

# An algebraic approach to invariant preserving integrators: The case of quadratic and Hamiltonian invariants

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**Summary** In this article, conditions for the preservation of quadratic and Hamiltonian invariants by numerical methods which can be written as B-series are derived in a purely algebraical way. The existence of a *modified* invariant is also investigated and turns out to be equivalent, up to a conjugation, to the preservation of the exact invariant. A striking corollary is that a *symplectic* method is formally conjugate to a method that preserves the Hamiltonian exactly. Another surprising consequence is that the underlying one-step method of a symmetric multistep scheme is formally conjugate to a symplectic P-series when applied to Newton's equations of motion.

## 1 Introduction

Given a  $n$ -dimensional system of differential equations

$$y'(x) = f(y(x)), \tag{1}$$

a B-series  $B(a)$  is a formal expression of the form

$$\begin{aligned} B(a) &= id_{\mathbb{R}^n} + \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} a(t) F(t) \\ &= id_{\mathbb{R}^n} + ha(\bullet)f(\bullet) + h^2a(\mathcal{J})(f'f)(\bullet) + \dots \end{aligned} \tag{2}$$

where the index set  $\mathcal{T} = \{\bullet, \mathcal{J}, \mathcal{V}, \mathcal{J}'\dots\}$  is the set of rooted trees, and for each rooted tree  $t$ ,  $|t|$  and  $\sigma(t)$  are fixed positive integers<sup>1</sup>,  $F(t)$  is a map from  $\mathbb{R}^n$  to  $\mathbb{R}^n$  obtained from  $f$  and its partial derivatives, and where  $a$  is a function defined on  $\mathcal{T}$  which characterizes the B-series itself. The concept of B-series was introduced in [HW74], following the pioneering work of John Butcher [But69, But72], and is now exposed in various textbooks and articles, though possibly with different normalizations [CSS94, HNW93, HLW02].

B-series play a central role in the numerical analysis of ordinary differential equations as they may represent most numerical methods for solving the initial value problem

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<sup>1</sup> For illustration, first values are  $|\bullet| = 1$ ,  $|\mathcal{J}| = 2$ ,  $|\mathcal{J}'| = 3$ ,  $\sigma(\bullet) = 1$ ,  $\sigma(\mathcal{J}) = 1$ ,  $\sigma(\mathcal{J}') = 1$ ,  $\sigma(\mathcal{V}) = 2$ .

associated with (1). For instance, it is known [But87] that the numerical flow of a Runge-Kutta method can be expanded as a B-series with coefficients  $a$  depending only on the specific method, or, that multistep methods possess an underlying B-series method [HL04, Kir86]. A further remarkable result of Calvo and Sanz-Serna [CSS94] gives an algebraic characterization of symplectic B-series. More recently, an expression of the Lie-derivative of a B-series has been derived in terms of  $a$ , making some aspects of backward analysis easier [Hai99].

Following the same trend, we aim in this paper at characterizing B-series integrators that preserve quadratic or Hamiltonian invariants. In this context arises a new type of series, introduced by the third author in [Mur99] and embedding B-series (and Lie-derivatives along a vector field represented by a B-series) as a particular case. They are of the form

$$S(\alpha) = \sum_{u \in \mathcal{F}} \frac{h^{|u|}}{\sigma(u)} \alpha(u) X(u) \quad (3)$$

where the index set  $\mathcal{F} = \{e, \bullet, \dots, \mathcal{J}, \dots, \mathcal{J}\bullet, \mathcal{V}, \mathcal{J}, \dots\}$  is now the set of forests,  $|u|$  and  $\sigma(u)$  are for each forest  $u \in \mathcal{F}$  fixed positive integers, and  $X(u)$  is a linear differential operator acting on smooth functions on  $\mathbb{R}^n$ , and where  $\alpha$  is a real function defined on  $\mathcal{F}$  which characterizes the S-series itself. In contrast with B-series, which are (formal) functions from  $\mathbb{R}^n$  to itself, S-series are (formal) differential operators acting on smooth functions  $g \in C^\infty(\mathbb{R}^n)$  (or more generally on smooth maps  $g \in C^\infty(\mathbb{R}^n, \mathbb{R}^m)$ ):

$$S(\alpha)[g] = \alpha(e)g + h\alpha(\bullet)g'f + h^2 \frac{\alpha(\bullet\bullet)}{2} g''(f, f) + h^2 \alpha(\mathcal{J})g'f'f + \dots$$

Assuming that a smooth function  $I$  is a first integral of (1), i.e. satisfies

$$\forall y \in \mathbb{R}^n, \left( \nabla I(y) \right)^T f(y) = 0, \quad (4)$$

preserving  $I$  for an integrator  $B(a)$  amounts to satisfying the condition

$$\forall y \in \mathbb{R}^n, \left( I \circ B(a) \right)(y) = I(y),$$

and it can be shown [Mur99], that

$$I \circ B(a) = S(\alpha)[I], \quad (5)$$

where  $\alpha$ , acting on  $\mathcal{F}$ , is uniquely defined in terms of  $a$ . The requirement of a B-series preserving the first integral  $I$  exactly can sometimes be relaxed by requiring the existence of a *modified invariant*  $\tilde{I}$  obtained as the action on  $I$  of S-series of the form:

$$\tilde{I} = S(\beta)[I] = I + h\beta(\bullet)I'f + \dots$$

**Definition 1** Consider a differential system of the form (1) for which there exists an invariant  $I$ . A **modified invariant**  $\tilde{I}$  of B-series  $B(a)$  is a (formal) series  $\mathcal{O}(h)$ -close to  $I$  of the form

$$\tilde{I} = S(\beta)[I], \quad (6)$$

where  $\beta$  is a function on  $\mathcal{F}$  (satisfying  $\beta(e) = 1$  so that  $\tilde{I} = I + \mathcal{O}(h)$ ), such that

$$\tilde{I} \circ B(a) \equiv \tilde{I}.$$

Using the formalism of S-series introduced with greater detail in Section 2, we derive algebraic conditions for a B-series integrator to *exactly* preserve quadratic and Hamiltonian invariants: in Section 3 we give alternative (algebraic) proofs of already known results:

1. B-series integrators preserve *quadratic* invariants if and only if they satisfy the *symplecticity* conditions (a result already proved for a general class of one-step methods [BS94]);
2. B-series integrators preserve *Hamiltonian* invariants for *Hamiltonian problems* if and only if they satisfy certain specific conditions (also derived in [FHP04]).

The analysis conducted to derive algebraic conditions for exact preservation of invariants serves as a guideline for the rest of the paper; in Section 4 we address the question of existence of *modified* invariants: under which conditions on the B-series integrator may one construct a modified invariant of the form (6)? It turns out that in each of the two aforementioned cases (quadratic and Hamiltonian invariants) such a construction is possible if and only if the method is conjugate to a method that preserves invariants exactly. To be more specific, we provide the proofs of the following results:

1. a B-series integrator possesses a modified invariant for all problems with a *quadratic* invariant if and only if it is conjugate to a *symplectic* method;
2. a B-series integrator possesses a modified Hamiltonian for all *Hamiltonian* problems if and only if it is conjugate to a method that preserves the Hamiltonian exactly;
3. a symplectic B-series is formally conjugate to a B-series that preserves the Hamiltonian exactly.

A surprising consequence of the last but one result (generalized to P-series) along with the results derived in [HL04] is given in Section 5: The underlying one-step method of any symmetric linear multistep method is formally conjugate to a method that is symplectic for Newton equations.

## 2 Basic tools

In this first section, we describe the basic algebraic tools that allow for the manipulation of S-series.

### 2.1 Rooted trees and forests

**Definition 2 (Rooted trees, Forests)** *The set of (rooted) trees  $\mathcal{T}$  and forests  $\mathcal{F}$  can be defined recursively by:*

1. *the forest  $e$  is the empty forest,*
2. *if  $u$  is a forest of  $\mathcal{F}$ , then  $t = [u]$  is a tree of  $\mathcal{T}$ ,*
3. *if  $t_1, \dots, t_n$  are  $n$  trees of  $\mathcal{T}$ , the forest  $u = t_1 \dots t_n$  is the commutative juxtaposition of  $t_1, \dots, t_n$ .*

*Given a forest  $u \in \mathcal{F}$ , we set  $ue = eu = u$ . Given a rooted tree  $t \in \mathcal{T}$ , we denote as  $B^-(t)$  the forest  $u \in \mathcal{F}$  such that  $t = [u]$ . Given two rooted trees  $t, z \in \mathcal{T}$ , we denote  $t \circ z = [B^-(t)z]$ .*

Of course, rooted trees and forest can be defined as graph-theoretical objects, where  $t = [t_1 \cdots t_m]$  is the rooted tree obtained by grafting the roots of  $t_1, \dots, t_m$  to a new vertex which become the root of  $t$ , and  $B^-(t)$  is the forest obtained from removing the root of the rooted tree  $t$ . The rooted tree  $t \circ z$  is obtained from  $t$  by grafting the rooted tree  $z$  to the root of  $t$ . The order of a tree is its number of vertices and is denoted by  $|t|$ . The order  $|u|$  of a forest  $u = t_1 \dots t_n$  is also the number of its vertices, i.e.  $|u| = |t_1| + \cdots + |t_n|$ . If  $u = t_1^{r_1} \dots t_n^{r_n}$  where  $t_1, \dots, t_n$  are pairwise distinct and are repeated respectively  $r_1, \dots, r_n$  times, then the symmetry  $\sigma$  of  $u$  is

$$\sigma(u) = r_1! \dots r_n! (\sigma(t_1))^{r_1} \dots (\sigma(t_n))^{r_n}.$$

By convention,  $\sigma(e) = 1$ . The symmetry  $\sigma(t)$  of a tree  $t = [u]$  is the symmetry of  $u$ .

*Example 1* For instance,

$$[\bullet \cdots \bullet] = \mathfrak{V} \mathfrak{V} \mathfrak{V}, \quad B^-(\mathfrak{V} \mathfrak{V} \mathfrak{V}) = \bullet \cdots \bullet, \quad \text{and } \sigma(\mathfrak{V} \mathfrak{V} \mathfrak{V}) = \sigma(\bullet \cdots \bullet) = 6.$$

Recall that the order in which trees appear in a forest does not matter: For instance,

$$\mathfrak{V} \mathfrak{V} \mathfrak{V} \mathfrak{V} \mathfrak{V} = \mathfrak{V} \mathfrak{V} \mathfrak{V} \mathfrak{V} \mathfrak{V}.$$

## 2.2 B-series, S-series and their composition

For a tree  $t \in \mathcal{T}$  the *elementary differential*  $F(t)$  is a mapping from  $\mathbb{R}^n$  to  $\mathbb{R}^n$ , defined recursively by:

$$F(\bullet)(y) = f(y), \quad F([t_1, \dots, t_n])(y) = f^{(n)}(y) \left( F(t_1)(y), \dots, F(t_n)(y) \right).$$

Similarly, if the right-hand side is of the form  $f(y) = J^{-1} \nabla H(y)$ , the *elementary Hamiltonian*  $H(t)$  is the mapping from  $\mathbb{R}^n$  to  $\mathbb{R}$ , defined recursively by:

$$H(\bullet)(y) = H(y), \quad H([t_1, \dots, t_n])(y) = H^{(n)}(y) \left( F(t_1)(y), \dots, F(t_n)(y) \right).$$

**Definition 3 (Differential operator associated to a forest [Mer57])** Consider a forest  $u = t_1 \dots t_k$  of  $\mathcal{F}$ . The differential operator  $X(u)$  associated to  $u$  is the map operating on smooth functions  $\mathcal{D} = C^\infty(\mathbb{R}^n; \mathbb{R}^m)$  defined as:

$$\begin{aligned} X(u) : \mathcal{D} &\rightarrow \mathcal{D} \\ g &\mapsto X(u)[g] = g^{(k)}(F(t_1), \dots, F(t_k)) \end{aligned}$$

*Example 2* For  $g \in \mathcal{D}$ , one has

$$X(e)[g] = g, \quad X(\bullet)[g] = g'f, \quad X(\mathfrak{J})[g] = g'f'f, \quad X(\mathfrak{J} \bullet \bullet) = g^{(3)}(f'f, f, f).$$

More generally, the relations

$$X(t)[id_{\mathbb{R}^n}] = F(t), \quad X(u)[f] = F([u]), \quad X(t_1 \dots t_n)[H] = H([t_1, \dots, t_n]),$$

hold true.

**Definition 4 (Series of differential operators [Mur99])** Let  $\alpha$  be a function on  $\mathcal{F}$ :

$$\begin{aligned}\alpha &: \mathcal{F} \rightarrow \mathbb{R} \\ u &\mapsto \alpha(u)\end{aligned}$$

We define  $S(\alpha)$ , the series of differential operators associated with  $\alpha$ , as the (formal) series:

$$S(\alpha) = \sum_{u \in \mathcal{F}} \frac{h^{|u|}}{\sigma(u)} \alpha(u) X(u). \quad (7)$$

Consider now the action of a map  $g \in \mathcal{D}$  on a B-series  $B(a)$ , the following formula can be obtained [Mur99]:

$$g \circ B(a) = \sum_{u \in \mathcal{F}} \frac{h^{|u|}}{\sigma(u)} \alpha(u) X(u)[g], \quad (8)$$

with

$$\alpha(e) = 1 \text{ and } \alpha(t_1 \dots t_m) = a(t_1) \cdots a(t_m).$$

It follows that a S-series can be associated to every B-series  $B(a)$ . Conversely, given a map  $\alpha$  from  $\mathcal{F}$  to  $\mathbb{R}$ , there exists a B-series  $B(a)$  such that, for every smooth function  $g$ ,  $S(\alpha)[g]$  can be seen as the action of  $g$  on  $B(a)$ , if and only if

$$\alpha(e) = 1 \text{ and } \forall (t_1, \dots, t_n) \in \mathcal{T}^n, \alpha(t_1 \dots t_n) = \alpha(t_1) \cdots \alpha(t_n). \quad (9)$$

In this case,  $a$  is simply defined by  $a(t) = \alpha(t)$  for all  $t \in \mathcal{T}$ .

**Lemma 1 (Composition of S-series)** Consider two maps  $\alpha, \beta : \mathcal{F} \rightarrow \mathbb{R}$  and let  $S(\alpha)$  and  $S(\beta)$  be the associated series of differential operators. Then the composition of the two series  $S(\alpha)$  and  $S(\beta)$  is again a series  $S(\alpha\beta)$ , i.e.

$$\forall g \in \mathcal{D}, S(\alpha) \left[ S(\beta)[g] \right] = \left( S(\alpha) S(\beta) \right) [g] = S(\alpha\beta)[g] \quad (10)$$

where the map  $\alpha\beta : \mathcal{F} \rightarrow \mathbb{R}$  is uniquely determined from the two maps  $\alpha, \beta : \mathcal{F} \rightarrow \mathbb{R}$ .

*Proof* For a proof, we refer to [Mur05].

The particular formula that gives the map  $\alpha\beta : \mathcal{F} \rightarrow \mathbb{R}$  in terms of the two maps  $\alpha, \beta : \mathcal{F} \rightarrow \mathbb{R}$  can be found in [Mur05]. Such formula is closely related to (actually, it is a generalization of) the well known formula of the composition of B-series [HNW93, HLW02]. For those familiar with the commutative Hopf algebra of rooted trees [Bro04, CK98],  $\alpha\beta = (\alpha \otimes \beta) \circ \Delta$ , where  $\Delta$  is the coproduct in such a Hopf algebra.

Instead of giving a precise formula for  $\alpha\beta$  in Lemma 1, we just give the particular case where  $\beta(\bullet) = 1$  and  $\beta(u) = 0$  whenever  $u \in \mathcal{F} \setminus \{\bullet\}$ .

**Lemma 2** For any map  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$ , we have

$$hS(\alpha)X(\bullet) = S(\alpha'),$$

where  $\alpha'$  is defined by

$$\begin{aligned}\alpha'(e) &= 0, \\ \forall u = t_1 \cdots t_m \in \mathcal{F}, \quad \alpha'(u) &= \sum_{i=1}^m \alpha \left( B^-(t_i) \prod_{j \neq i} t_j \right).\end{aligned}$$

It may be interesting to note that, if  $\alpha(u) = 0$  whenever  $u \in \mathcal{F} \setminus \mathcal{T}$ , then  $S(\alpha)$  represents a series of Lie operators of vector fields (that is, a series of first order linear differential operators), so that given a smooth function  $I : \mathbb{R}^d \rightarrow \mathbb{R}$ , the series  $S(\alpha)[I]$  represents the Lie-derivative  $I'(y)\tilde{f}_h(y)$  of  $I$  along the formal vector field

$$\tilde{f}_h = \sum_{t \in \mathcal{T}} \frac{h^{|t|}}{\sigma(t)} \alpha(t) F(t)(y).$$

Thus, according to Lemma 1, the Lie-derivative of a function  $S(\beta)[I]$  is precisely  $S(\alpha\beta)[I]$ . Lemma IX.9.1 in [HLW02] can thus be seen as a particular case of Lemma 1, with  $\beta(u) = 0$  whenever  $u \in \mathcal{F} \setminus \mathcal{T}$  and  $I = id_{\mathbb{R}^n}$ . It can be seen that the formula for  $\alpha\beta(t)$  simplifies due to the fact that  $\alpha(u)$  vanishes for  $u \notin \mathcal{T}$  (so that, using the notation in [HLW02],  $\alpha\beta(t)$  reduces to  $\partial_\beta\alpha(t)$ ). It can be seen that the series of Lie operators associated to the modified differential equations corresponding to a B-series method  $S(\alpha)$  ( $\alpha$  satisfying (9), so that it corresponds to a B-series  $B(a)$ ) can be interpreted [Mur05] as  $S(\log \alpha)$ . In [Mur05] and [CHV05], explicit expressions of  $\log \alpha(t)$  are given.

### 3 Preservation of exact invariants

Given a differential equation of the form (1), we suppose that there exists a function  $I(y)$  of  $y$ , which is kept invariant along any exact solution of (1). We wish to derive conditions for a B-series integrator  $B(a)$  to preserve  $I$ , i.e.

$$I = I \circ B(a) = S(\alpha)[I], \tag{11}$$

where the map  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  is determined from  $a$  by (9). Let  $id$  denote the function on  $\mathcal{F}$  defined as  $id(e) = 1$  and  $id(u) = 0$  if  $u \in \mathcal{T} \setminus \{e\}$ , so that  $I = S(id)[I]$ . Then, (11) can be equivalently written as  $S(\alpha - id)[I] = 0$ , or also, by applying the formal logarithm on both sides of (11) (and taking into account that  $\log id = 0$ ), as  $S(\log \alpha)[I] = 0$ .

For a fixed first integral  $I$  of (1), let  $\mathcal{I}$  be the set of maps  $\delta : \mathcal{F} \rightarrow \mathbb{R}$  such that  $S(\delta)[I] = 0$ . Then,  $\alpha - id \in \mathcal{I}$  (or alternatively  $\log \alpha \in \mathcal{I}$ ) characterizes the fact that the B-series integrator associated to  $S(\alpha)$  preserves the first integral  $I$ .

The function  $I$  being an invariant of (1), we have that  $(\nabla I)^T f = 0$ , that is to say, the Lie-derivative of  $I$  along any exact trajectory of (1) is null. This is nothing else but saying that

$$X(\bullet)[I] = 0. \tag{12}$$

By virtue of Lemma 2, for any series of differential operators  $S(\omega)$  ( $\omega$  being an arbitrary real function on  $\mathcal{F}$ ) we have

$$0 = S(\omega)[X(\bullet)[I]] = S(\omega')[I].$$

Thus, given a function  $\delta$  of  $\mathcal{F}$ , the existence of some  $\omega : \mathcal{F} \rightarrow \mathbb{R}$  such that  $\delta = \omega'$  guarantees that  $\delta \in \mathcal{I}$ .

### 3.1 Quadratic invariants

If now we assume that  $I(y)$  is quadratic in the variables  $y$ , then we have that  $X(t_1 \cdots t_m)[I] = 0$  if  $m > 2$  ( $t_1, \dots, t_m \in \mathcal{T}$ ). The precedent discussion then shows that, given  $\delta : \mathcal{F} \rightarrow \mathbb{R}$ , the existence of a function  $\omega : \mathcal{F} \rightarrow \mathbb{R}$  such that

$$\delta(t) = \omega'(t) = \omega(B^-(t)), \quad (13)$$

$$\delta(tz) = \omega'(tz) = \omega(B^-(t)z) + \omega(tB^-(z)), \quad \forall t, z \in \mathcal{T}, \quad (14)$$

implies that  $\delta \in \mathcal{I}$ .

Clearly, (13) is equivalent to  $\omega(u) = \delta([u])$  for all  $u \in \mathcal{F}$ , which uniquely determines  $\omega$  in terms of  $\delta$ . By using that to eliminate  $\omega$  from (14), we finally obtain that (13)–(14) is equivalent to  $\delta(tz) = \delta([B^-(t)z]) + \delta([tB^-(z)])$ . We thus have proven the following.

**Lemma 3** *Let  $I$  be a quadratic first integral of (1). If  $\delta : \mathcal{F} \rightarrow \mathbb{R}$  is such that*

$$\delta(tz) = \delta(t \circ z) + \delta(z \circ t), \quad \text{for all } t, z \in \mathcal{T},$$

*then,  $\delta \in \mathcal{I}$  (i.e.  $S(\delta)[I] = 0$ ).*

**Theorem 1** *A map  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  satisfying (9) is such that  $S(\alpha)[I] = I$  for all couples  $(f, I)$  of a vector field  $f$  and a first quadratic integral  $I$ , if and only if  $\alpha$  satisfies the condition*

$$\forall (t_1, t_2) \in \mathcal{T}^2, \quad \alpha(t_1)\alpha(t_2) = \alpha(t_1 \circ t_2) + \alpha(t_2 \circ t_1), \quad (15)$$

*Proof* According to Lemma 3, (15) implies that  $\alpha - id \in \mathcal{I}$ , thus proving the 'if' part. Notice that (15) is the known condition [CSS94] for a B-series integrator to be symplectic when applied to a Hamiltonian ODE (1) (see also [HLW02]). Thus, the 'only if' part follows from the necessity of the symplecticity condition in [CSS94] (since the symplecticity condition can be seen [BS94, HLW02] as the preservation of a particular quadratic first integral).

In terms of the coefficients of the modified differential equations, (15) can be equivalently written as

$$\forall (t_1, t_2) \in \mathcal{T}^2, \quad \log \alpha(t_1 \circ t_2) + \log \alpha(t_2 \circ t_1) = 0 \quad (16)$$

This can be directly obtained from the fact that (16) implies, according to Lemma 3 (together with  $\log \alpha(tz) = 0$  for all  $t, z \in \mathcal{T}$ ) that  $\log \alpha \in \mathcal{I}$ . Observe that (16) coincide with the conditions for a B-series vector field to be Hamiltonian [Hai94] (see also [HLW02]) when (1) is a Hamiltonian system.

### 3.2 Hamiltonian systems

We now turn our attention to systems of the form (1) with

$$f(y) = J^{-1} \nabla H(y), \quad (17)$$

and we explore the conditions under which a B-series integrator  $B(a)$  preserves exactly the Hamiltonian function, i.e.

$$H \circ B(a) = H. \quad (18)$$

In terms of S-series, this is equivalent to requiring that

$$S(\alpha)[H] = H \quad (19)$$

where  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  is determined from  $a : \mathcal{T} \rightarrow \mathbb{R}$  by (9).

Following the approach in the beginning of Section 3 for the first integral  $I = H$ , it is enough identifying the set  $\mathcal{I}$  of maps  $\delta : \mathcal{F} \rightarrow \mathbb{R}$  such that  $S(\delta)[H] = 0$ , so that a B-series  $B(a)$  will preserve the Hamiltonian function  $H$  if  $\alpha - id \in \mathcal{I}$  (or equivalently,  $\log \alpha \in \mathcal{I}$ ).

We first notice that a lot of forests  $u \in \mathcal{F}$  give rise to the same elementary differential. As a matter of fact,  $X(u)[H] = H([u])$ , and it is known [Hai94,HLW02] that

$$\forall (s, t) \in \mathcal{T}^2, H(s \circ t) = -H(t \circ s). \quad (20)$$

It is said that two trees  $z_e$  and  $z_f$  are equivalent, and we write  $z_e \sim z_f$ , if there exists a finite sequence of trees  $t_0 = z_e, t_1, \dots, t_{n-1}, t_n = z_f$  such that for any pair of consecutive trees  $(t_i, t_{i+1})$  there exist  $r$  and  $s$  such that

$$t_i = s \circ r, \quad (21)$$

$$t_{i+1} = r \circ s. \quad (22)$$

Clearly,  $H(t) = \pm H(z)$  if  $t \sim z$ . Each equivalence class of rooted trees is identified with a tree where no root is specified, sometimes called *free trees*. Equivalence classes having a rooted tree  $t$  of the form  $t = z \circ z$  are referred as superfluous free trees, and  $H(t) = 0$  in that case (as  $H(z \circ z) = -H(z \circ z)$ ). Now, given a total order  $>$  on  $\mathcal{T}$ , a set  $\mathcal{HS} \subset \mathcal{T}$  of canonical representatives of the equivalence classes in  $\mathcal{T}/\sim$  corresponding to non-superfluous trees can be constructed as follows [Mur99]: Consider  $\mathcal{HS} = \cup_{n \geq 1} \mathcal{HS}_n$ , where  $\mathcal{HS}_1 = \{\bullet\}$ , and for  $n \geq 2$ ,  $\mathcal{HS}_n$  is such that  $t$  belongs to  $\mathcal{HS}_n$  if and only if  $t$  can not be written as

$$t = s_1 \circ s_2 \quad \text{with} \quad (s_1, s_2) \in \mathcal{T}^2 \quad \text{and} \quad s_1 \leq s_2.$$

The first of such sets (for a certain total order in  $\mathcal{T}$ ) are

$$\mathcal{HS}_1 = \{\bullet\}, \quad \mathcal{HS}_2 = \emptyset, \quad \mathcal{HS}_3 = \{\blacktriangledown\}, \quad \mathcal{HS}_4 = \{\blacktriangledown\}, \quad \mathcal{HS}_5 = \{\blacktriangledown, \blacktriangledown, \blacktriangledown\}.$$

We now turn back to our problem. Writing the S-series in terms of elementary Hamiltonians, we obtain:

$$\begin{aligned} S(\delta)[H] &= \sum_{u \in \mathcal{F}} \frac{h^{|u|}}{\sigma(u)} \delta(u) X(u)[H], \\ &= \sum_{t \in \mathcal{HS}} h^{|t|-1} H(t) \sum_{u \in \mathcal{F}, [u] \sim t} \frac{(-1)^{d([u])}}{\sigma(u)} \delta(u), \end{aligned}$$

where  $d([u])$  denotes the distance between the root of  $[u]$  and the root of  $t$ . We thus have proven the following.

**Lemma 4** *Let (1) be a Hamiltonian system with  $f = J^{-1} \nabla H$ . If  $\delta : \mathcal{F} \rightarrow \mathbb{R}$  is such that*

$$\sum_{u \in \mathcal{F}, [u] \sim t} \frac{(-1)^{d([u])}}{\sigma(u)} \delta(u) = 0 \quad (23)$$

*for all  $t \in \mathcal{HS}$ , then  $S(\delta)[H] = 0$ .*



If it is required that  $S(\delta)[H] = 0$  for all Hamiltonian systems, then, the fact that the elementary Hamiltonians  $H(t), t \in \mathcal{HS}$  are independent [HLW02] shows that (23) is a necessary condition. We finally get the following result:

**Theorem 2** *Consider a B-series integrator associated to the S-series  $S(\alpha)$  ( $\alpha$  satisfying (9)). It holds that  $S(\alpha)(H) = H$  for all Hamiltonian system  $f = J^{-1}\nabla H$ , if and only if the following condition holds:*

$$\forall t \in \bigcup_{n \geq 2} \mathcal{HS}_n, \quad \sum_{u \in \mathcal{F}, [u] \sim t} (-1)^{d([u])} \frac{\alpha(u)}{\sigma(u)} = 0. \quad (24)$$

An equivalent characterization of B-series integrators  $B(\alpha)$  preserving the Hamiltonian function is obtained in terms of the coefficients of the modified differential equation in [FHP04]. Using our notation, the authors arrive to the equivalent condition

$$\forall t \in \bigcup_{n \geq 2} \mathcal{HS}_n, \quad \sum_{z \in \mathcal{T}, [z] \sim t} (-1)^{d([z])} \frac{\log \alpha(z)}{\sigma(z)} = 0. \quad (25)$$

This can be obtained using our approach by equivalently considering  $S(\log \alpha)[H] = 0$  instead of  $S(\alpha)[H] = H$ , and noting that  $\log \alpha(u) = 0$  for forests  $u$  with more than one tree.

Next result shows in particular ( $\gamma \equiv 0$ ) that there exist B-series (apart from B-series corresponding to a rescaling of the exact flow of (1)) preserving  $H$  for any Hamiltonian system  $f = J^{-1}\nabla H$ .

**Lemma 5** *Given an arbitrary  $\beta : \mathcal{F} \rightarrow \mathbb{R}$ , there exists  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  satisfying (9) such that*

$$\forall t \in \bigcup_{n \geq 2} \mathcal{HS}_n, \quad \sum_{u \in \mathcal{F}, [u] \sim t} (-1)^{d([u])} \left( \frac{\alpha(u) - \beta(u)}{\sigma(u)} \right) = 0. \quad (26)$$

*Proof* The proof proceeds by induction on the order: assume that  $\alpha$  is determined for all rooted trees  $z \in \mathcal{T}$  with  $|z| < p$  and consider  $s \in \mathcal{T}$  with  $|s| = p$ : either  $[s]$  belongs to the class of a superfluous free tree, in which case the term  $\alpha([s])$  never appears in conditions (26) and can be defined arbitrarily, or there exists a unique  $t \in \mathcal{HS}_{p+1}$  such that  $[s] \sim t$ , in which case  $\alpha([s])$  appears once and only once in equations (26) for trees  $t \in \mathcal{HS}_{p+1}$ . As a result, if for a given  $t \in \mathcal{HS}_{p+1}$ , (26) involves  $k \geq 2$  trees of order  $p$ , then  $\alpha$  can be defined arbitrarily for  $k - 1$  of them, while the last one, say  $\alpha([s])$ , has to be defined as

$$\alpha([s]) = - \sum_{u \in \mathcal{F}/\{s\}, [u] \sim t} (-1)^{d([u])} \left( \frac{\alpha(u) - \beta(u)}{\sigma(u)} \right) + (-1)^{d([s])} \frac{\beta([s])}{\sigma(s)}.$$

Hence, conditions (26) can be solved for all trees of  $\mathcal{HS}_{p+1}$ , and the required result follows by induction.

**Theorem 3** *Suppose a B-series integrator associated to  $S(\alpha)$  satisfies both condition (15) for the preservation of quadratic invariants and condition (24) for the preservation of exact Hamiltonians. Then it is the B-series of a scaled exact flow.*

*Proof* The proof simplifies slightly by considering  $\beta = \log \alpha$ , which by assumption has to satisfy (25) and (16).

We choose the set  $\mathcal{HS}$  of canonical representatives of non-superfluous free trees in such a way that, for each equivalence class, its representative is a tree of the form  $[\bullet^k v]$  ( $v \in \mathcal{F}$ ,  $k \geq 1$ ) with maximized  $k$ . Condition (16) implies that,

$$t \in \mathcal{HS} \text{ and } z \sim t \implies \beta(z) = (-1)^{d(z)} \beta(t). \quad (27)$$

We first note that condition (25) for  $t = [\bullet^{k+1}] \in \mathcal{HS}$  just reads  $-\beta([\bullet^{k+1}])/\sigma([\bullet^{k+1}]) = 0$ . We will prove on induction on  $|v|$  that  $\beta(z) = 0$  for  $z = [\bullet^k v] \in \mathcal{HS}$ .

Given  $z = [\bullet^k v] \in \mathcal{HS}$ , it holds that  $t = [\bullet^{k+1} v] \in \mathcal{HS}$ , and if  $[s] \sim t$ , then either  $s = z = [\bullet^k v]$  or  $s \sim [\bullet^{k+1} u] \in \mathcal{HS}$  (with  $|u| = |v| - 1$ ), and thus (25) reads, taking (27) into account,

$$\sum_{s \in \mathcal{T}, [s] \sim t} (-1)^{d([s])} \frac{\beta(s)}{\sigma(s)} = -\frac{\beta([\bullet^k v])}{\sigma([\bullet^k v])} + \sum_u (-1)^{d([s]) + d(s)} \frac{\beta([\bullet^{k+1} u])}{\sigma([\bullet^{k+1} u])} = 0,$$

(where  $u \in \mathcal{F}$  is such that  $s \sim [\bullet^{k+1} u]$  and  $[s] \sim t$ , and thus  $|u| < |v|$ ), and by induction argument  $\beta(z) = 0$ .

#### 4 Preservation of modified invariants

In this section, we investigate the conditions under which  $B(a)$  preserves a modified invariant of the form  $\tilde{I} = S(\beta)[I]$ . In that case, although the B-series integrator does not preserve exactly the invariant  $I$ , it will be approximately preserved.

If there exist two B-series  $B(b)$  and  $B(\bar{a})$  such that  $B(b) \circ B(a) = B(\bar{a}) \circ B(b)$  (so that the integrator  $B(a)$  is formally conjugate to  $B(\bar{a})$ ) and  $B(\bar{a})$  preserves exactly the first integral  $I$ , then

$$I = I \circ B(\bar{a}) \implies I \circ B(b) = I \circ B(\bar{a}) \circ B(b) = I \circ B(b) \circ B(a),$$

and thus, the B-series  $B(a)$  preserves the modified invariant  $\tilde{I} = I \circ B(b) = S(\beta)[I]$ . Conversely, if  $B(a)$  has a modified first integral of the form  $\tilde{I} = I \circ B(b)$ , then the B-series integrator  $B(a)$  is formally conjugate to a B-series ( $B(\bar{a}) = B(b) \circ B(a) \circ B(b)^{-1}$ ) that preserves exactly the invariant  $I$ . Obviously, in that case, the modified invariant  $\tilde{I} = S(\beta)[I]$  is such that

$$\beta(e) = 1 \text{ and } \beta(t_1 \dots t_m) = b(t_1) \cdots b(t_m). \quad (28)$$

However, one may think that there exist B-series  $B(a)$  having a modified first integral  $I = S(\beta)$  ( $\beta$  not being of the form (28)) without  $B(a)$  being formally conjugate to a B-series that preserves exactly the invariant  $I$ . We will show that this is not the case in the two specific situations considered in this paper (that is, for quadratic invariants, and for the Hamiltonian function of a Hamiltonian system).

#### 4.1 Quadratic invariants

**Theorem 4** Consider a vector field  $f$  having a quadratic first integral  $I$ . A B-series integrator  $B(a)$  has a modified first integral of the form  $\tilde{I} = S(\beta)[I]$  when applied to (1) if and only if  $B(a)$  is formally conjugate to a B-series that preserves the first integral  $I$  exactly.

*Proof* From the discussion at the beginning of Section 4, we only need to prove that, for an arbitrary  $\beta : \mathcal{F} \rightarrow \mathbb{R}$ , there exists  $b : \mathcal{T} \rightarrow \mathbb{R}$  such that  $S(\beta)[I] = I \circ B(b)$ . That is,  $S(\delta)[I] = 0$  where  $\delta : \mathcal{F} \rightarrow \mathbb{R}$  is given by

$$\delta(e) = 0 \text{ and } \delta(t_1 \dots t_m) = \beta(t_1 \dots t_m) - b(t_1) \cdots b(t_m).$$

According to Lemma 3, it is sufficient to show the existence of  $b : \mathcal{T} \rightarrow \mathbb{R}$  such that

$$b(t_2 \circ t_1) + b(t_1 \circ t_2) = \beta(t_2 \circ t_1) + \beta(t_1 \circ t_2) + b(t_1)b(t_2) - \beta(t_1 t_2) \quad (29)$$

for arbitrary trees  $t_1, t_2 \in \mathcal{T}$ . Such  $b$  can be constructed as follows: We set  $b(t) = 0$  for all  $t \in \mathcal{HS}$ . The equalities (29) then uniquely determine the value  $b(t)$  for any  $t \in \mathcal{T} \setminus \mathcal{HS}$  in terms of the values of  $\beta$  and the values of  $b(z)$  for rooted trees  $z$  with  $|z| < |t|$ .

Theorem 4, together with Theorem 1 and the remark that follows to it, implies that a B-series integrator  $B(a)$  has a modified first integral of the form  $\tilde{I} = S(\beta)[I]$  for all couples  $(f, I)$  of a vector field  $f$  and a quadratic first integral  $I$ , if and only if  $B(a)$  is formally conjugate to a symplectic B-series.

#### 4.2 Hamiltonian invariants

**Theorem 5** Consider a Hamiltonian system (1) with  $f = J^{-1}\nabla H$ . A B-series integrator  $B(a)$  has a modified first integral of the form  $\tilde{H} = S(\beta)[H]$  when applied to (1) if and only if  $B(a)$  is formally conjugate to a B-series that preserves  $H$  exactly.

*Proof* As in the proof of Theorem 4, we only need to prove that, for an arbitrary  $\beta : \mathcal{F} \rightarrow \mathbb{R}$ , there exists  $b : \mathcal{T} \rightarrow \mathbb{R}$  such that  $S(\beta)[I] = I \circ B(\beta)$ , which directly follows from Lemma 5.

**Corollary 1** A symplectic B-series is formally conjugate to a B-series that preserves exactly  $H$  for all Hamiltonian systems  $f = J^{-1}\nabla H$ .

### 5 Extension to P-series methods

All the results obtained for B-series methods can now be generalized to P-series methods. In this section, we thus consider partitioned systems of the form

$$\begin{aligned} \dot{p} &= f(p, q), \\ \dot{q} &= g(p, q). \end{aligned} \quad (30)$$

The corresponding trees are now two-coloured trees (black and white)

$$t = [t_1, \dots, t_m, z_1, \dots, z_n] \bullet \quad \text{and} \quad z = [t_1, \dots, t_m, z_1, \dots, z_n] \circ$$

obtained by joining the roots of  $t_1, \dots, t_m, z_1, \dots, z_n$  to a black vertex or to a white vertex (see for instance [HLW02] pp. 62). As a convention, we use  $t$  for trees with a black root,  $z$  for trees with a white root, and  $s$  for trees with root of arbitrary colour. Elementary differentials can be defined accordingly

$$\begin{aligned} F(\bullet) &= f, & F(\circ) &= g, \\ F([t_1, \dots, t_m, z_1, \dots, z_n] \bullet) &= \left( \partial_p^m \partial_q^n f \right) \left( F(t_1), \dots, F(t_m), F(z_1), \dots, F(z_n) \right), \\ F([t_1, \dots, t_m, z_1, \dots, z_n] \circ) &= \left( \partial_p^m \partial_q^n g \right) \left( F(t_1), \dots, F(t_m), F(z_1), \dots, F(z_n) \right), \end{aligned}$$

where we have omitted the obvious arguments  $p$  and  $q$ . We consider forests  $u = t_1 \dots t_m z_1 \dots z_n$  of two-coloured trees and the corresponding action of the operator  $X(u)$  on a function  $I(p, q)$  as follows:

$$X(u)[I] = \left( \partial_p^m \partial_q^n I \right) (F(t_1), \dots, F(t_m), F(z_1), \dots, F(z_n)).$$

The construction of two-coloured trees follows step-by-step the construction for one-coloured trees of Section 2. In the present section,  $\mathcal{T}$  and  $\mathcal{F}$  denote the sets of two-coloured rooted trees and forests respectively. Series of differential operators are defined accordingly. Of course, P-series integrators are associated to S-series  $S(\alpha)$  with  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  satisfying (9). For a P-series  $P(a)$  (with  $a : \mathcal{T} \rightarrow \mathbb{R}$ ), it holds for arbitrary smooth functions  $g \in C^\infty(\mathbb{R}^n)$  that  $g \circ P(a) = S(\alpha)[g]$ , where  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  is determined from  $a$  by (9).

A generalization for Lemma 1 of composition of S-series also holds [Mur05]. We next state the particular case where  $\beta(\bullet) = \beta(\circ) = 1$  and  $\beta(u) = 0$  whenever  $u \in \mathcal{F}$  with  $|u| > 1$ .

**Lemma 6** *For any map  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$ , we have*

$$hS(\alpha)(X(\bullet) + X(\circ)) = S(\alpha'),$$

where  $\alpha'$  is defined by

$$\begin{aligned} \alpha'(e) &= 0, \\ \forall u = s_1 \dots s_m \in \mathcal{F}, \quad \alpha'(u) &= \sum_{i=1}^m \alpha \left( B^-(s_i) \prod_{j \neq i} s_j \right). \end{aligned}$$

Thus, proceeding as in Section 3, one sees that, given a first integral  $I$  of the partitioned system (30), and a map  $\delta : \mathcal{F} \rightarrow \mathbb{R}$ ,  $S(\delta)[I] = 0$  if there exists a map  $\omega : \mathcal{F} \rightarrow \mathbb{R}$  such that  $\delta = \omega'$ . If  $I$  is a quadratic first integral, it is sufficient that  $\delta(u) = \omega'(u)$  for forests with less than three trees. If in addition  $I$  is of the form  $I(p, q) = p^T Dq$ , then the existence of a map  $\omega : \mathcal{F} \rightarrow \mathbb{R}$  such that  $\delta(u) = \omega'(u)$  for forests with one tree and for forests of the form  $u = tz$ . This can be used to prove the following result.

**Theorem 6** *Given a map  $\alpha : \mathcal{F} \rightarrow \mathbb{R}$  satisfying (9), it holds that  $S(\alpha)[I] = I$  for all partitioned systems (30) having a quadratic first integral of the form  $I(p, q) = p^T Dq$ , if and only if*

$$\alpha(t)\alpha(z) = \alpha(t \circ z) + \alpha(z \circ t), \quad \alpha([u] \bullet) = \alpha([u] \circ) \quad (31)$$

for any two-coloured tree  $t$  with black root, for any two-coloured tree  $z$  with white root, and for arbitrary two-coloured forests  $u$ .

The conditions obtained in Theorem 6 are known [HLW02] to be the necessary and sufficient conditions for a P-series integrator  $P(\alpha)$  to be symplectic when applied to Hamiltonian systems of the form (30) with

$$f(p, q) = -\nabla_q H(p, q), \quad g(p, q) = \nabla_p H(p, q). \quad (32)$$

It may be worth mentioning that a similar result holds for arbitrary quadratic first integrals (not necessarily of the form  $I(p, q) = p^T Dq$ ), only that in that case (31) must be considered for trees  $t$  and  $z$  with roots of arbitrary colour, which can be seen to imply that the map  $\alpha$  is colour blind, so that  $P(\alpha)$  is then a B-series (see [HLW02]).

**Theorem 7** *Consider a partitioned system (30) having a quadratic first integral  $I$ . A P-series integrator  $P(a)$  has a modified first integral of the form  $\tilde{I} = S(\beta)[I]$  when applied to (30) if and only if  $P(a)$  is formally conjugate to a P-series that preserves the first integral  $I$  exactly.*

*Proof* The proof is very similar to that of Theorem 4, and it is sufficient to show the existence of  $b : \mathcal{T} \rightarrow \mathbb{R}$  such that

$$b(t \circ z) + b(z \circ t) = \beta(t \circ z) + \beta(z \circ t) + b(t)b(z) - \beta(tz), \quad (33)$$

$$b([u] \bullet) - \beta([u] \bullet) = b([u] \circ) - \beta([u] \circ), \quad (34)$$

for any two-coloured tree  $t$  with black root, for any two-coloured tree  $z$  with white root, and for arbitrary two-coloured forests  $u$ . Now, instead of the equivalence relation on the set of rooted trees (as given in Subsection 3.2) induced by the conditions for symplectic B-series, we need to resort to the analogous equivalence relation (see for instance Definition IX.10.3 in [HLW02]) on the set of two-coloured trees induced by condition (15). It is then straightforward to check that one can arbitrarily choose the value of  $b(s)$  (for instance  $b(s) = 0$ ) of one two-coloured tree  $s$  per equivalence class of two-coloured trees of order  $n$ , and then (33) and (34) uniquely determine the value of  $b$  for the remaining two-coloured trees of order  $n$  in terms of the values of  $b$  for two-coloured trees of smaller order.

Theorem 7 thus implies the following result.

**Corollary 2** *A P-series integrator  $P(a)$  has a modified first integral of the form  $\tilde{I} = S(\gamma)[I]$  for all partitioned systems (30) having a quadratic first integral  $I$ , if and only if  $P(a)$  is formally conjugate to a symplectic P-series.*

If a P-series method is applied to a *separable* partitioned system of the form

$$\begin{cases} \dot{p} = f(q), \\ \dot{q} = g(p), \end{cases} \quad (35)$$

then elementary differentials  $F$  of two-coloured trees having two adjacent vertices of the same colour vanish, and their coefficients play no longer a role. We will refer to such trees as *vanishing* trees. We thus have that, for the conservation by a P-series method of all quadratic first integrals  $I(p, q) = p^T Dq$  of separable partitioned systems, it is sufficient that the conditions in Theorem 6 hold with the coefficients of vanishing trees considered as free parameters. The conditions thus obtained by eliminating the free parameters are known (see [HLW02] pp. 199) to be necessary and sufficient for a P-series method to be symplectic when applied to a separable Hamiltonian system. Actually, it can be seen

that such conditions are also necessary for the conservation of all quadratic first integrals  $I(p, q) = p^T Dq$  of separable partitioned systems.

Using exactly the same arguments, one can show that a P-series method satisfies all quadratic first integrals  $I(p, q) = p^T Dq$  of partitioned systems of the form

$$\begin{cases} \dot{p} = f(q), \\ \dot{q} = p, \end{cases} \quad (36)$$

if and only if it is symplectic when applied to Newton equations of the form (36) with  $f(q) = -\nabla U(q)$ .

The considerations above together with Theorem 7 imply the following.

**Theorem 8** *A P-series integrator  $P(a)$  has a modified first integral  $\tilde{I} = S(\beta)[I]$  for all equations of the form (35) (resp. (36)) having a quadratic first integral  $I(p, q) = p^T Dq$  if and only if  $P(a)$  is formally conjugate to a P-series that is symplectic when applied to Hamiltonian systems of the form (35) with  $f(q) = -\nabla U(q)$ ,  $g(p) = \nabla T(p)$  (resp. (36) with  $f(q) = -\nabla U(q)$ ).*

**Theorem 9 (Hairer, Lubich in [HL04])** *The underlying P-series of any symmetric linear multistep method has a modified first integral of the form  $\tilde{I} = S(\beta)[I]$  for all Newton equations of the form (36) with  $f = -\nabla U$  having a quadratic first integral  $I(p, q) = p^T Dq$ .*

**Corollary 3** *The underlying P-series of any symmetric linear multistep method is formally conjugate to a P-series which is symplectic for Newton equations of the form (36) with  $f = -\nabla U$ .*

Corollary 3 implies, as a consequence of (3), the following statement, directly proven in [HL04]: The underlying P-series  $P(a)$  of any symmetric partitioned linear multistep method admits a modified Hamiltonian of the form  $\tilde{H} = S(\tilde{\beta})[H]$ . As a matter of fact, it can be assumed that  $\beta$  in the statement of Theorem 9 is of the form (28), so that the P-series obtained as the composition  $P(b) \circ P(a) \circ P(b)^{-1}$  is symplectic when applied to Newton equations, and by standard backward error analysis, it can be formally considered as the exact flow of a Hamiltonian system with Hamiltonian function  $\tilde{H} = S(\gamma)[H]$ . In particular, the P-series  $P(b) \circ P(a) \circ P(b)^{-1}$  admits  $\tilde{H}$  as a modified first integral, that is,

$$S(\gamma)[H] \circ P(b) \circ P(a) \circ P(b)^{-1} = S(\gamma)[H].$$

But we have that  $S(\gamma)[H] \circ P(b) \circ P(a) \circ P(b)^{-1} = S(\beta^{-1}\alpha\beta\gamma)[H]$ , and finally

$$S(\gamma)[H] = S(\beta^{-1}\alpha\beta\gamma)[H] \implies S(\beta\gamma)[H] = S(\alpha\beta\gamma)[H] = S(\beta\gamma)[H] \circ P(a),$$

which shows that  $S(\tilde{\beta})[H]$ , with  $\tilde{\beta} = \beta\gamma$ , is a modified first integral of the P-series  $P(a)$ .

Finally, we can prove the following analog of Theorem 5 for Hamiltonian systems (systems of the form (30) with (32)).

**Theorem 10** *A P-series integrator has a modified first integral of the form  $\tilde{H} = S(\gamma)[H]$  when applied to Hamiltonian systems if and only if it is formally conjugate to a P-series that preserves  $H$  exactly.*

Thus, a symplectic P-series is formally conjugate to a P-series that preserves the Hamiltonian exactly.

## References

- [Bro04] Ch. Brouder. Trees, renormalization and differential equations. *BIT*, 44(3):425–438, 2004.
- [BS94] P. B. Bochev and C. Scovel. On quadratic invariants and symplectic structure. *BIT*, 34:337–345, 1994.
- [But69] J. C. Butcher. The effective order of Runge-Kutta methods. In J. Ll. Morris, editor, *Proceedings of Conference on the Numerical Solution of Differential Equations*, volume 109 of *Lecture Notes in Math.*, pages 133–139, 1969.
- [But72] J. C. Butcher. An algebraic theory of integration methods. *Math. Comput.*, 26:79–106, 1972.
- [But87] J. C. Butcher. *The Numerical Analysis of Ordinary Differential Equations. Runge-Kutta and General Linear Methods*. John Wiley & Sons, Chichester, 1987.
- [CHV05] P. Chartier, E. Hairer, and G. Vilmart. A substitution law for B-series vector fields. Technical Report 5498, INRIA, France, 2005.
- [CK98] A. Connes and D. Kreimer. Hopf algebras, renormalization and noncommutative geometry. *Commun. Math. Phys.*, 199, 1998.
- [CSS94] M. P. Calvo and J. M. Sanz-Serna. Canonical B-series. *Numer. Math.*, 67:161–175, 1994.
- [FHP04] E. Faou, E. Hairer, and T. L. Pham. Energy conservation with non-symplectic methods: examples and counter-examples. *BIT*, 44:699–709, 2004.
- [Hai94] E. Hairer. Backward analysis of numerical integrators and symplectic methods. *Annals of Numerical Mathematics*, 1:107–132, 1994.
- [Hai99] E. Hairer. Backward error analysis for multistep methods. *Numer. Math.*, 84:199–232, 1999.
- [HL04] E. Hairer and C. Lubich. Symmetric multistep methods over long times. *Numer. Math.*, 97:699–723, 2004.
- [HLW02] E. Hairer, C. Lubich, and G. Wanner. *Geometric Numerical Integration. Structure-Preserving Algorithms for Ordinary Differential Equations*. Springer Series in Computational Mathematics 31. Springer, Berlin, 2002.
- [HNW93] E. Hairer, S. P. Nørsett, and G. Wanner. *Solving Ordinary Differential Equations I. Nonstiff Problems*. Springer Series in Computational Mathematics 8. Springer, Berlin, 2 edition, 1993.
- [HW74] E. Hairer and G. Wanner. On the Butcher group and general multi-value methods. *Computing*, 13:1–15, 1974.
- [Kir86] U. Kirchgraber. Multi-step methods are essentially one-step methods. *Numer. Math.*, 48:85–90, 1986.
- [Mer57] R. H. Merson. An operational method for the study of integration processes. In *Proc. Symp. Data Processing Weapons Research Establishment*, pages 110–1 to 110–25, Salisbury Australia, 1957.
- [Mur99] A. Murua. Formal series and numerical integrators, Part i: Systems of ODEs and symplectic integrators. *Applied Numerical Mathematics*, 29:221–251, 1999.
- [Mur05] A. Murua. The Hopf algebra of rooted trees, free Lie algebras, and Lie series. *accepted for publication in FOCM*, 2005.