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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 Hamitonian 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 $B(\alpha)$ is a formal expression of the form

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

where the index set $\mathcal{T} = \{\bullet, [\bullet], [\bullet,\bullet], [[\bullet]], \cdots\}$ is the set of rooted trees, and for each rooted tree t, $|t|$ and $\sigma(t)$ are fixed positive integers[1], $F(t)$ 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 $|\bullet| = 1$, $|[\bullet]| = 2$, $|[[\bullet]]| = 3$, $\sigma(\bullet) = 1$, $\sigma([\bullet]) = 1$, $\sigma([[\bullet]]) = 1$, $\sigma([\bullet,\bullet]) = 2$.

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

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

where the index set $\mathcal{F} = \{e, \bullet, \bullet\,\bullet, [\bullet], \bullet\,\bullet\,\bullet, [\bullet]\,\bullet, [\bullet,\bullet], [[\bullet]], \cdots\}$ 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 funcions 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 $g \in C^\infty(\mathbb{R}^n, \mathbb{R}^m)$):

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

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

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

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

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

and it can be shown [Mur99], that

$$I \circ B(a) = S(\alpha)[I], \tag{5}$$

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:

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

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*

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

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 [FHP05]).

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 $t_1, \ldots, t_n$ are n trees of $\mathcal{T}$, the forest $u = t_1 \ldots t_n$ is the commutative juxtaposition of $t_1, \ldots, t_n$.*

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. $|u| = |t_1| + \cdots + |t_m|$. If $u = t_1^{r_1} \dots t_n^{r_n}$ where t_1, ..., t_n are pairwise distinct and are repeated respectively r_1, ..., 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,

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

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

$$[\bullet\bullet\bullet]\,[\bullet\bullet]\,[\bullet[\bullet]] = [\bullet\bullet]\,[\bullet[\bullet]]\,[\bullet\bullet\bullet].$$

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:

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

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:

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

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:*

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

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

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

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 $\mathcal{F}$:*

$$\alpha : \mathcal{F} \to \mathbb{R}$$
$$u \mapsto \alpha(u)$$

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

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

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

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

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

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

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 $\alpha, \beta : \mathcal{F} \to \mathbb{R}$ 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.*

$$\forall\, g \in \mathcal{D},\ S(\alpha)\Big[S(\beta)[g]\Big] = \Big(S(\alpha)S(\beta)\Big)[g] = S(\alpha\beta)[g] \tag{10}$$

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

Proof For a proof, we refer to [Mur06].

The particular formula that gives the map $\alpha\beta : \mathcal{F} \to \mathbb{R}$ in terms of the two maps $\alpha, \beta : \mathcal{F} \to \mathbb{R}$ can be found in [Mur06]. 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 $u \in \mathcal{F}\backslash\{\bullet\}$.

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

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

where α' is defined by

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

It may be interesting to note that, if $\alpha(u) = 0$ whenever $u \in \mathcal{F}\backslash\mathcal{T}$, 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 $I : \mathbb{R}^d \to \mathbb{R}$, 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 $u \in \mathcal{F}\backslash\mathcal{T}$ 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 [Mur06] as $S(\log\alpha)$. In [Mur06] 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 $\alpha : \mathcal{F} \to \mathbb{R}$ is determined from a by (9). Let id denote the function on $\mathcal{F}$ defined as $id(e) = 1$ and $id(u) = 0$ if $u \in \mathcal{T}\backslash\{e\}$, 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 $\delta : \mathcal{F} \to \mathbb{R}$ 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 $\omega : \mathcal{F} \to \mathbb{R}$ 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 $\delta : \mathcal{F} \to \mathbb{R}$, the existence of a function $\omega : \mathcal{F} \to \mathbb{R}$ such that

$$\delta(t) = \omega'(t) = \omega(B^-(t)), \tag{13}$$

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

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 $\delta : \mathcal{F} \to \mathbb{R}$ is such that*

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

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

Theorem 1 *A map $\alpha : \mathcal{F} \to \mathbb{R}$ 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*

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

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 symplecticness 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 modifed differential equations, (15) can be equivalently written as

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

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

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

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

$$H \circ B(a) = H. \tag{18}$$

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

$$S(\alpha)[H] = H \tag{19}$$

where $\alpha : \mathcal{F} \to \mathbb{R}$ is determined from $a : \mathcal{T} \to \mathbb{R}$ 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 $\delta : \mathcal{F} \to \mathbb{R}$ 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

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

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 $t_0 = z_e, t_1, \ldots, t_{n-1}, t_n = z_f$ such that for any pair of consecutive trees (t_i, t_{i+1}) there exist r and s such that

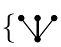
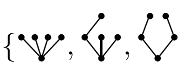
$$t_i = s \circ r, \tag{21}$$

$$t_{i+1} = r \circ s. \tag{22}$$

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 clases 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

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

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* $\delta : \mathcal{F} \to \mathbb{R}$ *is such that*

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

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:*

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

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 [FHP05]. Using our notation, the authors arrive to the equivalent condition

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

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 $\beta:\mathcal{F}\to\mathbb{R}$, there exists $\alpha:\mathcal{F}\to\mathbb{R}$ satisfying (9) such that*

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

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

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

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,

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

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

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

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

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

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 $B(\beta)$ 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 $\beta : \mathcal{F} \to \mathbb{R}$, there exists $b : \mathcal{T} \to \mathbb{R}$ such that $S(\beta)[I] = I \circ B(\beta)$. That is, $S(\delta)[I] = 0$ where $\delta : \mathcal{F} \to \mathbb{R}$ 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 $b : \mathcal{T} \to \mathbb{R}$ such that

$$b(t_2 \circ t_1) + b(t_1 \circ t_2) = \beta(t_2 \circ t_1) + \beta(t_1 \circ t_2) + b(t_1)b(t_2) - \beta(t_1 t_2) \tag{29}$$

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 $t \in \mathcal{T} \backslash \mathcal{HS}$ 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 $\beta : \mathcal{F} \to \mathbb{R}$, there exists $b : \mathcal{T} \to \mathbb{R}$ 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

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

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 $t_1, \ldots, t_m, z_1, \ldots, z_n$ 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

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

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

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

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 $\alpha : \mathcal{F} \to \mathbb{R}$ satisfying (9). For a P-series $P(a)$ (with $a : \mathcal{T} \to \mathbb{R}$), it holds for arbitrary smooth functions $g \in C^\infty(\mathbb{R}^n)$ that $g \circ P(a) = S(\alpha)[g]$, where $\alpha : \mathcal{F} \to \mathbb{R}$ is determined from a by (9).

A generalization for Lemma 1 of composition of S-series also holds [Mur06]. 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 $\alpha : \mathcal{F} \to \mathbb{R}$, we have*

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

where α' is defined by

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

Thus, proceeding as in Section 3, one sees that, given a first integral I of the partitioned system (30), and a map $\delta : \mathcal{F} \to \mathbb{R}$, $S(\delta)[I] = 0$ if there exists a map $\omega : \mathcal{F} \to \mathbb{R}$ 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 $I(p, q) = p^T D q$, then the existence of a map $\omega : \mathcal{F} \to \mathbb{R}$ 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 $\alpha : \mathcal{F} \to \mathbb{R}$ satisfying* (9)*, it holds that $S(\alpha)[I] = I$ for all partitioned systems* (30) *having a quadratic first integral of the form $I(p, q) = p^T D q$, 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

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

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 $b : \mathcal{T} \to \mathbb{R}$ such that

$$b(t \circ z) + b(z \circ t) = \beta(t \circ z) + \beta(z \circ t) + b(t)b(z) - \beta(tz), \tag{33}$$

$$b([u]_\bullet) - \beta([u]_\bullet) = b([u]_\circ) - \beta([u]_\circ), \tag{34}$$

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-coloroured 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

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

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

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

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 t 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

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

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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