

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

$$y'(x) = f(y(x)), \quad (1)$$

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

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

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 integers¹, $F(t)$ 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

¹ 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 $\mathcal{F} = \{e, \bullet, \bullet\bullet, \mathcal{J}, \bullet\bullet\bullet, \mathcal{J}\bullet, \mathcal{V}, \mathcal{J}\mathcal{J}, \dots\}$ 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 α 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 α , 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 β 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 σ 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 α 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 α , 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 α 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 Δ 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 α' 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 $S(\alpha)$ (α 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 $S(\omega)$ (ω being an arbitrary real function on \mathcal{F}) we have

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

Thus, given a function δ 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 ω in terms of δ . By using that to eliminate ω 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 α 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 $S(\alpha)$ (α 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 α 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 α 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 $I = S(\beta)$ (β 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 β 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 α' 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*

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

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 α 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 β 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.

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