FREE INTEGRO-DIFFERENTIAL ALGEBRAS AND GRÖBNER-SHIRSHOV BASES

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Abstract. The notion of commutative integro-differential algebra was introduced for the algebraic study of boundary problems for linear ordinary differential equations. Its noncommutative analog achieves a similar purpose for linear systems of such equations. In both cases, free objects are crucial for analyzing the underlying algebraic structures, e.g. of the (matrix) functions.

In this paper we apply the method of Gröbner-Shirshov bases to construct the free (noncommutative) integro-differential algebra on a set. The construction is from the free Rota-Baxter algebra on the free differential algebra on the set modulo the differential Rota-Baxter ideal generated by the noncommutative integration by parts formula. In order to obtain a canonical basis for this quotient, we first reduce to the case when the set is finite. Then in order to obtain the monomial order needed for the Composition-Diamond Lemma, we consider the free Rota-Baxter algebra on the truncated free differential algebra. A Composition-Diamond Lemma is proved in this context, and a Gröbner-Shirshov basis is found for the corresponding differential Rota-Baxter ideal.

Contents

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1. Introduction

1.1. **Commutative Setting.** An *integro-differential algebra* (R, d, P) is an algebraic abstraction of the familiar setting of calculus, where one employs a notion of differentiation d together with a notion of integration P on some (real or complex) algebra of functions.

For understanding the motivation behind this abstraction, let us first consider the (R, d). This is the familiar setting of *differential algebra* as set up in the work of Ritt [29, 30] and Kolchin [26]. The idea is to capture the structure of (polynomially) nonlinear differential equations from a purely algebraic viewpoint. If one speaks of solutions in this context, one usually means elements in a suitable differential field $\bar{R}$ extending R. In particular, in differential Galois theory, an “integral” of $f \in R$ is taken as an element $u \in \bar{R}$ such that $d(u) = f$.

In applications, however, differential equations often come together with *boundary conditions* (for simplicity here we include also initial conditions under this term). Incorporating these into the algebraic model requires some modifications: Assuming every $f \in R$ has an integral $u \in R$, the condition $d(u) = f$ becomes $d \circ P = 1_R$, and it is natural to assume that the operator $P\colon f \mapsto u$ is linear. In the standard setting $R = C^\infty(\mathbb{R})$ we have $d(u) = u'$ and $P(f) = \int_a^x f(\xi)\, d\xi$ for some initial point $a \in \mathbb{R}$. This leads us to expect some further properties of P:

- The Fundamental Theorem of Calculus tells us that P is a right inverse of d, as noted above. But it also tells us that P is *not* a left inverse; rather, we have $P \circ d = 1_R - E_a$ in the standard setting, where E_a is the *evaluation* $u \mapsto u(a)$. Note that E_a is a multiplicative functional on R.
- Just like d satisfies the product rule (also known as the Leibniz law), so P satisfies the well-known *integration by parts* rule. In its strong form, this is the rule $P(f d(g)) = fg - P(d(f)g) - E(f)E(g)$; in its weak form it is given by $P(f)P(g) = P(fP(g)) + P(P(f)g)$. Both can be verified immediately in the standard setting; for their distinction in general see below.

We will now explain briefly why both of these properties are instrumental for treating *boundary problems* (differential equations with boundary conditions) on an algebraic level. We restrict ourselves to the classical case of two-point boundary problems for a linear ordinary differential equations. For this and the more general setting of Stieltjes boundary condititions, we refer to [31].

If R is an arbitrary $\mathbf{k}$-algebra, we can define an *evaluation* as a multiplicative linear functional $R \to \mathbf{k}$. In the case of a two-point boundary problem over $[a, b] \subset \mathbb{R}$, one will have two evaluations $E_a\colon u \mapsto u(a)$ and $E_b\colon u \mapsto u(b)$. A boundary condition like $2u(a) - 3u'(a) + u'(b) = 0$ then translates to $\beta(u) = 0$ with the linear functional $\beta = 2E_a - 3E_a d + E_b d$.

We can now define a general boundary problem over (R, d, E_a, E_b) as the task of finding for given $f \in R$ the solution $u \in R$ of

$$\boxed{\begin{array}{l} Tu = f, \\ \beta_1(u) = \cdots = \beta_n(u) = 0, \end{array}}$$

where $T \in R[d]$ is a monic linear differential operator of order n and the boundary conditions β_i are linear functionals built from d and the evaluations E_a, E_b as above, with differentiation order below n. We call the boundary problem (1.1) *regular* if there is a unique solution $u \in R$ for every $f \in R$. In this case, the association $f \mapsto u$ gives rise to linear map $G\colon R \to R$ known as the *Green’s operator* of (1.1).

It turns out [31, Thm. 26] that the Green's operator G of (1.1) can be computed algebraically from a given fundamental system of T. Moreover, G can be written in the form of an integral operator $u = \int_a^b g(x,\xi)\, f(\xi)\, d\xi$, where $g(x,\xi)$ is the so-called *Green's function* of (1.1). More precisely, defining the operator ring generated by $R[d]$, the integral operator P and the evaluations E_a, E_b, modulo suitable relations, G can be written as an element of this quotient ring, with g as its canonical representative. We observe that a *single* integration is sufficient for undoing n differentiations—this is achieved by collapsing n integrations into one, using integration by parts as one of the relations.

In fact, the relations contain two different rules that encode *integration by parts*: The rewrite rule $\int f \int \to \ldots$ encapsulates the weak form $P(f)P(g) = P(fP(g)) + P(P(f)g)$ while the rewrite rule $\int f \partial \to \ldots$ encodes the strong form $P(fd(g)) = fg - P(d(f)g) - E(f)E(g)$. The former contracts multiple integrations into one, the purpose of latter is to eliminate derivatives from the Green's operator.

In concluding this brief account on the algebraic treatment of boundary problems, let us note that the operator ring is much more general than the usual Green's functions. Extending two-point conditions to *Stieltjes boundary conditions* leads to a threefold generalization: More than two point evaluations can be used, definite integrals may appear, and the differentiation order need not be lower than that of T. In this case, G is still representable as an element of the operator ring, and as before it may be computed from a given fundamental system of T.

Let us now turn to the distinction between the "weak" form (also called Rota-Baxter axiom) and the "strong" form (called the hybrid Rota-Baxter axiom) of integration by parts. Since the former does not involve the derivation d, it can be used to encode an algebraic structure (R, P) with just an integral—this leads to the important notion of a Rota-Baxter algebra, introduced below in a more general context in Def. 2.1(b). Rota-Baxter algebras form an extremely rich structure with important applications in combinatorics, physics (Yang-Baxter equation, renormalization theory), and probability; see [20] for a detailed survey. Here we restrict our interest to the interaction between the Rota-Baxter operator P and the derivation d. If this interaction is only given by the section axiom $d \circ P = 1_R$, one speaks of a *differential Rota-Baxter algebra*, introduced formally in Def. 2.1(c) below. Intuitively, this is a weak coupling between the differential algebra (R, d) and the Rota-Baxter algebra (R, P).

In contrast, the hybrid Rota-Baxter axiom involves P as well as d, and it creates a stronger coupling between d and P. In fact, one checks immediately that it implies the Rota-Baxter axiom, but the converse is not in general true as one sees from Example 3 in [31]. An *integro-differential algebra* (R, d, P) is then defined as a differential ring (R, d) with a right inverse P of d that satisfies the hybrid Rota-Baxter axiom; see Def. 2.1(d) for the more general setting. Hence every integro-differential algebra is also a differential Rota-Baxter algebra but generally not vice versa. The crucial difference between the two categories can be expressed in various equivalent ways [22, Thm. 2.5] of which we shall mention only two. An integro-differential algebra (R, d, P) is a differential Rota-Baxter algebra satisfying one of the following equivalent extra conditions:

- The projector $E := 1_R - P \circ d$ is *multiplicative*. So if additionally $\ker d = \mathbf{k}$ as is typically the case in an ordinary differential algebra, then E deserves to be called an "evaluation". This is the situation we had observed before in the standard setting.
- The image $P(R)$ is not only a subalgebra (as in any Rota-Baxter algebra) but an *ideal* of R. As a consequence, this excludes the possibility that (R, d) has the structure of a differential field so common in differential Galois theory (see above).

In many “natural” examples—such as the standard setting described above—the notions of differential Rota-Baxter algebra and integro-differential algebra actually coincide. However, their differences are borne out fully when it comes to constructing the corresponding *free objects*: For differential Rota-Baxter algebras, this works in the same way as for the free Rota-Baxter algebra (only with differential instead of plain monomials). Due to the tighter differential/Rota-Baxter coupling, the construction of the free integro-differential algebra is significantly more complex. Two different methods have been used to this end: In [22] an artificial evaluation is set up while in [18] Gröbner-Shirshov bases are employed.

Free objects are useful in many ways. In the case of the free integro-differential algebra, we mention the following two *applications*, where we think of the R as function spaces similar to the standard setting:

- It allows to build up integro-differential subalgebras $R \subset C^\infty(\mathbb{R})$ by *adjoining* new functions. For example, we can create the subalgebra of exponentials $R = \mathbb{R}[e^x]$ by forming the free integro-differential algebra in one indeterminate e and passing to the quotient modulo the integro-differential ideal generated by $P(e)-e+1$. Note that this implies the differential relation $d(e) = e$ and the initial value $E(e) = 1$.
- It attaches a rigorous meaning to the intuitive notion of *purely algebraic manipulations of integro(-differential) equations*. For example, in the proof of the Picard-Lindelöf theorem, one transforms a given initial value problem for a differential equation into an equivalent integral equation.

Intuitively, one should think of the elements in a free integro-differential as an integro-differential generalization of differential polynomials (with trivial derivation on the coefficients).

1.2. **Noncommutative Setting.** Up to now we have thought of the ring R as commutative but the above considerations—in particular the applications of the free integro-differential algebra—will also make sense without the assumption of commutativity. In fact, the noncommutative standard example is the (real or complex) *matrix algebra* $R = C^\infty(\mathbb{R})^{n\times n}$, and this forms the basis for two-point (and more general) boundary problems for linear systems of ordinary differential equations. Hence we may think of the (noncommutative) free object as the substrate for adjoining matrix functions and manipulating systems of integro-differential equations (the usual situation of the Picard-Lindelöf theorem).

This can immediately be generalized. The *matrix functor* assigns to an arbitrary (commutative or noncommutative) integro-differential algebra (R, d, P) the (necessarily noncommutative) integro-differential algebra $(R^{n\times n}, \bar{d}, \bar{P})$ whose derivation $\bar{d}$ and Rota-Baxter operator $\bar{P}$ are defined coordinatewise; the same is true for the transport of morphisms from $R \to S$ to $R^{n\times n} \to S^{n\times n}$.

Another familiar functor from the category of integro-differential algebras to itself is given by the construction of *noncommutative polynomials* $R\langle x_1, \ldots, x_k\rangle$ over a commutative integro-differential algebra (R, d, P), where the $x_1, \ldots, x_k$ are assumed to commute with the coefficients in R but not amongst themselves. The derivation and Rota-Baxter operator, as well as the transport of morphisms, are defined coefficientwise.

The construction of $R\langle x_1, \ldots, x_k\rangle$ models some extensions of a commutative integro-differential algebra to a larger noncommutative one: In some cases, the larger algebra will be a quotient of $R\langle x_1, \ldots, x_k\rangle$. A typical case is given by extending $R = C^\infty(\mathbb{R})$ to $R[i, j, k] := R\langle i, j, k\rangle/I$ where I is the ideal generated by the familiar relations $i^2 = j^2 = k^2 = -1$ and $ij = k, jk = i, ki = j$ with their anticommutative counterparts. Obviously $R[i, j, k]$ can be seen as an algebraic model for smooth *quaternion-valued functions* of a real variable. (Finding the right notions of differentiation and integration for functions of a quaternion variable is a far more delicate process, giving rise to the *quaternion calculus* [15]. It would be interesting to investigate this in the frame of noncommutative integro-differential algebras but this is beyond the scope of the current paper.)

Finally, let us mention a potential application in combinatorics: In *species theory* [2], the usage of derivations and so-called combinatorial differential equations [27] is well-established. Algebraically, the isomorphism classes of species form a differential semiring that can be extended to a differential ring by introducing so-called virtual species. Using the more restricted setting of linear species, it is also possible to introduce an integral operator [2, 28], thus endowing the class of virtual linear species with the structure of an integro-differential ring. Since species can be extended to a noncommutative setting [14], it would be interesting to see how an integro-differential structure can be set up in this case.

1.3. **Structure of the Paper.** In this paper we construct free integro-differential algebras. This construction, built on an earlier construction of free differential Rota-Baxter algebras [21], is obtained by applying the method of Gröbner bases or Gröbner-Shirshov bases. The method has its origin in the works of Buchberger [12], Hironaka [25], Shirshov [32] and Zhukov [33]. Even though it has been fundamental for many years in commutative algebra, associative algebra, algebraic geometry and computational algebra [3, 4]. It has only recently shown how comprehensive the method of Gröbner-Shirshov bases can be, through the large number of algebraic structures that the method has been successfully applied to. See [5, 6, 8, 11] for further details. The method is especially useful in constructing free objects in various categories, including the alternative constructions of free Rota-Baxter algebras and free differential Rota-Baxter algebras [7, 9]. In the recent paper [18], this method is applied to construct the free commutative integro-differential algebras.

The layout of the paper is as follows. In *Section 2*, we give the definition of integro-differential algebra and summarize the construction of free differential Rota-Baxter algebras as a preparation for the construction of free (noncommutative) integro-differential algebras. In *Section 3*, we set up a weakly monomial order on differential Rota-Baxter monomials of order n. In *Section 4*, we prove the Composition-Diamond Lemma for free differential Rota-Baxter algebras of order n. In *Section 5*, we prove that the differential Rota-Baxter ideal of the free differential Rota-Baxter algebra that defines the relations for free integro-differential algebras possesses a Gröbner-Shirshov basis. Therefore we can apply the Composition-Diamond Lemma to obtain a canonical basis, identified as the set of functional monomials, for the free integro-differential algebra of order n. We then show that the order n pieces form a direct system whose functional monomials accumulate to a canonical basis of the free integro-differential algebra on a finite set X. Finally, we prove that for an arbitrary set X, the inclusions of the finite subsets of X into X also preserve the functional monomials, which allows us to take their union as a canonical basis of the free integro-differential algebra on X.

2. Free integro-differential algebras

We recall the definitions of algebras with various differential and integral operators and the constructions of the free objects in the corresponding categories. See [17, 22] for further details and examples.

2.1. **The definitions.** We recall the algebraic structures considered in this paper. We also introduce variations with bounded derivation order that will be needed later. Algebras considered in this paper are assumed to be unitary, unless specified otherwise.

Definition 2.1. Let $\mathbf{k}$ be a unitary commutative ring. Let $\lambda \in \mathbf{k}$ be fixed.

(a) A **differential k-algebra of weight λ** (also called a **λ-differential k-algebra**) is an associative $\mathbf{k}$-algebra R together with a linear operator $d\colon R \to R$ such that

$$d(1) = 0,\ d(uv) = d(u)v + ud(v) + \lambda d(u)d(v) \text{ for all } u, v \in R. \tag{1}$$

(b) A **Rota-Baxter k-algebra of weight λ** is an associative $\mathbf{k}$-algebra R together with a linear operator $P\colon R \to R$ such that

$$P(u)P(v) = P(uP(v)) + P(P(u)v) + \lambda P(uv) \text{ for all } u, v \in R. \tag{2}$$

(c) A **differential Rota-Baxter k-algebra of weight λ** (also called a **λ-differential Rota-Baxter k-algebra**) is a differential $\mathbf{k}$-algebra (R, d) of weight λ and a Rota-Baxter operator P of weight λ such that

$$d \circ P = \mathrm{id}. \tag{3}$$

(d) An **integro-differential k-algebra of weight λ** (also called a **λ-integro-differential k-algebra**) is a differential $\mathbf{k}$-algebra (R, d) of weight λ with a linear operator $P\colon R \to R$ that satisfies Eq. (3) and such that

$$\begin{aligned} P(d(u)P(v)) &= uP(v) - P(uv) - \lambda P(d(u)v) \text{ for all } u, v \in R,\\ P(P(u)d(v)) &= P(u)v - P(uv) - \lambda P(ud(v)) \text{ for all } u, v \in R. \end{aligned} \tag{4}$$

Eqs. (2), (3) and (4) are called the **Rota-Baxter axiom**, **section axiom** and **integration by parts axiom**, respectively. See [22] for the equivalent conditions for the integration by parts axiom in various forms.

2.2. **Free differential algebras.** We first recall the construction of free differential algebras and introduce their order n variations. For a set Y, let $M(Y)$ be the free monoid on Y with identity 1, and let $S(Y)$ be the free semigroup on Y. Thus elements in $M(Y)$ are words, plus the identity 1, from the alphabet set Y. Further the noncommutative polynomial algebra $\mathbf{k}\langle Y\rangle$ on Y is the semigroup algebra $\mathbf{k}M(Y)$.

Theorem 2.2. (a) *Let Y be a set with a map $d_0\colon Y \to Y$. Extend d_0 to $d\colon \mathbf{k}\langle Y\rangle \to \mathbf{k}\langle Y\rangle$ as follows. Let $w = u_1 \cdots u_k, u_i \in Y, 1 \leq i \leq k$, be a word from the alphabet set Y. Recursively define*

$$d(w) = d_0(u_1)u_2 \cdots u_k + u_1 d(u_2 \cdots u_k) + \lambda d_0(u_1) d(u_2 \cdots u_k). \tag{5}$$

Explicitly, we have

$$d(w) = \sum_{\emptyset \neq I \subseteq [k]} \lambda^{|I|-1} d_I(u_1) \cdots d_I(u_k), \quad d_I(u_i) := d_{w,I}(u_i) = \begin{cases} d(u_i), & i \in I,\\ u_i, & i \notin I. \end{cases} \tag{6}$$

Further define $d(1) = 0$ and then extend d to $\mathbf{k}\langle Y\rangle$ by linearity. Then $(\mathbf{k}\langle Y\rangle, d)$ is a differential algebra of weight λ.

(b) *Let X be a set. Let $Y := \Delta X := \{x^{(n)} \mid x \in X, n \geq 0\}$ with the map $d_0\colon \Delta X \to \Delta X, x^{(n)} \mapsto x^{(n+1)}$. Then with the extension d of d_0 as in Eq. (5), $(\mathbf{k}\langle \Delta X\rangle, d)$ is the free differential algebra of weight λ on the set X.*

(c) *For a given $n \geq 1$, let $\Delta X^{(n+1)} := \left\{x^{(k)} \,\middle|\, x \in X, k \geq n+1\right\}$. Then $\mathbf{k}\langle \Delta X\rangle \Delta X^{(n+1)} \mathbf{k}\langle \Delta X\rangle$ is the differential ideal I_n of $\mathbf{k}\langle \Delta X\rangle$ generated by the set $\{x^{(n+1)} \mid x \in X\}$. The quotient differential algebra $\mathbf{k}\langle \Delta X\rangle / I_n$ is of order n and has a canonical basis given by*

$$\Delta_n X := \{x^{(k)} \mid x \in X, k \leq n\},$$

thus giving a differential algebra isomorphism $\mathbf{k}\langle \Delta X\rangle / I_n \cong \mathbf{k}\langle \Delta_n X\rangle$*, called the* **differential polynomial algebra of order** n*. Here the differential structure on the later algebra is given by*

$$d(x^{(i)}) = \begin{cases} x^{(i+1)}, & 1 \leq i \leq n-1, \\ 0, & i = n. \end{cases}$$

Proof. Item (a) is a generalization of Item (b) from [21] and can be proved in the same way. Item (c) is a direct consequence of Item (b). □

2.3. **Free operated algebras.** We now recall the construction of the free operated algebra on a set X that has the free (differential) Rota-Baxter algebra as a quotient [9, 19, 20, 23]. At the same time, the explicit construction of free Rota-Baxter algebras and free differential Rota-Baxter algebras in Theorem 2.5 can be realized on a submodule of the free operated algebra spanned by reduced words under a rewriting rule defined by the Rota-Baxter axiom.

Definition 2.3. An **operated monoid (resp. k-algebra) with operator set** Ω is a monoid (resp. $\mathbf{k}$-algebra) G together with maps $\alpha_\omega \colon G \to G, \omega \in \Omega$. A homomorphism between operated monoids (resp. $\mathbf{k}$-algebras) $(G, \{\alpha_\omega\}_\omega)$ and $(H, \{\beta_\omega\}_\omega)$ is a monoid (resp. $\mathbf{k}$-algebra) homomorphism $f \colon G \to H$ such that $f \circ \alpha_\omega = \beta_\omega \circ f$ for $\omega \in \Omega$.

We next construct the free objects in the category of operated monoids.

Fix a set Y. We define monoids $\mathfrak{M}_{\Omega,n} := \mathfrak{M}_{\Omega,n}(Y)$ for $n \geq 0$ by the following recursion. We use the notation $\sqcup$ for disjoint union.

First denote $\mathfrak{M}_{\Omega,0} := M(Y)$. Let $\lfloor M(Y)\rfloor_\omega := \{\lfloor u\rfloor_\omega \,|\, u \in M(Y)\}, \omega \in \Omega$, be disjoint sets in bijection with and disjoint from $M(Y)$. Then define

$$\mathfrak{M}_{\Omega,1} := M(Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor M(Y)\rfloor_\omega)).$$

Note that elements in $\lfloor M(Y)\rfloor_\omega$ are only symbols indexed by elements in $M(Y)$. For example, $\lfloor 1\rfloor_\omega$ is not the identity, but a new symbol. The inclusion $Y \hookrightarrow Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor \mathfrak{M}_{\Omega,0}\rfloor_\omega)$ induces a monomorphism $i_{0,1} \colon \mathfrak{M}_{\Omega,0} = M(Y) \hookrightarrow \mathfrak{M}_{\Omega,1} = M(Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor \mathfrak{M}_{\Omega,0}\rfloor_\omega))$ of free monoids through which we identify $\mathfrak{M}_{\Omega,0}$ with its image in $\mathfrak{M}_{\Omega,1}$. Inductively assume that $\mathfrak{M}_{\Omega,m-1}$ has been defined for $m \geq 2$ and that the embedding

$$i_{m-2,m-1} \colon \mathfrak{M}_{\Omega,m-2} \hookrightarrow \mathfrak{M}_{\Omega,m-1}$$

has been obtained. We then define

$$\mathfrak{M}_{\Omega,m} := M(Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor \mathfrak{M}_{\Omega,m-1}\rfloor_\omega)).$$

We also have the injection

$$\lfloor \mathfrak{M}_{\Omega,m-2}\rfloor_\omega \hookrightarrow \lfloor \mathfrak{M}_{\Omega,m-1}\rfloor_\omega, \;\; \omega \in \Omega.$$

Thus by the freeness of $\mathfrak{M}_{\Omega,m-1} = M(Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor \mathfrak{M}_{\Omega,m-2}\rfloor_\omega))$ as a free commutative monoid, we have

$$\mathfrak{M}_{\Omega,m-1} = M(Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor \mathfrak{M}_{\Omega,m-2}\rfloor_\omega)) \hookrightarrow M(Y \sqcup (\sqcup_{\omega\in\Omega} \lfloor \mathfrak{M}_{\Omega,m-1}\rfloor_\omega)) = \mathfrak{M}_{\Omega,m}.$$

We finally define the monoid

$$\mathfrak{M}_\Omega(Y) := \bigcup_{m\geq 0} \mathfrak{M}_{\Omega,m} = \varinjlim \mathfrak{M}_{\Omega,m}.$$

When Ω is a singleton, the subscript Ω will be suppressed. Elements in $\mathfrak{M}_\Omega(Y)$ are called **bracketed monomials** in Y. Defining

$$\lfloor\ \rfloor_\omega\colon \mathfrak{M}_\Omega(Y)\to\mathfrak{M}_\Omega(Y), u\mapsto \lfloor u\rfloor_\omega,\ \omega\in\Omega,$$

then $(\mathfrak{M}_\Omega(Y),\{\lfloor\ \rfloor_\omega\}_{\omega\in\Omega})$ is an operated monoid and its linear span $(\mathbf{k}\mathfrak{M}_\Omega(Y),\lfloor\ \rfloor_{\omega\in\Omega})$ is an operated $\mathbf{k}$-algebra.

Proposition 2.4. ([19]) *Let $j_Y\colon Y\hookrightarrow \mathfrak{M}_\Omega(Y)$ denote the natural embedding. Then the triple $(\mathbf{k}\mathfrak{M}_\Omega(Y),\{\lfloor\ \rfloor_\omega\}_\omega, j_Y)$ is the free operated $\mathbf{k}$-algebra on Y. More precisely, for any operated $\mathbf{k}$-algebra R and any set map $f\colon Y\to R$, there is a unique extension of f to a homomorphism $\overline{f}\colon \mathbf{k}\mathfrak{M}_\Omega(Y)\to R$ of operated $\mathbf{k}$-algebras.*

2.4. **The construction of free Rota-Baxter algebras.** Consider $\mathfrak{M}_\Omega(Y)$ with $\Omega=\{\omega\}$ being a singleton. Denote $P(u):=\lfloor u\rfloor:=\lfloor u\rfloor_\omega, u\in\mathfrak{M}(Y)$. For a nonempty set Y and nonempty subsets U and V of $\mathfrak{M}(Y)$, define the **alternating products of** U **and** V to be the following subsets of $\mathfrak{M}(Y)$

$$\Lambda(U,V):=\left(\bigcup_{r\geq 0}(UP(V))^rU\right)\bigcup\left(\bigcup_{r\geq 1}(UP(V))^r\right)\bigcup\left(\bigcup_{r\geq 0}(P(V)U)^rP(V)\right)\bigcup\left(\bigcup_{r\geq 1}(P(V)U)^r\right). \tag{7}$$

With these notations, define $\Lambda_0(Y)=M(Y)$ to be the free monoid on Y and, for $m\geq 1$, define

$$\Lambda_m(Y)=\Lambda(S(Y),\Lambda_{m-1}(Y))\cup\{1\}.$$

Then $\Lambda_m(Y), m\geq 0$, define an increasing sequence and we define the set of **Rota-Baxter words** to be

$$\mathcal{R}(Y):=\Lambda_\infty(Y):=\cup_{m\geq 0}\Lambda_m(Y).$$

Each $1\neq u\in\mathcal{R}(Y)$ can be uniquely expressed as $u=u_1\cdots u_m$, where $u_1,\cdots,u_m$ are alternately in $S(Y)$ and $P(\mathcal{R}(Y))$. The **depth** $\operatorname{dep}(u)$ of u is defined to be the least $m\geq 0$ such that u is contained in $\Lambda_m(Y)$. Define

$$P_Y\colon \mathcal{R}(Y)\to\mathcal{R}(Y),\quad u\mapsto\lfloor u\rfloor,\quad u\in\mathcal{R}(Y).$$

Let $I_{\rm RB}(Y)$ denote the operated ideal of $\mathbf{k}\mathfrak{M}(Y)$ generated by elements of the form

$$\lfloor u\rfloor\lfloor v\rfloor-\lfloor u\lfloor v\rfloor\rfloor-\lfloor\lfloor u\rfloor v\rfloor-\lambda\lfloor uv\rfloor,\quad u,v\in\mathbf{k}\mathfrak{M}(Y).$$

By [16, 20] where $\mathbf{k}\mathcal{R}(Y)$ is denoted by $Ш^{NC}(Y)$, the composition

$$\mathbf{k}\mathcal{R}(Y)\to\mathbf{k}\mathfrak{M}(Y)\to\mathbf{k}\mathfrak{M}(Y)/I_{\rm RB}(Y) \tag{8}$$

is a bijection. Hence (the coset representatives of) the words in $\mathcal{R}(Y)$ form a linear basis of the free Rota-Baxter algebra on Y. Further, write

$$\operatorname{Red}:=\alpha\circ\eta\colon \mathbf{k}\mathfrak{M}(Y)\to\mathbf{k}\mathfrak{M}(Y)/I_{\rm RB}(Y)\to\mathbf{k}\mathcal{R}(Y), \tag{9}$$

where $\eta:\mathbf{k}\mathfrak{M}(Y)\to\mathbf{k}\mathfrak{M}(Y)/I_{\rm RB}$ is the quotient map and $\alpha:\mathbf{k}\mathfrak{M}(Y)/I_{\rm RB}\to\mathbf{k}\mathcal{R}(Y)$ is the inverse of the linear bijection in Eq. (8).

Define a product $\diamond$ on $\mathbf{k}\mathcal{R}(Y)$ as follows. Let $u=u_1u_2\cdots u_s$ and $v=v_1v_2\cdots v_t$ be two Rota-Baxter words, where u_i for $1\leq i\leq s$ and v_j for $1\leq j\leq t$ are alternately in $S(Y)$ and $\lfloor\mathcal{R}(Y)\rfloor$.

(a) If $s=t=1$ and hence $u,v\in S(Y)\cup\lfloor\mathcal{R}(Y)\rfloor$, then define

$$u\diamond v:=\begin{cases} uv, & u \text{ or } v\in S(Y),\\ \operatorname{Red}(\lfloor\tilde{u}\rfloor\lfloor\tilde{v}\rfloor)=\operatorname{Red}(\lfloor B(\tilde{u},\tilde{v})\rfloor)=\lfloor\operatorname{Red}(B(\tilde{u},\tilde{v}))\rfloor, & u=\lfloor\tilde{u}\rfloor, v=\lfloor\tilde{v}\rfloor\in\lfloor\mathcal{R}(Y)\rfloor,\end{cases} \tag{10}$$

where $B(\tilde{u},\tilde{v})=\tilde{u}\lfloor\tilde{v}\rfloor+\lfloor\tilde{u}\rfloor\tilde{v}+\lambda\tilde{u}\,\tilde{v}$.

(b) If $s > 1$ or $t > 1$, then define

$$u\diamond v := u_1u_2\cdots(u_s\diamond v_1)v_2\cdots v_t,$$

where $u_s\diamond v_1$ is defined by Eq. (10) and the remaining products are given by concatenation together with $\mathbf{k}$-linearity when $u_s\diamond v_1$ is a linear combination.

We call $\mathcal{R}(\Delta X)$ the set of **differential Rota-Baxter (DRB) monomials** on X.

Theorem 2.5. (a) ([16]) *Let Y be a set. Then $(\mathbf{k}\mathcal{R}(Y), \diamond, P_Y)$ is the free Rota-Baxter algebra on Y.*

(b) ([21]) *Let X be a set and $(\mathbf{k}\langle\Delta X\rangle, d)$ the differential algebra of weight λ on X in Theorem 2.2.(b). There is a unique extension $d_{\Delta X}$ of d to $\mathbf{k}\mathcal{R}(\Delta X)$ such that $(\mathbf{k}\mathcal{R}(\Delta X), d_{\Delta X}, P_{\Delta X})$, together with $j_X\colon \mathbf{k}\langle\Delta X\rangle \hookrightarrow \mathbf{k}\mathcal{R}(\Delta X)$, is the free differential Rota-Baxter $\mathbf{k}$-algebra of weight λ on the differential algebra $\mathbf{k}\langle\Delta X\rangle$.*

In the same fashion, one obtains $\mathcal{R}(\Delta_n X))$, called the set of **DRB monomials of order** n on X, as a basis of $\mathbf{k}\mathcal{R}(\Delta_n X)$ by applying (a) to $Y := \Delta_n X, n \geq 1$. We note that in $\mathbf{k}\mathcal{R}(\Delta_n X)$, the property $d^{n+1}(u) = 0$ only applies to $u \in X$. For example, taking $n = 2$, then $d^2(x) = 0$. But $d(\lfloor x\rfloor) = x$ and hence $d^2(\lfloor x\rfloor) = d(x) = x^{(1)} \neq 0$.

2.5. **Free integro-differential algebras.** By the universal property of $\mathbf{k}\mathfrak{M}(Y)$, we obtain the following conclusion from general principles of universal algebra [1, 13].

Proposition 2.6. *Let X be a set. Let $\Omega = \{d, P\}$ and denote $d(u) := \lfloor u\rfloor_d, P(u) := \lfloor u\rfloor_P$. Let $J_{\rm ID} = J_{{\rm ID},X}$ be the operated ideal of $\mathbf{k}\mathfrak{M}_\Omega(X)$ generated by the set*

$$\left\{\begin{array}{l} d(uv) - d(u)v - ud(v) - \lambda d(u)d(v),\\ d(1),\\ (d\circ P)(u) - u,\\ P(d(u)P(v)) - uP(v) + P(uv) + \lambda P(d(u)v),\\ P(P(u)d(v)) - P(u)v + P(uv) + \lambda P(ud(v)) \end{array}\middle|\ u, v \in \mathfrak{M}_\Omega(X)\right\}.$$

Then the quotient operated algebra $\mathbf{k}\mathfrak{M}_\Omega(X)/J_{\rm ID}$, with the quotient of the operator d and P, is the free integro-differential algebra on X.

Our main purpose in this paper is to give an explicit construction of the free integro-differential algebra by determining a canonical subset of $\mathfrak{M}_\Omega(X)$. The construction is given in Theorem 5.15.

We will achieve this construction in several steps. First let $J_{\rm DRB} = J_{{\rm DRB},X}$ denote the operated ideal of $\mathbf{k}\mathfrak{M}_\Omega(X)$ generated by the set

$$\left\{\begin{array}{l} d(uv) - d(u)v - ud(v) - \lambda d(u)d(v),\\ d(1),\\ (d\circ P)(u) - u,\\ P(u)P(v) - P(uP(v)) - P(P(u)v) - \lambda P(uv) \end{array}\middle|\ u, v \in \mathfrak{M}_\Omega(X)\right\}.$$

Then the quotient operated algebra $\mathbf{k}\mathfrak{M}_\Omega(X)/J_{\rm DRB}$, with the quotient operators d and P, is the free differential Rota-Baxter algebra on X. Its explicit construction is given in [21] and recalled in Theorem 2.5:

$$\mathbf{k}\mathfrak{M}_\Omega(X)/J_{\rm DRB} \cong \mathbf{k}\mathcal{R}(\Delta X),$$

as the free Rota-Baxter algebra on the free differential algebra $\mathbf{k}\langle\Delta X\rangle$ on X.

Let $I_{\rm ID}$ denote the image of $J_{\rm ID}$ under the quotient map $\mathbf{k}\mathfrak{M}_\Omega(X) \to \mathbf{k}\mathcal{R}(\Delta X)$, then we have

$$\mathbf{k}\mathfrak{M}_\Omega(X)/J_{\rm ID} \cong \mathbf{k}\mathcal{R}(\Delta X)/I_{\rm ID}.$$

Further, $I_{\rm ID}$ is the differential Rota-Baxter ideal of $\mathcal{R}(\Delta X)$ generated by the set

$$\left\{ \begin{array}{l} P(d(u)P(v)) - uP(v) + P(uv) + \lambda P(d(u)v), \\ P(P(u)d(v)) - P(u)v + P(uv) + \lambda P(ud(v)) \end{array} \;\middle|\; u, v \in \mathcal{R}(\Delta X) \right\}.$$

Thus to obtain an explicit construction of the free integro-differential algebra $\mathbf{k}\mathfrak{M}_\Omega(X)/J_{\rm ID}$ by providing a canonical subset of $\mathfrak{M}_\Omega(X)$ as a basis (of coset representatives) of the quotient, we just need to determine a canonical subset of $\mathcal{R}(\Delta X)$ as a basis of the quotient $\mathbf{k}\mathcal{R}(\Delta X)/I_{\rm ID}$.

However, in order to apply the Gröbner-Shirshov basis method, we need a monomial (well) order on $\mathcal{R}(\Delta X)$ which is easily seen to be nonexistent: Suppose $x > P(x)$, then we have $x > P(x) > \cdots > P^n(x) > \cdots$ leading to an infinite descending chain. Suppose $P(x) > x$, then we have $x > d(x)$, again leading to an infinite descending chain $x > d(x) \cdots > x^{(n)} > \cdots$. To overcome this difficulty, we consider, for each $n \geq 1$, the free Rota-Baxter algebra $\mathbf{k}\mathcal{R}(\Delta_n X)$ on the truncated differential algebra $\mathbf{k}[\Delta_n X]$ in Theorem 2.2.(c) and construct an explicit basis of the quotient $\mathbf{k}\mathcal{R}(\Delta_n X)/I_{{\rm ID},n}$ where $I_{{\rm ID},n}$ is the differential Rota-Baxter ideal of the Rota-Baxter algebra $\mathbf{k}\mathcal{R}(\Delta_n X)$ generated by the set

$$\left\{ \begin{array}{l} \phi_1(u,v) := P(d(u)P(v)) - uP(v) + P(uv) + \lambda P(d(u)v), \\ \phi_2(u,v) := P(P(u)d(v)) - P(u)v + P(uv) + \lambda P(ud(v)) \end{array} \;\middle|\; u, v \in \mathcal{R}(\Delta_n X) \right\}. \tag{11}$$

Then as n goes to infinity, the above explicit basis will give the desired basis of $\mathbf{k}\mathcal{R}(\Delta X)/I_{\rm ID}$ and hence of $\mathbf{k}\mathfrak{M}_\Omega(X)/J_{\rm ID}$. See the proof of Theorem 5.15 for details of this last step.

3. Weakly monomial order

Write $\mathcal{R}_n := \mathcal{R}(\Delta_n X)$.

Definition 3.1. Let X be a set, $\star$ a symbol not in X and $\Delta_n X^\star := \Delta_n(X \cup \{\star\})$.

(a) By a **$\star$-DRB monomial on** $\Delta_n X$, we mean any expression in $\mathcal{R}(\Delta_n X^\star)$ with exactly one occurrence of $\star$. The set of all $\star$-DRB monomials on $\Delta_n X$ is denoted by $\mathcal{R}_n^\star$.

(b) For $q \in \mathcal{R}_n^\star$ and $u \in \mathcal{R}_n$, we define

$$q|_u := q|_{\star \mapsto u}$$

to be the bracketed monomial in $\mathfrak{M}(\Delta_n X)$ obtained by replacing the letter $\star$ in q by u, and call $q|_u$ a **u-monomial on** $\Delta_n X$.

(c) For $s = \sum_i c_i u_i \in \mathbf{k}\mathcal{R}_n$, where $c_i \in \mathbf{k}$, $u_i \in \mathcal{R}_n$ and $q \in \mathcal{R}_n^\star$, we define

$$q|_s := \sum_i c_i q|_{u_i},$$

which is in $\mathbf{k}\mathfrak{M}(\Delta_n X)$. We call $q|_s$ an **s-monomial** on $\Delta_n X$. This applies in particular when s is a monomial.

We note that a $\star$-DRB monomial q is a DRB monomial in $\Delta_n X^\star$ while the u-monomial $q|_u$ might not be a DRB monomial. For example, for $q = P(x)\star \in \mathcal{R}_n^\star$ and $u = P(x) \in \mathcal{R}_n$ where $x \in X$, the u-monomial $q|_u = P(x)P(x)$ is no longer in $\mathcal{R}_n$.

Lemma 3.2. *Let S be a subset of $\mathbf{k}\mathcal{R}_n$ and* Id(S) *be the differential Rota-Baxter ideal of $\mathbf{k}\mathcal{R}_n$ generated by S. Then*

$$\mathrm{Id}(S) = \left\{ \sum_i c_i q_i|_{s_i} \;\middle|\; c_i \in \mathbf{k}, q_i \in \mathcal{R}_n^\star, s_i \in S \right\}.$$

Proof. It is easy to see that the right hand side is contained in the left side. On the other hand, the right hand side is already an operated ideal of $\mathbf{k}\mathcal{R}_n$ containing S. □

Definition 3.3. If $q = p|_{d^\ell(\star)}$ for some $p \in \mathcal{R}^\star(\Delta_n X)$ and $\ell \in \mathbb{Z}_{\geq 1}$, then we call q a **type I $\star$-DRB monomial**. Let $\mathcal{R}^\star_{n,\mathrm{I}}$ denote the set of type I $\star$-DRB monomials on $\Delta_n X$ and call

$$\mathcal{R}^\star_{n,\mathrm{II}} := \mathcal{R}^\star_n \setminus \mathcal{R}^\star_{n,\mathrm{I}}$$

the set of **type II $\star$-DRB monomials**.

Definition 3.4. Let $<$ be a linear order on $\mathcal{R}(\Delta_n X)$, $q \in \mathcal{R}^\star_n$ and $s \in \mathbf{k}\mathcal{R}_n$.

(a) For any $0 \neq f \in \mathbf{k}\mathcal{R}_n$, let $\overline{f}$ denote the leading term of f: $f = c\overline{f} + \sum_i c_i u_i$, where $0 \neq c, c_i \in \mathbf{k}$, $u_i \in \mathcal{R}_n$, $u_i < \overline{f}$. Furthermore, f is called **monic** if $c = 1$.

(b) Write

$$\overline{q|_s} := \overline{\mathrm{Red}(q|_s)},$$

where $\mathrm{Red}\colon \mathbf{k}\mathfrak{M}(\Delta_n X) \to \mathbf{k}\mathcal{R}_n$ is the reduction map in Eq. (9).

(c) The element $q|_s \in \mathbf{k}\mathcal{R}_n$ is called **normal** if $q|_{\overline{s}}$ is in $\mathcal{R}_n$. In other words, if $\mathrm{Red}(q|_{\overline{s}}) = q|_{\overline{s}}$.

Remark 3.5. (a) By definition, $q|_s$ is normal if and only if $q|_{\overline{s}}$ is normal if and only if the $\overline{s}$-DRB monomial $q|_{\overline{s}}$ is already a DRB monomial, that is, no further reduction in $\mathbf{k}\mathcal{R}_n$ is possible.

(b) Examples of not normal (abnormal) s-DRB monomials are

(i) $q = \star P(x)$ and $\overline{s} = P(x)$, giving $q|_s = P(x)P(x)$, which is reduced to $P(xP(y)) + P(P(x)y) + \lambda P(xy)$ in $\mathbf{k}\mathcal{R}_n$;

(ii) $q = d(\star)$ and $\overline{s} = P(x)$, giving $q|_{\overline{s}} = d(P(x))$, which is reduced to x in $\mathbf{k}\mathcal{R}_n$;

(iii) $q = d(\star)$ and $\overline{s} = x^2$, giving $q|_{\overline{s}} = d(x^2)$, which is reduced to $2xx^{(1)} + \lambda(x^{(1)})^2$ in $\mathbf{k}\mathcal{R}_n$;

(iv) $q = d^n(\star)$ and $\overline{s} = d(x)$, giving $q|_{\overline{s}} = d^{n+1}(s)$, which is reduced to 0 in $\mathbf{k}\mathcal{R}_n$.

Definition 3.6. A **weakly monomial order** on $\mathcal{R}_n$ is a well order $<$ satisfying

$$u < v \Rightarrow \overline{q|_u} < \overline{q|_v} \text{ if either } q \in \mathcal{R}^\star_{n,\mathrm{II}}, \text{ or } q \in \mathcal{R}^\star_{n,\mathrm{I}} \text{ and } q|_v \text{ is normal}$$

for $u, v \in \mathcal{R}_n$.

Let X be a well-ordered set. Let $n \geq 0$ be given. First, we extend the order on X to ΔX and $\Delta_n X$. For $x_0^{(i_0)}, x_1^{(i_1)} \in \Delta X$ (resp. $\Delta_n X$) with $x_0, x_1 \in X$, define

$$x_0^{(i_0)} < x_1^{(i_1)} \left(\text{resp. } x_0^{(i_0)} <_n x_1^{(i_1)}\right) \Leftrightarrow (x_0, -i_0) < (x_1, -i_1) \quad \text{lexicographically.} \tag{12}$$

For example $x^{(2)} < x^{(1)} < x$. Also, $x_1 < x_2$ implies $x_1^{(2)} < x_2^{(2)}$. Then by [1], the order $<_n$ is a well order on $\Delta_n X$. Next, we extend the well order on $\Delta_n X$ to a weakly monomial order on $\mathcal{R}_n$.

We adapt the order defined in [7] to the case when the set is taken to be $\Delta_n X$ and when the order is restricted to $\mathcal{R}_n$. For any $u \in \mathcal{R}_n$ and for a set $T \subseteq \Delta_n X \cup \{P\}$, denote by $\deg_T(u)$ the number of occurrences of $t \in T$ in u. Let

$$\deg(u) = (\deg_{P \cup \Delta_n X}(u), \deg_P(u)).$$

We order $\deg(u)$ lexicographically. If $u \in \Delta_n X \cup P(\mathcal{R}_n)$, then u is called **indecomposable**. For any $u \in \mathcal{R}_n$, u has a **standard form:**

$$u = u_0 \cdots u_k, \text{ where } u_0, \cdots, u_k \text{ are indecomposable.} \tag{13}$$

Now we set up an order $<_n$ on $\mathcal{R}_n$ as follows. Let $u, v \in \mathcal{R}_n$. If $\deg(u) < \deg(v)$, then $u <_n v$. If $\deg(u) = \deg(v) = (m_1, m_2)$, then we define $u <_n v$ by induction on (m_1, m_2) which is at least

$(1,0)$. If $(m_1,m_2)=(1,0)$, that is, $u,v\in\Delta_nX$, we use the order in Eq (12). Let $(m_1,m_2)>(1,0)$ be given, and assume the order is defined for all $(m_1',m_2')<(m_1,m_2)$ and consider u,v with $\deg(u)=\deg(v)=(m_1,m_2)$. If $u,v\in P(\mathcal{R}_n)$, say $u=P(\tilde{u})$ and $v=P(\tilde{v})$, then define $u<_n v$ if and only if $\tilde{u}<_n\tilde{v}$ where the latter is defined by the induction hypothesis. Otherwise, let $u=u_0\cdots u_k$ and $v=v_0\cdots v_\ell$ be the standard forms with $k>0$ or $\ell>0$. Then define $u<_n v$ if and only if $(u_0,\cdots,u_k)<(v_0,\cdots,v_\ell)$ lexicographically. Here the latter is again defined by the induction hypothesis.

We next show that the order $<_n$ defined above is a weakly monomial order on $\mathcal{R}_n$. Recall the following lemma from [7] on $\mathcal{R}(X)$ which still applies when it is restricted to $\mathcal{R}_n$.

Lemma 3.7. *([7] Lemma 3.3) If $u<_n v$ with $u,v\in\mathcal{R}_n$, then $\overline{uw}<_n\overline{vw}$ and $\overline{wu}<_n\overline{wv}$ for any $w\in\mathcal{R}_n$.*

Lemma 3.8. *Let $\ell\geq 1$ and $s\in\mathcal{R}_n$. Then $d^\ell(\star)|_s$ is normal if and only if $s\in\Delta_{n-\ell}X$.*

Proof. If $s\in\Delta_{n-\ell}X$, then $d^\ell(s)$ is in Δ_nX and hence $d^\ell(\star)|_s$ is normal. Conversely, if $s\notin\Delta_{n-\ell}X$, then either $s\notin\Delta_nX$ or $s\in\Delta_nX\setminus\Delta_{n-\ell}X$. In both cases we have that $d^\ell(\star)|_s$ is not normal. See Remark 3.5. □

Lemma 3.9. *Let $u,v\in\mathcal{R}_n$ and $\ell\in\mathbb{Z}_{\geq 1}$. If $u<_n v$ and $d^\ell(\star)|_v$ is normal, then $\overline{d^\ell(u)}<_n\overline{d^\ell(v)}$.*

Proof. We prove the result by induction on ℓ. We first consider $\ell=1$ and prove $\overline{d(u)}<_n\overline{d(v)}$. Since $d(\star)|_v$ is normal, we have $v=x_1^{(i_1)}\in\Delta_{n-1}X$ by Lemma 3.8. Since $u<_n v$, by the definition of $<_n$, we have $u=x_2^{(i_2)}\in\Delta_nX$ with either $x_2<x_1$ or $x_1=x_2$ and $i_2>i_1$. Hence $\overline{d(u)}<_n\overline{d(v)}$.

Next, suppose the result holds for $1\leq m<\ell$. Then by the induction hypothesis, we have

$$\overline{d^\ell(u)}=\overline{d(d^{\ell-1}(u))}=\overline{d(\overline{d^{\ell-1}(u)})}<_n\overline{d(\overline{d^{\ell-1}(v)})}=\overline{d(d^{\ell-1}(v))}=\overline{d^\ell(v)}.$$

□

Proposition 3.10. *The order $<_n$ is a weakly monomial order on $\mathcal{R}_n$.*

Proof. Let $u,v\in\mathcal{R}_n$ with $u<_n v$ and $q\in\mathcal{R}_n^\star$. Depending on the location of the symbol $\star$, we have the following three cases to consider.

Case 1. Suppose the symbol $\star$ in q is not contained in P or d. Then $q=s\star t$ where $s,t\in\mathcal{R}_n$. This case is covered by Lemma 3.7

Case 2. Suppose the symbol $\star$ is contained in P. Then $q=sP(p)t$ for some $s,t\in\mathcal{R}_n$ and $p\in\mathcal{R}_n^\star$. This case can be verified by induction on $\operatorname{dep}(q)$ and the fact that, for $u,v\in\mathcal{R}_n$, $u<_n v$ implies $P(u)<_n P(v)$ by the definition of $<_n$.

Case 3. The symbol $\star$ is contained in d, that is, $q\in\mathcal{R}_{n,\mathrm{I}}^\star$. Then $q=p|_{d^\ell(\star)}$ for some $p\in\mathcal{R}_n^\star$ and $\ell\in\mathbb{Z}_{\geq 1}$. Take such ℓ maximal so that $p\in\mathcal{R}_{n,\mathrm{II}}^\star$. We need to show that if $u<_n v$ and $q|_v$ is normal, then $\overline{q|_u}<_n\overline{q|_v}$. But if $q|_v$ is normal then $d^\ell(\star)|_v$ is normal. Then by Lemma 3.9, we have $\overline{d^\ell(u)}<_n\overline{d^\ell(v)}$. Then by Cases 1 and 2, we have $\overline{q|_u}=\overline{p|_{\overline{d^\ell(u)}}}<_n\overline{p|_{\overline{d^\ell(v)}}}=\overline{q|_v}$. This completes the proof. □

We shall use the weakly monomial order $<_n$ on $\mathcal{R}_n$ throughout the rest of this paper. The following consequence of Proposition 3.10 will be applied in Section 4.

Lemma 3.11. *Let $q\in\mathcal{R}_n^\star$ and let $s\in\mathbf{k}\mathcal{R}_n$ be monic. If $q|_s$ is normal, then $\overline{q|_s}=q|_{\overline{s}}$.*

Proof. Let $s = \overline{s} + \sum_i c_i s_i$ with $0 \neq c_i \in \mathbf{k}$ and $s_i <_n \overline{s}$. Then $q|_s = q|_{\overline{s}} + \sum_i c_i q|_{s_i}$. Since $q|_s$ is normal, it follows that $q|_{\overline{s}} \in \mathcal{R}_n$ and so $\overline{q|_{\overline{s}}} = q|_{\overline{s}}$. We have the following two cases to consider.

Case 1. $q \in \mathcal{R}^{\star}_{n,\mathrm{II}}$. Then $\overline{q|_{s_i}} <_n \overline{q|_{\overline{s}}} = q|_{\overline{s}}$ by Definition 3.6 and Proposition 3.10. Hence $\overline{q|_s} = \overline{q|_{\overline{s}}} = q|_{\overline{s}}$.

Case 2. $q \in \mathcal{R}^{\star}_{n,\mathrm{I}}$. Since $q|_s$ is mormal, we have $q|_{\overline{s}}$ is normal and so $\overline{q|_{s_i}} < \overline{q|_{\overline{s}}} = q|_{\overline{s}}$ by Definition 3.6 and Proposition 3.10. Hence $\overline{q|_s} = q|_{\overline{s}}$. □

4. Composition-Diamond lemma

In this section, we shall establish the Composition-Diamond lemma for the order n free differential Rota-Baxter algebra $\mathbf{k}\mathcal{R}_n$.

Definition 4.1. Let X be a set, $\star_1$, $\star_2$ two distinct symbols not in X and $\Delta_n X^{\star_1,\star_2} := \Delta_n(X \cup \{\star_1, \star_2\})$.

(a) We define $\mathcal{R}(\Delta_n X^{\star_1,\star_2})$ in the same way as for $\mathcal{R}(\Delta_n X)$ with X replaced by $X \cup \{\star_1, \star_2\}$.

(b) We define a $(\star_1, \star_2)$**-DRB monomial on** $\Delta_n X$ to be an expression in $\mathcal{R}(\Delta_n X^{\star_1,\star_2})$ with exactly one occurrence of $\star_1$ and exactly one occurrence of $\star_2$. The set of all $(\star_1, \star_2)$-DRB monomials on $\Delta_n X$ is denoted by $\mathcal{R}_n^{\star_1,\star_2}$.

(c) For $q \in \mathcal{R}_n^{\star_1,\star_2}$ and $u_1, u_2 \in \mathbf{k}\mathcal{R}_n$, we define

$$q|_{u_1,u_2} := q|_{\star_1 \mapsto u_1, \star_2 \mapsto u_2}$$

to be the bracketed monomial obtained by replacing the letter $\star_1$ (resp. $\star_2$) in q by u_1 (resp. u_2) and call it a (u_1, u_2)**-monomial on** $\Delta_n X$.

(d) The element $q|_{u_1,u_2}$ is called **normal** if $q|_{\overline{u}_1,\overline{u}_2}$ is in $\mathcal{R}_n$. In other words, if $\mathrm{Red}(q|_{\overline{u}_1,\overline{u}_2}) = q|_{\overline{u}_1,\overline{u}_2}$.

A (u_1, u_2)-DRB monomial on $\Delta_n X$ can also be recursively defined by $q|_{u_1,u_2} := (q^{\star_1}|_{u_1})|_{u_2}$, where $q^{\star_1}$ is q when q is regarded as a $\star_1$-DRB monomial on the set $\Delta_n X^{\star_2}$. Then $q^{\star_1}|_{u_1}$ is in $\mathcal{R}^{\star_2}(\Delta_n X)$. Similarly, we have $q|_{u_1,u_2} := (q^{\star_2}|_{u_2})|_{u_1}$.

Definition 4.2. (a) Let $u, w \in \mathcal{R}_n$. We call u a **subword** of w if there is a $q \in \mathcal{R}_n^{\star}$ such that $w = q|_u$.

(b) Let u_1 and u_2 be two subwords of w. Then u_1 and u_2 are called **separated** if $u_1, u_2 \in \mathcal{R}_n$ and there is a $q \in \mathcal{R}^{\star_1,\star_2}(\Delta_n X)$ such that $w = q|_{u_1,u_2}$.

(c) Let $u = u_1 \cdots u_k \in \mathcal{R}_n$ be the standard form. The integer k is called the **breadth** of u and is denoted by $\mathrm{bre}(u)$.

(d) Let $f, g \in \mathcal{R}_n$. A pair (u, v) with $u, v \in \mathcal{R}_n$ is called an **intersection pair** for (f, g) if $w := fu = vg$ or $w := uf = gv$ is a differential Rota-Baxter monomial and satisfies $\max\{\mathrm{bre}(f), \mathrm{bre}(g)\} < \mathrm{bre}(w) < \mathrm{bre}(f) + \mathrm{bre}(g)$. Then we call f and g **overlapping**.

There are three kinds of compositions.

Definition 4.3. Let $f, g \in \mathbf{k}\mathcal{R}_n$ be monic with respect to $<_n$.

(a) If $\overline{f} \in \mathcal{R}_n P(\mathcal{R}_n)$, then define a **composition of right multiplication** to be fu where $u \in P(\mathcal{R}_n)\mathcal{R}_n$. We similarly define a **composition of left multiplication**.

(b) If there is an intersection pair (u, v) for $(\overline{f}, \overline{g})$ with $w := \overline{f}u = v\overline{g}$ (resp. $w := u\overline{f} = \overline{g}v$), then we define

$$(f, g)_w := (f, g)_w^{u,v} := fu - vg \text{ (resp. } uf - gv)$$

and call it an **intersection composition** of f and g.

(c) If there exists a $q \in \mathcal{R}_n^\star$ such that $w := \overline{f} = q|_{\overline{g}}$, then we define $(f,g)_w := (f,g)_w^q := f - q|_g$ and call it an **inclusion composition** of f and g with respect to q. Note that if this is the case, then $q|_g$ is normal.

In the last two cases, $(f,g)_w$ is called the **ambiguity** of the composition.

Definition 4.4. Let $S \subseteq \mathbf{k}\mathcal{R}_n$ be a set of monic differential Rota-Baxter polynomials and $w \in \mathcal{R}_n$.

(a) An element g in $\mathbf{k}\mathcal{R}_n$ is called **trivial modulo** $[S]$ if $g = \sum_i c_i q_i|_{s_i}$, where, for each i, we have $0 \neq c_i \in \mathbf{k}$, $q_i \in \mathcal{R}_n^\star$, $s_i \in S$ such that $q_i|_{s_i}$ is normal and $q_i|_{\overline{s_i}} \leq_n \overline{g}$. If this is the case, we write $g \equiv 0 \bmod [S]$.
(b) The composition of right (resp. left) multiplication fu (resp. uf) is called **trivial modulo** $[S]$ if $fu \equiv 0 \bmod [S]$ (resp. $uf \equiv 0 \bmod [S]$).
(c) For $u, v \in \mathbf{k}\mathcal{R}_n$, we call u and v **congruent modulo** $[S, w]$ and denote this by

$$u \equiv v \bmod [S, w]$$

if $u - v = 0$, or if $u - v = \sum_i c_i q_i|_{s_i}$, where $0 \neq c_i \in \mathbf{k}$, $q_i \in \mathcal{R}_n^\star$, $s_i \in S$ such that $q_i|_{s_i}$ is normal and $q_i|_{\overline{s_i}} <_n w$.
(d) For $f, g \in \mathbf{k}\mathcal{R}_n$ and suitable u, v or q that give an intersection composition $(f,g)_w^{u,v}$ or an including composition $(f,g)_w^q$, the composition is called **trivial modulo** $[S, w]$ if

$$(f,g)_w^{u,v} \text{ or } (f,g)_w^q \equiv 0 \bmod [S, w].$$

(e) The set $S \subseteq \mathbf{k}\mathcal{R}_n$ is a **Gröbner-Shirshov basis** if all compositions of right multiplication and left multiplication are trivial modulo $[S]$, and, for $f, g \in S$, all intersection compositions $(f,g)_w^{u,v}$ and all inclusion compositions $(f,g)_w^q$ are trivial modulo $[S, w]$.

We give some preparatory lemmas before establishing the Composition-Diamond Lemma.

Lemma 4.5. *Let $S \subseteq \mathbf{k}\mathcal{R}_n$ with $d(S) \subseteq S$. If each composition of left multiplication and right multiplication of S is trivial modulo $[S]$, then $q|_s$ is trivial modulo $[S]$ for every $q \in \mathcal{R}_n^\star$ and $s \in S$.*

Proof. We have the following two cases to consider.
Case 1. $q \in \mathcal{R}_{n,\mathrm{II}}^\star$. This case is similar to the proof of Lemma 3.6 in [7].
Case 2. $q \in \mathcal{R}_{n,\mathrm{I}}^\star$. Then $q = p|_{d^\ell(\star)}$ for some $p \in \mathcal{R}_n^\star$ and $\ell \geq 1$. Choose such an ℓ to be maximal so that p is in $\mathcal{R}_{n,\mathrm{II}}^\star$. Since $d(S) \subseteq S$, by Case 1 that has been proved above, the result holds. □

Lemma 4.6. *Let $S \subseteq \mathbf{k}\mathcal{R}_n$ with $d(S) \subseteq S$ be a Gröbner-Shirshov basis. Let $s_1, s_2 \in S$, $q_1, q_2 \in \mathcal{R}_n^\star$ and $w \in \mathcal{R}_n$ such that $w = q_1|_{\overline{s_1}} = q_2|_{\overline{s_2}}$, where $q_i|_{s_i}$ is normal for $i = 1, 2$. If $\overline{s_1}$ and $\overline{s_2}$ are separated in w, then $q_1|_{s_1} \equiv q_2|_{s_2}$ mod $[S, w]$.*

Proof. Let $q \in \mathcal{R}_n^{\star_1,\star_2}$ be the $(\star_1, \star_2)$-DRB monomial obtained by replacing the occurrence of $\overline{s_1}$ in w by $\star_1$ and the occurrence of $\overline{s_2}$ in w by $\star_2$. Then we have

$$q^{\star_1}|_{\overline{s_1}} = q_2, q^{\star_2}|_{\overline{s_2}} = q_1 \text{ and } q|_{\overline{s_1},\overline{s_2}} = q_1|_{\overline{s_1}} = q_2|_{\overline{s_2}},$$

where in the first two equalities, we have identified $\mathcal{R}_n^{\star_2}$ and $\mathcal{R}_n^{\star_1}$ with $\mathcal{R}_n^\star$. Let $s_1 - \overline{s_1} = \sum_i c_i u_i$ and $s_2 - \overline{s_2} = \sum_j d_j v_j$ with $0 \neq c_i, d_j \in \mathbf{k}$ and $u_i, v_j \in \mathcal{R}_n$ such that $u_i <_n \overline{s_1}$ and $v_j <_n \overline{s_2}$. Then by the linearity of s_1 and s_2 in $q|_{s_1,s_2}$, we have

$$\begin{aligned} q_1|_{s_1} - q_2|_{s_2} &= (q^{\star_2}|_{\overline{s_2}})|_{s_1} - (q^{\star_1}|_{\overline{s_1}})|_{s_2} \\ &= q|_{s_1,\overline{s_2}} - q|_{\overline{s_1},s_2} \end{aligned}$$

$$\begin{aligned}
&= q|_{s_1,\overline{s_2}} - q|_{s_1,s_2} + q|_{s_1,s_2} - q|_{\overline{s_1},s_2}\\
&= -q|_{s_1,s_2-\overline{s_2}} + q|_{s_1-\overline{s_1},s_2}\\
&= -(q^{\star_2}|_{s_2-\overline{s_2}})|_{s_1} + (q^{\star_1}|_{s_1-\overline{s_1}})|_{s_2}\\
&= -\sum_j d_j(q^{\star_2}|_{v_j})|_{s_1} + \sum_i c_i(q^{\star_1}|_{u_i})|_{s_2}\\
&= -\sum_j d_j q|_{s_1,v_j} + \sum_i c_i q|_{u_i,s_2}.
\end{aligned}$$

From Lemma 4.5, for each j, we may suppose that

$$q|_{s_1,v_j} = (q|_{s_1})|_{v_j} = \sum_\ell d_{j\ell} p_\ell|_{v_{j\ell}},$$

where $0 \neq d_{j\ell} \in \mathbf{k}$, $p_\ell \in \mathcal{R}_n^\star$, $v_{j\ell} \in S$ such that $p_\ell|_{v_{j\ell}}$ is normal and $\overline{p_\ell|_{v_{j\ell}}} \leq_n \overline{(q|_{s_1})|_{v_j}} = \overline{q|_{s_1,v_j}}$. Since $(q^{\star_1}|_{s_1})|_{\overline{s_2}} = q|_{s_1,\overline{s_2}} = (q^{\star_2}|_{\overline{s_2}})|_{s_1} = q_1|_{s_1}$ is normal and $v_j <_n \overline{s_2}$, by Definition 3.6 and Proposition 3.10, we have

$$\overline{q|_{s_1,v_j}} = \overline{(q^{\star_1}|_{s_1})|_{v_j}} <_n \overline{(q^{\star_1}|_{s_1})|_{\overline{s_2}}} = \overline{q_1|_{s_1}} = q_1|_{\overline{s_1}} = w.$$

So we have

$$\overline{p_\ell|_{v_{j\ell}}} \leq_n w.$$

With a similar argument to the case of $q|_{u_i,s_2}$, we can obtain that $q_1|_{s_1} \equiv q_2|_{s_2} \mod [S,w]$. □

For $k \geq 1$, write $\mathfrak{M}_k := \mathfrak{M}_{\Omega,k}(\Delta_n X)$ where $\Omega = \{d, P\}$. For $q \in \mathcal{R}_n^\star$, we define the **depth** $\operatorname{dep}_\star(q)$ **of** $\star$ **in** q by induction on $k \geq 0$ such that $q \in \mathcal{R}_n^\star \cap \mathfrak{M}_k$. Let $k = 0$. Then $q \in M(\Delta_n X^\star)$ and we define $\operatorname{dep}_\star(q) = 0$. Suppose $\operatorname{dep}_\star(q)$ has been defined for $q \in \mathcal{R}_n^\star \cap \mathfrak{M}_m, m \geq 0$, and consider $q \in \mathcal{R}_n^\star \cap \mathfrak{M}_{m+1}$. Then we have $q = q_1 \cdots q_\ell$ with each q_i in $\Delta_n X \cup \{\star\}$ or $\lfloor \mathfrak{M}(\Delta_n X^\star)\rfloor \cap \mathfrak{M}_{m+1}, 1 \leq i \leq \ell$, and with $\star$ appearing in a unique q_i. Suppose the unique q_i is in $\Delta_n X \cup \{\star\}$. Then define $\operatorname{dep}_\star(q) = 0$. Suppose the unique q_i is in $\lfloor \mathfrak{M}(\Delta_n X^\star)\rfloor \cap \mathfrak{M}_{m+1}$. Then $q_i = \lfloor \tilde{q}_i \rfloor$ with $\tilde{q}_i \in \mathfrak{M}(\Delta_n X^\star) \cap \mathfrak{M}_m$. Thus $\tilde{q}_i$ is in $\mathcal{R}_n^\star \cap \mathfrak{M}_m$ and $\operatorname{dep}_\star(\tilde{q}_i)$ is defined by the induction hypothesis. We then define $\operatorname{dep}_\star(q) := \operatorname{dep}_\star(\tilde{q}_i) + 1$. For example, $\operatorname{dep}_\star(q) = 1$ if $q = P(\star)$ and $\operatorname{dep}_\star(q) = 2$ if $q = P(xP(\star))$.

For the purpose of the proof the next lemma, we describe the relative location of two bracketed subwords in the more precise notion of placements (or occurrences [10]) in a bracketed word. See [24] for details. But note that we focus on words in $\mathcal{R}_n$ as a subset of $\mathfrak{M}(\Delta_n X)$.

Definition 4.7. Let $w, u \in \mathcal{R}_n$ and $q \in \mathcal{R}_n^\star$ be such that $w = q|_u$. Then we call the pair (u, q) a **placement** (or **occurrence**) of u in w.

The pair (u, q) corresponds to the pair (q, u) in [10, Chapter 2] where q is called the prefix. We note that a placement (u, q) gives an appearance of u as a subword or subterm of $w = q|_u$. A placement is more precise than a subword since a placement emphasizes the location of a subword. For example $u = x$ has two appearances in $w = x\lfloor x\rfloor$ which are differentiated by the two placements (u, q_1) and (u, q_2) where $q_1 = \star\lfloor x\rfloor$ and $x\lfloor\star\rfloor$.

Definition 4.8. Let $w, u_1, u_2 \in \mathcal{R}_n$ and $q_1, q_2 \in \mathcal{R}_n^\star$ be such that

$$q_1|_{u_1} = w = q_2|_{u_2}. \tag{14}$$

The two placements (u_1, q_1) and (u_2, q_2) are said to be

(a) **separated** if there exists an element q in $\mathcal{R}_n^{\star_1,\star_2}$ and $a, b \in \mathcal{R}_n$ such that $q_1|_{\star_1} = q|_{\star_1, b}$, $q_2|_{\star_2} = q|_{a, \star_2}$ and $w = q|_{a, b}$;
(b) **nested** if there exists an element q in $\mathcal{R}_n^\star$ such that either $q_2 = q_1|_q$ or $q_1 = q_2|_q$;
(c) **intersecting** if there exist an element q in $\mathcal{R}_n^\star$ and elements a, b, c in $\mathcal{R}_n\backslash\{1\}$ such that $w = q|_{abc}$ and either
  (i) $q_1 = q|_{\star c}, q_2 = q|_{a\star}$; or
  (ii) $q_1 = q|_{a\star}, q_2 = q|_{\star c}$.

By taking $u = abc$, it is easy to see that (u_1, q_1) and (u_2, q_2) are intersecting (in case (i)) if and only if there are $v_1, v_2 \in \mathcal{R}_n$ such that $w = q|_u$, $u := u_1v_1 = v_2u_2$ and

$$\max\{\mathrm{bre}(u_1), \mathrm{bre}(u_2)\} < \mathrm{bre}(u) < \mathrm{bre}(u_1) + \mathrm{bre}(u_2).$$

This corresponds to the above definition via the relations $(u, v_1, v_2) = (abc, c, a)$.

Theorem 4.9. [24, Theorem 4.11] *Let w be a bracketed word in $\mathcal{R}_n$. For any two placements (u_1, q_1) and (u_2, q_2) in w, exactly one of the following is true:*

(a) *(u_1, q_1) and (u_2, q_2) are separated;*
(b) *(u_1, q_1) and (u_2, q_2) are nested;*
(c) *(u_1, q_1) and (u_2, q_2) are intersecting.*

Now we are ready to prove the next result.

Lemma 4.10. *Let $S \subseteq \mathbf{k}\mathcal{R}_n$ with $d(S) \subseteq S$. If S is a Gröbner-Shirshov basis, then for each pair $s_1, s_2 \in S$ for which there exist $q_1, q_2 \in \mathcal{R}_n^\star$ and $w \in \mathcal{R}_n$ such that $w = q_1|_{\overline{s_1}} = q_2|_{\overline{s_2}}$ with $q_1|_{s_1}$ and $q_2|_{s_2}$ normal, we have $q_1|_{s_1} \equiv q_2|_{s_2} \bmod [S, w]$.*

Proof. Let $s_1, s_2 \in S$, $q_1, q_2 \in \mathcal{R}_n^\star$ and $w \in \mathcal{R}_n$ be such that $w = q_1|_{\overline{s_1}} = q_2|_{\overline{s_2}}$. Let $(\overline{s_1}, q_1)$ and $(\overline{s_2}, q_2)$ be the corresponding placements of w. By Theorem 4.9, according to the relative location of the placements $(q_1, \overline{s_1})$ and $(q_2, \overline{s_2})$ in w, we have the following three cases to consider.

Case 1. The placements $(\overline{s_1}, q_1)$ and $(\overline{s_2}, q_2)$ are separated in w. This case is covered by Lemma 4.6.

Case 2. The placements $(\overline{s_1}, q_1)$ and $(\overline{s_2}, q_2)$ are intersecting in w. We only need to consider Case (i) of overlapping since the proof of Case (ii) is similar. Then by the remark after Definition 4.8, there are $u, v \in \mathcal{R}_n$ such that $w_1 := \overline{s_1}u = v\overline{s_2}$ is a subword in w, where

$$\max\{\mathrm{bre}(\overline{s_1}), \mathrm{bre}(\overline{s_2})\} < \mathrm{bre}(w_1) < \mathrm{bre}(\overline{s_1}) + \mathrm{bre}(\overline{s_2}).$$

Since S is a Gröbner-Shirshov basis, we have

$$s_1u - vs_2 = \sum_j c_j p_j|_{t_j},$$

where $0 \neq c_j \in \mathbf{k}$, $t_j \in S$, $p_j \in \mathcal{R}_n^\star$ such that $p_j|_{t_j}$ is normal and $\overline{p_j|_{t_j}} = p_j|_{\overline{t_j}} <_n \overline{s_1}u = v\overline{s_2} = w_1$.

Let $q \in \mathcal{R}_n^{\star_1,\star_2}$ be obtained from q_1 by replacing $\star$ by $\star_1$, and the u on the right of $\star$ by $\star_2$. Let $p \in \mathcal{R}_n^\star$ be obtained from q by replacing $\star_1\star_2$ by $\star$. Then we have

$$q^{\star_2}|_u = q_1, q^{\star_1}|_v = q_2 \text{ and } p|_{\overline{s_1}u} = q|_{\overline{s_1}, u} = q_1|_{\overline{s_1}} = w,$$

where in the first two equalities, we have identified $\mathcal{R}_n^{\star_2}$ and $\mathcal{R}_n^{\star_1}$ with $\mathcal{R}_n^\star$. Thus we have

$$q_1|_{s_1} - q_2|_{s_2} = (q^{\star_2}|_u)|_{s_1} - (q^{\star_1}|_v)|_{s_2} = p|_{s_1u - vs_2} = \sum_j c_j p|_{p_j|_{t_j}} = \sum_j c_j \tilde{p}_j|_{t_j},$$

where $\tilde{p}_j := p|_{p_j} \in \mathcal{R}_n^\star$. By Lemma 4.5, for each j, we may suppose that

$$\tilde{p}_j|_{t_j} = \sum_\ell c_{j\ell} p_{j\ell}|_{t_{j\ell}},$$

where $0 \neq c_{j\ell} \in \mathbf{k}$, $t_{jl} \in S$, $p_{jl} \in \mathcal{R}_n^\star$, $p_{j\ell}|_{t_{j\ell}}$ is normal and $\overline{p_{j\ell}|_{t_{j\ell}}} \leq_n \overline{\tilde{p}_j|_{t_j}}$. So

$$q_1|_{s_1} - q_2|_{s_2} = \sum_j c_j \tilde{p}_j|_{t_j} = \sum_{j,\ell} c_j c_{j\ell} p_{j\ell}|_{t_{j\ell}}.$$

Since $\overline{p_j|_{t_j}} <_n w_1$ and $p|_{w_1} = w \in \mathcal{R}_n$ is normal, by Definition 3.6, we have

$$\overline{\tilde{p}_j|_{t_j}} = \overline{p|_{p_j|_{t_j}}} = \overline{p|_{\overline{p_j|_{t_j}}}} <_n \overline{p|_{w_1}} = p|_{w_1} = w$$

and so

$$\overline{p_{j\ell}|_{t_{j\ell}}} \leq_n \overline{\tilde{p}_j|_{t_j}} <_n w.$$

Hence

$$q_1|_{s_1} \equiv q_2|_{s_2} \mod [S, w].$$

Case 3. The placements $(\overline{s_1}, q_1)$ and $(\overline{s_2}, q_2)$ are nested. Without loss of generality, we may suppose $q_2 = q_1|_q$ for some $q \in \mathcal{R}_n^\star$. Then $q_1|_{\overline{s_1}} = q_2|_{\overline{s_2}} = (q_1|_q)|_{\overline{s_2}}$ and hence $\overline{s_1} = q|_{\overline{s_2}}$. Since $\overline{s_1} = q|_{\overline{s_2}} \in \mathcal{R}_n$, it follows that $q|_{s_2}$ is normal by Definition 3.4 and $\overline{q|_{s_2}} = q|_{\overline{s_2}}$. For the inclusion composition $(s_1, s_2)^q_{\overline{s_1}}$, since S is a Gröbner-Shirshov basis, we have

$$(s_1, s_2)^q_{\overline{s_1}} = s_1 - q|_{s_2} = \sum_j c_j p_j|_{t_j},$$

where $0 \neq c_j \in \mathbf{k}$, $p_j \in \mathcal{R}_n^\star$, $t_j \in S$ and $p_j|_{t_j}$ is normal with $\overline{p_j|_{t_j}} <_n \overline{s_1}$. Thus

$$q_2|_{s_2} - q_1|_{s_1} = q_1|_{q|_{s_2}} - q_1|_{s_1} = -q_1|_{s_1 - q|_{s_2}} = -\sum_j c_j q_1|_{p_j|_{t_j}} = -\sum_j c_j \tilde{p}_j|_{t_j},$$

where $\tilde{p}_j := q_1|_{p_j} \in \mathcal{R}_n^\star$. By Lemma 4.5, for each j, we may write

$$\tilde{p}_j|_{t_j} = \sum_\ell c_{j\ell} p_{j\ell}|_{t_{j\ell}},$$

where $0 \neq c_{j\ell} \in \mathbf{k}$, $p_{j\ell}|_{t_{j\ell}}$ is normal and $\overline{p_{j\ell}|_{t_{j\ell}}} \leq_n \overline{\tilde{p}_j|_{t_j}}$. So

$$q_2|_{s_2} - q_1|_{s_1} = -\sum_{j,\ell} c_j c_{j\ell} p_{j\ell}|_{t_{j\ell}}.$$

Since $\overline{p_j|_{t_j}} <_n \overline{s_1}$ and $q_1|_{\overline{s_1}} = w \in \mathcal{R}_n$ is normal, by Definition 3.6, we have

$$\overline{\tilde{p}_j|_{t_j}} = \overline{q_1|_{p_j|_{t_j}}} = \overline{q_1|_{\overline{p_j|_{t_j}}}} <_n \overline{q_1|_{\overline{s_1}}} = q_1|_{\overline{s_1}} = w$$

and so $\overline{p_{j\ell}|_{t_{j\ell}}} \leq_n \overline{\tilde{p}_j|_{t_j}} <_n w$. Hence $q_2|_{s_2} - q_1|_{s_1} \equiv 0 \mod [S, w]$.

This completes the proof of Lemma 4.10. ◻

Lemma 4.11. *Let $S \subseteq \mathbf{k}\mathcal{R}_n$ with $d(S) \subseteq S$ and $\mathrm{Irr(S)} := \mathcal{R}_n \setminus \{q|_{\overline{s}} \mid q \in \mathcal{R}_n^\star, s \in S, q|_s$ is normal $\}$. Then any $f \in \mathbf{k}\mathcal{R}_n$ has an expression*

$$f = \sum_i c_i u_i + \sum_j d_j q_j|_{s_j},$$

where for each i, j, we have $0 \neq c_i, d_j \in \mathbf{k}, u_i \in \mathrm{Irr(S)}, \overline{u_i} \leq_n \overline{f}$, $q_j \in \mathcal{R}_n^\star$, $s_j \in S$ such that $q_j|_{s_j}$ is normal and $q_j|_{\overline{s_j}} \leq_n \overline{f}$.

Proof. Suppose the lemma does not hold and let f be a counterexample with $\overline{f}$ minimal. Write $f = \sum_i c_i u_i$ where $0 \neq c_i \in \mathbf{k}$, $u_i \in \mathcal{R}_n$ and $u_1 >_n u_2 >_n \cdots$. If $u_1 \in \mathrm{Irr(S)}$, then let $f_1 := f - c_1 u_1$. If $u_1 \notin \mathrm{Irr}(S)$, that is, there exists $s_1 \in S$ such that $u_1 = q_1|_{\overline{s_1}}$ and $q_1|_{s_1}$ is normal, then let $f_1 := f - c_1 q_1|_{s_1}$. In both cases $\overline{f_1} <_n \overline{f}$. By the minimality of f, we have that f_1 has the desired expression. Then f also has the desired expression. This is a contradiction. □

Now we are ready to derive the Composition-Diamond Lemma.

Theorem 4.12. *(Composition-Diamond Lemma) Let S be a set of monic DRB polynomials in $\mathbf{k}\mathcal{R}_n$ with $d(S) \subseteq S$ and $\mathrm{Id}(S)$ the differential Rota-Baxter ideal of $\mathbf{k}\mathcal{R}_n$ generated by S. Then the following conditions are equivalent:*

(a) *S is a Gröbner-Shirshov basis in $\mathbf{k}\mathcal{R}_n$.*
(b) *If $0 \neq f \in \mathrm{Id}(S)$, then $\overline{f} = q|_{\overline{s}}$ for some $q \in \mathcal{R}_n^\star$, $s \in S$ and $q|_s$ is normal.*
(c) *$\mathrm{Irr(S)} = \mathcal{R}_n \setminus \{q|_{\overline{s}} \mid q \in \mathcal{R}_n^\star, s \in S, q|_s$ is normal$\}$ is a $\mathbf{k}$-basis of $\mathbf{k}\mathcal{R}_n/\mathrm{Id}(S)$. In other words, $\mathbf{k}\mathrm{Irr}(S) \oplus \mathrm{Id}(S) = \mathbf{k}\mathcal{R}_n$.*

Proof. (a) ⇒ (b): Let $0 \neq f \in \mathrm{Id}(S)$. Then by Lemmas 3.2 and 4.5,

$$f = \sum_{i=1}^k c_i q_i|_{s_i}, \text{ where } 0 \neq c_i \in \mathbf{k}, q_i \in \mathcal{R}_n^\star, s_i \in S, q_i|_{s_i} \text{ is normal}, 1 \leq i \leq k. \tag{15}$$

Let $w_i = q_i|_{\overline{s_i}}, 1 \leq i \leq k$. We rearrange them in non-increasing order by

$$w_1 = w_2 = \cdots = w_m >_n w_{m+1} \geq_n \cdots \geq_n w_k.$$

If for each $0 \neq f \in \mathrm{Id}(S)$, there is a choice of the above sum such that $m = 1$, then $\overline{f} = q_1|_{\overline{s_1}}$ and we are done. So suppose the implication (a) ⇒ (b) does not hold. Then there is an $0 \neq f \in \mathrm{Id}(S)$ such that for any expression in Eq. (15), we have that $m \geq 2$. Fix such an f and choose an expression in Eq. (15) such that $q_1|_{\overline{s_1}}$ is minimal and then with $m \geq 2$ minimal, that is, with the fewest $q_i|_{s_i}$ such that $q_i|_{\overline{s_i}} = q_1|_{\overline{s_1}}$. Since $m \geq 2$, we have $q_1|_{\overline{s_1}} = w_1 = w_2 = q_2|_{\overline{s_2}}$.

Since S is a Gröbner-Shirshov basis in $\mathbf{k}\mathcal{R}_n$, by Lemma 4.10, we have

$$q_2|_{s_2} - q_1|_{s_1} = \sum_j d_j p_j|_{r_j},$$

where each $0 \neq d_j \in \mathbf{k}$, $r_j \in S$, $p_j \in \mathcal{R}_n^\star$ and $p_j|_{r_j}$ are normal with $p_j|_{\overline{r_j}} <_n w_1$. Hence

$$f = \sum_{i=1}^k c_i q_i|_{s_i} = (c_1 + c_2) q_1|_{s_1} + c_3 q_3|_{s_3} + \cdots + c_m q_m|_{s_m} + \sum_{i=m+1}^k c_i q_i|_{s_i} + \sum_j c_2 d_j p_j|_{r_j}.$$

By the minimality of m, we must have $c_1 + c_2 = c_3 = \cdots = c_m = 0$. Then we obtain an expression of f in the form of Eq. (15) for which $q_1|_{\overline{s_1}}$ is even smaller, a contradiction.

(b) ⇒ (c): Obviously $0 \in \mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S) \subseteq \mathbf{k}\mathcal{R}_n$. Suppose the inclusion is proper. Then $\mathbf{k}\mathcal{R}_n \setminus (\mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S))$ contains only nonzero elements. Let $f \in \mathbf{k}\mathcal{R}_n \setminus (\mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S))$ be such that

$$\overline{f} = \min\{\overline{g} \mid g \in \mathbf{k}\mathcal{R}_n \setminus (\mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S))\}.$$

Case 1. $\overline{f} \in \mathrm{Irr(S)}$. Then $f \neq \overline{f}$ since $f \notin \mathrm{Irr(S)}$. By $\overline{f - \overline{f}} <_n \overline{f}$ and the minimality of $\overline{f}$, we must have

$$f - \overline{f} \in \mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S)$$

and so

$$f \in \mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S),$$

a contradiction.

Case 2. $\overline{f} \notin \mathrm{Irr(S)}$. Then by the definition of Irr(S), we have $\overline{f} = q|_{\overline{s}}$ for some $q \in \mathcal{R}^\star(\Delta X)$, $s \in S$ and $q|_s$ is normal. Thus $\overline{q|_s} = q|_{\overline{s}} = \overline{f}$ and so $\overline{f - q|_s} <_n \overline{f}$. If $f = q|_s$, then $f \in \mathrm{Id}(S)$, a contradiction. If $f \neq q|_s$, then $f - q|_s \neq 0$ with $\overline{f - q|_s} <_n \overline{f}$. By the minimality of $\overline{f}$, we have

$$f - q|_s \in \mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S).$$

This implies that

$$f \in \mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S),$$

again a contradiction.

Hence $\mathbf{k}\mathrm{Irr}(S) + \mathrm{Id}(S) = \mathbf{k}\mathcal{R}_n$. Suppose $\mathbf{k}\mathrm{Irr}(S) \cap \mathrm{Id}(S) \neq 0$ and let $0 \neq f \in \mathbf{k}\mathrm{Irr(S)} \cap \mathrm{Id}(S)$. Then by $f \in \mathrm{Irr(S)}$, we may assume that

$$f = c_1 v_1 + c_2 v_2 + \cdots + c_k v_k,$$

where $v_1 >_n v_2 >_n \cdots >_n v_k \in \mathrm{Irr(S)}$. Since $f \in \mathrm{Id}(S)$, by Item (b), we have $v_1 = \overline{f} = q|_{\overline{s}}$ for some $q \in \mathcal{R}_n^\star$, $s \in S$ and $q|_s$ is normal. This is a contradiction to the definition of Irr(S). Therefore $\mathbf{k}\mathrm{Irr}(S) \oplus \mathrm{Id}(S) = \mathbf{k}\mathcal{R}_n$ and Irr(S) is a $\mathbf{k}$-basis of $\mathbf{k}\mathcal{R}(\Delta X)/\mathrm{Id}(S)$.

(c) ⇒ (a) : Suppose $f, g \in S$ give an intersection or inclusion composition. With the notations in the definitions of compositions, let $F = fu$ and $G = vg$ in the case of intersection composition and let $F = f$ and $G = q|_g$ in the case of inclusion composition. Then we have $w := \overline{F} = \overline{G}$. If $(f, g)_w = F - G = 0$, there is nothing to prove. If $(f, g)_w \neq 0$, we have

$$(f, g)_w = \sum_{i=1}^{k} c_i u_i, \quad 0 \neq c_i \in \mathbf{k}, u_1 >_n u_2 >_n \cdots >_n u_k \in \mathcal{R}_n.$$

Then $u_i <_n \overline{F} = \overline{G} = w$. Since $(f, g)_w \in \mathrm{Id}(S)$ and $\mathbf{k}\mathrm{Irr}(S) \cap \mathrm{Id}(S) = 0$ by Item (c), we have $u_i \notin \mathrm{Irr(S)}$ for $i = 1, \cdots, k$. So by the definition of Irr(S), there are $q_i \in \mathcal{R}_n^\star$, $s_i \in S$ such that $u_i = q_i|_{\overline{s_i}}$ and $q_i|_{s_i}$ is normal for each $1 \leq i \leq k$. Since $\overline{q_i|_{s_i}} = q_i|_{\overline{s_i}} = u_i <_n w$, we have $(f, g)_w \equiv 0 \mod [S, w]$.

For any composition of right multiplication fu where $f \in S$, $\overline{f} \in \mathcal{R}_n P(\mathcal{R}_n)$ and $u \in P(\mathcal{R}_n)$, we have $fu \in \mathrm{Id}(S)$. By Item (c), we have $\mathbf{k}\mathrm{Irr}(S) \cap \mathrm{Id}(S) = 0$. This implies from Lemma 4.11 that $fu = \sum_j d_j q_j|_{s_j}$, where $0 \neq d_j \in \mathbf{k}$, $s_j \in S$ such that $q_j \in \mathcal{R}_n^\star$, $q_j|_{s_j}$ is normal and $q_j|_{\overline{s_j}} \leq_n \overline{fu}$. Thus $fu \equiv 0 \mod [S]$. With a similar argument, we can show that the compositions of left multiplication are trivial $[S]$.

Therefore S is a Gröbner-Shirshov basis. □

5. Gröbner-Shirshov bases and free integro-differential algebras

In this section we begin with a finite set X and $n \geq 1$ and prove that the idea $I_{\mathrm{ID},n}$ of $\mathbf{k}\mathcal{R}_n$ possesses a Gröbner-Shirshov basis. This is done in Section 5.1. Then in Section 5.2, we apply the Composition-Diamond Lemma in Theorem 4.12 to construct a canonical basis for $\mathbf{k}\mathcal{R}_n/I_{\mathrm{ID,n}}$. Letting n to go to infinity, we obtain a canonical basis of the free integro-differential algebra $\mathbf{k}\mathcal{R}(\Delta X)/I_{\mathrm{ID}}$ on the finite set X. Finally for any well-ordered set X, by showing that the canonical basis of the free integro-differential algebra on each finite subset of X is compatible with the inclusions of the subsets of X, we obtain a canonical basis of the free integro-differential algebra on X.

5.1. **Gröbner-Shirshov basis.** In this subsection, X is a finite set. Let

$$S_n := \{\phi_1(u,v), \phi_2(u,v) \mid u, v \in \mathcal{R}_n\}$$

be the set of generators in Eq. (11) corresponding to the integration by parts axiom Eq. (4). Then $I_{\mathrm{ID,n}}$ is the differential Rota-Baxter ideal $\mathrm{Id}(S_n)$ of $\mathbf{k}\mathcal{R}_n$ generated by S_n.

Remark 5.1. Let $u = 1$. Then $\phi_1(u,v) = \phi_1(1,v) = 0$ is in S_n. By Eqs. (1) and (3), we have

$$d(\phi_1(u,v)) = d(u)P(v) - d(uP(v)) + uv + \lambda d(u)v = 0, \tag{16}$$

and hence is in S_n. Similarly, $d(\phi_2(u,v)) = 0$. So $d(S_n) \subseteq S_n$.

Next, we show that S_n is a Gröbner-Shirshov basis of the differential Rota-Baxter ideal $I_{\mathrm{ID},n} = \mathrm{Id}(S_n) \subseteq \mathbf{k}\mathcal{R}_n$.

Lemma 5.2. *Let $u = u_0u_1\cdots u_k \in M(\Delta X)$ with $u_0,\cdots,u_k \in \Delta X$. Then $\overline{d(u)} = u_0u_1\cdots u_{k-1}d(u_k)$. If $u \in M(\Delta_n X)$, then $\overline{d(u)} = u_0u_1\cdots u_{k-1}d(u_k)$ provided $u_k \in \Delta_{n-1}X$.*

Proof. This follows from Eq. (6) and the definitions of the order on ΔX. □

Let $\mathcal{A}_d := \{\overline{d(u)} \mid u \in S(\Delta X)\}$, $\mathcal{A}_{n,d} := \mathcal{A}_d \cap M(\Delta_n X)$ and

$$\mathcal{Z}_n := \{x_0^{(n)}\cdots x_k^{(n)} \mid x_0,\cdots,x_k \in X, k \geq 0\}. \tag{17}$$

Note that $d(u) = 0$ for $u \in M(\Delta_n X)$ if and only if $u = 1$ or $u \in \mathcal{Z}_n$.

Lemma 5.3. *We have*

$$\left\{\overline{\phi_1(u,v)} \mid u, v \in \mathcal{R}_n\right\} = P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n)) \bigcup \left(\bigcup_{r\geq 1} P(\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^r P(\mathcal{R}_n))\right)$$
$$\bigcup \left(P((\Lambda(\mathcal{Z}_n,\mathcal{R}_n) \setminus P(\mathcal{R}_n))\mathcal{R}_n) \bigcap \mathcal{R}_n\right) \bigcup \{0\}.$$

Here we take the intersection with $\mathcal{R}_n$ to ensure that the right hand side is in $\mathcal{R}_n$.

Proof. We first show that the left hand side of the equation is contained in the right hand side. If $u = 1$, then $\phi_1(u,v) = 0 = \overline{\phi_1(u,v)}$. If $u \in P(\mathcal{R}_n)$, let $u = P(u_0)$ for some $u_0 \in \mathcal{R}_n$, then

$$\phi_1(u,v) = P(u_0P(v)) - P(u_0)P(v) + P(P(u_0)v) + \lambda P(u_0v) = 0$$

and so $\overline{\phi_1(u,v)} = 0$. Suppose that $u \neq 1$ and $u \notin P(\mathcal{R}_n)$. Note that

$$\deg_{\Delta_n X}(\overline{P(d(u)P(v))}) = \deg_{\Delta_n X}(\overline{uP(v)}) = \deg_{\Delta_n X}(\overline{P(uv)}) = \deg_{\Delta_n X}(\overline{P(d(u)v)}).$$

Case 1. $\deg_P(\overline{d(u)}) = \deg_P(u)$. Then

$$\deg_P(\overline{P(d(u)P(v))}) > \deg_P(\overline{uP(v)}), \deg_P(\overline{P(uv)}), \deg_P(\overline{P(d(u)v)})$$

and so $\overline{\phi_1(u,v)} = \overline{P(d(u)P(v))} = P(\overline{d(u)P(v)})$. According to Eq. (7), we have four subcases to consider. Consider first that $u = u_0P(\tilde{u}_0)\cdots u_kP(\tilde{u}_k)u_{k+1}$ with $u_0,\cdots,u_{k+1} \in S(\Delta_n X)$ and $\tilde{u}_0,\cdots,\tilde{u}_{k+1} \in \mathcal{R}_n$. Since $\deg_P(\overline{d(u)}) = \deg_P(u)$, there is at least one u_i with $0 \le i \le k+1$ such that $u_i \notin \mathcal{Z}_n$. If $u_{k+1} \notin \mathcal{Z}_n$, then $d(u_{k+1}) \neq 0$ and

$$\overline{\phi_1(u,v)} = P(\overline{d(u)P(v)}) = P(u_0P(\tilde{u}_0)\cdots u_kP(\tilde{u}_k)\overline{d(u_{k+1})}P(v)) \in P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n)).$$

If $u_{k+1} \in \mathcal{Z}_n$, suppose that u_i with $0 \le i \le k$ is right most such that $u_i \notin \mathcal{Z}_n$, then

$$\overline{d(u)} = u_0P(\tilde{u}_0)\cdots u_{i-1}P(\tilde{u}_{i-1})\overline{d(u_i)}P(\tilde{u}_i)u_{i+1}P(\tilde{u}_{i+1})\cdots u_kP(\tilde{u}_k)u_{k+1}$$

and so

$$\overline{\phi_1(u,v)} = P(\overline{d(u)}P(v)) \in \cup_{r\ge 1}P(\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^rP(\mathcal{R}_n)).$$

For the other subcases, with a similar argument, we can obtain that

$$\overline{\phi_1(u,v)} \in P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n)) \cup \left(\cup_{r\ge 1} P(\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^rP(\mathcal{R}_n))\right).$$

Case 2. $\deg_P(\overline{d(u)}) \neq \deg_P(u)$. Then $u \in \Lambda(\mathcal{Z}_n,\mathcal{R}_n) \setminus P(\mathcal{R}_n)$ and $\deg_P(\overline{d(u)}) = \deg_P(u) - 1$. So

$$\deg_P(\overline{P(d(u)P(v))}) = \deg_P(\overline{uP(v)}) = \deg_P(\overline{P(uv)}) = \deg_P(\overline{P(d(u)v)}) + 1.$$

If $u \notin \mathcal{R}_nP(\mathcal{R}_n)$, then $\overline{uP(v)} = uP(v)$ and $\overline{P(uv)} = P(uv)$. By the definition of $<_n$, we have $uP(v) <_n P(uv)$. If $u \in \mathcal{R}_nP(\mathcal{R}_n)$, let $u = u_0P(u_1)$ with $u_0, u_1 \in \mathcal{R}_n$. Then by the definition of $<_n$, we have

$$\overline{uP(v)} = \overline{u_0P(u_1)P(v)} = u_0P(\overline{P(u_1)v}) <_n P(\overline{u_0P(u_1)v}) = \overline{P(uv)}$$

Since $\overline{d(u)} <_n u$, we have $\overline{P(d(u)P(v))}, \overline{P((d(u)v)} <_n \overline{P(uv)}$. Hence $\overline{\phi_1(u,v)} = \overline{P(uv)} = P(\overline{uv}) \in P(\Lambda(\mathcal{Z}_n,\mathcal{R}_n)\mathcal{R}_n)$.

We next prove the reverse inclusion. If $w = P(u_0\overline{d(u_1)}P(v)) \in P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n))$ with $u_0, v \in \mathcal{R}_n$ and $\overline{d(u_1)} \in \mathcal{A}_{n,d}$, let $u = u_0u_1$. Then $\overline{d(u)} = u_0\overline{d(u_1)}$ and

$$\overline{\phi_1(u,v)} = \overline{P(d(u)P(v))} = P(\overline{d(u)}P(v)) = P(u_0\overline{d(u_1)}P(v)) = w.$$

If

$$w = P(u_0\overline{d(u_1)}u_2P(v)) \in \cup_{r\ge 1}P(\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^rP(\mathcal{R}_n))$$

with $u_0, v \in \mathcal{R}_n$, $\overline{d(u_1)} \in \mathcal{A}_{n,d}$ and $u_2 \in \cup_{r\ge 1}(P(\mathcal{R}_n)\mathcal{Z}_n)^r$, let $u = u_0u_1u_2$. Then $\overline{d(u)} = u_0\overline{d(u_1)}u_2$ and

$$\overline{\phi_1(u,v)} = \overline{P(d(u)P(v))} = P(\overline{d(u)}P(v)) = P(u_0\overline{d(u_1)}u_2P(v)) = w.$$

If $w = P(uv) \in P(\Lambda(\mathcal{Z}_n,\mathcal{R}_n)\mathcal{R}_n)$ with $u \in \Lambda(\mathcal{Z}_n,\mathcal{R}_n)$ and $v \in \mathcal{R}_n$, then $\overline{\phi_1(u,v)} = P(uv) = w$. □

Lemma 5.4. *We have*

$$\left\{\overline{\phi_2(u,v)} \mid u,v \in \mathcal{R}_n\right\} = \mathcal{R}_n \bigcap \Bigg(P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}) \bigcup \Big(\bigcup_{r\ge 1} P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^r) \Big)$$

$$\bigcup \Big(\bigcup_{r\ge 1} P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^rP(\mathcal{R}_n)) \Big) \bigcup P\Big(\mathcal{R}_n(\Lambda(\mathcal{Z}_n,\mathcal{R}_n) \setminus P(\mathcal{R}_n))\Big) \Bigg) \bigcup \{0\}.$$

Here we take the intersection with $\mathcal{R}_n$ to ensure that the right hand side is in $\mathcal{R}_n$.

Proof. The proof is similar to that of Lemma 5.3. □

Note that only the first union components of Lemmas 5.3 and 5.4 do not involve $\mathcal{Z}_n$. Thus we have

Proposition 5.5. $\{\overline{\phi_1(u,v)}, \overline{\phi_2(u,v)} \mid u, v \in \mathcal{R}_n\} = P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n)) \cup P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}) \cup \epsilon(\Delta_n X)$, *where*

$$\begin{aligned}\epsilon(\Delta_n X) \ := \ & \mathcal{R}_n \bigcap \Bigg(\Big(\bigcup_{r\geq 1} P(\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^r P(\mathcal{R}_n)) \Big) \bigcup P\Big((\Lambda(\mathcal{Z}_n, \mathcal{R}_n) \setminus P(\mathcal{R}_n))\mathcal{R}_n \Big) \\ & \bigcup \Big(\bigcup_{r\geq 1} P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^r) \Big) \\ & \bigcup \Big(\bigcup_{r\geq 1} P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}(P(\mathcal{R}_n)\mathcal{Z}_n)^r P(\mathcal{R}_n)) \Big) \bigcup P\Big(\mathcal{R}_n(\Lambda(\mathcal{Z}_n, \mathcal{R}_n) \setminus P(\mathcal{R}_n)) \Big) \Bigg) \bigcup \{0\}.\end{aligned}$$

Every term in $\epsilon(\Delta_n X)$ has a factor in $\mathcal{Z}_n$ and will thus disappear as n goes to infinity.

Lemma 5.6. *The compositions of multiplication are trivial modulo* $[S_n]$.

Proof. Let $f \in S_n$. Then $f = \phi_1(u,v)$ or $f = \phi_2(u,v)$ for some $u, v \in \mathcal{R}_n$. We only consider the case when

$$f = \phi_1(u,v) = P(d(u)P(v)) - uP(v) + P(uv) + \lambda P(d(u)v), \ u, v \in \mathcal{R}_n,$$

since the case for $f = \phi_2(u,v)$ is similar. It is sufficient to show that $\phi_1(u,v)P(w)$ and $P(w)\phi_1(u,v)$ are trivial modulo $[S_n]$. We first show that $\phi_1(u,v)P(w)$ is trivial modulo $[S_n]$. Note that $\overline{\phi_1(u,v)} \in P(\mathcal{R}_n)$. From Eq. (2) we obtain

$$\begin{aligned}\phi_1(u,v)P(w) =& P(d(u)P(v))P(w) - uP(v)P(w) + P(uv)P(w) + \lambda P(d(u)v)P(w) \\ =& P(P(d(u)P(v))w) + P(d(u)P(v)P(w)) + \lambda P(d(u)P(v)w) \\ & - uP(v)P(w) + P(uv)P(w) + \lambda P(d(u)v)P(w) \\ =& P(P(d(u)P(v))w) + P(d(u)P(P(v)w + vP(w) + \lambda vw)) + \lambda P(d(u)P(v)w) \\ & - uP(P(v)w) - uP(vP(w)) - \lambda uP(vw) + P(P(uv)w) + P(uvP(w)) \\ & + \lambda P(uvw) + \lambda P(P(d(u)v)w) + \lambda P(d(u)vP(w)) + \lambda^2 P(d(u)vw).\end{aligned} \tag{18}$$

By the definition of $\phi_1(u,v)$, we have

$$P(P(d(u)P(v))w) = P(\phi_1(u,v)w) + P(uP(v)w) - P(P(uv)w) - \lambda P(P(d(u)v)w), \tag{19}$$

and

$$\begin{aligned}& P(d(u)P(P(v)w + vP(w) + \lambda vw)) \\ =& \phi_1(u, P(v)w + vP(w) + \lambda vw) + uP(P(v)w + vP(w) + \lambda vw) \\ & - P(u(P(v)w + vP(w) + \lambda vw)) - \lambda P(d(u)(P(v)w + vP(w) + \lambda vw)) \\ =& \phi_1(u, P(v)w + vP(w) + \lambda vw) + uP(P(v)w) + uP(vP(w)) + \lambda uP(vw) - P(uP(v)w) \\ & - P(uvP(w)) - \lambda P(uvw) - \lambda P(d(u)P(v)w) - \lambda P(d(u)vP(w)) - \lambda^2 P(d(u)vw)\end{aligned} \tag{20}$$

Substituting Eqs. (19) and (20) into Eq. (18), we have

$$\begin{aligned}\phi_1(u,v)P(w) &= P(\phi_1(u,v)w) + \phi_1(u, P(v)w + vP(w) + \lambda vw) \\ &= P(\phi_1(u,v)w) + \phi_1(u, P(v)w) + \phi_1(u, vP(w)) + \lambda\phi_1(u, vw).\end{aligned}$$

The last three terms are already in S_n and hence are of the form $q|_s$ with $q = \star$ and $s \in S_n$. So to show that they are trivial modulo $[S]$ we just need to bound the leading terms.

Note that

$$\overline{P(aP(b))}, \overline{P(P(a)b)}, \overline{P(ab)} \leq_n \overline{P(a)P(b)} \text{ for } a, b \in \mathcal{R}_n.$$

If $\deg_P(u) = \deg_P(\overline{d(u)})$, that is, if we are in Case 1 of Lemma 5.3, then we have

$$\begin{aligned}
\overline{\phi_1(u, P(v)w)} &= \overline{P(d(u)P(P(v)w))} \leq_n \overline{P(d(u)P(v)P(w))} \leq_n \overline{P(d(u)P(v))P(w)} = \overline{\phi_1(u, v)P(w)},\\
\overline{\phi_1(u, vP(w))} &= \overline{P(d(u)P(vP(w)))} \leq_n \overline{P(d(u)P(v)P(w))} \leq_n \overline{P(d(u)P(v))P(w)} = \overline{\phi_1(u, v)P(w)},\\
\overline{\phi_1(u, vw)} &= \overline{P(d(u)P(vw))} \leq_n \overline{P(d(u)P(v)P(w))} \leq_n \overline{P(d(u)P(v))P(w)} = \overline{\phi_1(u, v)P(w)}.
\end{aligned}$$

If $\deg_P(u) \neq \deg_P(\overline{d(u)})$, that is, if we are in Case 2 of Lemma 5.3, then we have

$$\begin{aligned}
\overline{\phi_1(u, P(v)w)} &= \overline{P(uP(v)w)} \leq_n \overline{P(P(uv)w)} \leq_n \overline{P(uv)P(w)} = \overline{\phi_1(u, v)P(w)},\\
\overline{\phi_1(u, vP(w))} &= \overline{P(uvP(w))} \leq_n \overline{P(uv)P(w)} = \overline{\phi_1(u, v)P(w)},\\
\overline{\phi_1(u, vw)} &= \overline{P(uvw)} \leq_n \overline{P(uv)P(w)} = \overline{\phi_1(u, v)P(w)}.
\end{aligned}$$

Thus

$$\phi_1(u, P(v)w) + \phi_1(u, vP(w)) + \lambda\phi_1(u, vw) \equiv 0 \bmod [S_n, \overline{\phi_1(u, v)P(w)}\,]$$

and so $\phi_1(u, v)P(w) \equiv 0 \bmod [S_n]$ if and only if $P(\phi_1(u, v)w) \equiv 0 \bmod [S_n, \overline{\phi_1(u, v)P(w)}\,]$. Let $w = w_1w_2 \cdots w_k$ be the standard decomposition of w. We prove the latter statement by induction on $\mathrm{dep}(w_1)$.

If $\mathrm{dep}(w_1) = 0$, that is, $w_1 \in M(\Delta_n X)$, let $q := P(\star w) \in \mathcal{R}_n^\star$. Then

$$q|_{\phi_1(u,v)} = P(\phi_1(u, v)w) = P(\phi_1(u, v)w_1w_2 \cdots w_k)$$

and $q|_{\phi_1(u,v)}$ is normal by $w_1 \in M(\Delta_n X)$. If $\deg_P(u) = \deg_P(\overline{d(u)})$, then

$$\overline{P(\phi_1(u, v)w)} = \overline{P(P(d(u)P(v))w)} \leq_n \overline{P(d(u)P(v))P(w)} = \overline{\phi_1(u, v)P(w)},$$

If $\deg_P(u) \neq \deg_P(\overline{d(u)})$, then

$$\overline{P(\phi_1(u, v)w)} = \overline{P(P(uv)w)} \leq_n \overline{P(uv)P(w)} = \overline{\phi_1(u, v)P(w)}.$$

Hence $P(\phi_1(u, v)w) \equiv 0 \bmod [S_n]$.

If $\mathrm{dep}(w_1) > 0$, we may suppose $w_1 = P(\tilde{w})$ with $\tilde{w} \in \mathcal{R}_n$. Then $w_2 \in \Delta_n X$, as $w = w_1w_2 \cdots w_k$ is the standard decomposition of w. Since $\mathrm{dep}(\tilde{w}) < \mathrm{dep}(w_1)$, by the induction hypothesis, we may assume that

$$\phi_1(u, v)P(\tilde{w}) = \sum_i c_i p_i|_{s_i},$$

where $0 \neq c_i \in \mathbf{k}, p_i \in \mathcal{R}_n^\star, s_i \in S_n$, $p_i|_{s_i}$ is normal and $\overline{p_i|_{s_i}} \leq \overline{\phi_1(u, v)P(\tilde{w})}$. Let $q_i := P(p_iw_2 \cdots w_k)$. Since $p_i|_{s_i}$ is normal and $w_2 \in \Delta_n X$, it follows that $q_i|_{s_i}$ is normal. Furthermore, we have

$$\begin{aligned}
P(\phi_1(u, v)w) &= P(\phi_1(u, v)w_1w_2 \cdots w_k) = P(\phi_1(u, v)P(\tilde{w})w_2 \cdots w_k)\\
&= \sum_i c_i P(p_i|_{s_i} w_2 \cdots w_k) = \sum_i c_i q_i|_{s_i}
\end{aligned}$$

and

$$\overline{q_i|_{s_i}} = \overline{P(p_i|_{s_i} w_2 \cdots w_k)} \leq_n \overline{P(\phi_1(u, v)P(\tilde{w})w_2 \cdots w_k)} = \overline{P(\phi_1(u, v)w)} \leq_n \overline{\phi_1(u, v)P(w)}.$$

Therefore $P(\phi_1(u, v)w) \equiv 0 \bmod [S_n, \overline{\phi_1(u, v)P(w)}]$. This completes the induction. Hence $\phi_1(u, v)P(w) \equiv 0 \bmod [S_n]$, as needed.

With a similar argument, we can show that $P(w)\phi_1(u,v) \equiv 0 \bmod [S_n]$. □

Lemma 5.7. *There are no intersection compositions in S_n.*

Proof. Let $f, g \in S_n$. By Lemmas 5.3 and 5.4, we have $\operatorname{bre}(\overline{f}) = 1 = \operatorname{bre}(\overline{g})$. Suppose $w := \overline{f}u = v\overline{g}$ gives an intersection composition. Then by the definition of intersection composition, we have $1 < \operatorname{bre}(w) < 2$. This is a contradiction. Thus there are no intersection compositions in S_n. □

Lemma 5.8. *The including compositions in S_n are trivial.*

Proof. We first list all possible inclusion compositions from $f, g \in S_n$, namely those $f, g \in S_n$ such that $w := \overline{f} = q|_{\overline{g}}$ for some $q \in \mathfrak{R}_n^\star$.

We begin with the case when $q = \star$. Then we have $w := \overline{f} = \overline{g}$. From Lemmas 5.3 and 5.4, we must have

$$f = \phi_1(u,v) = g, \text{ or } f = \phi_2(u,v) = g.$$

Hence $f - g$ is trivial modulo $[S_n, w]$, as needed.

We next consider the case when $q \neq \star$. We need $\overline{f} = q|_{\overline{g}}$ where $\overline{f}$ is of the form $\overline{P(w)}$ with $w = d(u)P(v)$, $w = P(u)d(v)$ or $w = uv$ while $\overline{g}$ is also of the form $P(d(r)P(s))$, $P(P(r)d(s))$ or $P(rs)$. Thus q is of the forms

$$P(d(p)P(v)),\ P(d(u)P(p)),\ P(P(p)d(v)),\ P(P(u)d(p)),\ P(pv),\ P(up),\ P(d(u)\star),\ P(\star d(v)),$$

where $p \in \mathfrak{R}_n^\star$ and where the $\star$ in p or by itself is replaced by $\overline{g}$ which can be of the forms $P(d(r)P(s))$, $P(P(r)d(s))$ or $P(rs)$. Thus there are 24 possibilities. The last two cases in the displayed list occur when the P in $P(q)$ and the P in $\overline{g}$ coincide. Thus all the including compositions $\overline{f} = q|_{\overline{g}}$ with $q \neq \star$ are of the forms

$$P(d(p|_{\overline{g}})P(v)), P(d(u)P(p|_{\overline{g}})), P(P(p|_{\overline{g}})d(v)), P(P(u)d(p|_{\overline{g}})), P(p|_{\overline{g}}v), P(up|_{\overline{g}}), P(d(u)\star|_{\overline{g}}), P(\star|_{\overline{g}}d(v)),$$

with $\overline{g} = P(d(r)P(s)), P(P(r)d(s))$ or $P(rs)$.

With a similar argument as in [18, Lemma 5.7], we can show the triviality of the ambiguities of the compositions

$$P(d(u)P(p|_{P(d(r)P(s))})),\ P(d(p|_{P(d(r)P(s))})P(v)),\ P(d(u)P(d(r)P(s))),\ P(P(d(r)P(s))d(v)).$$

We next check that the ambiguity of the composition $P(d(u)P(p|_{P(P(v)d(w))}))$ is trivial. This is the case when $w = \overline{f} = q|_{\overline{g}}$ where $q = P(d(u)P(p))$ for some $p \in \mathfrak{R}_n^\star$. Then f and g of S_n are of the form

$$f = \phi_1(u,v) = P(d(u)P(v)) - uP(v) + P(uv) + \lambda P(d(u)v),$$
$$g = \phi_2(r,s) = P(P(r)d(s)) - P(r)s + P(rs) + \lambda P(rd(s)),$$

where $\overline{f} = \overline{P(d(u)P(v))}$ and $\overline{g} = \overline{P(P(r)d(s))}$. Further $v = p|_{\overline{g}} = p|_{\overline{\phi_2(r,s)}} = p|_{\overline{P(P(r)d(s))}}$ for some $p \in \mathfrak{R}_n^\star$ and

$$w = \overline{f} = \overline{\phi_1(u,v)} = \overline{P(d(u)P(v))} = \overline{P(d(u)P(p|_{\overline{g}}))} = \overline{q|_{\overline{g}}} = q|_{\overline{g}}$$

with $q = P(d(u)P(p)) \in \mathfrak{R}_n^\star$ and $q|_g$ being normal. Then

$$f = \phi_1(u,v) = P(d(u)P(p|_{P(P(r)d(s))})) - uP(p|_{P(P(r)d(s))}) + P(up|_{P(P(r)d(s))}) + \lambda P(d(u)p|_{P(P(r)d(s))})$$

and

$$q|_g = q|_{\phi_2(r,s)} = P(d(u)P(p|_{P(P(r)d(s))})) - P(d(u)P(p|_{P(r)s})) + P(d(u)P(p|_{P(rs)})) + \lambda P(d(u)P(p|_{P(rd(s))})).$$

So we have

$$(f,g)_w = f - q|_g = -\,uP(p|_{P(P(r)d(s))}) + P(up|_{P(P(r)d(s))}) + \lambda P(d(u)p|_{P(P(r)d(s))}) + P(d(u)P(p|_{P(r)s})) - P(d(u)P(p|_{P(rs)})) - \lambda P(d(u)P(p|_{P(rd(s))})). \tag{21}$$

From the definition of $\phi_1(u,v)$ and $\phi_2(r,s)$, we have

$$\begin{aligned}
-uP(p|_{P(P(r)d(s))}) &= -uP(p|_{\phi_2(r,s)}) - uP(p|_{P(r)s}) + uP(p|_{P(rs)}) + \lambda uP(p|_{P(rd(s))}),\\
P(up|_{P(P(r)d(s))}) &= P(up|_{\phi_2(r,s)}) + P(up|_{P(r)s}) - P(up|_{P(rs)}) - \lambda P(up|_{P(rd(s))}),\\
\lambda P(d(u)p|_{P(P(r)d(s))}) &= \lambda P(d(u)p|_{\phi_2(r,s)}) + \lambda P(d(u)p|_{P(r)s}) - \lambda P(d(u)p|_{P(rs)}) - \lambda^2 P(d(u)p|_{P(rd(s))}),\\
P(d(u)P(p|_{P(r)s})) &= \phi_1(u,p|_{P(r)s}) + uP(p|_{P(r)s}) - P(up|_{P(r)s}) - \lambda P(d(u)p|_{P(r)s}),\\
-P(d(u)P(p|_{P(rs)})) &= -\phi_1(u,p|_{P(rs)}) - uP(p|_{P(rs)}) + P(up|_{P(rs)}) + \lambda P(d(u)p|_{P(rs)}),\\
-\lambda P(d(u)P(p|_{P(rd(s))})) &= -\lambda\phi_1(u,p|_{P(rd(s))}) - \lambda uP(p|_{P(rd(s))}) + \lambda P(up|_{P(rd(s))}) + \lambda^2 P(d(u)p|_{P(rd(s))}).
\end{aligned} \tag{22}$$

From Eqs. (21) and (22), it follows that

$$(f,g)_w = -uP(p|_{\phi_2(r,s)}) + P(up|_{\phi_2(r,s)}) + \lambda P(d(u)p|_{\phi_2(r,s)}) + \phi_1(u,p|_{P(r)s}) - \phi_1(u,p|_{P(rs)}) - \lambda\phi_1(u,p|_{P(rd(s))}).$$

By Lemma 3.2, we have

$$uP(p|_{\phi_2(r,s)}),\ P(up|_{\phi_2(r,s)}),\ P(d(u)p|_{\phi_2(r,s)}) \in \mathrm{Id}(S_n)$$

and

$$\phi_1(u,p|_{P(r)s}),\ \phi_1(u,p|_{P(rs)}),\ \phi_1(u,p|_{P(rd(s))}) \in S_n \subseteq \mathrm{Id}(S_n).$$

Since

$$\overline{uP(p|_{\phi_2(r,s)})},\ \overline{P(up|_{\phi_2(r,s)})},\ \overline{P(d(u)p|_{\phi_2(r,s)})} <_n \overline{\phi_1(u,p|_{\phi_2(r,s)})} = \overline{\phi_1(u,v)} = w$$

and

$$\overline{\phi_1(u,p|_{P(r)s})},\ \overline{\phi_1(u,p|_{P(rs)})},\ \overline{\phi_1(u,p|_{P(rd(s))})} <_n \overline{\phi_1(u,p|_{\overline{\phi_2(r,s)}})} = \overline{\phi_1(u,v)} = w,$$

we conclude that $(f,g)_w \equiv 0 \bmod [S_n, w]$.

Next, we check that the ambiguity of composition $P(P(u)d(q|_{P(d(v)P(w))}))$ is trivial. This is the case when $w = \overline{f} = q|_{\overline{g}}$ for some $q = P(P(u)d(p))$ for some $p \in \mathfrak{R}_n^\star$. Then the two elements f and g of S_n are of the form

$$\begin{aligned}
f &= \phi_2(u,v) = P(P(u)d(v)) - P(u)v + P(uv) + \lambda P(ud(v)),\\
g &= \phi_1(r,s) = P(d(r)P(s)) - rP(s) + P(rs) + \lambda P(d(r)s),
\end{aligned}$$

where $\overline{f} = \overline{P(P(u)d(v))}$ and $\overline{g} = \overline{P(d(r)P(s))}$. Thus $v = p|_{\overline{g}} = p|_{\overline{\phi_1(r,s)}} = p|_{\overline{P(d(r)P(s))}}$ for some $p \in \mathfrak{R}_n^\star$ and

$$w = \overline{f} = \overline{\phi_2(u,v)} = \overline{P(P(u)d(v))} = \overline{P(P(u)d(p|_{\overline{g}}))} = \overline{q|_{\overline{g}}} = q|_{\overline{g}}$$

with $q = P(P(u)d(p)) \in \mathfrak{R}_n^\star$ and $q|_g$ being normal. Then

$$f = \phi_2(u,v) = P(P(u)d(p|_{P(d(r)P(s))})) - P(u)p|_{P(d(r)P(s))} + P(up|_{P(d(r)P(s))}) + \lambda P(ud(p|_{P(d(r)P(s))}))$$

and

$$q|_g = q|_{\phi_1(r,s)} = P(P(u)d(p|_{P(d(r)P(s))})) - P(P(u)d(p|_{rP(s)})) + P(P(u)d(p|_{P(rs)})) + \lambda P(P(u)d(p|_{P(d(r)s)})).$$

So we have

$$\begin{aligned}
(f,g)_w &= f - q|_g\\
&= -\,P(u)p|_{P(d(r)P(s))} + P(up|_{P(d(r)P(s))}) + \lambda P(ud(p|_{P(d(r)P(s))}))\\
&\quad + P(P(u)d(p|_{rP(s)})) - P(P(u)d(p|_{P(rs)})) - \lambda P(P(u)d(p|_{P(d(r)s)})).
\end{aligned} \tag{23}$$

By the definition of $\phi_1(r,s)$ and $\phi_2(u,v)$, we have

$$\begin{aligned}
-P(u)p|_{P(d(r)P(s))} &= -P(u)p|_{\phi_1(r,s)} - P(u)p|_{rP(s)} + P(u)p|_{P(rs)} + \lambda P(u)p|_{P(d(r)s)},\\
P(up|_{P(d(r)P(s))}) &= P(up|_{\phi_1(r,s)}) + P(up|_{rP(s)}) - P(up|_{P(rs)}) - \lambda P(up|_{P(d(r)s)}),\\
\lambda P(ud(p|_{P(d(r)P(s))})) &= \lambda P(ud(p|_{\phi_1(r,s)})) + \lambda P(ud(p|_{rP(s)})) - \lambda P(ud(p|_{P(rs)})) - \lambda^2 P(ud(p|_{P(d(r)s)})),\\
P(P(u)d(p|_{rP(s)})) &= \phi_2(u, p|_{rP(s)}) + P(u)p|_{rP(s)} - P(up|_{rP(s)}) - \lambda P(ud(p|_{rP(s)})),\\
-P(P(u)d(p|_{P(rs)})) &= -\phi_2(u, p|_{P(rs)}) - P(u)p|_{P(rs)} + P(up|_{P(rs)}) + \lambda P(ud(p|_{P(rs)})),\\
-\lambda P(P(u)d(p|_{P(d(r)s)})) &= -\lambda\phi_2(u, p|_{P(d(r)s)}) - \lambda P(u)p|_{P(d(r)s)} + \lambda P(up|_{P(d(r)s)}) + \lambda^2 P(ud(p|_{P(d(r)s)})).
\end{aligned}$$

Then Eq. (23) becomes

$$(f,g)_w = -P(u)p|_{\phi_1(r,s)} + P(up|_{\phi_1(r,s)}) + \lambda P(ud(p|_{\phi_1(r,s)})) + \phi_2(u, p|_{rP(s)}) - \phi_2(u, p|_{P(rs)}) - \lambda\phi_2(u, p|_{P(d(r)s)}).$$

From Lemma 3.2, we have

$$P(u)p|_{\phi_1(r,s)}, P(up|_{\phi_1(r,s)}), P(ud(p|_{\phi_1(r,s)})) \in \mathrm{Id}(S_n)$$

and

$$\phi_2(u, p|_{rP(s)}), \phi_2(u, p|_{P(rs)}), \phi_2(u, p|_{P(d(r)s)}) \in S_n \subseteq \mathrm{Id}(S_n).$$

Since

$$\overline{P(u)p|_{\phi_1(r,s)}},\ \overline{P(up|_{\phi_1(r,s)})},\ \overline{P(ud(p|_{\phi_1(r,s)}))} <_n \overline{\phi_2(u, p|_{\phi_1(r,s)})} = \overline{\phi_2(u,v)} = w$$

and

$$\overline{\phi_2(u, p|_{rP(s)})},\ \overline{\phi_2(u, p|_{P(rs)})},\ \overline{\phi_2(u, p|_{P(d(r)s)})} <_n \overline{\phi_2(u, p|_{\overline{\phi_1(r,s)}})} = \overline{\phi_2(u,v)} = w,$$

we have that $(f,g)_w \equiv 0 \mod [S_n, w]$.

We last check the ambiguity of composition $P(p|_{P(d(r)P(s))}v)$ is trivial. This is the case when $w = \overline{f} = \overline{q|_g}$, where $q = P(pv)$ for some $p \in \mathfrak{R}_n^\star$. Then f and g of S_n are of the form

$$\begin{aligned}
f &= \phi_1(p|_{P(d(r)P(s))}, v) = P(p|_{P(d(r)P(s))}v) + P(d(p|_{P(d(r)P(s))})P(v)) - p|_{P(d(r)P(s))}P(v) + \lambda P(d(p|_{P(d(r)P(s))})v)\\
g &= \phi_1(r,s) = P(d(r)P(s)) - rP(s) + P(rs) - \lambda P(d(r)s),
\end{aligned}$$

where $\overline{f} = \overline{P(p|_{P(d(r)P(s))}v)}$ and $\overline{g} = \overline{P(d(r)P(s))}$. Then

$$\begin{aligned}
(f,g)_w &= f - q|_g\\
&= P(d(p|_{P(d(r)P(s))})P(v)) - p|_{P(d(r)P(s))}P(v) + \lambda P(d(p|_{P(d(r)P(s))})v)\\
&\quad + P(p|_{rP(s)}v) - P(p|_{P(rs)}v) - \lambda P(p|_{P(d(r)s)}v).
\end{aligned} \tag{24}$$

Since

$$\begin{aligned}
P(d(p|_{P(d(r)P(s))})P(v)) &= P(d(p|_{\phi_1(r,s)})P(v)) + P(d(p|_{rP(s)})P(v)) - P(d(p|_{P(rs)})P(v)) - \lambda P(d(p|_{P(d(r)s)})P(v))\\
-p|_{P(d(r)P(s))}P(v) &= -p|_{\phi_1(r,s)}P(v) - p|_{rP(s)}P(v) + p|_{P(rs)}P(v) + \lambda p|_{P(d(r)s)}P(v)\\
\lambda P(d(p|_{P(d(r)P(s))})v) &= \lambda P(d(p|_{\phi_1(r,s)})v) + \lambda P(d(p|_{rP(s)})v) - \lambda P(d(p|_{P(rs)})v) - \lambda^2 P(d(p|_{P(d(r)s)})v)\\
P(p|_{rP(s)}v) &= \phi_1(p|_{rP(s)}, v) - P(d(p|_{rP(s)})P(v)) + p|_{rP(s)}P(v) - \lambda P(d(p|_{rP(s)})v)\\
-P(p|_{P(rs)}v) &= -\phi_1(p|_{P(rs)}, v) + P(d(p|_{P(rs)})P(v)) - p|_{P(rs)}P(v) + \lambda P(d(p|_{P(rs)})v)\\
-\lambda P(p|_{P(d(r)s)}v) &= -\lambda\phi_1(p|_{P(d(r)s)}, v) + \lambda P(d(p|_{P(d(r)s)})P(v)) - \lambda p|_{P(d(r)s)}P(v) + \lambda^2 P(d(p|_{P(d(r)s)})v),
\end{aligned}$$

Eq. (24) becomes

$$f - q|_g = P(d(p|_{\phi_1(r,s)})P(v)) - p|_{\phi_1(r,s)}P(v) + \lambda P(d(p|_{\phi_1(r,s)})v) + \phi_1(p|_{rP(s)}, v) - \phi_1(p|_{P(rs)}, v) - \lambda\phi_1(p|_{P(d(r)s)}, v).$$

From Lemma 3.2, we have

$$P(d(p|_{\phi_1(r,s)})P(v)),\ p|_{\phi_1(r,s)}P(v),\ P(d(p|_{\phi_1(r,s)})v) \in \mathrm{Id}(S_n)$$

and

$$\phi_1(p|_{rP(s)}, v), \phi_1(p|_{P(rs)}, v), \phi_1(p|_{P(d(r)s)}, v) \in S_n \subseteq \mathrm{Id}(S_n).$$

Since

$$\overline{P(d(p|_{\phi_1(r,s)})P(v))}, \overline{p|_{\phi_1(r,s)}P(v)}, \overline{P(d(p|_{\phi_1(r,s)})v)} <_n \overline{P(p|_{\phi_1(r,s)}v)} = \bar{f} = w$$

and

$$\overline{\phi_1(p|_{rP(s)}, v)}, \overline{\phi_1(p|_{P(rs)}, v)}, \overline{\phi_1(p|_{P(d(r)s)}, v)} <_n \overline{\phi_1(p|_{P(d(r)P(s))}, v)} = \overline{q|_g} = w,$$

we have that $(f, g)_w \equiv 0 \bmod [S_n, w]$.

With a similar argument, we can show the triviality of the ambiguities of the other compositions. □

By Lemmas 5.6, 5.7 and 5.8, it follows immediately that

Theorem 5.9. *S_n is a Gröbner-Shirshov basis in $\mathbf{k}\mathcal{R}_n$. Hence $\mathrm{Irr}(S_n)$ in Theorem 4.12 is a $\mathbf{k}$-basis of $\mathbf{k}\mathcal{R}_n/\mathrm{Id}(S_n)$.*

5.2. **Bases for free integro-differential algebras.** We next identify $\mathrm{Irr}(S_n)$ and thus obtaining a canonical basis of $\mathbf{k}\mathcal{R}_n/\mathrm{Id}(S_n)$.

For any $u, v \in M(\Delta_n X)$, let $u = u_1 \cdots u_\ell$ and $v = v_1 \cdots v_m$ with $u_i, v_j \in \Delta X, 1 \leq i \leq \ell, 1 \leq j \leq m$. Note that, by the definition of $<_n$, we have

$$u <_n v \Leftrightarrow \begin{cases} \ell < m, \\ \text{or } \ell = m \text{ and } \exists 1 \leq i_0 \leq \ell \text{ such that } u_i = v_i \text{ for } 1 \leq i < i_0 \text{ and } u_{i_0} < v_{i_0}, \end{cases}$$

We now introduce the key concept to identify $\mathrm{Irr}(S_n)$.

Definition 5.10. For any $u \in M(\Delta X)$, u has a unique decomposition

$$u = u_0 \cdots u_k, \text{ where } u_0, \cdots, u_k \in \Delta X.$$

Call u **functional** if either $u = 1$ or $u_k \in X$. Write

$$\mathcal{A}_f := \{u \in M(\Delta X) \,|\, u \text{ is functional }\},\ \mathcal{A}_{n,f} := \mathcal{A}_f \cap M(\Delta_n X)) \text{ and } A_f := \mathbf{k}\mathcal{A}_f.$$

Lemma 5.11. *$M(\Delta X) = \mathcal{A}_d \sqcup \mathcal{A}_f$ and $M(\Delta_n X) = \mathcal{A}_{n,d} \sqcup \mathcal{A}_{n,f}$.*

Proof. First we show that $\mathcal{A}_d \cap \mathcal{A}_f = \emptyset$. Let $\overline{d(u)} \in \mathcal{A}_d$ with $u \in S(\Delta X)$. Suppose $u = u_0 \cdots u_k$, where $u_0, \cdots, u_k \in \Delta X$. Then by Lemma 5.2, we have $\overline{d(u)} = u_0 \cdots u_{k-1} d(u_k)$. So $\overline{d(u)} \notin \mathcal{A}_f$. Next we show that $M(\Delta X) = \mathcal{A}_d \cup \mathcal{A}_f$. Let $u \in M(\Delta X) \setminus \mathcal{A}_f$. From the definition of being functional, we may suppose that

$$u = u_0 \cdots u_{k-1} u_k, \text{ where } u_0, \cdots, u_{k-1} \in \Delta X, u_k \in \Delta X \setminus X.$$

Suppose $u_k = x^{(\ell)}$ for some $x \in X$ and $\ell \geq 1$. Let $v = u_0 \cdots u_{k-1} x^{(\ell-1)}$. By Lemma 5.2, we have $u = \overline{d(v)} \in \mathcal{A}_d$. Hence $M(\Delta X) = \mathcal{A}_d \sqcup \mathcal{A}_f$.

Since $M(\Delta_n X) \subseteq M(\Delta X)$ and $M(\Delta X) = \mathcal{A}_d \sqcup \mathcal{A}_f$, we have that $M(\Delta_n X) = \mathcal{A}_{n,d} \sqcup \mathcal{A}_{n,f}$. □

We now give the notion to identify the canonical basis of $\mathbf{k}\mathcal{R}(\Delta X)/I_{\mathrm{Id}}$. Write $\mathcal{A}^0_{n,f} := \mathcal{A}_{n,f} \setminus \{1\}$.

Definition 5.12. Let $\mathcal{B}(\Delta_n X)$ denote the subset of $\mathcal{R}_n$ consisting of those $w \in \mathcal{R}_n$ with

(a) if w has a subword $P(u_1 u_2 P(u_3))$ with $u_1, u_3 \in \mathcal{R}_n$ and $u_2 \in S(\Delta_n X)$, then u_2 is in $\mathcal{A}^0_{n,f}$;

(b) if w has a subword $P(P(u_1) u_2 u_3)$ with $u_1, u_2 \in \mathcal{R}_n$ and $u_3 \in S(\Delta_n X)$, then u_3 is in $\mathcal{A}^0_{n,f}$.

The subset $\mathcal{R}_n$ can be defined by the following recursion based on the observation that restrictions on an element in $\mathcal{B}(\Delta_n X)$ is imposed only to its subwords inside P.

For a nonempty set Y and nonempty subsets U and V of $\mathfrak{M}(Y)$, define the following subset of $\Lambda(U,V)$:

$$\Lambda'(U,V) := \left(\bigcup_{r\geq 0}(UP(V))^r U\right) \bigcup \left(\bigcup_{r\geq 0}(UP(V))^r \mathcal{A}^0_{n,f} P(V)\right)$$
$$\bigcup \left(\bigcup_{r\geq 0}(P(V)U)^r P(V)\mathcal{A}^0_{n,f} P(V)\right) \bigcup \left(\bigcup_{r\geq 0}(P(V)U)^r P(V)\mathcal{A}^0_{n,f}\right).$$

We define a sequence $\mathcal{B}_m := \mathcal{B}(\Delta_n X)_m, m \geq 0$, by taking

$$\mathcal{B}_0 := \mathcal{B}'_0 := M(\Delta_n X),$$

and for $m \geq 0$, recursively defining

$$\mathcal{B}_{m+1} := \Lambda(S(\Delta_n X), \mathcal{B}'_m),\ \mathcal{B}'_{m+1} := \Lambda'(S(\Delta_n X), \mathcal{B}'_m).$$

Then $\mathcal{B}_m$, $m \geq 0$, define an increasing sequence and we define

$$\mathcal{B}(\Delta_n X) := \varinjlim \mathcal{B}_m = \cup_{m\geq 0}\mathcal{B}_m.$$

Proposition 5.13. *We have*

$$\operatorname{Irr}(S_n) = \mathcal{B}(\Delta_n X) \setminus \left\{ q|_s \,\middle|\, q \in \mathcal{R}^\star_n, s \in \epsilon(\Delta_n X) \text{ and } q|_s \text{ is normal} \right\}.$$

Proof. By Theorems 4.12 and 5.9, we have

$$\operatorname{Irr}(S_n) = \mathcal{R}_n \setminus \left\{ q|_s \,\middle|\, q \in \mathcal{R}^\star_n, s \in \left\{ \overline{\phi_1(u,v)}, \overline{\phi_2(u,v)} \,\middle|\, u,v \in \mathcal{R}_n \right\} \text{ and } q|_s \text{ is normal} \right\}.$$

By Proposition 5.5, we have

$$\left\{ \overline{\phi_1(u,v)}, \overline{\phi_2(u,v)} \,\middle|\, u,v \in \mathcal{R}_n \right\} = P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n)) \cup P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}) \cup \epsilon(\Delta_n X).$$

The first and second union components correspond to restrictions imposed in items (a) and (b) of Definition 5.12 respectively.

$$\mathcal{B}(\Delta_n X) = \mathcal{R}_n \setminus \left\{ q|_s \,\middle|\, q \in \mathcal{R}^\star_n, s \in P(\mathcal{R}_n\mathcal{A}_{n,d}P(\mathcal{R}_n)) \cup P(P(\mathcal{R}_n)\mathcal{R}_n\mathcal{A}_{n,d}), q|_s \text{ is normal} \right\}.$$

Thus we have

$$\operatorname{Irr}(S_n) = \mathcal{B}(\Delta_n X) \setminus \left\{ q|_s \,\middle|\, q \in \mathcal{R}^\star_n, s \in \epsilon(\Delta_n X) \text{ and } q|_s \text{ is normal} \right\},$$

and the proposition follows. □

Let

$$S := \{\phi_1(u,v), \phi_2(u,v) \mid u,v \in \mathcal{R}(\Delta X)\} \tag{25}$$

be the set of generators corresponding to the integration by parts axiom Eq. (4). Then, with a similar argument to Eq.(16), we have $d(S) \subseteq S$.

Lemma 5.14. *Let $I_{\mathrm{ID},n}$ (resp. I_{ID}) be the differential Rota-Baxter ideal of $\mathbf{k}\mathcal{R}_n$ (resp. $\mathbf{k}\mathcal{R}(\Delta X)$) generated by S_n (resp. S). Then as $\mathbf{k}$-modules we have $I_{\mathrm{ID},1} \subseteq I_{\mathrm{ID},2} \subseteq \cdots \subseteq I_{\mathrm{ID}} = \cup_{n\geq 1} I_{\mathrm{ID},n}$ and $I_{\mathrm{ID},n} = I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n$.*

Proof. Since $S_n \subseteq S_{n+1}$ and $\mathbf{k}\mathcal{R}_n \subseteq \mathbf{k}\mathcal{R}_{n+1}$ for any $n \geq 1$, we have $I_{\mathrm{ID},1} \subseteq I_{\mathrm{ID},2} \subseteq \cdots$ and $I_{\mathrm{ID}} = \cup_{n\geq 1} I_{\mathrm{ID},n}$. We next show $I_{\mathrm{ID},n} = I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n$. Obviously, $I_{\mathrm{ID},n} \subseteq I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n$. So we only need to verify $I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n \subseteq I_{\mathrm{ID},n}$. By Theorem 5.9, we have $\mathbf{k}\mathcal{R}_n = \mathbf{k}\mathrm{Irr}(S_n) \oplus I_{\mathrm{ID},n}$. Also $\mathbf{k}\mathrm{Irr}(S_1) \subseteq \mathbf{k}\mathrm{Irr}(S_2) \subseteq \cdots$. Let $n \geq 1$ and $k \geq 0$. Since $\mathbf{k}\mathrm{Irr}(S_{n+k}) \cap I_{\mathrm{ID},n+k} = 0$ and $\mathbf{k}\mathrm{Irr}(S_n) \subseteq \mathbf{k}\mathrm{Irr}(S_{n+k})$, we have $\mathbf{k}\mathrm{Irr}(S_n) \cap I_{\mathrm{ID},n+k} = 0$. Since $I_{\mathrm{ID},n} \subseteq I_{\mathrm{ID},n+k}$, by the modular law we have

$$I_{\mathrm{ID},n+k} \cap \mathbf{k}\mathcal{R}_n = I_{\mathrm{ID},n+k} \cap (\mathbf{k}\mathrm{Irr}(S_n) \oplus I_{\mathrm{ID},n}) = (I_{\mathrm{ID},n+k} \cap \mathbf{k}\mathrm{Irr}(S_n)) \oplus I_{\mathrm{ID},n} = I_{\mathrm{ID},n}. \tag{26}$$

Let $u \in I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n$. By $I_{\mathrm{ID}} = \cup_{n\geq 1} I_{\mathrm{ID},n}$, we have $u \in I_{\mathrm{ID},N}$ for some $N \in \mathbb{Z}_{\geq 1}$. If $N \geq n$, then $u \in I_{\mathrm{ID},N} \cap \mathbf{k}\mathcal{R}_n = I_{\mathrm{ID},n}$ by Eq. (26). If $N < n$, then $u \in I_{\mathrm{ID},N} \subseteq I_{\mathrm{ID},n}$. Hence $I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n \subseteq I_{\mathrm{ID},n}$ and so $I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n = I_{\mathrm{ID},n}$. □

Still assuming that X is finite, we define

$$\mathcal{R}(\Delta X)_f := \varinjlim \mathcal{B}(\Delta_n X).$$

Write $\mathcal{A}_f^0 := \mathcal{A}_f \setminus \{1\}$. Then by Definition 5.12, $\mathcal{R}(\Delta X)_f \subseteq \mathcal{R}(\Delta X)$ consists of $w \in \mathcal{R}(\Delta X)$ with the properties that

(a) if w has a subword $P(u_1u_2P(u_3))$ with $u_1, u_3 \in \mathcal{R}(\Delta X)$ and $u_2 \in S(\Delta X)$, then u_2 is in $\mathcal{A}_f^0$;
(b) if w has a subword $P(P(u_1)u_2u_3)$ with $u_1, u_2 \in \mathcal{R}(\Delta X)$ and $u_3 \in S(\Delta X)$, then u_3 is in $\mathcal{A}_f^0$.

Now we are ready to prove the main result of this paper.

Theorem 5.15. *Let X be a nonempty well-ordered set, $\mathbf{k}\mathcal{R}(\Delta X)$ the free differential Rota-Baxter algebra on X and I_{ID} the ideal of $\mathbf{k}\mathcal{R}(\Delta X)$ generated by S defined in Eq. (25). Then the composition*

$$\mathbf{k}\mathcal{R}(\Delta X)_f \hookrightarrow \mathbf{k}\mathcal{R}(\Delta X) \to \mathbf{k}\mathcal{R}(\Delta X)/I_{\mathrm{ID}}$$

of the inclusion and the quotient map is a linear isomorphism. In other words, as $\mathbf{k}$-modules

$$\mathbf{k}\mathcal{R}(\Delta X) \cong \mathbf{k}\mathcal{R}(\Delta X)_f \oplus I_{\mathrm{ID}}.$$

Proof. First assume that X is a finite ordered set. By Theorem 4.12 and Lemma 5.14 we have

$$\mathbf{k}\mathrm{Irr}(S_n) \cong \mathbf{k}\mathcal{R}_n/I_{\mathrm{ID},n} = \mathbf{k}\mathcal{R}_n/(I_{\mathrm{ID}} \cap \mathbf{k}\mathcal{R}_n) \cong (\mathbf{k}\mathcal{R}_n + I_{\mathrm{ID}})/I_{\mathrm{ID}}$$

From Proposition 5.13 we have

$$\mathcal{B}(\Delta_n X) \hookrightarrow \mathrm{Irr}(S_{n+1}) \hookrightarrow \mathcal{B}(\Delta_{n+1} X).$$

Thus when n goes to infinity, we have $\varinjlim \mathcal{B}(\Delta_n X) = \varinjlim \mathrm{Irr}(S_n)$. Therefore we have

$$\mathbf{k}\mathcal{R}(\Delta X)_f = \varinjlim (\mathbf{k}\mathcal{B}(\Delta_n X)) = \varinjlim (\mathbf{k}\mathrm{Irr}(S_n)) \cong \varinjlim ((\mathbf{k}\mathcal{R}_n + I_{\mathrm{ID}})/I_{\mathrm{ID}}) = \mathbf{k}\mathcal{R}(\Delta X)/I_{\mathrm{ID}},$$

since $\varinjlim \mathcal{R}_n = \mathcal{R}(\Delta X)$.

Now let X be a given nonempty well-ordered set and $u \in \mathbf{k}\mathcal{R}(\Delta X)$. Then there is a finite *ordered* subset $Y \subseteq X$ such that u is in $\mathbf{k}\mathcal{R}(\Delta Y)$. Then by the case of finite sets proved above, $u \in \mathbf{k}\mathcal{R}(\Delta Y)_f + I_{Y,\mathrm{ID}}$. By definition, we have $\mathbf{k}\mathcal{R}(\Delta Y)_f \subseteq \mathbf{k}\mathcal{R}(\Delta X)_f$ and $I_{Y,\mathrm{ID}} \subseteq I_{\mathrm{ID}}$. Hence $u \in \mathbf{k}\mathcal{R}(\Delta X)_f + I_{\mathrm{ID}}$. This proves $\mathbf{k}\mathcal{R}(\Delta X) = \mathbf{k}\mathcal{R}(\Delta X)_f + I_{\mathrm{ID}}$.

Further, if $0 \neq u$ is in I_{ID}, then there is a finite ordered subset $Y \subseteq X$ such that u is in $I_{Y,\mathrm{ID}}$. Thus $u \notin \mathbf{k}\mathcal{R}(\Delta Y)_f$ since $\mathbf{k}\mathcal{R}(\Delta Y)_f \cap I_{Y,\mathrm{ID}} = 0$. By the definition of $\mathbf{k}\mathcal{R}(\Delta X)_f$, we have $\mathbf{k}\mathcal{R}(\Delta Y) \cap \mathbf{k}\mathcal{R}(\Delta X)_f = \mathbf{k}\mathcal{R}(\Delta Y)_f$. Therefore $u \notin \mathbf{k}\mathcal{R}(\Delta X)_f$. This proves $\mathbf{k}\mathcal{R}(\Delta X) = \mathbf{k}\mathcal{R}(\Delta X)_f \oplus I_{X,\mathrm{ID}}$. □

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