ALGEBRAIC STRUCTURE OF AROMATIC B-SERIES

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ABSTRACT. Aromatic B-series are a generalization of B-series. Some of the algebraic structures on B-series can be defined analogically for aromatic B-series. This paper derives combinatorial formulas for the composition and substitution laws for aromatic B-series.

1. Introduction. B-series have long been an important tool for studying numerical integrators for ordinary differential equations. These series have an interesting and rich algebraic structure.

A generalization of B-series is formed by the aromatic B-series, introduced by Munthe-Kaas and Verdier.

The purpose of the present paper is to describe algebraic structures on aromatic B-series corresponding to known algebraic structures on normal B-series.

Superficially, an aromatic B-series represents a vector field. It is also interesting to study aromatic S-series, which can represent scalar functions, vector fields, higher degree differential operators or linear combinations thereof.¹

In particular:
- Theorem 5.1 describes the composition law of aromatic S-series.
- Theorem 5.2 describes how aromatic S-series arise from aromatic B-series.
- Theorem 6.3 describes the substitution law for aromatic B-series.

The structure of the paper is as follows: Section 2 provides a background describing ordinary B-series and some of their algebraic structure. Section 3 defines aromatic forests, aromatic B-series and the generalization aromatic S-series. Section 4 and section 5 develop the combinatorial formulas for composing aromatic S-series and, by extension, aromatic B-series. Section 6 studies the substitution law on aromatic B-series and S-series, as well as the interaction between the substitution and composition laws. Section 7 is an application of the substitution law to define a pseudo-volume-preserving aromatic B-series method.

2. Background. The use of formal series as a tool for studying integrators of ordinary differential equations has a long and successful history, see e.g. [21] for an overview.

The most commonly known example are the Butcher series or B-series. These were originally introduced by Butcher [3, 4] and by Hairer and Wanner [11] as a tool

¹(Nonaromatic) S-series are also defined, but cannot represent non-constant scalar functions.
to study Runge–Kutta methods for the numerical solution of ordinary differential equations.

B-series have a deep algebraic structure, see for instance Manchon [14]. B-series also arise naturally in other fields of mathematics, Brouder [2] pointed out an important link to the work by Connes and Kreimer [8], which was originally written in the context of renormalization.

See also [12, Section III] for an introduction to B-series, and [15] for a review of the history of B-series.

In the context of numerical integrators, B-series arise as follows: Let $k \in \{\mathbb{R}, \mathbb{C}\}$ and let $f$ be a smooth vector field on a finite dimensional $k$-vector space $W$ defining the ODE

$$\dot{x} = f(x).$$

For a large class of one-step integrators (including the exact “integrator” and all Runge–Kutta methods) the following holds: When the integrator is applied to (1) and the result of one step with the integrator is expanded as a power series in the step size $h$, all terms occurring in the series expansion are formed by combining derivatives of $f$, e.g.

$$f'f'''(f'f,f,f)$$

where $f' = \frac{df}{dx}$ is the Jacobian of $f$ and $f''' = \frac{d^3f}{dx^3}$ is the third derivative of $f$, viewed as a trilinear map $f''' : W^3 \to W$.

Such expressions are called elementary differentials, and the set of all elementary differentials is in a one-to-one correspondence to the set of non-planar rooted trees, here denoted $T$.

For instance, for the elementary differential above,

$$f'f'''(f'f,f,f) = F_f \left( \begin{array}{c} \tau \\ \psi \end{array} \right),$$

where $F_f$ is the bijective function from $T$ to the set of elementary differentials formed from $f$.

For a specific vector field $f$ and tree $\tau$, $F_f(\tau)$ is again vector field over $W$.

A $B$-series is defined as a formal sum of elementary differentials, that is, a series of the form

$$B_f(a) = \sum_{\tau \in T} a(\tau) \sigma(\tau) F_f(\tau),$$

where $a : T \to k$, and the normalization factors $\sigma : T \to k$ are defined such that $\sigma(\tau)$ is equal to the cardinality of the symmetry group of the tree $\tau$.

A $B$-series integrator is a numerical integrator such that each individual step of the integrator can be expanded as a B-series

$$x_{k+1} = x_k + B_f(a)(x_k) = [id + B_f(a)](x_k).$$

(Here the step size $h$ is subsumed into the vector field $f$.)

As mentioned above the class of such method includes all Runge–Kutta methods and the exact “method” defined by exactly following the vector field.

B-series have a rich algebraic structure that has been studied by many authors. We will briefly cover some of the structure here, see e.g. [5, 6, 14, 18] for proofs and more background.
The algebraic structure of B-series can be described in terms of certain algebraic objects called Hopf algebras. See Appendix B for a brief introduction to Hopf algebras.

The Connes–Kreimer Hopf algebra $H_F$ is the Hopf algebra over rooted forests, i.e. multisets of rooted trees $\mathcal{F}$. It is convenient to extend the definition of $F_f$ to forests, where the resulting product of elementary differentials is viewed as a differential operator on smooth functions $C^\infty(W)$, e.g.

$$F_f(\tau_1 \tau_2)[g] = g''[F_f(\tau_1), F_f(\tau_2)]$$

and

$$F_f(1)[g] = g,$$

where $1$ denotes the empty forest.

We denote the algebraic dual of $H_F$ by $H^*$. The elements of $H^*$ are formal series indexed by rooted forests.

The dual of a Hopf algebra is naturally an associative, unital algebra with a product given by the dual of the coproduct, known as the convolution product:

$$a \cdot b(x) = \mu_k \circ (a \otimes b) \circ \Delta(x), \quad (3)$$

where $\mu_k$ denotes multiplication in $k$ and $\Delta$ denotes the coproduct in the Hopf algebra.

For a fixed vector field $f$, $a \in H^*_F$ can be identified with a formal series of differential operators acting on functions in $C^\infty(W)$,

$$S_f(a) = \sum_{\phi \in \mathcal{F}} \frac{a(\phi)}{\sigma(\phi)} F_f(\phi), \quad (4)$$

where $\sigma(\phi)$ is the cardinality of the symmetry group of $\phi$. Such series were named $S$-series by Murua [18].

It turns out that the convolution product in $H^*_F$ corresponds to composition of formal series of differential operators

$$S_f(a_1 \cdot a_2) = S_f(a_1) \circ S_f(a_2).$$

Of special importance are the characters of $H_F$, that is to say the linear maps $a: H_F \to k$ satisfying

$$a(xy) = a(x)a(y), \quad \text{and} \quad a(1) = 1,$$

where $1$ denotes the empty forest.

It can be verified that the set of characters form a group under the convolution product with identity given by the co-unit in $H_F$. We will denote this group by $G(H_F)$.

There is a natural one-to-one correspondence between B-series and characters of $H_F$: For $a: \mathcal{T} \to k$, there is a unique character $\kappa(a): H_F \to k$ that agrees with $a$ on $\mathcal{T}$.

$$\kappa(a) = \sum_{\phi \in \mathcal{F}} \frac{a(\phi)}{\sigma(\phi)} F_f(\phi)$$

The group of characters is an infinite dimensional Lie group [1], and its Lie algebra is formed by the infinitesimal characters of $H_F$, that is morphisms $b: H_F \to k$, satisfying

$$b(xy) = b(x)c(y) + c(x)b(y),$$

where $c: H_F \to k$ is the counit of $H_F$.  

It can be verified that the set of infinitesimal characters forms a Lie algebra under anti-symmetrization of the convolution product.

We will denote the Lie algebra of infinitesimal characters \( \mathfrak{g}(H_\pi) \).

Infinitesimal characters correspond to formal series of vector fields on \( W \). For example, the modified vector fields of numerical integrators used in backward error analysis are given by the logarithm associated with the product (3), or, equivalently with the Lie group logarithm on the group of characters.

2.1. The composition and substitution product. As we have seen above, composition of two S-series correspond to the convolution product on \( H^*_\pi \).

There is another product on S-series, the substitution product.

The substitution product \( \ast : \mathfrak{g}(H_\pi) \times H^*_\pi \rightarrow H^*_\pi \), arises from replacing the vector field \( f \) in an S-series with a B-series \( B_f(b) \).

\[
S_f(b \ast a) = S_{B_f(b)}(a).
\]

The substitution product can be described in terms of the \textit{rooted tree bialgebra} \( \bar{H} \), which is isomorphic to \( H^*_\pi \) as an algebra. Calaque, Ebrahimi-Fard and Manchon [5] described a compatible coproduct \( \Delta \) on \( \bar{H} \), as well as a left \( \bar{H} \)-comodule map \( H_\pi \rightarrow \bar{H} \otimes H_\pi \).

We will denote the set of characters of \( \bar{H} \) by \( G(\bar{H}) \), although it is only a monoid. The substitution product \( b \ast a \) can defined as either:

1. The dual of \( \Delta \) when both arguments are in \( G(\bar{H}) \), or
2. The dual of the comodule map, when \( b \in G(\bar{H}) \), \( a \in H^*_\pi \).

The interaction between the substitution and convolution products is defined via these two descriptions of \( \ast \), as well as that any character \( b \in G(\bar{H}) \) defines an algebra automorphism \( H^*_\pi \rightarrow H^*_\pi \) by \( a \mapsto b \ast a \).

3. Aromatic B-series. McLachlan et.al. [16] classified the B-series methods as exactly the integrators equivariant under all affine maps, including maps between affine spaces of non-equal dimension.

Munthe-Kaas and Verdier had earlier [17] showed that a larger class of methods, \textit{Aromatic Butcher series methods}, are equivariant under all \textit{invertible} affine maps.

Series related to the aromatic Butcher series (aromatic B-series) had been studied already by Iserles, Quispel and Tse [13], and by Chartier and Murua [7].

The crucial difference between B-series and aromatic Butcher series is that in the aromatic case, \textit{trace operations} are also allowed in forming elementary differentials, e.g. \( \text{tr}(f')f = (\text{div } f)f \).

On the combinatorial side, these new elementary differentials are obtained by replacing the set of rooted trees with a larger set of directed graphs, e.g.

\[
\text{tr}(f')f = F_f(\ast). \]

For our purposes, a \textit{directed graph} \( \gamma = (V, E) \) is defined by a finite set of \textit{vertices or nodes} \( V \), and a set of \textit{edges} \( E \subseteq V \times V \). We say that the edge \((v_1, v_2)\) goes out of \( v_1 \) and into \( v_2 \). A \textit{subgraph} of \( \gamma \), is another directed graph \((W, F)\) where \( W \subseteq V \), \( F \subseteq W \times W \cap E \). In this definition of graph, we allow the empty graph with 0 vertices, and self-loops.

On a given graph, we define the \textit{direct predecessor} function \( \pi_\gamma \) from \( V \) to the power set of \( V \) by \( v_1 \in \pi_\gamma(v_2) \) iff \( (v_1, v_2) \in E \).

Two graphs are \textit{equivalent} and we write \( \gamma_1 = (V_1, E_1) \simeq (V_2, E_2) = \gamma_2 \) if there exists a bijection \( g : V_1 \rightarrow V_2 \) such that \((g \times g)(E_1) = E_2 \).
The automorphism group of a directed graph is the set of permutations $g: V \rightarrow V$ satisfying that $(g \times g)(E) = E$.

Aromatic elementary differentials correspond to equivalence classes of directed graphs satisfying an additional criterion.

**Definition 3.1.** An aromatic forest is an equivalence class of directed graphs where each node has at most one outgoing edge. We denote the set of aromatic forests as $A\mathcal{F}$. A root of an aromatic forest is a node with zero outgoing edges. The set of roots of the aromatic forest $\phi$ is denoted $r(\phi)$.

We will occasionally refer to aromatic forests as graphs (as opposed to equivalence classes of graphs). Take these statements to mean a member of the equivalence class, the independence of choice of member is either obvious or explicitly stated.

It follows from the definition that an aromatic forest consists of connected components, each of which has either (a) one root, in which case the connected component is a rooted tree, or (b) no roots, in which case it contains exactly one cycle and is called an aroma.

**Definition 3.2.** We define the following subsets of $A\mathcal{F}$:

- $A = \{1, 2, 3, \ldots\}$, the set of aromatic forests with no roots.
- $A' = \{1, 2, 3, \ldots\}$, the set of connected aromatic forests with no roots, or aromas.
- $A\mathcal{T} = \{1, 2, 3, \ldots\}$, the set of aromatic forests with exactly one root.
- $T = \{1, 2, 3, \ldots\}$, the set of rooted trees, or connected aromatic forests with exactly one root.
- $F$, the set of loopless aromatic forests, which are (unordered) multisets of rooted trees. The set $F$ is also called forests.
- $F_k$, the set of forests with exactly $k$ roots.

We note that $A\mathcal{F} = A \times F$.

For a fixed vector field $f$ on a finite dimensional vector space $W$, an aromatic forest defines an elementary differential operator acting on smooth functions on $W$.

**Definition 3.3.** Let $\phi = (V, E)$ be an aromatic forest, and $f$ a smooth vector field on $W$. The elementary differential operator $F_f(\phi)$ is an differential operator acting on smooth functions on $W$, defined as follows: For each node $p \in V$, form the factor $f_{I_{\pi(p)}}^p$, where $I_{\pi(p)} = i_{q_1}i_{q_2}\ldots$ is the multiindex defined by the direct predecessor function on $\phi$, that is $q_1, q_2, \ldots$ are the vertices such that $(q_j, p) \in E$. The upper index on $f$ corresponds to the vector components of $f$ and the lower are partial derivatives with respect to the coordinate directions, $f_{i_{q_1}i_{q_2}\ldots}^p = \partial^m f^p_i / \partial x_{i_{q_1}} \cdots \partial x_{i_{q_m}}$. Then, for each root $s$, form the factor $\partial_s = \partial / \partial x_{i_s}$. Finally, multiply the factors and sum over repeated indices.

**Example 1** (Elementary differential operator). Let $\gamma$ be the tree with indices
(in this picture, i, j, k, . . . are used in place of $i_p$ for $p \in V(\gamma)$.) Then $F_f(\gamma) = f^1 f^j f^m f^{i_m} f^{k} \partial^i_n$.

When $\phi$ contains no aromas, the elementary differential operator $F_f(\phi)$ corresponds to the product of elementary differential operators referenced in section 2.

In general, an elementary differential operator $F_f(\phi)$ is a differential operator of degree $|\gamma(\phi)|$. Thus, if $\gamma \in A$, $F_f(\gamma)$ is a scalar field. If $\phi = \gamma \tau_1 \tau_2 \cdots \tau_r$, where $\gamma \in A$, $\tau_i \in T$, then $F_f(\phi) = F_f(\gamma) F_f(\tau_1) \cdots F_f(\tau_r)$ is the product of the scalar field $F_f(\gamma)$ and $r$ vector fields $F_f(\tau_1), \ldots, F_f(\tau_r)$.

The action of $F_f(\tau)$ on a smooth function $g$ over $W$ is

$$F_f(\phi)[g] = F_f(\gamma) g^{(r)}(F_f(\tau_1), \ldots, F_f(\tau_r)),$$

where $g^{(r)}$ is the $r$th derivative of $g$.

An elementary differential operator $F_f(\phi)$ can be considered to be a $|\phi|$-linear function of vector fields $E_\phi$ evaluated on $|\phi|$ copies of $f$.

$$E_\phi(f, f, \ldots, f) = F_f(\phi),$$

(5)

where each argument of $E_\phi$ is identified with a vertex in the graph $\phi$.

In [17], aromatic B-series methods are defined as integrators whose series expansions only contain terms of the form $F_f(\tau)$ where $\tau$ is an aromatic tree.

Definition 3.4. Let $a : AT \to k$ and $f$ be a smooth vector field on the finite-dimensional vector space $W$. The aromatic B-series $B_f(a)$ is the formal series

$$B_f(a) = \sum_{\tau \in AT} a(\tau) F_f(\tau).$$

The normalization constant $a$ is here defined, for an aromatic tree $\tau$, to be the cardinality of $G_\tau$, the graph automorphism group of $\tau$.

For later use, we also define $\sigma(\phi)$ for an aromatic forest $\phi$ to be the cardinality of $G_\phi$.

An aromatic B-series method is an integrator whose update map is given by

$$y_{k+1} = y_k + B_f(a)(y_k)$$

In the formula for the aromatic B-series method, the step size parameter $h$ is subsumed into the vector field $f$.

To be able to compose aromatic B-series, we want to describe the effect of such an integrator to a function, i.e. evaluate $g(y + B_f(a)(y))$ for smooth $g$. To do this, we introduce aromatic S-series, which mirror normal S-series (4).

Definition 3.5. Let $a : AF \to k$, and $f$ be a smooth vector field on a finite dimensional vector space $W$. Let the aromatic S-series of $a$ be the formal series of differential operators acting on smooth functions $g \in C^\infty(W)$ defined by

$$S_f(a)[g] = \sum_{\phi \in AF} \frac{a(\phi)}{\sigma(\phi)} F_f(\phi)[g].$$

For an aromatic B-series $B_f(a)$, where $a : AT \to k$, there is a corresponding aromatic S-series $S_f(\kappa(a))$. The action of $S_f(\kappa(a))$ on a smooth function $g$, is calculated by expanding $g(y + B_f(a)(y))$ as a Taylor series around $y$. Obtaining the coefficients of $\kappa(a)$ will require some algebraic machinery which will be developed in the next section.

For now, we define the composition product of two S-series.
Definition 3.6. For $a, b: \mathcal{AF} \to \mathbb{k}$, define the composition product $a \cdot b$ to be the aromatic B-series defined by its action on smooth functions $S_f(a \cdot b)[g] = S_f(a)[S_f(b)[g]]$.

The building block of the composition product is the composition of two elementary differential operators.

Definition 3.7. The composition of two aromatic forests $\phi_1 \circ \phi_2$ is the formal sum of aromatic forests defined as follows: Let $\ast$ be a dummy node not contained in either $V(\phi_1)$ or $V(\phi_2)$ and $(V(\phi_1) \cup \ast)^r(\phi_1)$ the set of functions $\rho: r(\phi_1) \to V(\phi_2) \cup \ast$. Let $\phi_1 \circ \phi_2 = \sum_{\rho \in (V(\phi_2) \cup \ast)^r(\phi_1)} \Phi(\phi_1, \phi_2, \rho)$, where $\Phi(\phi_1, \phi_2, \rho)$ is the aromatic forest with nodes $V(\phi_1) \cup V(\phi_2)$ and edges $E(\phi_1) \cup E(\phi_2) \cup E_\rho$, where $E_\rho = \{(p, \rho(p)) \text{ s.t. } p \in r(\phi_1), \rho(p) \neq \ast\}$.

Informally, the composition product is formed by the sum over all possible ways to add edges from some (possibly none) roots of $\phi_1$ to the nodes of $\phi_2$.

Example 2. In this example, the nodes are colored to more clearly separate the two factors.

\[ \ast \circ \ast = \boxdot_{\ast \circ \ast} \]

Lemma 3.8. When $g$ is a smooth function over $W$, the equality $F_f(\phi_1)[F_f(\phi_2)[g]] = F_f(\phi_1 \circ \phi_2)[g].$

Proof. By Definition 3.3 $F_f(\phi_1)$ is a sum of products of the form $F_f(\phi_1) = \prod_{p \in V(\phi_1)} f_{\tau(\phi_1)}^{p} \prod_{s \in r(\phi_1)} \partial_s,$

and similar for $\phi_2$. Use the product rule to expand

$$ F_f(\phi_1)[F_f(\phi_2)[g]] = \prod_{p \in V(\phi_1)} f_{\tau(\phi_1)}^{p} \prod_{s \in r(\phi_1)} \partial_s \left[ \prod_{q \in V(\phi_2)} \prod_{t \in r(\phi_2)} f_{\tau(\phi_2)}^{q} g_t \right]. $$

The result is a sum of terms, where in each term, each of the operators $\partial_s$ is applied to (a) one of the factors $f_{\tau(\phi_1)}^{p}$ or (b) one of the factors $g_t$. Referring to the definition of the elementary differential operators and the composition, case (a) corresponds to adding an edge $s \rightarrow q$, while (b) corresponds to not adding an edge from $s$. The sum is then taken over all possible choices. \qed

4. Coalgebra structure. We will be interested in series indexed by aromatic forests, and composition of such series.

A convenient environment for studying series indexed by elements of a certain set $S$ is the dual space of the free vector space over $S$. Let

$$ C_A = \bigoplus_{\gamma \in A} \mathbb{k}\gamma, \quad H_F = \bigoplus_{\omega \in \mathcal{F}} \mathbb{k}\omega \quad \text{and} \quad C_{\mathcal{AF}} = C_A \otimes H_F = \bigoplus_{\phi \in \mathcal{AF}} \mathbb{k}\phi, \quad (6) $$

denote the free vector spaces over the sets $A, \mathcal{F}$ and $\mathcal{AF}$. $H_F$, when equipped with the correct structure, is the Connes–Kreimer Hopf algebra from B-series theory.

$C_A$ is the vector space of commutative polynomials in the variables $A$. 
The algebraic dual spaces of the spaces in (6) are

\[ C^*_A = \prod_{\gamma \in A} k \gamma^*, \quad H^*_F = \prod_{\omega \in F} k \omega^* \text{ and } C^*_{AF} = \prod_{\phi \in AF} k \phi^*, \]

where \( \gamma^*, \omega^* \) and \( \phi^* \) denote elements in the respective dual bases. An element \( a \in C^*_A \) is identified with the formal series

\[ \sum_{\gamma \in A} \frac{a(\gamma)}{\sigma(\gamma)} \gamma. \]

Correspondingly for elements in \( H^*_F \) and \( C^*_{AF} \).

In the following, we will describe coalgebra\(^2\) structures on \( C_A, H_F \) and \( C_{AF} \).

We recall that a coalgebra is a vector space equipped with a coproduct \( \Delta: C \to C \otimes C \) and a counit \( \epsilon: C \to k \). Following Sweedler [22], the coproduct is written \( \Delta(c) = \sum_{(c)} c(1) \otimes c(2) \). For a precise definition of a coalgebra, see Appendix B or [22].

\( C_A \) is the dual of the algebra of formal power series in the variables \( A' \). Let \( a \in C^*_A \) be identified with the formal infinite series \( \sum_{\gamma \in A} \frac{a(\gamma)}{\sigma(\gamma)} \gamma \) and correspondingly for \( b \in C^*_A \) be defined by

\[ \sum_{\gamma \in A} \frac{a \cdot b(\gamma)}{\sigma(\gamma)} \gamma = \left( \sum_{\gamma_1} \frac{a(\gamma_1)}{\sigma(\gamma_1)} \gamma_1 \right) \left( \sum_{\gamma_2} \frac{b(\gamma_2)}{\sigma(\gamma_2)} \gamma_2 \right), \]

where the right hand side is the formal multiplication of series.

It is clear that \( a \cdot b(\gamma) \) is a finite sum of terms of the form \( a(\gamma_1) b(\gamma_2) \), and we define the coproduct \( \Delta_A(\gamma) = \sum_{(\gamma)} \gamma_1 \otimes \gamma_2 \) by

\[ a \cdot b(\gamma) = \sum_{(\gamma)} a(\gamma_1) b(\gamma_2). \]

Coassociativity of \( \Delta_A \) follows from associativity of formal commutative multiplication of series. The counit \( \epsilon_A \) is given by \( 1^*: C_A \to k \).

**Example 3.**

\[ \Delta_A(\begin{array}{c} \bullet \otimes \bullet \otimes \bullet \\ \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus 2 \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \end{array}) = \]

\[ 1 \otimes \bullet \otimes \bullet \otimes \bullet \oplus 2 \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus 2 \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus \bullet \otimes \bullet \otimes \bullet \oplus 1. \]

The coproduct of \( H_F \) is the dual of the Grossman–Larson product as defined in [8]. Both \( C_A \) and \( H_F \) are graded connected coalgebras where the grading is induced by the number of vertices of the graphs, and \( (C_A)_0 = (H_F)_0 = k1 \simeq k \).

Since \( C_{AF} = C_A \otimes H_F \), we can identify

\[ (C_A \otimes H_F)^* \simeq \text{Hom}_k(H_F, C^*_A), \]

where \( \text{Hom}_k(H_F, C^*_A) \) denotes linear functions from \( H_F \) to \( C^*_A \), in the usual way: \( a: C_A \otimes H_F \to k \) is mapped to \( a^*: H_F \to C^*_A \) by

\[ \langle a^*(\phi), c \rangle = a(c \otimes \phi). \]

\( H_F \) with the commutative concatenation product is an algebra, while \( C^*_A \) is the algebra of series in the variables \( A' \).

\(^2\)All (co)algebras considered in this paper are (co)associative and (co)unital, and we will omit the qualifiers.
In other words, series indexed by aromatic forests can be identified with linear maps between algebras $H_F \to C_H^*$. We will see later that series corresponding to algebra morphisms $H_F \to C_H^*$, or $C_A$-valued characters of $H_F$, play a special role.

Definition 4.1. An admissible partition $p_\phi$ of an aromatic forest $\phi$ is a partition of the graph $\phi$ into two (possibly empty) subgraphs $R(p_\phi)$ and $P^*(p_\phi)$, such that no edge in $\phi$ go from $R(p_\phi)$ to $P^*(p_\phi)$.

The graded coproduct is defined on aromatic forests as

$$\Delta_{AF}(\phi) = \sum_{(\phi)} \phi(1) \otimes \phi(2) = \sum_{p_\phi} P^*(p_\phi) \otimes R(p_\phi), \quad (9)$$

and extended linearly to $C_{AF}$.

$\Delta_{AF}$ is calculated for small aromatic forests in Appendix A.

The counit is defined by $\epsilon(\phi) = 1$ if $\phi = 1$, $\epsilon(\phi) = 0$ otherwise.

Theorem 4.2. $(C_{AF}, \Delta_{AF}, \epsilon)$ is a graded coalgebra.

Proof. That $\Delta_{AF}$ is ccoassociative follows from the observation that $(\Delta \otimes \text{id}) \circ \Delta$ and $(\text{id} \otimes \Delta) \circ \Delta$ both can be interpreted as the splitting of $\phi$ in three parts $\phi_1, \phi_2, \phi_3$ such that no edges goes from $\phi_3$ to $\phi_2$ nor from $\phi_2$ to $\phi_1$. The counital property follows from

$$\sum_{p_\phi} \epsilon(P^*(p_\phi))R(p_\phi) = \epsilon(1)\phi = \phi,$$

and

$$\sum_{p_\phi} P^*(p_\phi)\epsilon(R(p_\phi)) = \phi\epsilon(1) = \phi.$$

Finally, the grading is induced by the number of nodes of $\phi$. \qed

We note that as a vector space $C_{AF} = C_A \otimes H_F$, but $\Delta_{AF}$ is not the coproduct inherited from this product.

$C_{AF}$ can be made into an commutative, but not co-commutative Hopf algebra by adjoining the commutative concatenation product $\sqcup$. However, this structure is not as closely connected to aromatic B-series integrators as the Connes–Kreimer Hopf algebra is to B-series integrators, as will be seen in section 5.

Theorem 4.3. $(C_{AF}, \sqcup, \Delta_{AF}, \epsilon)$ is a graded, connected, commutative bialgebra, thus also a commutative Hopf algebra.

Proof. The compatibility conditions are straight-forward to check, and the existence of an antipode follows from Theorem B.1. \qed

5. The composition law. We are now ready to tackle the composition of aromatic S-series. Recall that for normal S-series, the composition corresponds to the dual of the coproduct in $H_F$.

The coproduct in $C_{AF}$ has been designed so that this correspondence also holds between aromatic S-series and the coproduct $\Delta_{AF}$.

In Definition 3.5, an aromatic S-series was defined by a function $a: \mathcal{AF} \to k$. By a slight misuse of notation we extend $a$ linearly to a linear function $a: C_{AF} \to k$.

Theorem 5.1. Let $a, b \in C_{AF}^*$, $f$ a smooth vector field on $W$, and $g$ a smooth function on $W$. Then

$$S_f(b)[S_f(a)[g]] = S_f(b \cdot a)[g], \quad (10)$$
where
\[ b \cdot a(\phi) = (b \otimes a)(\Delta_{A,F}(\phi)) = \sum_{(\phi)} b(P_*^*(\rho_{\phi}))a(R(\rho_{\phi})). \] (11)

**Proof.** The composition of two aromatic S-series \( S_f(b) \circ S_f(a) \) is a series of compositions of elementary differential operators.

Using Lemma 3.8, the composition of two elementary differential operators becomes a finite sum of elementary differential operators. Thus, the composition of two aromatic S-series is an aromatic S-series.

What needs to be proven is that this aromatic S-series is equal to the S-series \( S_f(b \cdot a) \), where \( b \cdot a \) is given by the convolution product (11).

The technique used in the proof is to write both sides of (10) as a *triple* sum over aromatic forests, where the coefficients are non-zero if and only if the third forest \( \psi \) occurs as a term in the composition of the first two \( \phi_2 \circ \phi_1 \), or equivalently that \( \phi_1 \otimes \phi_2 \) occurs as a term in \( \Delta_{A,F}(\psi) \). Finally, the non-zero terms are shown to be equal by a use of the orbit-isotropy theorem [10, Theorem 16.16]

We start with the composition \( S_f(b)[S_f(a)[g]] \):

\[
S_f(b)[S_f(a)[g]] = \sum_{\phi_2 \in A,F} b(\phi_2)F_f(\phi_2) \left[ \sum_{\phi_1 \in A,F} a(\phi_1)F_f(\phi_1)[g] \right].
\]

Using Lemma 3.8, we rewrite

\[
S_f(b)[S_f(a)[g]] = \sum_{\phi_2 \in A,F} \frac{b(\phi_2)}{\sigma(\phi_2)}F_f(\phi_2) \left[ \sum_{\phi_1 \in A,F} \frac{a(\phi_1)}{\sigma(\phi_1)}F_f(\phi_1)[g] \right].
\]

(12)

where \( M_1(\phi_1,\phi_2,\psi) \) is the multiplicity of \( \psi \) in

\[ \phi_2 \circ \phi_1 = \sum_{\rho \in (V(\phi_1) \cup *)^r(\phi_2)} \Phi(\phi_2,\phi_1,\rho). \]

We continue with \( S_f(b \cdot a)[g] \):

\[
S_f(b \cdot a)[g] = \sum_{\psi \in A,F} \frac{b \cdot a(\psi)}{\sigma(\psi)}F_f(\psi)[g]
\]

\[
= \sum_{\psi \in A,F} \frac{b(\psi_{(1)})a(\psi_{(2)})}{\sigma(\psi)}F_f(\psi)[g]
\]

(13)

where \( M_2(\phi_1,\phi_2,\psi) \) is the multiplicity of \( \phi_1 \otimes \phi_2 \) in \( \Delta_{C}(\psi) \).
The claim is true if
\[ \frac{M_1(\phi_1, \phi_2, \psi)}{\sigma(\phi_1)\sigma(\phi_2)} = \frac{M_2(\phi_1, \phi_2, \psi)}{\sigma(\psi)}, \]
for all \( \phi_1, \phi_2, \psi \). We proceed by proving this equality.

(1) \( M_1 = 0 \Leftrightarrow M_2 = 0 \): If edges can be added from \( \phi_2 \) to \( \phi_1 \) to form \( \psi \), the splitting of \( \psi \) into \( \phi_1 \) and \( \phi_2 \) is an admissible partition and vice versa.

(2) If \( M_1, M_2 \neq 0 \), \( \frac{\sigma(\phi_1)\sigma(\phi_2)}{M_1(\phi_1, \phi_2, \psi)} \) and \( \frac{\sigma(\psi)}{M_2(\phi_1, \phi_2, \psi)} \) are equal to the cardinality of subgroups of, respectively, \( G_{\phi_1} \times G_{\phi_2} \) and \( G_{\psi} \) and we will prove that these subgroups are isomorphic.

For the remainder of the proof, let \( \phi_1, \phi_2, \psi, \rho', p'_{\psi} \) be such that
\[ \Phi(\phi_2, \phi_1, \rho') = \psi \quad \text{and} \quad P^*(p'_{\psi}) \otimes R(p'_{\psi}) = \phi_1 \otimes \phi_2. \]

Let \( G_{\phi_1} \times G_{\phi_2} \) act on \( (V(\phi_1) \cup \star)^{r(\phi_2)} \) from the left by setting
\[ (g_1, g_2) \cdot \rho(p) = g_1 \circ \rho \circ g_2^{-1}(p), \]
where we define \( g_1(\star) = \star \).

Now, \( \Phi(\phi_2, \phi_1, \rho') \simeq \Phi(\phi_2, \phi_1, (g_1, g_2) \cdot \rho') \) as graphs, and \( M_1(\phi_1, \phi_2, \psi) \) is the size of the orbit of \( \rho' \) under the action of \( G_{\phi_1} \times G_{\phi_2} \). The orbit-isotropy theorem yields that \( \frac{\sigma(\phi_1)\sigma(\phi_2)}{M_1(\phi_1, \phi_2, \psi)} \) is the size of the isotropy group of \( \rho' \) under the same action. We call this group \( H_1 \).

The admissible partition of \( \psi, p_{\psi} \) is fully defined by the set of vertices forming the subgraph \( R(p_{\psi}) \). We let \( G_{\psi} \) act on the set of admissible partitions of \( \psi \) by its action on the subgraph \( R(\psi) \). (That is, by considering the simultaneous action on the set of vertices \( R(\psi) \).) Since \( G_{\psi} \) acts on \( \psi \) by graph isomorphisms, the restriction of the action to a subgraph is a graph isomorphism of the subgraph. Therefore, \( R(g \cdot p'_{\psi}) \simeq R(p'_{\psi}) \) and \( P^*(g \cdot p'_{\psi}) \simeq P^*(p'_{\psi}) \) as graphs, and \( M_2(\phi_1, \phi_2, \psi) \) is the size of the orbit of \( p'_{\psi} \) under the action of \( G \). The orbit-isotropy theorem yields that \( \frac{\sigma(\psi)}{M_2(\phi_1, \phi_2, \psi)} \) is the size of the isotropy subgroup of \( p'_{\psi} \) under the same action. We call this group \( H_2 \).

We now prove that \( H_1 \simeq H_2 \) as groups. Let \((g_1, g_2) \in H_1 \) i.e. \( g_1 \circ \rho = \rho' \circ g_2 \rvert_{r(\phi_2)}. \)

Now, define the action of \((g_1, g_2)\) on \( \psi = \Phi(\phi_2, \phi_1, \rho') \) by letting \( g_1, g_2 \) act on the subgraphs \( \phi_1, \phi_2 \). This is a graph automorphism of \( \psi \) because for \((r, \rho'(r)) \in E_{\rho'}, (g_2(r), g_1 \circ \rho'(r)) = (g_2(r), \rho' \circ g_2(r)) \in E_{\rho'}^p \). It is in \( H_2 \) because \((g_1, g_2)\) maps \( R(p_{\psi}) \simeq \phi_1 \) to \( R(p_{\psi}) \).

The converse isomorphism \( H_2 \rightarrow H_1 \) follows from considering \( g \in H_2 \) and doing the appropriate restrictions to get \((g_1, g_2) \in G_{\phi_1} \times G_{\phi_2}. \) For \((p, \rho(p)) \in E(\psi)\), we get \((g_2(p), g_1 \circ \rho(p)) \in E(\psi). \) As \( g_2(p) \in \phi_2, g_1 \circ \rho(p) \in \phi_1, \) we must have \( g_1 \circ \rho(p) = \rho \circ g_2(p). \) Therefore \((g_1, g_2) \in H_1. \)

As \( H_1 \simeq H_2, \) we get
\[ \frac{\sigma(\phi_1)\sigma(\phi_2)}{M_1(\phi_1, \phi_2, \psi)} = |H_1| = |H_2| = \frac{\sigma(\psi)}{M_2(\phi_1, \phi_2, \psi)}, \]
and the claim follows.

\[ \square \]

Theorem 5.1 says that the composition product \( C^*_{AF} \otimes C^*_{AF} \rightarrow C^*_{AF} \) is the dual of the coproduct in \( C_{AF}. \) As the dual space of a graded connected coalgebra, the invertible elements of \( C_{AF} \) are \( \{a \in C_{AF} \text{ s.t. } a(1) \neq 0\}, \) and the inverse is given
We have that
\[ a^{-1}(1) = 1/a(1), \quad a^{-1}(\phi) = -\frac{a(\phi) + \sum_{\phi'} a(\phi') a^{-1}(\phi'')}{a(1)}, \]
where \( \sum_{\phi'} \phi' \otimes \phi'' = \Delta(\phi) - 1 \otimes \phi - \phi \otimes 1 \) is the reduced coproduct.

We proceed by describing the aromatic S-series arising from aromatic B-series in Theorem 5.2.

Recall that for ordinary B-series, these correspond to \( k \)-valued characters of \( H_F \).

However for aromatic B-series, the corresponding elements turn out not to be characters of \( C_{A\! F} \) with the natural algebra structure described in Theorem 4.3.

Rather, they are algebra morphisms \( H_F \to C_{A!}^{\mu} \).

The proof closely follows a similar proof for B-series in [18].

**Theorem 5.2.** Extend \( a:C_{A\! T} \to k \) to a function \( \kappa(a):C_{A\! F} \to k \) by requiring that \( \kappa(a) \) and \( a \) coincide on \( A\! T \), and that \( \kappa(a)^\top:H_F \to C_{A!}^{\mu} \), defined as in (8), is an algebra morphism. Then \( g(y + B_f(a)(y)) = S_f(\kappa(a))[g](y) \).

**Proof.** We have that \( A\! T = A \times T \), so we can rewrite the sum
\[ B_f(a) = \sum_{\tau \in A\! T} \frac{a(\tau)}{\sigma(\tau)} F_f(\tau) = \sum_{\theta \in T} \sum_{\gamma \in A} \frac{a(\gamma \theta)}{\sigma(\gamma \theta)} F_f(\gamma \theta). \]

Now, we make two observations: (i) \( F_f(\gamma \theta) = F_f(\gamma) F_f(\theta) \). (ii) The automorphism group of \( \gamma \theta \) cannot mix connected components with 0 and 1 root, so \( \sigma(\gamma \theta) = \sigma(\gamma) \sigma(\theta) \). Collecting terms, we can write
\[ B_f(a) = \sum_{\theta \in T} \left[ \sum_{\gamma \in A} \frac{a(\gamma \theta)}{\sigma(\gamma)} F_f(\gamma) \right] \frac{1}{\sigma(\theta)} F_f(\theta). \]

The sum inside the brackets is a formal series of scalar functions and can be expressed as series indexed by the aromas \( A \):
\[ S_f(a^\top(\theta)) = \sum_{\gamma \in A} \frac{a(\gamma \theta)}{\sigma(\gamma)} F_f(\gamma), \]
where \( a^\top(\theta):C_A \to k \) is defined by \( \langle a^\top(\theta), \gamma \rangle = a(\gamma \theta) \) as in (8).

We can now write
\[ B_f(a) = \sum_{\theta \in T} \frac{S_f(a^\top(\theta))}{\sigma(\theta)} F_f(\theta). \]

We see that this is simply the expression for a regular B-series, with the constant coefficient \( a(\theta) \) replaced by a \( y \)-dependent scalar value \( S_f(a^\top(\theta)) \).

Now, let \( g \) be a smooth function, and expand \( g(y + B_f(a)(y)) \) using Taylor’s theorem.
\[ g(y + B_f(a)(y)) = g(y) + \sum_{k=1}^{\infty} \frac{1}{k!} g^{(k)}(y)(B_f(a)(y), \ldots, B_f(a)(y)). \]
The multi-linearity of \( g^{(k)}(y) \) allows us to rewrite the above equation. Suppressing the dependence of \( y \), we get

\[
g(y + B_f(a)(y)) = g(y) + \sum_{k=1}^{\infty} \sum_{(u_1, \ldots, u_k) \in T^k} S_f(a^\top(u_1)) \cdots S_f(a^\top(u_k)) g^{(k)}(F_f(u_1), \ldots, F_f(u_k))
\]

In the above equation, \( u_1 \cdots u_k \) is a \( k \)-tuple of rooted trees, \( \nu \) is the number of distinct trees among \( u_1, \ldots, u_k \), and \( \mu_1, \ldots, \mu_\nu \) are the multiplicities of each distinct tree.

If \( \phi = u_1 \cdots u_m \), the symmetry group \( G_\phi \) is the semidirect product of permuting identical trees among \( u_1, \ldots, u_m \) and \( G_{u_1} \times \cdots \times G_{u_m} \), so

\[
\sigma(\phi) = \mu_1! \cdots \mu_\nu! \sigma(u_1) \cdots \sigma(u_k).
\]

We define \( \kappa(a)^\top : H_F \to C_A^* \) to be an algebra morphism by

\[
\kappa(a)^\top(\phi) = a^\top(u_1) \cdots a^\top(u_k),
\]

where the product is taken in \( C_A^* \). For \( \phi = 1 \), this simplifies to the empty product \( \kappa(a)^\top(1) = \epsilon_A \).

For any \( \gamma_1, \gamma_2 \in A \), we have \( F_f(\gamma_1 \gamma_2) = F_f(\gamma_1) F_f(\gamma_2) \). Consequently, we have

\[
S_f(\kappa(a)^\top(\phi)) = S_f(a^\top(u_1)) \cdots S_f(a^\top(u_k)),
\]

and

\[
g(y + B_f(a)(y)) = \sum_{\phi \in F} \frac{S_f(\kappa(a)^\top(\phi))(y)}{\sigma(\phi)} F_f(\phi)[g](y). \quad \square
\]

The aromatic S-series \( \kappa(a) \) appearing in Theorem 5.2 are, in general, not characters of \( (C_A^*, \sqcup) \) with values in \( k \). To see this, consider the aromatic graph \( \mathcal{\bullet} \).

The requirement that \( \kappa(a)^\top : C_F \to C_A^* \) is an algebra morphism implies that

\[
\kappa(a)(\mathcal{\bullet}) = \langle \kappa(a)^\top(1), \mathcal{\bullet} \rangle = \langle \epsilon_A, \mathcal{\bullet} \rangle = 0,
\]

on the other hand, \( \kappa(a)(\mathcal{\bullet}) = a(\mathcal{\bullet}) \) can be nonzero.

The S-series in Theorem 5.2 are characters of \( H_F \) with values in \( C_A^* \), and such characters form a group when equipped with the convolution product

\[
a^\top \cdot b^\top : \tau \mapsto \sum_{\tau(1)} a^\top(\tau(1)) \cdot b^\top(\tau(2)).
\]

However, the composition product of aromatic S-series described in Theorem 5.1 is a different product.

6. Substitution law. In this section, we study the substitution law, that is, the operation of substituting the vector field \( f \) in an aromatic S-series with another vector field\(^3\) \( \tilde{f} \) itself expressed as a B-series \( \tilde{f} = B_f(b) \).

The combinatorial formulas and algebraic properties for the substitution law in the case of ordinary B-series were described in [5, 6]. In the latter, the substitution law is also described as the dual of a coproduct in a bialgebra \( \tilde{H} \).

In the present paper, only the combinatorial formulas are described for aromatic B-series.

\(^3\) or formal sum of vector fields.
Definition 6.1. A partition $p^\phi$ of an aromatic forest $\phi$ is a partition of the graph $\phi$ into subgraphs $P(p^\phi) = \{\theta_1, \ldots, \theta_m\}$ such that $\theta_1, \ldots, \theta_m \in \mathcal{AT}$. We view $P(p^\phi)$ as a multiset of aromatic trees. The set of partitions of $\phi$ is denoted $\mathcal{P}(\phi)$. The skeleton $\chi(p^\phi)$ of a partition is the aromatic forest which is obtained by collapsing each of the subgraphs in $P(p^\phi)$ to a single node.

Constructively, a partition is defined by cutting a subset of the edges in $\phi$, obtaining a set of connected components, and then adjoining each rootless connected component, (i.e. aroma) to a connected component with root (i.e. a rooted tree).

Definition 6.2. For the purposes of the proof, we also define a labeled partition $p^*\phi$ as a partition where we assign each subgraph $\theta_1, \ldots, \theta_m$ to a vertex of the skeleton $\chi(p^\phi)$. For a labeled partition, we let $P(p^*\phi) = (\theta_1, \ldots, \theta_m)$ be a sequence of aromatic trees. The set of labeled partitions of $\phi$ is written as $\mathcal{P}^*(\phi)$.

For a partition $p^\phi$, the number of possible labellings is $\sigma(\chi(p^\phi))$.

We illustrate partitions and labeled partitions with an example.

Example 4. Let $\phi$ be the aromatic graph:

(i) Cutting the edge $4 \rightarrow 5$ leaves the connected subgraphs

which both are trees. The skeleton is

(ii) Cutting the edge $2 \rightarrow 4$ leaves the connected subgraphs

The connected components are two trees and an aroma, and there is a choice in which rooted tree to adjoin the aroma to. If we choose $P(\phi) = \{\lambda \tau_1, \tau_2\}$, then the skeleton is
If we choose $P(\phi) = \{\tau_1, \lambda \tau_2\}$, then the skeleton is

$\begin{array}{c}
\tau_1 \\
\lambda \tau_2
\end{array}$

**Theorem 6.3.** Let $b : AT \to k$ be an aromatic B-series and $a : AF \to k$ be an aromatic S-series, then $S_{B_j(b)}(a)$ can be expressed as an aromatic B-series in $f$, $S_{B_j(b)}(a) = S_f(b \ast a)$ with coefficients

$$b \ast a(\phi) = \sum_{p^\phi \in P(\phi)} a(\chi(p^\phi)) \prod_{\theta \in S(p^\phi)} b(\theta). \quad (14)$$

We prove the theorem for $a = \gamma^*$ where $\gamma$ is an arbitrary aromatic forest with $|\gamma| = m$. The full theorem follows from linearity in $a$.

Let $\tilde{f} = B_f(b)$. The method used in the proof consists of writing $F_f(\gamma)$ as an $m$-linear function $E_\gamma$ evaluated at $m$ copies of $\tilde{f}$ and its derivatives.

This function is then expanded by writing $\tilde{f} = B_f(b)$ as a sum over $AT$. The result is an $m$-tuple sum over aromatic trees $AT$. The terms in this sum are of the form

$$E_\gamma(F_f(\theta_1), F_f(\theta_2), \ldots, F_f(\theta_m))$$

where $\theta_1, \ldots, \theta_m$ are aromatic trees, and $E_\gamma$ specifies how derivatives of its arguments shall be combined to form a differential operator. This resulting differential operator $E_\gamma(F_f(\theta_1), F_f(\theta_2), \ldots, F_f(\theta_m))$ is eventually an affine equivariant function of $f$ and a finite linear combination of elementary differentials of the form $F_f(\phi)$.

Then equal terms in the entire sum are collected. Proving equality to $S_f(b \ast a)$ is done by an application of the orbit-isotropy theorem.

**Proof.** By the definition of S-series (Definition 3.5) $S_f(\gamma) = \frac{1}{\sigma(\gamma)} F_f(\gamma)$, and, by the definition of elementary differential operator (Definition 3.3)

$$F_f(\gamma) = E_\gamma(\tilde{f}, \tilde{f}, \ldots, \tilde{f}) = \prod_{j \in V(\gamma)} \tilde{f}_{I_\gamma(j)}^j \prod_{k \in r(\gamma)} \partial_k,$$

where Einstein’s summation convention is used.

Now,

$$\tilde{f} = \sum_{\theta \in AT} \frac{b(\theta)}{\sigma(\theta)} F_f(\theta),$$

so

$$F_f(\gamma) = \sum_{\theta_1} \sum_{\theta_2} \cdots \sum_{\theta_m} \frac{b(\theta_1) b(\theta_2) \cdots b(\theta_m)}{\sigma(\theta_1) \sigma(\theta_2) \cdots \sigma(\theta_m)} E_\gamma(F_f(\theta_1), F_f(\theta_2), \ldots, F_f(\theta_m))$$

$$= \sum_{\theta_1} \cdots \sum_{\theta_m} \prod_{j \in V(\gamma)} \frac{b(\theta_j)}{\sigma(\theta_j)} F_f(\theta_j) I_{\gamma(j)}^j \prod_{k \in r(\gamma)} \partial_k,$$

where each of the sums goes over $\theta_k \in AT$. In the above equation, each of $F_f(\theta_j) I_{\gamma(j)}^j$ corresponds to taking derivatives of the elementary differential operators $F_f(\theta)$.

These derivatives are then combined according to $E_\gamma$. The resulting expression is a sum of elementary differential operators corresponding to aromatic forests.
The graphs of these aromatic forests are formed from the graphs \( \theta_1, \ldots, \theta_m \) in the following manner: For each edge \( e_i = (u, v) \) in \( E(\gamma) \), choose a vertex in \( \theta_v \) and add an edge from the root of \( \theta_u \) to that vertex. The sum is then taken over all possible choices of vertices.

We can denote the aromatic forest formed by a particular choice of vertices by

\[
\Gamma(\theta_1, \ldots, \theta_m; j_1, \ldots, j_n) = \Gamma(\Theta; j).
\]

where \( j_1, j_2, \ldots, j_n \) are the vertices chosen for edges \( e_1, \ldots, e_n \in E(\gamma) \). Recall that for \( e_i = (u, v) \), we are restricted to choosing \( j_i \) in \( \theta_v \).

With this notation,

\[
S_f(a) = \frac{1}{\sigma(\gamma)} \sum_{\Theta \in \mathcal{AT}} \sum_{\phi} \prod_{l} b(\gamma, \Theta, \phi) \prod_{i} \frac{b(\theta_i)}{\sigma(\theta_i)} F_f(\Gamma(\Theta; j)),
\]

where the sum \( \sum_{\phi} \) goes over all possible choices of vertices.

We now collect equal terms. Collecting \( j \) for which \( \Gamma(\Theta; j) = \phi \) are equal, we get

\[
S_g(a) = \frac{1}{\sigma(\gamma)} \sum_{\Theta \in \mathcal{AT}} \sum_{\phi} M_1(\gamma, \Theta, \phi) \prod_{i} b(\theta_i) \prod_{i} \frac{b(\theta_i)}{\sigma(\theta_i)} F_f(\phi), \tag{15}
\]

where \( M_1(\gamma, \Theta, \phi) \) counts the number of \( j \) such that \( \Gamma(\Theta; j) = \phi \).

What we seek to prove is that \( S_g(a) \) is equal to

\[
S_f(b \ast a) = \sum_{\phi} \frac{1}{\sigma(\phi)} \sum_{p^* \in P(\phi)} \prod_{\chi(p^*)=\gamma} b(\theta) F_f(\phi).
\]

We rewrite this by extending the sum over all labeled partitions, and dividing by \( \sigma(\gamma) \) to compensate. (Recall Definition 6.2.)

\[
S_f(b \ast a) = \sum_{\phi} \frac{1}{\sigma(\phi)\sigma(\gamma)} \sum_{p^* \in P(\phi) \in S(\gamma)} \prod_{\chi(p^*)=\gamma} b(\theta) F_f(\phi).
\]

Collecting terms for which \( P(p^* \phi) = (\theta_1, \ldots, \theta_m) = \Theta \), we get

\[
B_f(b \ast a) = \sum_{\phi} \frac{1}{\sigma(\phi)\sigma(\gamma)} \sum_{\Theta} M_2(\gamma, \Theta, \phi) \prod_{i} b(\theta_i) F_f(\phi), \tag{16}
\]

where \( M_2(\gamma, \Theta, \phi) \) counts the number of labeled partitions \( p^* \phi \) such that \( P(p^* \phi) = \Theta \).

Comparing (15) with (16), \( S_g(a) = S_f(b \ast a) \) provided that

\[
\frac{M_2(\gamma, \Theta, \phi)}{\sigma(\phi)} = \frac{M_1(\gamma, \Theta, \phi)}{\prod \sigma(\theta_i)}. \tag{17}
\]

We proceed by proving that, when nonzero, either side of (17) can be identified with the reciprocal of the cardinality of an isotropy subgroup. Furthermore, we will show that the two isotropy subgroups are isomorphic.

We begin by showing that \( M_1 \) and \( M_2 \) are nonzero simultaneously.

Let \( \gamma, \Theta = (\theta_1, \ldots, \theta_m), \phi \) be given. If there is no way of adding edges to the graphs \( \theta_1, \ldots, \theta_m \) that results in \( \phi \), there is also no way to obtain \( \theta_1, \ldots, \theta_m \) by cutting edges in \( \phi \) and vice versa. In this case, \( M_1 = M_2 = 0 \).

If non-zero, we can identify each side of the equation (17) with the reciprocal of the cardinality of subgroups of symmetry groups:
(i) $G_\phi$ acts on labeled partitions of $\phi$ in a natural manner. Let $p^{*\phi}$ be such that $\chi(p^{*\phi}) = \gamma$, and $P(p^{*\phi}) = (\theta_1, \ldots, \theta_m)$. The action of $G_\phi$ conserves both $\chi(p^{*\phi})$ and $P(p^{*\phi}) = (\theta_1, \ldots, \theta_m)$, and all partitions satisfying $P(p^{*\phi}) = \Theta$ is obtained in this manner. Therefore, $M_2(\gamma, \Theta, \phi)$ is the size of the orbit of $p^{*\phi}$ under the $G_\phi$ action.

By the orbit-isotropy theorem, $\frac{\sigma(\phi)}{M_2(\gamma, \Theta, \phi)}$ is the size of the isotropy subgroup of $p^{*\phi}$, that is: the subgroup of $G_\phi$ which does not mix the vertex subsets corresponding to $\theta_1, \ldots, \theta_m$, and in addition, within each vertex subset $V(\theta_i)$, any vertex whose in-degree is higher in $\phi$ than in $\theta_i$, has to be fixed under the subgroup.

(ii) $j$ denotes a sequence of vertices in $\theta_1, \ldots, \theta_m$ with some restrictions, $G_{\theta_1} \times \cdots \times G_{\theta_m}$ acts on the set of such sequences by moving the vertices within each subgraph. Let $j$ be such that $\Gamma(\Theta, j) = \phi$. The action of $G_{\theta_1} \times \cdots \times G_{\theta_m}$ preserves $\Gamma(\Theta, j)$, and all sequences satisfying the requirement are obtained in this manner. Therefore $M_1(\gamma, \Theta, \phi)$ is the size of the orbit of $j$ under the action of $G_{\theta_1} \times \cdots \times G_{\theta_m}$.

By the orbit-isotropy theorem, $\frac{\prod_{\sigma(\phi)} M_1(\gamma, \Theta, \phi)}{M_1(\gamma, \Theta, \phi)}$ is the size of the isotropy group of $j$ under this action, that is the subgroup of $G_{\theta_1} \times \cdots \times G_{\theta_m}$ which, in each component preserves $j \cap V(\theta_i)$.

Since the vertices in $j$ are exactly those which have higher in-degree in $\phi$ than in $\theta_i$, the two subgroups described in (i) and (ii) are isomorphic.

The composition and substitution laws are two algebraic operations on aromatic S-series. The natural question is how they interact.

For B-series, [6] describes the interaction in terms of the operations themselves. The same properties hold for aromatic S-series, as summed up in the following proposition.

**Proposition 1.** (a) $(C^*_A, \tau)$ forms a monoid with identity $\bullet$ which acts on $C^*_B$ by algebra morphisms, in particular, the following identities hold for $a, a_1, a_2 \in C^*_A, b, c \in C^*_A$, $\alpha_1, \alpha_2 \in k$.

\[
\begin{align*}
   b \ast (a_1a_1 + a_1a_1) &= a_1b \ast a_1 + a_2b \ast a_1, \\
   c \ast (b \ast a) &= (c \ast b) \ast a, \\
   b \ast \bullet &= b, \\
   \bullet \ast a &= a, \\
   b \ast (a_1 \cdot a_2) &= (b \ast a_1) \cdot (b \ast a_2), \\
   b \ast a^{-1} &= (b \ast a)^{-1}.
\end{align*}
\]

(b) The set $\{b \in C^*_A \text{ s.t. } b(\bullet) \neq 0\}$ with operation $\ast$ forms a group.

**Proof.** (a) All of the formulas follows from $S_f(b \ast a) = S_{B_f(\phi)}(a)$, and $S_f(a \cdot b) = S_{f}(b) \circ S_{f}(a)$.

(b) From (a) we know that $\bullet$ is both a right and left identity on $C^*_A$. The right inverse of an element $b \in C^*_A$, $b(\bullet) \neq 0$ is given by

\[
b^{-1}(\bullet) = \frac{1}{b(\bullet)}.
\]

\[
b^{-1}(\gamma) = -\frac{1}{b(\bullet)} \sum_{p^0 \in P(\phi)} b(\chi(p^0)) \prod_{\theta \in P(p^0)} b^{-1}(\theta),
\]

\[
b^{-1}(\tau) = -\frac{1}{b(\bullet)} \sum_{p^0 \in P(\phi)} b(\chi(p^0)) \prod_{\theta \in P(p^0)} b^{-1}(\theta),
\]

\[
b^{-1}(\theta) = -\frac{1}{b(\bullet)} \sum_{p^0 \in P(\phi)} b(\chi(p^0)) \prod_{\theta \in P(p^0)} b^{-1}(\theta),
\]
where in the last sum, the trivial partition with $\chi(p^\phi) = \bullet, P(p^\phi) = \tau$ is omitted. All elements in $\{b \in C^\tau_{\mathcal{AT}} \text{ s.t. } b(\bullet) \neq 0\}$ allow a right inverse in the same set, therefore a right inverse is also a left inverse.

\[\square\]

In the nonaromatic case, the interaction between the composition and substitution products was described on the bialgebraic side via two bialgebras interacting.

The description of the substitution law as the dual of a coproduct in a fitting bialgebra and the corresponding interaction between $C_{\mathcal{AT}}^\tau$ and this bialgebra remains unsolved.

6.1. Divergence of aromatic B-series. A special case of the substitution law is the divergence of an aromatic B-series. Recall that $F_{\mathcal{J}}(\phi) = \text{tr} f' = \text{div} f$, so the divergence of $f$ is given by $S_f(\phi^*) = F_f(\phi)$.

Let $\tilde{f} = B_f(b)$ be an aromatic B-series. By Theorem 6.3 the divergence of $\tilde{f}$ is given by

$$\text{div} \tilde{f} = S_f(\phi^*)$$

$$= S_f(b * \phi^*),$$

and we define $\nabla b := b * \phi^*$.

By (14), we have

$$\nabla b(\phi) = \sum_{p^\phi \in P(\phi)} \phi^*(\chi(p^\phi)) \prod_{\theta \in S(p^\phi)} b(\theta).$$

In this case, we only get non-zero values when $\chi(p^\phi) = \bullet$, thus $\phi$ can not have any roots, and $P(p^\phi)$ can only consist of a single aromatic tree.

$$\nabla b(\phi) = \sum_{v \in V(\phi)} b(\phi_v),$$

where $\phi_v$ is the aromatic tree obtained by deleting the edge going out of $v$. This formula, specialized for B-series, appears in the papers by Iserles, Quispel and Tse [13], and the paper by Chartier and Murua [7].

Now, assume that $f$ is a divergence-free vector field $\text{div} f = F_f(\phi) = 0$, and that we apply an aromatic B-series method (i.e. an affine-equivariant, local numerical method) to the differential equation $\dot{y} = f(y)$. The modified vector field given by $B_f(b)$, and the method is volume-preserving if $\nabla b = b * \phi^*$ is non-zero only on $\phi \in \mathcal{AT}$ that have $\phi$ as a subgraph.

7. Affine-equivariant pseudo-volume-preserving integrators. One question raised by Munthe-Kaas and Verdier [17] is the existence of volume-preserving aromatic B-series methods.

Volume-preserving methods are well known in the literature, see for instance [9, 20], but all such methods rely on some partition of the vector field along coordinate axes, and are therefore not equivariant under invertible affine maps, and are therefore not aromatic B-series methods.

It is known that B-series methods cannot be volume-preserving (apart from the exact integrator) [7, 13] but that aromatic B-series methods can be [17]. However, it has so far not been possible to find an equation defining the update map for a volume-preserving aromatic B-series method.

While this question remains unanswered, with the computational tools developed in this paper, one can at least find methods that are pseudo-volume-preserving.
That is, that methods that preserves the volume with a higher order of accuracy than the order of the method itself.

One approach is as follows:

Let \( \tilde{f} \) be a preprocessed vector field

\[
\tilde{f} = B_f(b),
\]

where \( B_f(b) \) is an expression that can be efficiently computed from \( f \), for example a linear combination involving \( f \), \((f')f \), \((f')^2 \), \( \text{tr}((f')^2) f \), \ldots. Then integrate

\[
\dot{x} = \tilde{f}(x)
\]

using a standard Runge–Kutta method or other B-series method with B-series \( B_f(a) \).

If \( B_f(b) \) is chosen properly, the resulting integrator can preserve the volume form to higher order than the original B-series method given by \( B_f(a) \).

An example of a method which is second order, but preserves volume to fourth order is detailed below.

**Example 5.** We base our method on the implicit midpoint method, whose modified vector field is \( B_f(a) \), where

\[
a = \ast + \frac{1}{12} \left( \ast \ast - \mathbf{V} \ast \right) + \text{remainder}.
\]

Here the remainder contains terms of order 5 and higher.

And define a pre-processed vector field by

\[
\tilde{f}(y) = f(y) + \frac{h^2}{12} \left( \frac{1}{2} \text{tr}(f'(y)^2) - f'(y)^2 \right) f(y).
\]

In the notation of aromatic B-series, \( \tilde{f} = B_f(b) \) where

\[
b = \ast + \frac{1}{12} \mathcal{O} \ast - \frac{1}{12} \mathbf{f}.
\]

The integrator is defined by substituting \( F \) for \( f \) in the implicit midpoint method

\[
y_{n+1} = y_n + hF \left( \frac{y_n + y_{n+1}}{2} \right).
\]

(19)

Implementing this method requires evaluating the Jacobian \( f'(y) \) and solving a non-linear equation.

The modified vector field of (19) is \( B_f(b \ast a) \) and the divergence of the modified vector field is \( B_f(b \ast a \ast \mathcal{O}^*) \), which we can calculate for the smallest rootless graphs. Using (14),

\[
b \ast a = \ast + \frac{1}{12} \left( \mathcal{O} \ast - \mathbf{V} \ast \right) + \text{remainder},
\]

and

\[
b \ast a \ast \mathcal{O}^* = \mathcal{O}^* - \frac{1}{12} \mathbf{O}^* + \text{remainder},
\]

where the remainders contain terms of 5th order or higher.

If \( f \) is divergence free, \( F_f \) sends any aromatic forest containing the subgraph \( \mathcal{O} \) to 0, so we see that while \( B_f(b \ast a) \) agrees to \( f \) to second order, \( \text{div} B_f(b \ast a) = S_f(b \ast a \ast \mathcal{O}^*) \) disappears to fourth order. The integrator (19), while second order, conserves volume to fourth order.
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The graphs of the aromatic trees were generated in two different ways: Most of the trees were generated using Håkon Marthinsen’s planarforest package http://hmarthinsen.github.io/planarforest/ and the author’s modification thereof. These in turn use the pythonTeX[19] package. The large tree in Example 1 was generated using Olivier Verdier’s etrees package.

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Appendix A. Tables for composition and substitution laws. In this appendix, we provide tables for the composition and substitution laws on aromatic B-series.

Appendix B. Coalgebras, bialgebras and Hopf algebras. See also [22] for an introduction to coalgebras, bialgebras, Hopf algebras.

Throughout this article, k is either \( \mathbb{R} \) or \( \mathbb{C} \), and all tensor products \( \otimes \) are taken over \( k \). An associative algebra over \( k \) is a vector space \( A \) over \( k \) equipped with an associative linear multiplication map \( \mu: A \otimes A \to A \), \( \mu: a \otimes b \mapsto ab \). It is unital if, in addition, there is a linear map \( u: k \to A \), called the unit such that for all \( \beta \in k, a \in A \), \( u(\beta)a = au(\beta) = \beta a \).

A is graded if \( A = \bigoplus_{n=0}^{\infty} A_n \) as a vector space and \( \mu(A_n, A_m) \subset A_{n+m} \).

A coassociative coalgebra over \( k \) is a vector space \( C \) equipped with a coproduct \( \Delta: C \to C \otimes C \). In the notation of Sweedler, we write \( \Delta(c) = \sum_{(c)} c(1) \otimes c(2) \).

The coproduct is linear and coassociative, that is
\[
(\Delta \otimes I) \circ \Delta = (I \otimes \Delta) \circ \Delta,
\]
where \( I \) is the identity map on \( C \), or equivalently
\[
\sum_{(c)} \Delta(c(1)) \otimes c(2) = \sum_{(c)} c(1) \otimes \Delta(c(2)).
\]

A coalgebra is counital if, in addition, there is a linear map \( \epsilon: C \to k \), called the counit such that for all \( c \in C \), \( \sum_{(c)} \epsilon(c(1))c(2) = c = \sum_{(c)} c(1)\epsilon(c(2)) \).

The (co)algebras considered in this paper are all both (co)associative and (co)-unital, and we will omit the qualifiers.

A coalgebra \( C \) is graded if \( C = \bigoplus_{n=0}^{\infty} C_n \) as a vector space and \( \Delta(C_n) \subset \bigoplus_{k+l=n} C_k \otimes C_l \). A coalgebra is connected if \( C_0 \cong k \).

For \( V,W \) algebras, respectively coalgebras, \( V \otimes W \) is again an algebra, respectively a coalgebra in a canonical way:
\[
(v_1 \otimes w_1)(v_2 \otimes w_2) = v_1v_2 \otimes w_1w_2
\]
or
\[
\Delta(v \otimes w) = \sum_{(v)} \sum_{(w)} v_{(1)} \otimes w_{(1)} \otimes v_{(2)} \otimes w_{(2)}
\]

A bialgebra \( B \) is simultaneously an algebra and coalgebra such that the maps \( \mu: B \otimes B \to B \) and \( u: k \to B \) are morphisms of counital coalgebras and \( \Delta: B \to B \otimes B \)
and \( c: B \to k \) are morphisms of unital algebras, that is, for all \( h, k \in B \),

\[
\Delta(hk) = \sum_{(h)} \sum_{(k)} h_{(1)}k_{(1)} \otimes h_{(2)}k_{(2)}
\]

\[
\Delta(u(1)) = u(1) \otimes u(1)
\]

\[
\epsilon(hk) = \epsilon(h)\epsilon(k)
\]

\[
\epsilon(u(1)) = 1
\]

\( B \) is graded if \( B = \bigoplus_{n=0}^{\infty} B_n \) is graded as an algebra and coalgebra, and connected if \( B_0 \simeq k \).

For \( C \) coalgebra and \( A \) algebra, \( \text{Hom}_k(C, A) \) equipped with the convolution product \( f \ast g = \mu_A \circ (f \otimes g) \circ \Delta_C \) is an algebra. The unit of the convolution product is \( u_A \circ \epsilon_C \).
| $\tau$ | $b + a(\tau)$ |
|-------|---------------|
| $\cdot$ | $a(\cdot)b(\cdot)$ |
| $\cdot \cdot$ | $a(\cdot)b(\cdot) + a(\cdot)b(\cdot)^2$ |
| $\cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + a(\cdot)b(\cdot)^2 + a(\cdot)b(\cdot)^3$ |
| $\cdot \cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + 2a(\cdot)b(\cdot)b(\cdot) + a(\cdot)b(\cdot)^3$ |
| $\cdot \cdot \cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + 2a(\cdot)b(\cdot)b(\cdot) + a(\cdot)b(\cdot)^3$ |
| $\cdot \cdot \cdot \cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + 2a(\cdot)b(\cdot)b(\cdot) + a(\cdot)b(\cdot)^3$ |
| $\cdot \cdot \cdot \cdot \cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + 2a(\cdot)b(\cdot)b(\cdot) + a(\cdot)b(\cdot)^3$ |
| $\cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + 2a(\cdot)b(\cdot)b(\cdot) + a(\cdot)b(\cdot)^3$ |
| $\cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot \cdot$ | $a(\cdot)b(\cdot) + 2a(\cdot)b(\cdot)b(\cdot) + a(\cdot)b(\cdot)^3$ |

For $B$ a bialgebra, $\text{Hom}_B(B, B)$ equipped with the convolution product is an algebra. If the convolution inverse of the identity map exists, it is called the antipode, and in this case the bialgebra is called a Hopf algebra.

**Theorem B.1.** [22] A graded, connected bialgebra is a graded Hopf algebra.

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\begin{table}[h]
\centering
\begin{tabular}{|c|c|}
\hline
$\lambda$ & $b \ast a(\lambda)$ \\
\hline
1 & $a(\mathbb{1})$ \\
$\mathbb{0}$ & $a(\mathbb{0})b(\mathbb{1}) + a(\mathbb{1})b(\mathbb{0}) + a(\mathbb{1})b(\mathbb{0})^2$ \\
$\mathbb{0}\mathbb{0}$ & $2a(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{1})^2$ \\
$\mathbb{0}\mathbb{0}\mathbb{0}$ & $2a(\mathbb{0})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{0})^2$ \\
$\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}$ & $2a(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{0})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{1})$ \\
$\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}$ & $3a(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{0})^2$ \\
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$\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}$ & $3a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0})b(\math{0}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{1})b(\mathbb{1})b(\mathbb{0}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{1})b(\mathbb{0})b(\mathbb{1}) + a(\mathbb{0})b(\mathbb{1})b(\mathbb{1})b(\mathbb{1})b(\mathbb{1})$ \\
$\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}\mathbb{0}$ & $3a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + 6a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{0}) + 6a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{1}) + 6a(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0}) + 6a(\mathbb{0})b(\mathbb{0})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + 6a(\mathbb{0})b(\mathbb{1})b(\mathbb{0})b(\mathbb{0})b(\mathbb{0})b(\mathbb{1}) + 6a(\math{0})b(\math{1})b(\math{1})b(\math{0})b(\math{0})b(\math{1})b(\math{0}) + 6a(\math{0})b(\math{1})b(\math{1})b(\math{0})b(\math{0})b(\math{1}) + 6a(\math{0})b(\math{1})b(\math{1})b(\math{1})b(\math{0})b(\math{0}) + 6a(\math{0})b(\math{1})b(\math{1})b(\math{1})b(\math{0})b(\math{1}) + 6a(\math{0})b(\math{1})b(\math{1})b(\math{1})b(\math{1})b(\math{0})$ \\
\hline
\end{tabular}
\caption{Substitution law (0 roots)}
\end{table}

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