THE CALCULUS OF VIRTUAL SPECIES AND $\mathbb{K}$-SPECIES.

by

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Introduction

In [3], Joyal introduces the category of species together with several operations such as $+, \cdot, \times, \circ$ and $'$. In [4], he states the substitution rule for virtual species. In this paper, we develop a method for proving the correctness of this rule; we also further study and extend some aspects of the theory of virtual species. In particular, we will

(1) Show that the ring of virtual species (resp d-species) is a unique factorization domain (**UFD**).

(2) Give a relation between $\times$ and $\circ$.

(3) Extend all the identities involving $+, \cdot, \times, \circ, '$, 0 and 1 to the setting of virtual species and, more generally, $\mathbb{K}$-species.

(4) Give some $\mathbb{K}$-species which are analogues of the logarithm and trigonometric functions.

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Chapter I : Background

§ I.1. Algebra

In this paper, "ring" always means commutative ring with 1.

Definition I.1.1. $(\mathbb{K}, 0, 1, +, \cdot)$ is a **half-ring** iff $(\mathbb{K}, +)$ and $(\mathbb{K}, \cdot)$ are commutative monoids and the two "distributive" laws: (1) $(a+b)c = ac + bc$; (2) $0c = 0$ hold in $\mathbb{K}$.

If $\mathbb{K}$ is a half-ring and $(\mathbb{M}, \cdot)$ is a monoid with the property that for each $m \in \mathbb{M}$, there are only finitely many pairs (m_1, m_2) such that $m = m_1 m_2$, then the set of all functions $f: \mathbb{M} \to \mathbb{K}$, denoted $\mathbb{K}[[\mathbb{M}]]$, gets a half-ring structure with pointwise addition and multiplication by convolution:

$$(f \cdot g)(m) \quad = \quad \sum_{m=m_1 \cdot m_2} f(m_1)\, g(m_2).$$

Obviously, $\mathbb{K}[[\mathbb{M}]]$ is a ring iff $\mathbb{K}$ is a ring. The map $\mathbb{M} \to \mathbb{K}[[\mathbb{M}]]$ sending each m to its characteristic function is an embedding of monoids if $\mathbb{K} \neq 0$, and it is customary to identify $\mathbb{M}$ with its image, and to write $\sum_{m \in \mathbb{M}} f(m)\, m$ instead of f, when this is convenient.

Let K, H be two groups of permutations of the finite sets F, E respectively. The **wreath product** $K \wr H$ is defined to be the group of permutations t of the set $F \times E$ which are of the form $t(f,e) = (\alpha(e)(f), h(e))$ where α is a function: $E \to K$ and $h \in H$. Thus t is determined by an element of H and a function α. So $|K \wr H| = |K|^{|E|} . |H|$. If G is a group of permutations of a set D, then $(K \wr H) \wr G = K \wr (H \wr G)$.

Example I.1.2. $2^{\S} \wr 2^{\S} = \mathbf{D}_4$ where $\mathbf{D}_4$ is the dihedral group of order 8.

Definition I.1.3. ([13]) Let $H \subset E_1^{\S} \times E_2^{\S} \times \cdots \times E_r^{\S}$ and $K_i \subset F_i^{\S}$ for $1 \leq i \leq r$. The **wreath product** $(K_1, K_2, \ldots, K_r) \wr H$ is defined to be the group of permutations t of the set $F_1 \times E_1 + F_2 \times E_2 + \cdots + F_r \times E_r$, which are of the form: For $1 \leq i \leq r$, $t(f_i, e_i) = (\varphi_i(e_i)(f_i), h(e_i))$ where φ_i is a function $E_i \to K_i$ and $h \in H$. Thus t is determined by an element of H and functions φ_i where $1 \leq i \leq r$.

So

$$|(K_1, K_2, \ldots, K_r) \wr H| \; = \; |K_1|^{|E_1|} . |K_2|^{|E_2|} \cdots |K_r|^{|E_r|} . |H| .$$

Given a finite set E, a partition π of E is a family E_i of non-empty subsets of E such that $E_i \cap E_j = \emptyset$ if $i \neq j$ and $\cup E_i = E$. Two partitions are equal iff they have the same elements. Let P[E] denote the set of all partitions of E. Let $\Sigma \underline{E}$ denote the disjoint union of $E_1, E_2, \ldots, E_d$ where $\underline{E} = (E_1, E_2, \ldots, E_d) \in \mathbf{B}^d$; We write $\Sigma \underline{E} = E_1 + E_2 + \cdots + E_d$.

§ I.2. Commutative algebra.

Definition I.2.1. ([13]). Let $\mathbb{R}$ be a ring. The **length** of any element r in $\mathbb{R}$, $\ell(r)$, is defined by: (a) $\ell(0) = \infty$; (b) $\ell(r) = 0$ if r is a unit; (c) otherwise, $\ell(r) = \sup\{k \mid r = x_1 \cdot x_2 \cdots x_k$ with x_i non-zero and non-unit$\}$.

Definition I.2.2. ([13]). Let $\mathbb{R}$ and $\mathbb{S}$ be two rings. A ring homomorphism $f: \mathbb{R} \to \mathbb{S}$ is called **local** if $f(r)$ unit in $\mathbb{S}$ implies r unit in $\mathbb{R}$ and is called **unit-surjective** if s unit in $\mathbb{S}$ implies $\exists\, r \in \mathbb{R}$ with $f(r) = s$.

Let $(\mathbb{R}_n)_{n\in\mathbb{N}}$ be a sequence of **UFD**'s and $(\alpha_n)_{n\in\mathbb{N}}$ be a sequence of local, unit-surjecive ring homomorphisms where $\alpha_n: \mathbb{R}_{n+1} \to \mathbb{R}_n$, and let $\langle \mathbb{R}, (\varphi_n)_{n\in\mathbb{N}} \rangle$ be the inverse limit of $\langle (\mathbb{R}_n)_{n\in\mathbb{N}}, (\alpha_n)_{n\in\mathbb{N}} \rangle$ where φ_n is the canonical homomorphism from $\mathbb{R}$ to $\mathbb{R}_n$. In fact φ_n is a local unit-surjective ring homomorphism. We often write r_n instead of $\varphi_n(r)$ for all $r \in \mathbb{R}$.

Proposition I.2.3. The inverse limit $\mathbb{R}$ of a sequence $\mathbb{R}_n$ of **UFD**'s and local, unit-surjective homomorphisms is an **UFD**.

Proof. Every non-zero and non-unit element r in $\mathbb{R}$ can be factored into a finite product of irreducible elements since $\ell(r) \le \ell(r_n)$ $\forall n$. If $r \in \mathbb{R}$ and $\ell(r) = 1$ then $\lim_{n\to\infty} \ell(r_n) = 1$. It can be proved that every irreductible element in $\mathbb{R}$ is a prime. So $\mathbb{R}$ is an **UFD**.

Proposition I.2.4. Let $(\mathbb{M}, \cdot)$ be a free commutative monoid and $\mathbb{R}$ be an **UFD** then $\mathbb{R}[\mathbb{M}]$ and $\mathbb{R}[[\mathbb{M}]]$ are **UFD**'s.

Chapter II : The concepts of species and $\mathbb{K}$-species

§ II.1. Group Sets

If X is a finite set, a permutation of X is a bijective map $g: X \to X$. Under the operation of composition, the set of all permutations of X forms a group $X\,\mathfrak{S}$. We have $|X\mathfrak{S}| = |X|!$, where we use $|\ |$ to denote cardinality. If G is a subgroup of $X\mathfrak{S}$, then we shall say that the pair (G,X) is a **group-set**. A subset Y of X is called a **G-invariant** subset if $g(Y) \subset Y$ for any $g \in G$. Let (G,X) be a group-set, U be a finite set containing X, and Y be a G-invariant subset of X. For any $g \in G$, the **extension of** g **to** U, g^U, is defined by: $g^U(u) = g(u)$ if $u \in X$; $g^U(u) = u$ otherwise. The **restriction of** g **to** Y, g_Y, is defined by: $g_Y(y) = g(y)$ if $y \in Y$. We denote $G^U = \{g^U \mid g \in G\}$ and $G_Y = \{g_Y \mid g \in G\}$.

Under the operation of composition, G^U and G_Y form groups and (G^U, U), (G_Y,Y) are group-sets. Since Y is a G-invariant subset of X, then $X - Y$ is a G-invariant subset of X and $(G_{X-Y}, X-Y)$ is a group-set.

Definition II.1.1 ([13]). Let (G,X) and (H,Y) be two group-sets. (H,Y) is called a **reducing group-set** of (G,X) if it satisfies the following conditions:

(a) Y is a G-invariant subset of X; (b) $H = G_Y$; (c) $H^X \subset G$.

Definition II.1.2 ([13]). Let (H,Y) and (K,Z) be two group-sets, then

(a) For any $h \in H$ and $k \in K$, let $h * k \in (Y+Z)!$ be defined by: $(h * k)(u) = h(u)$ if $u \in Y$; $(h*k)(u) = k(u)$ if $u \in Z$.
(b) Let $H * K$ denote the subgroup $\{h * k | h \in H, k \in K\}$ of $(Y + Z)!$.
(c) The group-set $(H * K, Y + Z)$ is called **external product** of the two group-sets (H,Y) and (K,Z) and is denoted : $(H * K, Y + Z) = (H,Y) * (K,Z)$.

From definition I.2, we find the group $H*K$ is the direct product of H^{Y+Z} and K^{Y+Z}. It is easy to check that the external product, $*$, satisfies the associative law.

Lemma II.1.3. If (G_Y,Y) is a reducing group-set of (G,X), then

(a) $(G_{X-Y}, X-Y)$ is a reducing group-set of (G,X); (b) $(G,X) = (G_Y,Y) * (G_{X-Y}, X-Y)$.

Lemma II.1.4. Let (G_Y,Y), (G_Z,Z) be two reducing group-sets of (G,X), then so is $(G_{Y\cap Z}, Y\cap Z)$.

Lemma II.1.5. If (H,Y) is a reducing group-set of (G,X) and (K,Z) is a reducing group-set of (H,Y), then (K,Z) is reducing group-set of (G,X).

Definition II.1.6. ([13]) A group-set (G,X) is called an **atomic group-set** if $X \neq \emptyset$ and (G,X) has no non-empty proper reducing group-set.

Proposition II.1.7. Every group-set (G,X) can be decomposed uniquely into an external product of atomic group-sets.

Let (G,X) and (H,Y) be two group-sets. We write $(G,X) \sim (H,Y)$ if there exists a bijection $f: Y \longrightarrow X$ such that $f^{-1}Gf = H$. It is easy to prove that $\sim$ is an equivalence relation. Let $\mathcal{G}$ be the set of equivalence classes of group - sets. We have:

Proposition II.1.8. $(\mathcal{G}, \cdot)$ is a free monoid.

§ II.2. Species

Let ***Sets*** be the category of (small) sets and maps and **B** be the category of finite sets and bijections.

Definition II.2.1 ([3]). A **species** is a functor $S: \mathbf{B} \to$ ***Sets***; and a **morphism** τ from species S to species T is a natural transformation from functor S to functor T.

If there is an isomorphism τ from species S to species T, then we write $S \approx T$. (and use the notation $S = T$ when we work "up to an isomorphism"). In what follows, the symbol S will be used sometimes to represent a species, and some other times to represent it's isomorphism class. The usage at a particular point in the text should be clear from the context. For any $E \in \mathbf{B}$ and any species S we write $S[E]$ for the image of E under S. Every element in $S[E]$ is called an S - structure on E.

The reader is referred to [3] (or [5]) for the definitions of the sum $S + T$, product $S \cdot T$, cartesian product $S \times T$, derivative S', and substitution $S \circ T$ (if $T[\varnothing] = \varnothing$), of two species S and T. They are summarized as follows:

Definition II.2.2 ([3]). For any $E \in \mathbf{B}$,

(a) $(S + T)[E] = S[E] + T[E]$ (b) $(S \cdot T)[E] = \sum_{E = E_1 + E_2} S[E_1] \times T[E_2]$.

(c) $(S \times T)[E] = S[E] \times T[E]$ (d) $S'[E] = S[E + 1]$

(d) $(S \circ T)[E] = \sum_{\pi \in P[E]} S[\pi] \times \prod_{C \in \pi} T[C]$

where $P[E]$ is the set of all partitions of E.

A species S is called a **subspecies** of the species U if $S[E] \subset U[E]$ for all finite sets E and the inclusion is a natural transformation. It is obvious that if S is a subspecies of U then there exists a unique species T such that $U = S + T$.

Example II.2.3. The zero species, 0, is defined by: $0[E] = \varnothing$ for any finite set E. 0 is the unit element for addition.

Example II.2.4. $1 = \mathbf{B}(\varnothing,-)$, so the species 1 satisfies $1[E] = \varnothing$ for any non-empty finite set E and $1[\varnothing] = \{*\}$; i.e. there is a unique 1-structure on the empty set. 1 is the unit element for multipliction.

Example II.2.5. $X = \mathbf{B}(\{*\},-)$, so $X[E] = \{*\}$ if $|E| = 1$; $X[E] = \varnothing$ if $|E| \neq 1$.

Example II.2.6. For $n \in \mathbb{N}$, write $\mathbf{n} = \{1, 2, ..., n\}$. We have $X^n = \mathbf{B}(\mathbf{n},-) = X \cdot X \cdots X$. More generally, let $H \subset \mathbf{n}!$; then we use X^n/H to denote the species $\mathbf{B}(\mathbf{n},-)/H$, i.e. $X^n/H[E]$ = the set of all "left cosets" of H in $\mathbf{B}(\mathbf{n}, E)$ where $\mathbf{B}(\mathbf{n}, E)$ is the set of all bijections from $\mathbf{n}$ to E ($\mathbf{B}(\mathbf{n}, E)$ is not a group). In fact $X^n/H[\mathbf{n}]$ = the set of all left cosets of H in $\mathbf{n}!$.

Example II.2.7. The exponential species $e^X = \mathbf{B}(-, \{*\})$ is defined by: $e^X[E] = \{*\}$ for any finite set E, i.e. there is a unique e^X-structure on any finite set. We have:

$$e^X = \sum_{n \geq 0} X^n / \mathbf{n}! \ .$$

A species U is called a **molecule** if $U \neq 0$, and $U = S + T$ implies either $S = 0$ or $T = 0$. Every species is a (possibly infinite) sum of its molecular subspecies. The molecules are of the type :

$$X^n/H \quad \text{where } H \text{ is a subgroup of } \mathbf{n}! \ .$$

It is easy to prove that $X^n/H = X^m/K$ iff $n = m$ and H, K are conjugate in $\mathbf{n}!$. Let $\mathcal{M}$ denote the set of isomorphism classes of all molecular species and $\mathcal{M}^*$ denote the set of isomorphism classes of all non-constant molecular species.

Proposition II.2.8 ([13]). Let $n, m \in \mathbb{N}$, $H \subset \mathbf{n}!$ and $K \subset \mathbf{m}!$, then:

(1) $X^n/H \cdot X^m/K = X^{n+m}/(H*K)$ where " $*$ " is the external product.

(2) $X^n/H \times X^m/K = \begin{cases} \sum_L |L|\,|A_L|\, X^n/L & \text{if } n = m; \text{ where } A_L = \{g \in \mathbf{n}! \mid gHg^{-1} \cap K = L\}. \\ 0 & \text{otherwise,} \end{cases}$

(3) $X^n/H \circ X^m/K = X^{mn}/(K \wr H)$ where " $\wr$ " is the wreath product.

(4) $(X^n/H)' = \sum_{e \in O_{n.H}} X^n/(H \cap (\mathbf{n}-\{e\})!)$ where $O_{n.H}$ denotes a complete set of representatives for the orbits of H in $\mathbf{n}$.

By propositions II.1.8 and II.2.8, we have

Proposition II.2.9. $(\mathcal{M}, \cdot)$ is a free commutative monoid.

Definition II.2.10. ([13]). A species S is called **finitary** if $S[E]$ is finite for all $E \in \mathbf{B}$. A finitary species S is called **strictly finite** if $\exists\, n > 0$ such that $S[E] = \emptyset$ for all $E \in \mathbf{B}$ with $|E| > n$.

The set of all finitary species (resp strictly finite species) forms a half-ring which is isomorphic to $\mathbb{N}[[\mathfrak{M}]]$ (resp $\mathbb{N}[\mathfrak{M}]$). The universal ring **V** (resp **SV**) containing this is called **the ring of virtual species** (or **$\mathbb{Z}$-species**). Every element in **V** can be represented as $S - T$ where S and T are two species. The ring **V** (resp **SV**) is isomorphic to $\mathbb{Z}[[\mathfrak{M}]]$ (resp $\mathbb{Z}[\mathfrak{M}]$). From propositions II.2.4 and II.2.9, we have

Theorem II.2.11. These two rings $\mathbb{Z}[[\mathfrak{M}]]$ and $\mathbb{Z}[\mathfrak{M}]$ are **UFD's.**

There are many identities involving $+, \cdot, \times, \circ, ', 0$ and 1 ([3],[5],[13]). Let S, T and U be species, then

(i) $(S + T) \circ U = (S \circ U) + (T \circ U)$;
(ii) $(S \cdot T) \circ U = (S \circ U) \cdot (T \circ U)$;
(iii) $(S \circ T) \circ U = S \circ (T \circ U)$;
(iv) $(S + T)' = S' + T'$;
(v) $(S \cdot T)' = S' \cdot T + S \cdot T'$;
(vi) $(S \times T)' = S' \times T'$;
(vii) $(S \circ T)' = (S' \circ T) \cdot T'$
... etc.

One objective is to extend all these identities to the setting of $\mathbb{K}$-species. This is done in chapter three.

§ II.3. d-species.

Definition II.3.1 ([3]). Let d be an integer > 0. A **d-species** is a functor $S: \mathbf{B}^d \longrightarrow$ ***Sets***; and a **morphism** τ from d-species S to d-species T is a natural transformation τ from functor S to functor T.

Let S, T be d-species and $T_1, T_2, \ldots, T_d$ be r-species (where $d, r \in \mathbb{N}$). The <u>sum</u> $S + T$, <u>product</u> $S \cdot T$, <u>cartesian product</u> $S \times T$, <u>partial derivatives</u> $(\partial S/\partial X_i)$, $1 \le i \le d$, and <u>substitution</u> $S \circ (T_1, T_2, \ldots, T_d)$ are defined as follows :

Definition II.3.2 ([3]). For any $\underline{E} = (E_1, E_2, \ldots, E_d) \in \mathbf{B}^d$ and $\underline{A} = (A_1, \ldots, A_r) \in \mathbf{B}^r$, define

(a) $(S + T)[\underline{E}] = S[\underline{E}] + T[\underline{E}]$
(b) $(S \cdot T)[\underline{E}] = \sum_{\underline{E} = \underline{D} + \underline{F}} S[\underline{D}] \times T[\underline{F}]$

where $\underline{E} = \underline{D} + \underline{F}$ means $E_i = D_i + F_i$ for $1 \le i \le d$,

(c) $(S \times T)[\underline{E}] = S[\underline{E}] \times T[\underline{E}]$
(d) $(\partial S/\partial X_i)[\underline{E}] = S[\underline{E} + \underline{e}_i]$

where $\underline{e}_i = (F_1, F_2, \ldots, F_d)$ with $F_i = \{*\}$ and $F_j = \varnothing$ if $i \neq j$, $1 \le i, j \le d$,

(d) $S \circ (T_1, \ldots, T_d)[\underline{A}] = \sum_{\pi \in P[\underline{A}]} \sum_{f: \pi \to \mathbf{d}} S[(f^{-1}(1), \ldots, f^{-1}(d)] \times \prod_{C \in \pi} T_{f(C)}[C \cap A_1, \ldots, C \cap A_r]$

where $P[\underline{A}]$ denotes the set of all partitions of $A_1 + \cdots + A_d$.

Example II.3.3. $X_i = \mathbf{B}^d(\underline{e}_i,-)$ where $\underline{e}_i = (F_1,F_2,\dots,F_d)$ with $F_i = \{*\}$ and $F_j = \varnothing$ if $i \neq j$. For $\underline{E} = (E_1,E_2,\dots,E_d) \in \mathbf{B}^d$, $X_i[\underline{E}] = \{*\}$ if $E_i = \underline{e}_i$; $X_i[\underline{E}] = \varnothing$ otherwise.

Example II.3.4. $X_1^{n_1} \cdot X_2^{n_2} \cdots X_d^{n_d} = \mathbf{B}^d(\underline{\mathbf{n}},-)$ where $\underline{\mathbf{n}} = (\mathbf{n}_1,\mathbf{n}_2,\dots,\mathbf{n}_d)$. and $\mathbf{B}^d(\underline{\mathbf{n}},\underline{E})$ is the set of all $(f_1,f_2,\dots,f_d)$ where all f_i are bijections from $\mathbf{n}_i$ to E_i. Note that $\mathbf{B}^d(\underline{\mathbf{n}},\underline{E})$ is empty unless $|E_i| = n_i$ for all i. More generally, let $H \subset \mathbf{n}_1! \times \mathbf{n}_2! \times \cdots \times \mathbf{n}_d!$, then $(X_1^{n_1} \cdot X_2^{n_2} \cdots X_d^{n_d}/H)[\underline{E}]$ is the set of all "left cosets" of H in $\mathbf{B}^d(\underline{\mathbf{n}},\underline{E})$; we often use $X_1^{n_1} \cdot X_2^{n_2} \cdots X_d^{n_d}/H$ to denote the d-species $\mathbf{B}^d(\underline{\mathbf{n}},-)/H$.

As in the single variable case, every d-species is uniquely a (possibly infinite) sum of its molecular d-subspecies. The molecular d-species are of the type:

$$X_1^{n_1} \cdot X_2^{n_2} \cdots X_d^{n_d}/H \qquad \text{where} \quad H \subset \mathbf{n}_1! \times \mathbf{n}_2! \times \cdots \times \mathbf{n}_d!.$$

Let $\mathfrak{M}_d$ be the set of all isomorphism classes of molecular d-species.

Definition II.3.5 ([13]). Let $n_i, m_i \in \mathbb{N}$ for $1 \le i \le d$, $H \subset \mathbf{n}_1! \times \cdots \times \mathbf{n}_d!$, $K \subset \mathbf{m}_1! \times \cdots \times \mathbf{m}_d!$. For any $h = (h_1, \dots, h_d) \in H$, $k = (k_1, \dots, k_d) \in K$ (h_i and k_i are the restriction of h, k to $\mathbf{n}_i$, $\mathbf{m}_i$ respectively for $1 \le i \le d$) and $u = (u_1,u_2,\dots,u_d) \in (\mathbf{n}_1+\mathbf{m}_1) \times \dots \times (\mathbf{n}_d+\mathbf{m}_d)$, we define: $(h *_d k)(u) = (g_1(u_1), g_2(u_2), \dots, g_d(u_d))$ where $g_i(u_i) = h_i(u_i)$ if $u_i \in \mathbf{n}_i$; $g_i(u_i) = k_i(u_i)$ if $u_i \in \mathbf{m}_i$ for $1 \le i \le d$, and $H *_d K = \{h *_d k \mid h \in H \text{ and } k \in K\}$.

From the above definition , we have

$$(X_1^{n_1} \cdots X_d^{n_d}/H) \cdot (X_1^{m_1} \cdots X_d^{m_d}/K) = X_1^{n_1+m_1} \cdots X_d^{n_d+m_d}/(H *_d K).$$

Lemma II.3.6. $(\mathfrak{M}_d, \cdot)$ is a free commutative monoid.

Theorem II.3.7. The ring of virtual finitary species $\mathbf{Z}[[\mathfrak{M}_d]]$ and the ring of virtual strictly finite species $\mathbf{Z}[\mathfrak{M}_d]$ are **UFD**'s.

Proposition II.3.8 ([13]). Let $n_i, m_i \in \mathbb{N}$, $K_i \subset \mathbf{m}_i!$ for $1 \le i \le d$, $H \subset \mathbf{n}_1! \times \cdots \times \mathbf{n}_d!$, and $K \subset \mathbf{m}_1! \times \cdots \times \mathbf{m}_d!$, then

$$(X_1^{n_1} \cdots X_d^{n_d}/H) \circ (X_1^{m_1}/K_1, \cdots, X_d^{m_d}/K_d) = (X_1^{n_1 m_1 + \cdots + n_d m_d}/(K_1, \dots, K_d) \wr H)$$

$$(X_1^{n_1} \cdots X_d^{n_d}/H) \times (X_1^{m_1} \cdots X_d^{m_d}/K) = \begin{cases} \sum_L |L| \cdot |A_{d,L}| \cdot (X_1^{n_1} \cdots X_d^{n_d}/L) & \text{if } m_i = n_i \text{ for } 1 \le i \le d; \\ 0 & \text{if } m_i \neq n_i \text{ for some i.} \end{cases}$$

where $A_{d,L} = \{ g \in \mathbf{n}_1! \times \mathbf{n}_2! \times \cdots \times \mathbf{n}_d! \mid gHg^{-1} \cap K = L \}$.

Just as in the case of one variable, there are many identities involving the operations $+, \cdot, \times, \circ$ and $'$ in d-species ([3]). We can also extend those identities of d-variable species to the setting of d-variable $\mathbb{K}$-species.

§ II.4. $\mathbb{K}$-species.

Let $\mathbb{K}$ be a half-ring. We can extend the operations $+, \cdot, \times$ and $'$ to the set

$$\mathbb{K}[[\mathfrak{M}]] = \{ \sum_{T\in\mathfrak{M}} a_T T \mid a_T \in \mathbb{K} \}$$

as follows:

$$\begin{array}{llcl}
(a) & (\sum_{T\in\mathfrak{M}} a_T T) + (\sum_{T\in\mathfrak{M}} b_T T) & = & \sum_{T\in\mathfrak{M}} (a_T + b_T) T \\
(b) & (\sum_{T\in\mathfrak{M}} a_T T) \cdot (\sum_{S\in\mathfrak{M}} b_S S) & = & \sum_{T,S\in\mathfrak{M}} (a_T \cdot b_S)(T \cdot S) \\
(c) & (\sum_{T\in\mathfrak{M}} a_T T) \times (\sum_{S\in\mathfrak{M}} b_S S) & = & \sum_{T,S\in\mathfrak{M}} (a_T \cdot b_S)(T \times S) \\
(d) & (\sum_{T\in\mathfrak{M}} a_T T)' & = & \sum_{T\in\mathfrak{M}} a_T T'.
\end{array}$$

Of course, the terms must be collected on the right sides of (b), (c), (d). It is possible to do so because: given a molecular species M, there are only finitely many pairs of molecular species (S,T) such that $M = S \cdot T$, finitely many pairs of molecular species (U,V) such that M is a subspecies of $U \times V$, and finitely many molecular species W such that M is a subspecies of W'.

Let σ be the unique half-ring homomorphism: $\mathbb{N} \to \mathbb{K}$; then σ induces a half-ring homomorphism $\hat{\sigma}$: $\mathbb{N}[[\mathfrak{M}]] \to \mathbb{K}[[\mathfrak{M}]]$. The homomorphism preserves $+$, $\cdot$, $\times$ and $'$. We hope to extend the concept of substitution, $\circ$, to $\mathbb{K}[[\mathfrak{M}]]$ in such a way that $\hat{\sigma}$ preserves $\circ$ and all the identities involving $+$, $\cdot$, $\times$, $\circ$, $'$ continue to hold.

Unfortunately it cannot succeed for all half-rings. For example:

(1) Let $\mathbb{K} = \mathbb{F}_2$, then $(X^2/2\mathfrak{y})\circ(X+X) = (X^2/2\mathfrak{y})\circ(0) = 0$, but $(X^2/2\mathfrak{y})\circ(X+X) = (X^2/2\mathfrak{y}) + X^2 + (X^2/2\mathfrak{y}) = X^2$. This is a contradiction.

(2) Let $\mathbb{K} = \mathbb{Z}[i]$. Let $(X^2/2\mathfrak{y})\circ(iX) = aX^2 + b(X^2/2\mathfrak{y})$ since $\deg((X^2/2\mathfrak{y})\circ(iX)) = 2$. (Here we are assuming a bit more about the extended substitution, namely that degrees multiply under substitution of $\mathbb{K}$-species of the form scalar times molecule.) More detailed computations show that $(a,b) = (i,(-1-i)/2)$ or $(i,(-1+i)/2)$. This is a contradiction since $b \notin \mathbb{Z}[i]$.

For examples above, we want $\binom{i}{2} = (-1-i)/2 \in \mathbb{K}$ if $i \in \mathbb{K}$. This suggests that some special half-rings, "binomial half-rings", will satisfy our desire.

Definition II.4.1 ([13]). A half-ring $\mathbb{K}$ is called a **binomial half-ring** if

(a) there exists a $\mathbb{Q}$-algebra $\mathbb{L}$ containing $\mathbb{K}$, and
(b) for every $a \in \mathbb{K}$ and $i \in \mathbb{N}$, $\binom{a}{i} = a(a-1)(a-2)\cdots(a-i+1)/i! \in \mathbb{K}$.

For example $\mathbb{N}$, $\mathbb{Z}$, $\mathbb{Q}$, $\mathbb{R}$, $\mathbb{C}$, $\mathbb{Q}[i]$ and $\mathbb{N} + \mathbb{Q}\varepsilon$ $(\varepsilon^2 = 0)$ are all binomial half-rings, but $\mathbb{F}_p$, p prime, and $\mathbb{Z}[i]$ are not binomial half-rings.

Definition II.4.2 ([13]). Let $\mathbb{K}$ be a binomial half-ring. A $\mathbb{K}$ - **species** is an element S of $\mathbb{K}[[\mathcal{M}]]$, i.e. a formal linear combination of the molecular species with coefficients in $\mathbb{K}$.

The concepts of species (resp. virtual species) and $\mathbb{N}$-species (resp. $\mathbb{Z}$-species) coincide.

Chapter III: The calculus of $\mathbb{K}$-species

§ III.1. Extension of substitution to $\mathbb{K}$-species.

In this section, $\mathbb{K}$ is a given binomial half-ring. We will define the operation $\circ$ for $\mathbb{K}$-species and prove that the identities in chapter II involving $\circ$ continue to hold.

Proposition III.1.1. Let T_1 and T_2 be two species, then $e^{T_1 + T_2} = e^{T_1} \cdot e^{T_2}$.

Notation III.1.2. a) Let $\mathbb{L}$ be a $\mathbb{Q}$-algebra, $a \in \mathbb{L}$ and $r_1, r_2, \ldots, r_n \in \mathbb{N}$. We write

$$\binom{a}{r_1, r_2, \ldots, r_n} = a(a-1)\cdots(a-\Sigma r+1) / r_1!\, r_2! \cdots r_n!$$

where Σr means $r_1 + r_2 + \cdots + r_n$.

b) Let $(p_j)_{j \in J}$ be a family of formal variables. We denote by $\mathbb{N}[\binom{p_j}{i}]$ the sub half-ring of $\mathbb{Q}[(p_j)_{j \in J}]$ generated by the polynomials $\binom{p_j}{i}$, $j \in J$, $i \in \mathbb{N}$.

Remark III.1.3. If $f((p_j)_{j \in J}) \in \mathbb{N}[\binom{p_j}{i}]$ and $(a_j)_{j \in J}$ is an arbitrary family of elements of the binomial half-ring $\mathbb{K}$, then $f((a_j)_{j \in J}) \in \mathbb{K}$.
We also have

$$\binom{a}{r_1, r_2, \ldots, r_n} = \binom{\Sigma r}{r_1, r_2, \ldots, r_n}\binom{a}{\Sigma r} \in \mathbb{N}[\binom{a}{i}].$$

Corollary III.1.4. For all $n \in \mathbb{N}$,

$$\mathbf{e}^{nX} = (\mathbf{e}^X)^n = \sum_{k\geq 0} \sum_{r_1+2r_2+\ldots+kr_k=k} \binom{n}{r_1, r_2, \ldots, r_k} (X/\mathbf{1}!)^{r_1} \cdot (X^2/\mathbf{2}!)^{r_2} \cdots (X^k/\mathbf{k}!)^{r_k}$$

$$= \sum_{M\in\mathfrak{M}} g_M(n)\, M$$

where all r_i are non-negative integers and all $g_M(p) \in \mathbb{N}[\binom{p}{i}]$.

Proposition III 1.5. $S \times \mathbf{e}^{nX} = S \circ (nX)$ for all $n \in \mathbb{N}$.

Proof. It is easy to show that for any $E \in \mathbf{B}$,

$$(S \circ (nX))[E] = S[E] \times \mathbf{n}^E$$

In particular for $S = \mathbf{e}^X$, this gives $\mathbf{e}^{nX}[E] = \mathbf{n}^E$. Substituting this back into the above equality gives

$$(S \circ (nX))[E] = S[E] \times \mathbf{e}^{nX}[E].$$

Naturality in E is easily verified, so the proof is completed. □

Lemma III 1.6. $(\sum_{A\in\mathfrak{M}_d} a_A A) \cdot (\sum_{A\in\mathfrak{M}_d} b_A A) = \sum_{A\in\mathfrak{M}_d} c_A A$, where $c_A = \sum_{A_1 \cdot A_2 = A} a_{A_1} b_{A_2}$ is a finite sum.

Lemma III 1.7. $(\sum_{A\in\mathfrak{M}_d} a_A A) \times (\sum_{A\in\mathfrak{M}_d} b_A A) = \sum_{A\in\mathfrak{M}_d} c_A A$, where $c_A = \sum_{A_1, A_2} n_{A,A_1,A_2} a_{A_1} b_{A_2}$ is a finite sum, with $n_{A,A_1,A_2} \in \mathbb{N}$ defined by $A_1 \times A_2 = \sum_{A\in\mathfrak{M}_d} n_{A,A_1,A_2} A$.

Proposition III 1.8. Let S be a species and $n\in\mathbb{N}$, then $S(nX) = \sum_{M\in\mathfrak{M}} f_M(n) M$ for some $f_M(p) \in \mathbb{N}[\binom{p}{i}]$.

Now, we can extend proposition III 1.8 to $\mathbb{K}$ - species:

Definition III 1.9. Let $\mathbb{K}$ be a binomial half-ring, $a \in \mathbb{K}$ and S be a $\mathbb{K}$-species. Then $S(aX) = \sum_{M\in\mathfrak{M}} f_M(a)\, M$ with $f_M(p)$ defined in proposition III 1.8.

Tables 4 and 5 give $S(-X)$ and $S(nX)$ for molecular species of small degree.

Lemma III 1.10. $X_1^{n_1} \cdots X_d^{n_d}/H \circ (X_1^{m_1}/K_1, \ldots, X_d^{m_d}/K_d) = X^{m_1 n_1 + m_2 n_2 + \cdots + m_d n_d}/((K_1, K_2, \cdots, K_d) \wr H)$ where $n_i, m_i \in \mathbb{N}$, $K_i \subset \mathbf{m}_i!$ for $1 \leq i \leq d$, and $H \subset \mathbf{n}_1! \times \mathbf{n}_2! \times \cdots \times \mathbf{n}_d!$.

Corollary III 1.11. Let $T_1, T_2, \ldots, T_d$ be d-species, then $e^{T_1+T_2+\ldots+T_d} = e^{T_1} \cdot e^{T_2} \ldots e^{T_d}$.

Lemma III 1.12. $e^X \circ (n_1 X_1 + \cdots + n_d X_d) = \sum_{A\in\mathfrak{M}_d} f_A(n_1, \ldots, n_d)\, A$

Similar arguments prove all the identites involving +, ·, ×, ∘, ', 0 and 1. Substitution for several-variable $\mathbb{K}$-species is defined in the analogous way and identities from actual species can be lifted to these by arguments similar to the one variable case.

§ III.2. The $\mathbb{K}$-species SIN, COS, and LG.

The trigonometric functions, cos x and sin x have properties such as $(\sin x)' = \cos x$, $(\cos x)' = -\sin x$ and $\sin^2 x + \cos^2 x = 1$. Here we try to find some special $\mathbb{K}$-species which have similar properties.

In fact, we can't find any $\mathbb{Z}$-species (=virtual species) which have the properties above. Suppose S and C are two $\mathbb{Z}$-species with $S_0 = 0$, $C_0 = 1$ such that $S' = C$, $C' = -S$ and $S \cdot S + C \cdot C = 1$.

Let $S = a_1X + a_2X^2 + a_3X^2/2! + \cdots$ and $C = 1 + b_1X + b_2X^2 + b_3X^2/2! + \cdots$. We have:

(i) $a_1 + (2a_2 + a_3)X + \ldots = 1 + b_1X + \cdots$, since $S' = C$;
(ii) $b_1 + (2b_2 + b_3)X + \ldots = -(a_1X + \cdots)$, since $C' = -S$;
(iii) $1 + 2b_1X + (a_1^2 + b_1^2 + 2b_2)X^2 + 2b_3X^2/2! + \cdots = 1$, since $S \cdot S + C \cdot C = 1$.

Comparing the coefficients of each molecular species on both sides, we have: $a_1 = 1$, $b_1 = 0$, and $a_1^2 + b_1^2 + 2b_2 = 1 + 2b_2 = 0$. This is a contradiction since $b_2 \notin \mathbb{Z}$.

Definition III.2.1. Let $\mathbb{K}$ be a binomial ring containing $\mathbb{Q}$, then

$$\mathbf{COS}\,X = 1/2\,(e^{iX} + e^{-iX}) \qquad \text{and} \qquad \mathbf{SIN}\,X = -i/2\,(e^{iX} + e^{-iX}).$$

Of course, in this definition, e^{iX} and e^{-iX} are both computed by substituting **i** for n in corollary III.1.4. Let the ring homomorphism $\sigma\colon \mathbb{Q}[\mathbf{i}] \to \mathbb{Q}[\mathbf{i}]$ be defined by: $a + b\mathbf{i} \mapsto a - b\mathbf{i}$. The induced homomorphism $\hat{\sigma}\colon \mathbb{Q}[\mathbf{i}][[\mathfrak{M}]] \to \mathbb{Q}[\mathbf{i}][[\mathfrak{M}]]$ fixes species **SIN** and species **COS**. So **SIN, COS** $\in \mathbb{Q}[[\mathfrak{M}]]$.

Proposition III.2.2. Let S be a $\mathbb{Z}$-species with $S_0 = 0$. If $e^X \circ S = 1$ then $S = 0$.

Proof. $1 = e^X \circ S = \sum_{n \geq 0} \sum_{r_1 + 2r_2 + \cdots + nr_n = n} ((X^{r_1}/r_1!) \circ (S_1)) \cdot ((X^{r_2}/r_2!) \circ (S_2)) \cdots ((X^{r_n}/r_n!) \circ (S_n))$ where $r_i \geq 0$ for all i. Comparing terms of degree n on both sides gives:

$$0 = \sum_{r_1 + 2r_2 + \cdots + nr_n = n} ((X^{r_1}/r_1!) \circ (S_1)) \cdot ((X^{r_2}/r_2!) \circ (S_2)) \cdots ((X^{r_n}/r_n!) \circ (S_n))$$

The n-th equation has highest term S_n (from $r_1 = \ldots = r_{n-1} = 0$, $r_n = 1$) and all lower where $f_A(p_1,\dots,p_d) \in \mathbb{N}[\binom{p_i}{j}]_{1\le i\le d}$

Lemma III.1.13. For any $n_1,n_2,\dots,n_d \in \mathbb{N}$ and d-species S, we have:

$$S \circ (n_1X_1, n_2X_2,\dots,n_dX_d) = S \times (e^X \circ (n_1X_1+\dots+n_dX_d)).$$

Lemma III.1.14. Let $M_1,\dots,M_d \in \mathfrak{M}^*$, then $(\sum_{A\in\mathfrak{M}_d} a_A A)\circ(M_1,\dots,M_d) = \sum_{B\in\mathfrak{M}} c_B B$ where $c_B = \sum (a_A \mid A \in \mathfrak{M}_d,\ A \circ (M_1, M_2, \dots, M_d) = B)$, a finite sum.

Lemma III.1.15. Let T be species, $A_j\in\mathfrak{M}^*$ for $1 \le j \le d$. Then we have $T\circ(n_1A_1+\dots+n_dA_d) = \sum_{B\in\mathfrak{M}} f_B(n_1,n_2,\dots,n_d)\, B$, where $f_B(p_1,p_2,\dots,p_d) \in \mathbb{N}[\binom{p_j}{i}]_{1\le j\le d}$ for all $B \in \mathfrak{M}$.

Remark III.1.16. Let S be a species and $S \circ (\sum_{A\in\mathfrak{M}} n_A A) = \sum_{B\in\mathfrak{M}} f_B((n_A)_{A\in\mathfrak{M}})\, B$ where f_B depends only on S and on the n_A's with $\deg A \le \deg B$. So we have:

Proposition III.1.17. Let T be a species, then

$$T \circ (\sum_{A\in\mathfrak{M}^*} n_A A) = \sum_{B\in\mathfrak{M}} f_B((n_A)_{A\in\mathfrak{M}})\, B \quad \text{where} \quad f_B((p_A)_{A\in\mathfrak{M}}) \in \mathbb{N}[\binom{p_A}{j}]_{A\in\mathfrak{M}}.$$

Definition III.1.18 ([13]). Let $\mathbb{K}$ be a binomial half-ring and S, T be two $\mathbb{K}$-species with $T = \sum_{A\in\mathfrak{M}^*} n_A A$ for $n_A\in \mathbb{K}$. The **substitution** of T in S, $S\circ T$, is defined by

$$\sum_{B\in\mathfrak{M}} f_B((n_A)_{A\in\mathfrak{M}})\, B \quad \text{with} \quad f_B((p_A)_{A\in\mathfrak{M}}) \text{ given in proposition III.1.17.}$$

If S is a $\mathbb{K}$-species, then $S = \sum_{n\in\mathbb{N}} \sum_H a_{nH} \cdot X^n/H$ where $a_{nH} \in \mathbb{K}$ and H ranges over representatives for the conjugacy classes of subgroups of $\mathbf{n}!$. S_n denotes the n-th term of the outer sum. (If S is an actual species, then $S_n[E] = S[E]$ if $|E| = n$; $S_n[E] = \emptyset$ if $|E| \ne n$.)

Theorem III.1.19. Let S, T and U be $\mathbb{K}$-species with $T_0 = U_0 = 0$, then

$$(S \circ T) \circ U = S \circ (T \circ U)$$

Proof. Let $S = \sum_{A\in\mathfrak{M}} s_A A$, $T = \sum_{B\in\mathfrak{M}} t_B B$ and $U = \sum_{C\in\mathfrak{M}} u_C C$. We have

$$(S \circ T) \circ U = \sum_{M\in\mathfrak{M}} f_M((s_A,t_B,u_C)_{A,B,C\in\mathfrak{M}})M, \quad S \circ (T \circ U) = \sum_{M\in\mathfrak{M}} g_M((s_A,t_B,u_C)_{A,B,C\in\mathfrak{M}})M$$

where $f_M((p_A,q_B,r_C)_{A,B,C\in\mathfrak{M}}),\ g_M((p_A,q_B,r_C)_{A,B,C\in\mathfrak{M}}) \in \mathbb{N}[\binom{p_A}{i},\binom{q_B}{j},\binom{r_C}{k}]_{A,B,C\in\mathfrak{M}}$.

By associativity of substitution for actual species, f_M and g_M agree when natural number are substituted for p_A, q_B and r_C, and hence they agree when arbitrary elements of $\mathbb{K}$ are substituted. □

terms involve only $S_1, S_2, \ldots, S_{n-1}$. The system of equations can be solved recursively. We have $S_n = 0$ for $n \geq 1$. i.e. $S = 0$. □

Corollary III.2.3. Let S, T be two $\mathbb{Z}$-species such that $S_0 = T_0 = 0$ and $e^X \circ S = e^X \circ T$ then $S = T$.

Definition III.2.4. The species $\mathbf{LG} = \sum_{k \geq 0} S_k$ is recursively defined by

$$S_0 = 0, \qquad S_1 = -X$$

and

$$\sum_{r_1+2r_2+\cdots+nr_n = n} ((X^{r_1}/\mathbf{r}_1!)\circ(S_1))\cdot((X^{r_2}/\mathbf{r}_2!)\circ(S_2))\cdots((X^{r_n}/\mathbf{r}_n!)\circ(S_n)) = 0, \quad n \geq 2.$$

Proposition III.2.5. $e^X \circ \mathbf{LG}\, X = 1 - X$.

Let $\mathbf{V}_i = \{T \in \mathbb{Z}[[\mathfrak{M}]] \mid T_0 = i\}$ then $T \mapsto e^T$ $(= e^X \circ T)$ gives a group homomorphism exp: $(\mathbf{V}_0, +) \rightarrow (\mathbf{V}_1, \cdot)$. From the propositions III.1.1, III.2.2 and III.2.5, we know that exp is a group isomorphism and that its inverse log is given by: $T \mapsto \mathbf{LG}(1 - T)$ (log is not a species).

Proposition III.2.6. $\mathbf{LG}(1 - S \cdot T) = \mathbf{LG}(1 - S) + \mathbf{LG}(1 - T)$ for any $S, T \in \mathbf{V}_1$.

NOTATION FOR TABLES

$\mathbf{n}!$ = The group of all permutations on $\mathbf{n}$; A_n = The group of all even permutations on $\mathbf{n}$; C_n = The cyclic subgroup of $\mathbf{n}!$ generated by (12...n); D_n = The dihedral group of order 2n; A·B = The direct product of group A and group B; K_4 = {id,(12)(34),(13)(24),(14)(23)}; H = {id, (12)(34)}; L = {id,(123),(132),(12)(45),(13)(45),(23)(45)} = $A_5 \cap$ Stabilizer {4,5}; T = The normalizer of C_5 = The affine group $\{ax + b \mid a,b \in \mathbb{F}_5, a \neq 0\}$ = {id, (12345), (13524), (14253), (15432), (2354), (25)(34), (2453), (1534), (13)(45), (1435), (1452), (15)(24), (1254), (1523), (12)(35), (1325), (1243), (14)(23), (1342)}.

The cartesian product between molecular species of degree ≤ 3

$X \times X = X$		
$X^2 \times X^2 = 2X^2$	$X^2 \times X^2/\mathbf{2}! = X^2$	$X^2/\mathbf{2}! \times X^2/\mathbf{2}! = X^2/\mathbf{2}!$
$X^3 \times X^3 = 6X^3$	$X^3 \times X^3/\mathbf{2}! = 3X^3$	$X^3 \times X^3/A_3 = 2X^3$
$X^3 \times X^3/\mathbf{3}! = X^3$		
$X^3/\mathbf{2}! \times X^3/\mathbf{2}! = X^3/\mathbf{2}! + X^3$	$X^3/\mathbf{2}! \times X^3/A_3 = X^3$	$X^3/\mathbf{2}! \times X^3/\mathbf{3}! = X^3/\mathbf{2}!$
$X^3/A_3 \times X^3/A_3 = 2X^3/A_3$	$X^3/A_3 \times X^3/\mathbf{3}! = X^3/A_3$	$X^3/\mathbf{3}! \times X^3/\mathbf{3}! = X^3/\mathbf{3}!$

Table I

The cartesian product between molecular species of degree 4

× cartesian product	$\frac{X^4}{4\underset{\cdot}{\nabla}}$	$\frac{X^4}{A_4}$	$\frac{X^4}{D_4}$	$\frac{X^4}{3\underset{\cdot}{\nabla}}$	$\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}$	$\frac{X^4}{K_4}$	$\frac{X^4}{C_4}$	$\frac{X^4}{A_3}$	$\frac{X^4}{2\underset{\cdot}{\nabla}}$	$\frac{X^4}{H}$	X^4
$\frac{X^4}{4\underset{\cdot}{\nabla}}$	$\frac{X^4}{4\underset{\cdot}{\nabla}}$	$\frac{X^4}{A_4}$	$\frac{X^4}{D_4}$	$\frac{X^4}{3\underset{\cdot}{\nabla}}$	$\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}$	$\frac{X^4}{K_4}$	$\frac{X^4}{C_4}$	$\frac{X^4}{A_3}$	$\frac{X^4}{2\underset{\cdot}{\nabla}}$	$\frac{X^4}{H}$	X^4
$\frac{X^4}{A_4}$	$\frac{X^4}{A_4}$	$2\frac{X^4}{A_4}$	$\frac{X^4}{K_4}$	$\frac{X^4}{A_3}$	$\frac{X^4}{H}$	$2\frac{X^4}{K_4}$	$\frac{X^4}{H}$	$2\frac{X^4}{A_3}$	X^4	$2\frac{X^4}{H}$	$2X^4$
$\frac{X^4}{D_4}$	$\frac{X^4}{D_4}$	$\frac{X^4}{K_4}$	$\frac{X^4}{D_4}+\frac{X^4}{K_4}$	$\frac{X^4}{2\underset{\cdot}{\nabla}}$	$\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}+\frac{X^4}{H}$	$3\frac{X^4}{K_4}$	$\frac{X^4}{C_4}+\frac{X^4}{H}$	X^4	$\frac{X^4}{2\underset{\cdot}{\nabla}}+X^4$	$3\frac{X^4}{H}$	$3X^4$
$\frac{X^4}{3\underset{\cdot}{\nabla}}$	$\frac{X^4}{3\underset{\cdot}{\nabla}}$	$\frac{X^4}{A_3}$	$\frac{X^4}{2\underset{\cdot}{\nabla}}$	$\frac{X^4}{3\underset{\cdot}{\nabla}}+\frac{X^4}{2\underset{\cdot}{\nabla}}$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}$	X^4	X^4	$\frac{X^4}{A_3}+X^4$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}+X^4$	$2X^4$	$4X^4$
$\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}$	$\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}$	$\frac{X^4}{H}$	$\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}+\frac{X^4}{H}$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}$	$2\frac{X^4}{2\underset{\cdot}{\nabla}2\underset{\cdot}{\nabla}}+X^4$	$3\frac{X^4}{H}$	$X^4+\frac{X^4}{H}$	$2X^4$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}+2X^4$	$2\frac{X^4}{H}+2X^4$	$6X^4$
$\frac{X^4}{K_4}$	$\frac{X^4}{K_4}$	$2\frac{X^4}{K_4}$	$3\frac{X^4}{K_4}$	X^4	$3\frac{X^4}{H}$	$6\frac{X^4}{K_4}$	$3\frac{X^4}{H}$	$2X^4$	$3X^4$	$6\frac{X^4}{H}$	$6X^4$
$\frac{X^4}{C_4}$	$\frac{X^4}{C_4}$	$\frac{X^4}{H}$	$\frac{X^4}{C_4}+\frac{X^4}{H}$	X^4	$X^4+\frac{X^4}{H}$	$3\frac{X^4}{H}$	$2\frac{X^4}{C_4}+X^4$	$2X^4$	$3X^4$	$2X^4+2\frac{X^4}{H}$	$6X^4$
$\frac{X^4}{A_3}$	$\frac{X^4}{A_3}$	$2\frac{X^4}{A_3}$	X^4	$\frac{X^4}{A_3}+X^4$	$2X^4$	$2X^4$	$2X^4$	$2\frac{X^4}{A_3}+2X^4$	$4X^4$	$4X^4$	$8X^4$
$\frac{X^4}{2\underset{\cdot}{\nabla}}$	$\frac{X^4}{2\underset{\cdot}{\nabla}}$	X^4	$\frac{X^4}{2\underset{\cdot}{\nabla}}+X^4$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}+X^4$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}+2X^4$	$3X^4$	$3X^4$	$4X^4$	$2\frac{X^4}{2\underset{\cdot}{\nabla}}+5X^4$	$6X^4$	$12X^4$
$\frac{X^4}{H}$	$\frac{X^4}{H}$	$2\frac{X^4}{H}$	$3\frac{X^4}{H}$	$2X^4$	$2\frac{X^4}{H}+2X^4$	$6\frac{X^4}{H}$	$2X^4+2\frac{X^4}{H}$	$4X^4$	$6X^4$	$4\frac{X^4}{H}+4X^4$	$12X^4$
X^4	X^4	$2X^4$	$3X^4$	$4X^4$	$6X^4$	$6X^4$	$6X^4$	$8X^4$	$12X^4$	$12X^4$	$24X^4$

Table 2

The derivative of molecular species of degree ≤ 5

Molecular	Derivative	Molecular	Derivative
1	0	X^5	$5X^4$
X	1	X^5/H	$X^4/H + 2X^4$
X^2	$2X$	$X^5/2\underset{\circ}{\nabla}$	$3X^4/2\underset{\circ}{\nabla} + X^4$
$X^2/2\underset{\circ}{\nabla}$	X	X^5/A_3	$2X^4/A_3 + X^4$
X^3	$3X^2$	X^5/C_4	$X^4/C_4 + X^4$
$X^3/2\underset{\circ}{\nabla}$	$X^2/2\underset{\circ}{\nabla} + X^2$	X^5/K_4	$X^4/K_4 + X^4$
X^3/A_3	X^2	$X^5/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}$	$X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla} + 2X^4/2\underset{\circ}{\nabla}$
$X^3/3\underset{\circ}{\nabla}$	$X^2/2\underset{\circ}{\nabla}$	X^5/C_5	X^4
X^4	$4X^3$	X^5/L	$X^4/A_3 + X^4/H$
X^4/H	$2X^3$	$X^5/A_3\cdot 2\underset{\circ}{\nabla}$	$X^4/A_3 + X^4/2\underset{\circ}{\nabla}$
$X^4/2\underset{\circ}{\nabla}$	$2X^3/2\underset{\circ}{\nabla} + X^3$	$X^5/3\underset{\circ}{\nabla}$	$2X^4/3\underset{\circ}{\nabla} + X^4/2\underset{\circ}{\nabla}$
X^4/A_3	$X^3/A_3 + X^3$	X^5/D_4	$X^4/D_4 + X^4/2\underset{\circ}{\nabla}$
X^4/C_4	X^3	X^5/D_5	X^4/H
X^4/K_4	X^3	$X^5/2\underset{\circ}{\nabla}\cdot 3\underset{\circ}{\nabla}$	$X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla} + X^4/3\underset{\circ}{\nabla}$
$X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}$	$2X^3/2\underset{\circ}{\nabla}$	X^5/A_4	$X^4/A_4 + X^4/A_3$
$X^4/3\underset{\circ}{\nabla}$	$X^3/3\underset{\circ}{\nabla} + X^3/2\underset{\circ}{\nabla}$	X^5/T	X^4/C_4
X^4/D_4	$X^3/2\underset{\circ}{\nabla}$	$X^5/4\underset{\circ}{\nabla}$	$X^4/3\underset{\circ}{\nabla} + X^4/4\underset{\circ}{\nabla}$
X^4/A_4	X^3/A_3	X^5/A_5	X^4/A_4
$X^4/4\underset{\circ}{\nabla}$	$X^3/3\underset{\circ}{\nabla}$	$X^5/5\underset{\circ}{\nabla}$	$X^4/4\underset{\circ}{\nabla}$

Table 3

The substitution of $-X$ in molecular species of degree ≤ 5

$1\circ(-X) = 1$	$X\circ(-X) = -X$
$X^2\circ(-X) = X^2$	$X^2/2\underset{\circ}{\nabla}\circ(-X) = X^2 - X^2/2\underset{\circ}{\nabla}$
$X^3\circ(-X) = -X^3$	$X^3/2\underset{\circ}{\nabla}\circ(-X) = X^3/2\underset{\circ}{\nabla} - X^3$
$X^3/A_3\circ(-X) = -X^3/A_3$	$X^3/3\underset{\circ}{\nabla}\circ(-X) = 2X^3/2\underset{\circ}{\nabla} - X^3 - X^3/3\underset{\circ}{\nabla}$
$X^4\circ(-X) = X^4$	$X^4/H\circ(-X) = X^4/H$
$X^4/2\underset{\circ}{\nabla}\circ(-X) = X^4 - X^4/2\underset{\circ}{\nabla}$	$X^4/A_3\circ(-X) = X^4/A_3$
$X^4/C_4\circ(-X) = X^4/H - X^4/C_4$	$X^4/K_4\circ(-X) = 3X^4/H - X^4 - X^4/K_4$
$X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}\circ(-X) = X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla} + X^4 - 2X^4/2\underset{\circ}{\nabla}$	$X^4/3\underset{\circ}{\nabla}\circ(-X) = X^4/3\underset{\circ}{\nabla} + X^4 - 2X^4/2\underset{\circ}{\nabla}$
$X^4/D_4\circ(-X) = X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla} + X^4/H - X^4/2\underset{\circ}{\nabla} - X^4/D_4$	$X^4/A_4\circ(-X) = 2X^4/A_3 + X^4/H - X^4 - X^4/A_4$
$X^4/4\underset{\circ}{\nabla}\circ(-X) = X^4/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla} + 2X^4/3\underset{\circ}{\nabla} + X^4 - 3X^4/2\underset{\circ}{\nabla} - X^4/4\underset{\circ}{\nabla}$	
$X^5\circ(-X) = -X^5$	$X^5/H\circ(-X) = -X^5/H$
$X^5/2\underset{\circ}{\nabla}\circ(-X) = X^5/2\underset{\circ}{\nabla} - X^5$	$X^5/A_3\circ(-X) = -X^5/A_3$
$X^5/C_4\circ(-X) = X^5/C_4 - X^5/H$	$X^5/K_4\circ(-X) = X^5/K_4 + X^5 - 3X^5/H$
$X^5/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}\circ(-X) = 2X^5/2\underset{\circ}{\nabla} - X^5 - X^5/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}$	$X^5/C_5\circ(-X) = -X^5/C_5$
$X^5/L\circ(-X) = X^5/L + X^5 - 2X^5/H - X^5/A_3$	$X^5/A_3\cdot 2\underset{\circ}{\nabla}\circ(-X) = X^5/2\underset{\circ}{\nabla}\cdot A_3 - X^5/A_3$
$X^5/3\underset{\circ}{\nabla}\circ(-X) = 2X^5/2\underset{\circ}{\nabla} - X^5 - X^5/3\underset{\circ}{\nabla}$	$X^5/D_4\circ(-X) = X^5/2\underset{\circ}{\nabla} + X^5/D_4 - X^5/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla} - X^5/H$
$X^5/D_5\circ(-X) = -X^5/D_5$	$X^5/T\circ(-X) = 2X^5/C_4 - X^5/T - X^5/H$
$X^5/2\underset{\circ}{\nabla}\cdot 3\underset{\circ}{\nabla}\circ(-X) = 3X^5/2\underset{\circ}{\nabla} + X^5/2\underset{\circ}{\nabla}\cdot 3\underset{\circ}{\nabla} - X^5/3\underset{\circ}{\nabla} - X^5 - 2X^5/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}$	
$X^5/A_4\circ(-X) = X^5 + X^5/A_4 - 2X^5/A_3 - X^5/H$	
$X^5/4\underset{\circ}{\nabla}\circ(-X) = 3X^5/2\underset{\circ}{\nabla} + X^5/4\underset{\circ}{\nabla} - 2X^5/3\underset{\circ}{\nabla} - X^5 - X^5/2\underset{\circ}{\nabla}\cdot 2\underset{\circ}{\nabla}$	
$X^5/A_5\circ(-X) = 2X^5 + 2X^5/A_4 + 2X^5/L - 3X^5/A_3 - 3X^5/H - X^5/A_5$	
$X^5/5\underset{\circ}{\nabla}\circ(-X) = 2X^5/2\underset{\circ}{\nabla}\cdot 3\underset{\circ}{\nabla} + 2X^5/4\underset{\circ}{\nabla} + 4X^5/2\underset{\circ}{\nabla} - 3X^5/3\underset{\circ}{\nabla} - X^5/5\underset{\circ}{\nabla} - X^5 - 3X^5/2\underset{\circ}{\nabla}$	

Table 4

The substitution of nX in molecular species of degree ≤ 4

$$1\circ(nX) = 1$$

$$X\circ(nX) = \binom{n}{1}X$$

$$X^2\circ(nX) = (\binom{n}{1}+2\binom{n}{2})X^2 = \binom{n}{1}^2X^2$$

$$X^2/2\mathbb{Z}\circ(nX) = \binom{n}{2}X^2+\binom{n}{1}X^2/2\mathbb{Z}$$

$$X^3\circ(nX) = (\binom{n}{1}+6\binom{n}{2}+6\binom{n}{3})X^3 = \binom{n}{1}^3X^3$$

$$X^3/2\mathbb{Z}\circ(nX) = (\binom{n}{1}+2\binom{n}{2})X^3/2\mathbb{Z}+(2\binom{n}{2}+3\binom{n}{3})X^3$$

$$X^3/A_3\circ(nX) = \binom{n}{1}X^3/A_3+(2\binom{n}{2}+2\binom{n}{3})X^3$$

$$X^3/3\mathbb{Z}\circ(nX) = 2\binom{n}{2}X^3/2\mathbb{Z}+\binom{n}{3}X^3+\binom{n}{1}X^3/3\mathbb{Z}$$

$$X^4\circ(nX) = (\binom{n}{1}+14\binom{n}{2}+36\binom{n}{3}+24\binom{n}{4})X^4 = \binom{n}{1}^4X^4$$

$$X^4/H\circ(nX) = (\binom{n}{1}+2\binom{n}{2})X^4/H+(6\binom{n}{2}+18\binom{n}{3}+12\binom{n}{4})X^4$$

$$X^4/2\mathbb{Z}\circ(nX) = (4\binom{n}{2}+15\binom{n}{3}+12\binom{n}{4})X^4+(\binom{n}{1}+6\binom{n}{2}+6\binom{n}{3})X^4/2\mathbb{Z}$$

$$X^4/A_3\circ(nX) = (4\binom{n}{2}+12\binom{n}{3}+8\binom{n}{4})X^4+(\binom{n}{1}+2\binom{n}{2})X^4/A_3$$

$$X^4/C_4\circ(nX) = \binom{n}{2}X^4/H+\binom{n}{1}X^4/C_4+(3\binom{n}{2}+9\binom{n}{3}+6\binom{n}{4})X^4$$

$$X^4/K_4\circ(nX) = 3\binom{n}{2}X^4/H+(2\binom{n}{2}+9\binom{n}{3}+6\binom{n}{4})X^4+\binom{n}{1}X^4/K_4$$

$$X^4/2\mathbb{Z}\cdot2\mathbb{Z}\circ(nX) = (\binom{n}{1}+2\binom{n}{2})X^4/2\mathbb{Z}\cdot2\mathbb{Z}+(\binom{n}{2}+6\binom{n}{3}+6\binom{n}{4})X^4+(4\binom{n}{2}+6\binom{n}{3})X^4/2\mathbb{Z}$$

$$X^4/3\mathbb{Z}\circ(nX) = (\binom{n}{1}+2\binom{n}{2})X^4/3\mathbb{Z}+(3\binom{n}{3}+4\binom{n}{4})X^4+(4\binom{n}{2}+6\binom{n}{3})X^4/2\mathbb{Z}$$

$$X^4/D_4\circ(nX) = \binom{n}{2}X^4/2\mathbb{Z}\cdot2\mathbb{Z}+\binom{n}{2}X^4/H+(2\binom{n}{2}+3\binom{n}{3})X^4/2\mathbb{Z}+\binom{n}{1}X^4/D_4+(3\binom{n}{3}+3\binom{n}{4})X^4$$

$$X^4/A_4\circ(nX) = 2\binom{n}{2}X^4/A_3+\binom{n}{2}X^4/H+(3\binom{n}{3}+2\binom{n}{4})X^4+\binom{n}{1}X^4/A_4$$

$$X^4/4\mathbb{Z}\circ(nX) = \binom{n}{2}X^4/2\mathbb{Z}\cdot2\mathbb{Z}+2\binom{n}{2}X^4/3\mathbb{Z}+\binom{n}{4}X^4+3\binom{n}{3}X^4/2\mathbb{Z}+\binom{n}{1}X^4/4\mathbb{Z}$$

Table 5

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