terms in its Taylor series expansion. One possible way around this is to truncate the Taylor series generated by the Lie transformations to order $P$ giving the following truncated map (denoted by $\mathcal{M}_P$):

$$\begin{aligned} \mathcal{M}_P z = M(1 + :f_3: + \cdots)(1 + :f_4: + \cdots) \cdots \\ \cdots (1 + :f_p: + \cdots) z. \end{aligned} \tag{5.19}$$

Here the power series is truncated in such a way that the highest order term generated is $z^{P-1}$. The truncated map $\mathcal{M}_P$ is called a symplectic jet of order $P$ (for a more precise definition, see [10]). Despite its name, $\mathcal{M}_P$ is not symplectic because of the truncation of the Taylor series. Therefore, it can lead to spurious damping or growth (as discussed earlier).

The basic idea behind the approaches followed [8, 10, 12] is to refactorize $\mathcal{M}_P$ [cf. eq. (5.19)] as a product of symplectic maps that can be evaluated exactly. This process of refactorizing $\mathcal{M}_P$ goes by the name of 'symplectic completion of symplectic jets'.

We begin this process by defining jolt maps. Consider the symplectic map given by $e^{:g(z):}$ where $g(z)$ is a function of the phase space variables $z$. It is called a jolt map if $:g(z):$ is a nilpotent operator of rank 2 i.e. if the following condition is satisfied

$$:g(z):^2 z = 0. \tag{5.20}$$

The function $g(z)$ is then called a jolt function. We note that jolt maps have only two non-zero terms in their Taylor series expansions [cf. eq. (5.3)]. Hence they can be evaluated exactly without any truncation. The term jolt map was first introduced in [12]. An example of jolt map [10] is given below:

$$e^{:\hat{R}f(q_1,q_2,q_3):}. \tag{5.21}$$

Here $f(q_1, q_2, q_3)$ is an $n$th degree polynomial in variables $q_1$, $q_2$, and $q_3$ and $\hat{R}$ is the Lie transformation corresponding to a $6 \times 6$ matrix $R$ belonging to any subgroup of $Sp(6, R)$. $\hat{R}$ is given by the following relation [cf. eq. (5.17)]

$$\hat{R}z_i = R_{ij}z_j = (Rz)_i. \tag{5.22}$$

Now we can formulate the problem [8]. Given the map $\mathcal{M}_P$, find another map $\mathcal{J}$ specified by the following product of $K$ jolt maps

$$\mathcal{J} = \hat{M}e^{:g_3^{(1)}+g_4^{(1)}+\cdots+g_P^{(1)}:}e^{:g_3^{(2)}+g_4^{(2)}+\cdots+g_P^{(2)}:}\ldots e^{:g_3^{(K)}+g_4^{(K)}+\cdots+g_P^{(K)}:} \tag{5.23}$$

such that this map agrees with $\mathcal{M}_P$ to order $P$ i.e.

$$\mathcal{J} \cong \mathcal{M}_P \quad \text{to order } P. \tag{5.24}$$

Here $g_n^{(i)}$'s are (homogeneous) jolt polynomials of degree $n$ given by the following relation

$$g_n^{(i)} = \beta_n^{(i)}\hat{R}_i q_1^n \quad i = 1, 2, \ldots, K, \tag{5.25}$$

where $\beta_n^{(i)}$ is a real coefficient. The matrices $R_i$ belong to a subgroup of $Sp(6, R)$ (including $Sp(6, R)$ itself) and $\hat{R}_i$ denotes the Lie transformation corresponding to these matrices [cf. eq. (5.22)]. Since $\mathcal{J}$ is given as a product of finite number of jolt maps, it can be evaluated exactly without any truncation. Thus it gives a symplectic approximation to $\mathcal{M}_P$ accurate to order $P$.

By comparing terms of same order in $\mathcal{M}_P$ and $\mathcal{J}$, the problem of obtaining a symplectic completion for $\mathcal{M}_P$ can be reduced to the following general problem: Given a $n$th degree homogeneous polynomial $f_n$ and $K$ matrices $R_i$, find the coefficients $\beta_n^{(i)}$'s such that the following condition is satisfied

$$\sum_{i=1}^{K} \beta_n^{(i)}\hat{R}_i q_1^n = f_n. \tag{5.26}$$

Typically, one has more $\beta_n^{(i)}$'s than there are equations. So, one imposes constraints on these coefficients. In [10], the sum of squares of these coefficients is minimized. A more sophisticated approach can be found in [12, 13].

To proceed further, following the approach given in [10], one goes to the continuum limit of the above problem. We get the following continuum problem: Given an $n$th degree homogeneous polynomial $f_n$ and a subgroup $G$ of $Sp(6, R)$ on which invariant integration is well defined, find the function $g(u)$ such that the following condition is satisfied

$$f_n = \int_G \mathrm{d}u\, g(u)\hat{R}(u)q_1^n. \tag{5.27}$$

Here $u$ denotes a general element of the group $G$ and $\hat{R}(u)$ denotes the Lie transformation corresponding to $u$. All integrations are invariant integrations performed over the group $G$. Again, an appropriate constraint on $g(u)$ is imposed.

This problem has been solved [10] by taking the group $G$ to be $SU(3)$. The solution is given by:

$$g(u) = \sum_{j,m} \frac{\mathrm{d}\phi_m^j}{\xi^j} \bar{\mathcal{D}}^j{}_{mm_j}(u), \quad j \leq n. \tag{5.28}$$

Here, $\xi_j$'s (all of which can be shown to be non-zero) and $\phi_m^j$'s are the coefficients

obtained by expanding $q_1^n$ and $f_n$ respectively in terms of $SU(3)$ basis vectors. Further, $\bar{\mathcal{D}}^j_{mm_j}(u)$'s are the complex conjugates of the usual $D$ matrices that occur in $SU(3)$ representation theory. Finally, $d$ is the dimension of the $SU(3)$ representation labeled by $j$.

Once the continuum solution has been obtained, one can go back to the discrete case by using discrete subgroups of $SU(3)$ or by quadrature formulas. See refs [10, 12, 13] for further details.

Now that a solution $g(u)$ has been obtained, we would like to reduce the number of jolt maps involved in the refactorization so that a fast numerical integration method is obtained. A substantial reduction can be achieved by splitting the integration over $SU(3)$ as an integration over $SO(3)$ followed by an integration over the coset space $SU(3)/SO(3)$. In ref. [10] it is shown that the number of jolt maps required by following this approach is less than that required by Irwin [8]. Irwin uses the group $U(1) \times U(1) \times U(1)$. However, there are still many theoretical problems regarding integration over coset spaces etc. which are not fully resolved. Work is still proceeding along these lines.

### 5.3 *Solvable map method*

In this approach [9,11], the symplectic map $\mathcal{M}$ is refactorized using the so-called 'solvable maps'.

Solvable maps [11] 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 explicitly. The Lie transformation $\exp(:aq_1^{l+2} + bq_1^{l+1}p_1:)$ is a simple example of a solvable map that is not a kick. One finds that

$$q_1' = \exp(:aq_1^{l+2} + bq_1^{l+1}p_1:)\, q_1 = \frac{q_1}{[1 + lbq_1^l]^{\frac{1}{l}}} \quad \text{for} \quad l \geq 1, \tag{5.29}$$

$$p_1' = \exp(:aq_1^{l+2} + bq_1^{l+1}p_1:)\, p_1 = \frac{E - a(q_1')^{l+2}}{b(q_1')^{l+1}}, \tag{5.30}$$

where

$$E = aq_1^{l+2} + bq_1^{l+1}p_1. \tag{5.31}$$

The basic idea behind the solvable map method is to represent each nonlinear factor $\exp(:f_n:)$ in $\mathcal{M}_P$ [cf. eq. (5.18)] as a product of solvable maps:

$$\exp(:f_n:) = \exp(:g_1:)\, \exp(:g_2:) \cdots \exp(:g_m:) \quad \text{for} \quad n \geq 3. \tag{5.32}$$

For example, consider the Lie representation of a general fourth order map in one dimension [cf. eq. (5.18)]:

$$\mathcal{M}_4 = \hat{M} \exp(:f_3:)\, \exp(:f_4:) \tag{5.33}$$

where

$$f_3 = a_1q_1^3 + a_2q_1^2p_1 + a_3q_1p_1^2 + a_4p_1^3, \tag{5.34}$$

$$f_4 = a_5q_1^4 + a_6q_1^3p_1 + \cdots + a_9p_1^4. \tag{5.35}$$

This can be represented in terms of solvable maps as given below:

$$\mathcal{M}_4 = \hat{M} \exp(:b_1 q_1^3 + b_2 q_1^2 p_1 :) \exp(:b_3 q_1 p_1^2 + b_4 p_1^3 :)$$
$$\exp(:b_5 q_1^4 + b_6 q_1^3 p_1 :) \exp(:b_7 q_1^2 p_1^2 :) \exp(:b_8 q_1 p_1^3 + b_9 p_1^4 :), \quad (5.36)$$

where

$$b_i = a_i \quad \text{for} \quad i = 1, 2, \ldots, 5 \quad \text{and} \quad i = 9, \quad (5.37)$$
$$b_6 = a_6 - 3a_1 a_3, \quad (5.38)$$
$$b_7 = a_7 - 9a_1 a_4/2 - 3a_2 a_3/2, \quad (5.39)$$
$$b_8 = a_8 - 3a_2 a_4. \quad (5.40)$$

Only some preliminary work has been done on this method. It needs a stronger theoretical foundation.

Another related approach is the monomial factorization method. See Refs [25, 26] for further details.

## 6. Summary

In this paper, we saw that if integration performed on a Hamiltonian system is not symplectic, one can draw wrong conclusions regarding the long-term stability of the system. We looked at various methods for symplectic integration. There is no single ideal method yet. Generating function methods suffer from the drawback that implicit equations have to be solved numerically during the process of integration with its attendent convergence problems. This can also lead to reduction in the speed of the algorithm. Symplectic RK methods are again implicit. Symplectic RKN methods can be explicit but are slow for long-term integration. This is especially so when one is integrating complicated systems like particle storage rings with thousands of components. Integration using symplectic maps can be very fast since one has to merely iterate the maps. Methods using Lie algebraic properties (like jolt factorization method and solvable map method) also give maps where the final values of variables are explicit functions of initial values. For these reasons, these approaches look most promising especially for long-term integration. However, some theoretical problems associated with these methods are not fully resolved.

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