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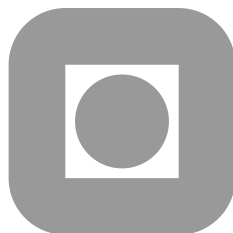
On conjugate B-series and their geometric structure

by

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On conjugate B-series and their geometric structure

Elena Celledoni,[§] Robert I McLachlan,[¶] Brynjulf Owren,^{*} and GRW Quispel^{||}

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The characterizations of B-series of symplectic and energy preserving integrators are well-known. The graded Lie algebra of B-series of modified vector fields include the Hamiltonian and energy preserving cases as Lie subalgebras, these spaces are relatively well understood. However, two other important classes are the integrators which are conjugate to Hamiltonian and energy preserving methods respectively. The modified vector fields of such methods do not form linear subspaces and the notion of a grading must be reconsidered. We suggest to study these spaces as filtrations, and viewing each element of the filtration as a vector bundle whose typical fiber replaces the graded homogeneous components. In particular, we shall study properties of these fibers, a particular result is that, in the energy preserving case, the fiber of degree n is a direct sum of the n th graded component of the Hamiltonian and energy preserving space. We also give formulas for the dimension of each fiber, thereby providing insight into the range of integrators which are conjugate to symplectic or energy preserving.

1 Introduction

In recent years the conservation of geometric properties in numerical integrators has attracted a lot of interest. Examples of such geometric properties are symplecticity, preservation of first integrals, and volume preservation. For Runge-Kutta methods some early and important results were: They conserve all linear invariants and there exists a subclass of methods which conserves quadratic invariants and symplecticity. No Runge-Kutta method conserves volume for every divergence free vector field. More recently, much attention has been given to a more general class of integrators which include the Runge-Kutta methods as a subclass. These are in general the schemes which can be expanded in a B -series, see e.g. [6]. Several families of integration methods belong to this class, usually denoted B -series methods, but one should keep in mind that not every B -series corresponds to a scheme of a known format. In particular, the exact solution of the ODE system can be expanded in a B -series. In the sequel we shall

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mostly consider properties of B -series without paying particular attention to whether each series corresponds to a computable integration scheme. This approach was taken for instance in [3, 4, 5] where results similar to those mentioned above for Runge-Kutta methods were proved in more generality. An important result was that for canonical Hamiltonian problems there exists a large class of B -series schemes which preserve the Hamiltonian. Later, it was observed by Quispel and McLaren [8] that the Average Vector Field (AVF) method is energy preserving for Hamiltonian problems. This scheme is defined as

$$y^{n+1} = y^n + h \int_0^1 f((1 - \xi)y^n + \xi y^{n+1}) d\xi$$

when applied to autonomous ODEs $y' = f(y)$. Note that the integral in the AVF method is calculated on the interval $[0, 1]$ for a real variable ξ . For many known Hamiltonian problems, this integral can be computed exactly a priori.

Insisting on the preservation of geometric structure in numerical integrators may sometimes cause the resulting schemes to be somewhat computational expensive or may alternatively exclude integrators that we know from experience have good long term properties. It may therefore be advantageous to relax on the preservation requirement by allowing for *conjugacy*. For an integrator represented as a map ϕ_h , one may take any consistent integrator χ_h and construct the conjugate scheme $\bar{\phi}_h = \chi_h \circ \phi_h \circ \chi_h^{-1}$. Applying this new scheme over N time steps results in the approximation $\bar{\phi}_h^N = \chi_h \circ \phi_h^N \circ \chi_h^{-1}$ showing that the long term behaviour of two conjugate methods does not depend on the number of time steps taken. It is of interest to understand the structure and richness of integrators which are conjugate to symplectic or energy preserving, and this will be discussed in what remains of this paper.

2 Preliminaries

The methods we consider are maps that may be formally expanded in a Taylor series. The integrator is a map ϕ_h so that a step is the iteration $y_{n+1} = \phi_h(y_n)$, where we have suppressed the dependence of the ODE vector field $f(y)$ in the notation. The sequence $\{y_n\}$ approximates the exact solution $y_n \approx y(x_n)$ at a discrete set of values $\{x_n\}$. For a system of ODEs written in autonomous form, $y' = f(y)$, we consider integrators having the expansion

$$\phi_h(y) = y + hf(y) + h^2 \frac{a(\bullet)}{1} f'f(y) + h^3 \frac{a(\mathfrak{Y})}{2} f''(f, f)(y) + \dots$$

As indicated, the terms of this infinite series are indexed by the set T of rooted trees, we write

$$\phi_h(y) = y + \sum_{t \in T} \frac{h^{|t|}}{\sigma(t)} a(t) F(t)(y), \quad (1)$$

where $|t|$ is the number of vertices in t . Each rooted tree is written recursively as either the one-node tree $\bullet \in T$, or in terms of its subtrees, $t = [t_1, \dots, t_m] \in T$ where each $t_i \in T$. Alternatively $t = [t_1^{r_1}, \dots, t_p^{r_p}]$ indicating that the subtree t_i occurs r_i times. With this notation, we can define the other functions appearing in (1). The symmetry coefficient $\sigma(t)$ can be defined recursively as

$$\sigma(\bullet) = 1, \quad \sigma([t_1^{r_1}, \dots, t_p^{r_p}]) = r_1! \cdots r_p! \sigma(t_1)^{r_1} \cdots \sigma(t_p)^{r_p}$$

The elementary differential $F(t)$ is similarly defined as

$$F(\bullet) = f, \quad F([t_1, \dots, t_m]) = f^{(m)}(F(t_1), \dots, F(t_m)), \quad (2)$$

and $a(t)$ is a coefficient particular to the map ϕ_h .

It is long known [6] that one may also formally represent any integrator map by means of a vector field $\tilde{f}_h(y)$, depending on the step size h . Letting $u(t)$ be the exact solution to the initial value problem $u' = \tilde{f}_h(u)$, $u(x_0) = u_0$, one has $u(x_n) = y_n$ for every n . The *modified vector field* $\tilde{f}_h(y)$ has the expansion

$$h\tilde{f}_h(y) = hf(y) + h^2f_2(y) + \dots$$

and by doing the formal calculations one is able to express the terms $f_j(y)$ by means of the same elementary differentials that appear in (1), that is,

$$h\tilde{f}_h = \sum_{t \in T} \frac{h^{|t|}}{\sigma(t)} b(t) F(t), \quad (3)$$

where the coefficients $b(t)$ have been derived from $a(t)$ in (1). For more details on such expansions and the relationship between the coefficients $a(t)$ and $b(t)$, see e.g. [1, 6]. In the rest of the paper we shall always work with the representation (3) rather than (1) for the methods we consider.

The Lie-Jacobi bracket between two smooth vector fields $X(y)$ and $Y(y)$ is again a vector field, we write $Z = \llbracket X, Y \rrbracket$. Using coordinates $y = (y^1, \dots, y^r)$, we may express $X(y)$ and $Y(y)$ as vectors with components $X^i(y)$, $Y^i(y)$, it is useful to reinterpret each vector field as a first order differential operator (derivation) $X := \sum_i X^i(y) \frac{\partial}{\partial y_i}$ and $Y := \sum_i Y^i(y) \frac{\partial}{\partial y_i}$. The Lie bracket between X and Y is simply the commutator

$$Z = \llbracket X, Y \rrbracket = XY - YX, \quad Z^i = \llbracket X, Y \rrbracket^i = \sum_{j=1}^r \left(X^j \frac{\partial Y^i}{\partial y^j} - Y^j \frac{\partial X^i}{\partial y^j} \right). \quad (4)$$

Let u and v be two rooted trees and $F(u)$ and $F(v)$ the corresponding elementary differentials, considered as vector fields. Combining (2) and (4) one finds that $\llbracket F(u), F(v) \rrbracket$ is a linear combination of vector fields $F(t_i)$ where $|t_i| = |u| + |v|$ for each i . In the rest of this paper, the particular ODE vector field f from which the elementary differentials are induced will not be of importance. We shall therefore simplify the notation and define the real vector space \mathcal{T} consisting of finite linear combinations of the elements of T . The step size h can be set to 1, since the powers of h are already encoded as the number of vertices in the tree t . Then we replace the series in (3) by

$$\sum_{t \in T} \frac{b(t)}{\sigma(t)} t \quad (5)$$

and we may think of b as a linear form on \mathcal{T} , thus $b \in \mathcal{T}^*$. One may further split the space \mathcal{T} into a direct sum of subspaces

$$\mathcal{T} = \bigoplus_{q>0} \mathcal{T}^q$$

where \mathcal{T}^q is the subspace of \mathcal{T} with basis $\{t \in T : |t| = q\}$. The Lie-Jacobi bracket (4) can be realized directly on \mathcal{T} . For $u, v \in T$, one defines $\llbracket u, v \rrbracket \in \mathcal{T}$ by adding together all trees

obtained by grafting u on each vertex of v and then subtracting all trees obtained by grafting v on each vertex of u , for example

$$\llbracket \mathfrak{V}, \mathfrak{V} \rrbracket = \mathfrak{V} \circ \mathfrak{V} + \mathfrak{V} \circ \mathfrak{V} + \mathfrak{V} \circ \mathfrak{V} - \mathfrak{V} \circ \mathfrak{V} - 2 \mathfrak{V} \circ \mathfrak{V}$$

This grafting procedure certainly respects the grading introduced above, in the sense that if $u \in \mathcal{T}^q$, $v \in \mathcal{T}^r$, then $\llbracket u, v \rrbracket \in \mathcal{T}^{q+r}$, this makes \mathcal{T} into a graded Lie algebra.

Another structure we shall make frequent use of is the Butcher product. It is a non-commutative product $\circ : T \times T \rightarrow T$ defined between two trees as follows: If $u = [u_1, \dots, u_m] \in T^q$ and $v \in T^r$ then $u \circ v = [u_1, \dots, u_m, v] \in T^{q+r}$. An example is

$$\mathfrak{V} \circ \mathfrak{V} = \mathfrak{V} \circ \mathfrak{V}$$

The product can be used to impose an equivalence relation on the rooted trees. A key observation is that for any two rooted trees u and v , $v \circ u$ is obtained from $u \circ v$ by shifting the position of the root to a neighbor vertex. Using the same example as above one may consider

$$\mathfrak{V} \circ \mathfrak{V} = \mathfrak{V} \circ \mathfrak{V} \quad \text{versus} \quad \mathfrak{V} \circ \mathfrak{V} = \mathfrak{V} \circ \mathfrak{V}$$

the second tree is obtained by shifting the root of the first tree one position up along the rightmost branch. Conversely, any two trees which differ just by such a root shift can be factored $u' \circ v'$ and $v' \circ u'$ so that we may define equivalence classes of trees known as free trees. Such a class consists of some rooted tree τ as well as any other rooted tree obtained from τ by shifting the root to some other vertex of τ . Free trees may therefore be associated to unrooted trees. The two related trees above belong to an equivalence class (free tree) with five elements

$$\dots \ni \{ \mathfrak{V}, \mathfrak{V}, \mathfrak{V}, \mathfrak{V}, \mathfrak{V} \}$$

For two rooted trees u and v belonging to the same free tree, we define the symmetric function $\kappa(u, v)$ to be the number of root shifts needed to obtain v from u . The bicentered unrooted trees are precisely the free trees which can be factorized as $u \circ u$ for some $u \in T$. We call these trees *superfluous* free trees. Any free tree which is not superfluous will be called *nonsuperfluous* in the sequel. An example of a superfluous free tree is $\mathfrak{V} \circ \mathfrak{V}$ where we can cut an edge to yield two copies of \mathfrak{V} . We shall denote the set of free trees by FT and the subset of nonsuperfluous free trees we call \overline{FT} and we use boldface letters for members of these sets.

2.1 B-series of symplectic integrators

The B -series corresponding to symplectic methods are those whose modified equation is Hamiltonian, this is a linear subspace of \mathcal{T} , in fact even a graded Lie subalgebra, we denote it by \mathcal{T}_Ω and its graded components $\mathcal{T}_\Omega^n \subseteq \mathcal{T}^n$. It is well known that a B -series with coefficients $b(t)$ as in (5) represents a Hamiltonian vector field if and only if the coefficients satisfy

$$b(u \circ v) + b(v \circ u) = 0, \quad \forall u, v \in T.$$

These equations only impose conditions between coefficients of rooted trees belonging to the same free tree, we get one independent condition for every root shift so in total there are $q - 1$

conditions for a free tree with q members. For superfluous trees, the factorization $t = u \circ u$ implies $b(t) = 0$ and inductively, any other tree t' in the same equivalence class must have $b(t') = 0$. For every non-superfluous free tree, $\mathbf{t} \in \overline{FT}$ the $q - 1$ conditions on the q members lead to precisely one basis element, this can be taken to be

$$\tau = \sum_{u \sim t} \frac{(-1)^{\kappa(t,u)}}{\sigma(u)} u, \quad t \in \pi^{-1}(\mathbf{t}), \quad \mathbf{t} \in \overline{FT}.$$

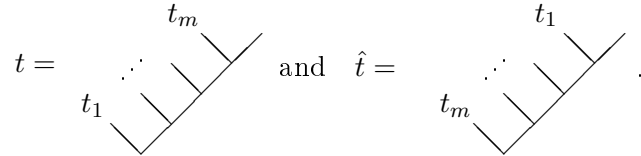
The representative $t \in \pi^{-1}(\mathbf{t})$ is arbitrary here.

2.2 B-series of energy preserving integrators

Similarly, we may consider methods ϕ_h which preserve the Hamiltonian, i.e. $H(y) = H(\phi_h(y))$ for all y in phase space. Assuming that ϕ_h has a modified vector field, we shall say that this belongs to the space \mathcal{T}_H . This space is also a graded linear subspace of \mathcal{T} , with graded components $\mathcal{T}_H^n \subset \mathcal{T}^n$. The conditions for a B-series like (5) to be energy preserving were derived in [3, 4], the conditions involving elements in \mathcal{T}^n are indexed by \overline{FT}^{n+1} . A condition corresponding to $\mathbf{t} \in \overline{FT}^{n+1}$ is derived as follows: Denote by $s_{\mathbf{t}}$ the subset of $\pi^{-1}(\mathbf{t})$ consisting of trees of the form $[t']$, i.e. those obtained by placing the root at a leaf. Let $[t]$ be some designated member of $\pi^{-1}(\mathbf{t})$. The condition corresponding to \mathbf{t} is

$$\sum_{[t'] \in s_{\mathbf{t}}} \frac{(-1)^{\kappa([t],[t'])}}{\sigma(t')} b(t') = 0$$

It is possible to find a basis for \mathcal{T}_H^n whose elements consist of linear combinations of at most two trees, these trees were given in [8], and in [2] it was proved to be a spanning set and a way of selecting a basis from this was indicated. The members of this spanning set are of the form $t + (-1)^m \hat{t}$ where t and \hat{t} are given as [2]



Here the symbols t_i are forests. The tree t is depicted by taking a pair consisting of the root and some leaf and pull them apart tightly so that the path between these two vertices form the "backbone" of the tree. On each node of this path zero or more trees are attached. To obtain \hat{t} one simply reverts the tree as shown in the figure.

3 Conjugate spaces

We proceed to consider B-series relevant for integrators which can be formally written as

$$\bar{\phi}_h = \chi_h \circ \phi_h \circ \chi_h^{-1}$$

See the theses by Leone [7] and Scully [9] for order conditions for such methods. Note also that conjugate methods have been studied in the context of effective order [1] and as methods

with processing. In more precise terms, we shall be interested in the modified vector fields of such methods and their formal series (5). In what follows, the map ϕ_h will typically be either symplectic or energy preserving, and the conjugation map χ_h can in principle be any map. We shall now represent the modified vector fields of the two maps χ_h, ϕ_h as \mathbf{u} and \mathbf{v} , writing

$$\mathbf{u} = \sum_{t \in T} \frac{u(t)}{\sigma(t)} t, \quad \mathbf{v} = \bullet + \sum_{|t| > 1} \frac{v(t)}{\sigma(t)} t,$$

so that the map $\bar{\phi}_h$ with modified field represented by \mathbf{w} obeys

$$\exp(\mathbf{w}) = \exp(\mathbf{u}) \exp(\mathbf{v}) \exp(-\mathbf{u})$$

from which we derive

$$\mathbf{w} = \exp(\mathbf{u}) \mathbf{v} \exp(-\mathbf{u}) = \exp(\text{ad}_{\mathbf{u}}) \mathbf{v} = \mathbf{v} + \llbracket \mathbf{u}, \mathbf{v} \rrbracket + \frac{1}{2} \llbracket \mathbf{u}, \llbracket \mathbf{u}, \mathbf{v} \rrbracket \rrbracket + \dots$$

Our interest lies in the characterization of all possible series \mathbf{w} of the above form, given that the series \mathbf{u} and \mathbf{v} are allowed to range over certain subsets or subspaces of the space \mathcal{T} . Such series do not form linear spaces, but some of their properties, as for instance their dimensions, can be understood by using two new linear spaces that we shall call $\mathcal{T}_{\bar{H}}^n$ and $\mathcal{T}_{\bar{\Omega}}^n$. We now let U and V be graded subspaces of \mathcal{T} such that

$$U = \bigoplus_{n > 0} U^n, \quad V = \bigoplus_{n > 0} V^n, \quad U^n = \mathcal{T}^n \cap U, \quad V^n = \mathcal{T}^n \cap V$$

We study elements of \mathcal{T} which are conjugations of elements of V by elements in U , following [2] we must then consider the set

$$\mathcal{M} = \{ \mathbf{w} = \exp(\text{ad}_{\mathbf{u}}) \mathbf{v}, \mathbf{u} \in U, \mathbf{v} \in V \}$$

where

$$\mathbf{w} = \exp(\text{ad}_{\mathbf{u}}) \mathbf{v} = \mathbf{v} + \llbracket \mathbf{u}, \mathbf{v} \rrbracket + \frac{1}{2} \llbracket \mathbf{u}, \llbracket \mathbf{u}, \mathbf{v} \rrbracket \rrbracket + \dots \quad (6)$$

\mathcal{M} is not a graded linear subspace of \mathcal{T} so we can not work with graded components as before. Instead we define a filtration through the quotient

$$G^n = \mathcal{T} / \bigoplus_{k > n} \mathcal{T}^k$$

We let $\mathcal{P}_n : \mathcal{T} \rightarrow G^n$ be the canonical projection and we consider the manifolds $\mathcal{M}^n = \mathcal{P}_n \mathcal{M}$ and their dimensions. We introduce the spaces $\mathcal{B}^n \subseteq G^n$ through

$$\mathcal{B}^n = \left\{ \mathbf{w} = \mathcal{P}_n \exp(\text{ad}_{\mathbf{u}}) \mathbf{v}, \mathbf{u} \in \bigoplus_{k \leq n-2} U^k, \mathbf{v} \in \bigoplus_{k \leq n-1} V^k \right\}$$

In fact, due to the grading on \mathcal{T} , we could have written \mathcal{M}^n in a similar way, just replacing the lower index bound in each direct sum by $n-1$ and n respectively. From this point, we assume $\bullet \in V$, and we consider only series $\mathbf{v} = \sum \mathbf{v}^k, \mathbf{v}^k \in V^k$, such that $\mathbf{v}^1 = \bullet$. Define

the projection $\pi : \mathcal{M}^n \rightarrow \mathcal{B}^n$ obtained simply by removing the $n - 1$ -component of \mathbf{u} and the n -component of \mathbf{v} . Precisely, if

$$\mathbf{w} = \mathcal{P}_n \exp(\text{ad}_{\mathbf{u}})\mathbf{v}, \quad \mathbf{u} = \sum_{k=1}^{n-1} \mathbf{u}^k, \quad \mathbf{v} = \bullet + \sum_{k=2}^n \mathbf{v}^k,$$

then

$$\pi \mathbf{w} = \mathcal{P}_n \exp(\text{ad}_{\bar{\mathbf{u}}})\bar{\mathbf{v}}, \quad \bar{\mathbf{u}} = \sum_{k=1}^{n-2} \mathbf{u}^k, \quad \bar{\mathbf{v}} = \bullet + \sum_{k=2}^{n-1} \mathbf{v}^k.$$

The triple $(\mathcal{M}^n, \mathcal{B}^n, \pi)$ forms a vector bundle with total space \mathcal{M}^n , base space \mathcal{B}^n and projection π . The typical fiber is $F^n = \pi^{-1}(x)$, and by construction this space is obtained simply by considering all terms of (6) which depend only on the $n - 1$ -component of u and the n -component of v ,

$$F^n = V^n + \llbracket U^{n-1}, \bullet \rrbracket.$$

Using the natural identification of G^n with $\mathcal{T}^1 \oplus \dots \oplus \mathcal{T}^n$ it is easy to see that $\dim \mathcal{B}^n \geq \dim \mathcal{M}^{n-1}$, thus,

$$\dim \mathcal{M}^n = \dim \mathcal{B}^n + \dim F^n \geq \dim \mathcal{M}^{n-1} + \dim F^n,$$

such that a lower bound for the dimension of \mathcal{M}^n can be obtained by summing up the dimensions of each F^k for $k = 1, \dots, n$.

One may say that the fibers F^k play a similar role for the conjugate spaces as do the graded components \mathcal{T}_Ω^n and \mathcal{T}_H^n for the Hamiltonian and energy preserving vector fields respectively. In our application we choose V to be either of \mathcal{T}_Ω or \mathcal{T}_H . The spaces we use to conjugate with can in principle be \mathcal{T} in both cases, but we find it reasonable to choose U to be a complement of \mathcal{T}_Ω in the Hamiltonian case and a complement of \mathcal{T}_H in the energy preserving case. We denote such complements $\mathcal{T}'_\Omega, \mathcal{T}'_H$ respectively. The corresponding manifold \mathcal{M} is characterized in terms of the bundles $(\mathcal{M}^n, \mathcal{B}^n, \pi)$ and the fibers F^n are denoted $\mathcal{T}'_\Omega^n, \mathcal{T}'_H^n$ respectively. In fact, in these two cases it is possible to prove that

$$\dim \mathcal{B}^n = \dim \mathcal{M}^{n-1}$$

and the dimension of \mathcal{M}^n is obtained by summing the dimensions of the fibers F^k for k from 1 to n , see [2].

4 Main results

The results presented here are mostly taken from [2] and are presented without proofs. The reader may keep in mind that there are three important properties of the map $\text{ad}_\bullet : t \mapsto \llbracket \bullet, t \rrbracket$ underlying many of the results used to characterize the conjugate fibers \mathcal{T}'_Ω^n and \mathcal{T}'_H^n . The first is that ad_\bullet is injective on \mathcal{T}^n , $n > 1$. The second is that $\text{ad}_\bullet^{-1}(\mathcal{T}'_\Omega^{n+1}) \subseteq \mathcal{T}'_\Omega^n$ (and similarly with \mathcal{T}'_Ω replaced by \mathcal{T}'_H). The third an explicitly given decomposition of $\text{ad}_\bullet(\tau)$ into the sum of two elements of \mathcal{T}'_Ω and \mathcal{T}'_H .

Theorem 1 *The dimension of \mathcal{T}'_H^n is*

$$\dim \mathcal{T}'_H^n = \dim \mathcal{T}'_H^n + \dim \mathcal{T}^{n-1} - \dim \mathcal{T}'_H^{n-1}.$$

Theorem 2 For $n > 2$,

$$\mathcal{T}_{\tilde{H}}^n = \mathcal{T}_{\Omega}^n \oplus \mathcal{T}_H^n$$

Theorem 3 $\mathcal{T}_{\tilde{\Omega}} \subset \mathcal{T}_{\tilde{H}}$.

Theorem 4

(i) From the four naturally-defined subspaces of B -series, namely \mathcal{T}_{Ω}^n , \mathcal{T}_H^n , $\mathcal{T}_{\tilde{\Omega}}^n$, and $\mathcal{T}_{\tilde{H}}^n$, precisely one new subspace can be constructed using the natural subspace operations of intersection and sum. This is $\mathcal{T}_{\Omega}^n \cap \mathcal{T}_H^n$, the energy-preserving conjugate-to-Hamiltonian B -series.

(ii) $\mathcal{T}_{\tilde{\Omega}}^n \cap \mathcal{T}_H^n$ is isomorphic to $\mathcal{T}_{\tilde{\Omega}}^{n-1}$, and an isomorphism is given by the map

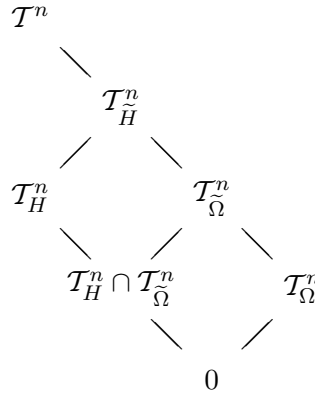
$$\mathcal{T}_{\tilde{\Omega}}^{n-1} \rightarrow \mathcal{T}_{\tilde{\Omega}}^n \cap \mathcal{T}_H^n, \quad t \mapsto \llbracket t, \bullet \rrbracket - X_{[t]} \quad (7)$$

(iii) Its dimension is

$$\dim \mathcal{T}_{\tilde{\Omega}}^n \cap \mathcal{T}_H^n = \dim \mathcal{T}^{n-1} - \dim \mathcal{T}_{\tilde{\Omega}}^{n-1}$$

(iv) There are B -series that are energy-preserving and conjugate-to-Hamiltonian, but are not the (reparameterized) flow of the original differential equation.

Theorem 5 The (Hasse) order diagram under inclusion for the linear spaces \mathcal{T}^n , \mathcal{T}_H^n , $\mathcal{T}_{\tilde{\Omega}}^n$, $\mathcal{T}_{\tilde{H}}^n$, and $\mathcal{T}_{\Omega}^n \cap \mathcal{T}_H^n$ for $n > 2$ is



and their dimensions up to order 10 are as given in Table 1. For $n = 1$ all these spaces are equal to $\text{span}(\bullet)$, while for $n = 2$ we have $\mathcal{T}^2 = \text{span}(\llbracket \bullet \rrbracket)$ and $\mathcal{T}_H^2 = \mathcal{T}_{\tilde{\Omega}}^2 = \mathcal{T}_{\tilde{H}}^2 = \mathcal{T}_{\tilde{\Omega}}^2 = \mathcal{T}_{\tilde{\Omega}}^2 \cap \mathcal{T}_H^2 = 0$.

References

- [1] J. C. Butcher. *Numerical methods for ordinary differential equations*. John Wiley & Sons Ltd, second edition, 2008.
- [2] E. Celledoni, R. I. McLachlan, B. Owren and GRW Quispel, Energy-preserving integrators and the structure of B -series, 2009. Submitted.

order	1	2	3	4	5	6	7	8	9	10
$\dim \mathcal{T}^n$	1	1	2	4	9	20	48	115	286	719
$\dim \mathcal{T}_\Omega^n$	1	0	1	1	3	4	11	19	47	97
$\dim \mathcal{T}_H^n$	1	0	1	1	5	9	29	68	189	484
$\dim \mathcal{T}_\Omega^n$	1	0	2	2	6	10	27	56	143	336
$\dim \mathcal{T}_H^n$	1	0	2	2	8	13	40	87	236	581
$\dim(\mathcal{T}_\Omega^n \cap \mathcal{T}_H^n)$	1	0	1	1	3	6	16	37	96	239

Table 1: Dimensions of the linear spaces spanned by the rooted trees and their 5 natural subspaces.

- [3] E Faou, E Hairer, and T-L Pham, Energy conservation with non-symplectic methods: examples and counter-examples, *BIT* **44** (2004) 699–709.
- [4] P Chartier, E Faou, and A Murua, An algebraic approach to invariant preserving integrators: The case of quadratic and Hamiltonian invariants, *Numer. Math.* **103** (2006), 575–590.
- [5] P Chartier and A Murua, Preserving first integrals and volume forms of additively split systems, *IMA Journal of Numerical Analysis* **27** (2007), 381–405.
- [6] E Hairer, Ch Lubich, and G Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. Structure-preserving algorithms for ordinary differential equations.
- [7] P Leone, Symplecticity and Symmetry of General Integration Methods, Thèse, Section de Mathématiques, Université de Genève, 2000.
- [8] G R W Quispel and D I McLaren, A new class of energy-preserving numerical integration methods, *J. Phys. A* **41** (2008) 045206 (7pp).
- [9] J E Scully, A search for improved numerical integration methods using rooted trees and splitting, MSc Thesis, La Trobe University, 2002.