Séminaire Lotharingien de Combinatoire **61A** (2009), Article B61Ag

GENERAL COMBINATORIAL DIFFERENTIAL OPERATORS

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A la mémoire de notre collègue et ami, Pierre Leroux

Abstract. Let $D = d/dX$. We develop a theory of combinatorial differential operators of the form $\Omega(X, D)$ where $\Omega(X, T)$ is a species of structures built on two sorts, X and T, of underlying elements. These operators act on species, $F(X)$, instead of functions. We show how to compose these operators, how to compute their adjoints and their counterparts in the context of underlying symmetric functions and power series. We also analyze how these operators behave when applied to products of species (generalized Leibniz rule) and other combinatorial operations. Special instances of these operators include: combinatorial finite difference operators, $\Phi(X, \Delta)$, corresponding the species $\Omega(X, T) = \Phi(X, E_+(T))$, where E_+ is the species of nonempty finite sets; pointing operators $\Lambda(XD)$, which are self-adjoint and correspond to the species $\Omega(X, T) = \Lambda(XT)$; and combinatorial Hammond differential operators, $\Theta(D)$, corresponding to the species $\Omega(X, T) = \Theta(T)$. We also give a table of all atomic differential operators $X^m D^k/K$ where K is a subgroup of $\mathbb{S}_m \times \mathbb{S}_k$ and $m + k \leq 7$.

Résumé. Soit $D = d/dX$. Nous développons une théorie d'opérateurs différentiels combinatoires de la forme $\Omega(X, D)$ où $\Omega(X, T)$ est une espèce de structures construite sur deux sortes, X et T, d'éléments sous-jacents. Ces opérateurs agissent sur des espèces, $F(X)$, plutôt que sur des fonctions. Nous montrons comment composer ces opérateurs, comment calculer leurs adjoints et les opérateurs qui leur correspondent dans le contexte des fonctions symétriques et des séries génératrices. Nous analysons aussi le comportement de ces opérateurs lorsqu'ils sont appliqués au produit d'espèces (règle de Leibniz) ainsi qu'à d'autres opérateurs combinatoires. Ces opérateurs incluent les opérateurs combinatoires de différences finies, $\Phi(X, \Delta)$, correspondant aux espèces $\Omega(X, T) = \Phi(X, E_+(T))$, où E_+ est l'espèce des ensembles finis non-vides, les opérateurs de pointage, $\Lambda(XD)$, qui sont auto-adjoints et les opérateurs différentiels combinatoires de Hammond, $\Theta(D)$, qui correspondent aux espèces $\Omega(X, T) = \Theta(T)$. Nous donnons également une table de tous les opérateurs différentiels atomiques $X^m D^k/K$ où K est un sous-groupe de $\mathbb{S}_m \times \mathbb{S}_k$ et $m + k \leq 7$.

With the support of NSERC (Canada).

Contents

1. Introduction

1.1. **The goal of this paper.** Let $D = d/dX$ denote the classical analytical derivation operator defined by

$$DF(X) = \frac{d}{dX}F(X) = F^{'}(X).$$

Higher order derivations $D^n = d^n/dX^n$ are obtained by iterating D. Alternatively, they can be visualized as lists of D's of the form

$$\underbrace{DDD\cdots D}_{n \text{ times}}.$$

But, a natural question is: what meaning can be given to circular arrangements or graphical arrangements of D's as in Figure 1?

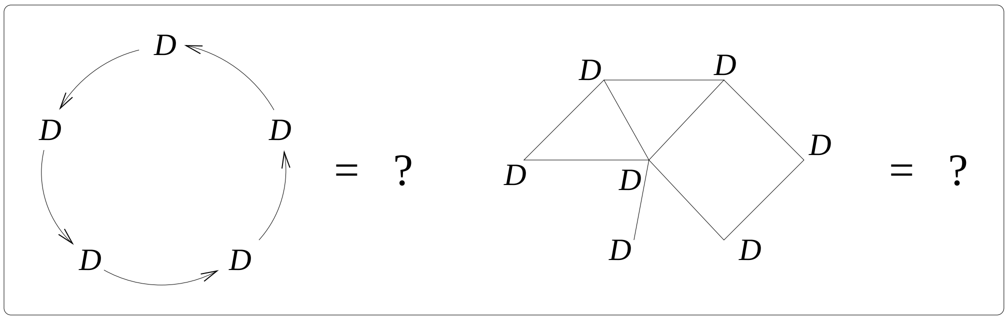


Figure 1. Circular and graphical arrangements of D's

More generally, what meaning can be given to circular or graphical arrangements of D's and X's as in Figure 2 where X is interpreted as the "multiplication by X" operator defined by $F(X) \mapsto XF(X)$? The purpose of this paper is to give an answer to these questions in the realm of species.

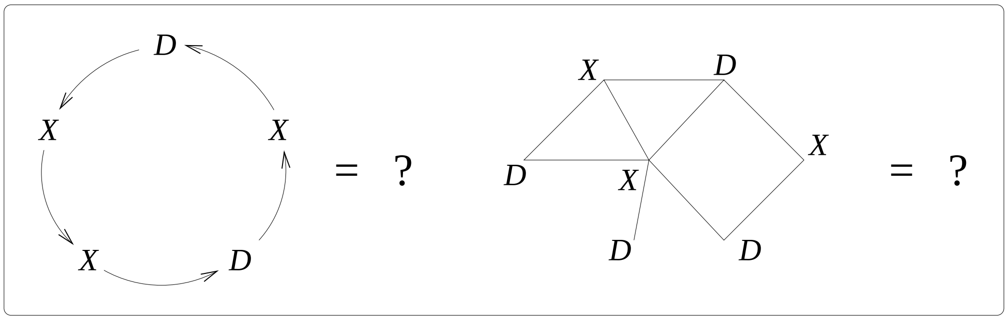


FIGURE 2. Circular and graphical arrangements of D's and X's

To achieve this goal, we will make use of partial cartesian products and substitutions of the form $T := 1$ to introduce general differential operators of the form $\Omega(X, D)$, where $\Omega(X, T)$ is an arbitrary two-sort species. These operators $\Omega(X, D)$ will transform species into species. For the benefit of the reader, we first recall some basic notions about species.

1.2. **Preliminary notions about species.** Informally, a combinatorial *species of structures* is a class of labelled structures which is closed under relabellings along bijections.[1] A structure belonging to a species F is called an *F-structure*. The set of F-structures on a finite underlying set U is assumed to be finite and is denoted by $F[U]$. Hence, $s \in F[U]$ means that s is an F-structure on U. Two F-structures s and t are said *isomorphic* if one can be obtained from the other one by a relabelling induced by a bijection between their underlying sets. More precisely, if $\beta : U \to V$ is such a bijection, the induced relabelling is denoted by $F[\beta] : F[U] \to F[V]$. An isomorphism class of F-structures is called an *unlabelled* F-structure. Two species F and G are equal (isomorphic), and we write $F = G$, if there exists a natural isomorphism (in the sense of theory of category) between them. This means that for each U, there exists a bijection $\alpha_U : F[U] \to G[U]$ such that $G[\beta]\alpha_U = \alpha_V F[\beta]$ for each bijection $\beta : U \to V$.

Several enumerative formal series can be associated to any species F. The most important one is the *cycle index series*, denoted $Z_F(x_1, x_2, x_3, \ldots)$, and is defined by

$$Z_F(x_1, x_2, x_3, \ldots) = \sum_{n\geq 0} \frac{1}{n!} \sum_{\sigma \in \mathbb{S}_n} \mathrm{fix} F[\sigma]\, x_1^{\sigma_1} x_2^{\sigma_2} x_3^{\sigma_3} \cdots = \sum_{n_1, n_2, \ldots} f_{n_1, n_2, \ldots} \frac{x_1^{n_1} x_2^{n_2} \cdots}{1^{n_1} n_1! 2^{n_2} n_2! \cdots} \tag{1}$$

where $\mathbb{S}_n$ denotes the symmetric group of order n, $\mathrm{fix}F[\sigma]$, the number of F-structures on $[n]$ left fixed under the action of the permutation $\sigma \in \mathbb{S}_n$, σ_i, $i \in \mathbb{N}^*$, is the number of cycles of length i of the permutation $\sigma \in \mathbb{S}_n$ and $f_{n_1,n_2,\ldots} = \mathrm{fix}F[\sigma]$ if σ is of type $1^{n_1} 2^{n_2} \cdots$. Other classical enumerative formal series, that is, the *exponential generating series* $F(x)$, which counts labeled F-structures, and the *tilda generating series* $\widetilde{F}(x)$, which counts the unlabeled F-structures. These series are obtained specializing the series Z_F,

$$F(x) = Z_F(x, 0, 0, \ldots) \qquad \text{and} \qquad \widetilde{F}(x) = Z_F(x, x^2, x^3, \ldots). \tag{2}$$

[1] Formally, a species of structures is a functor from the category of finite sets and bijections to the category of finite sets and functions, see [8].

Many combinatorial operations can be performed in the framework of the theory of species. The main ones are addition, product, substitution, pointing, cartesian product and derivation. For precise definitions of these operations, see [2]. However, in this paper we make an extensive use of the cartesian product and the derivation and we briefly recall their definitions. Let F and G be any species and U a finite set. The *derivative species* F' or DF of a species F is given by $F'[U] = F[U + \{*_U\}]$, where $*_U$ is an element chosen outside of the underlying set U. The *cartesian product* of F and G, denoted $F \times G$, is defined by $(F \times G)[U] = F[U] \times G[U]$.

The behaviour of the cycle index series according to the operations of derivation and of cartesian product is well known; see [2]. In particular, we have

$$Z_{F'}(x_1, x_2, x_3, \ldots) = \frac{\partial}{\partial x_1} Z_F(x_1, x_2, x_3, \ldots), \tag{3}$$

$$Z_{F\times G}(x_1, x_2, x_3, \ldots) = (Z_F \times Z_G)(x_1, x_2, x_3, \ldots), \tag{4}$$

where $Z_F \times Z_G$ means the *Hadamard* (coefficient by coefficient) *product* of the series Z_F and Z_G.

A *molecular species* M is a species possessing only one isomorphism type. This means that any two M-structures are always isomorphic. Such a species is characterized by the fact that it is indecomposable under the combinatorial sum:

$$M \text{ is molecular} \quad \Longleftrightarrow \quad (M = F + G \Longrightarrow F = 0 \text{ or } G = 0).$$

Any molecular species M can be written under the form of a quotient species $M = X^n/H$, where X^n represents the species of linear orders of length n and $H \leq \mathbb{S}_n$ is a subgroup of the symmetric group of order n. In fact, H is the *stabilizer* of any M-structure. Two molecular species X^n/H and X^m/K are equal (that is, isomorphic as species) if and only if $n = m$ and H and K are conjugate subgroups of $\mathbb{S}_n$. Furthermore, any species F can be uniquely expanded in terms of molecular species as follows:

$$F = \sum_{M \in \mathcal{M}} f_M M,$$

where $\mathcal{M}$ denotes the set of all molecular species and $f_M \in \mathbb{N}$ is the number of subspecies of F isomorphic to M. This expansion is unique and called the *molecular expansion* of the species F.

It is also possible to extend the notion of molecular species to the case of multi-sort species. For instance, for two-sort species, where the two sorts of elements of underlying sets are denoted X and T, each molecular species $M = M(X,T)$ can be written in the form $M(X,T) = X^nT^k/H$, where $H \leq \mathbb{S}_n^X \times \mathbb{S}_k^T$ is the stabilizer of any M-structure and $\mathbb{S}_n^X$ is the symmetric group of order n acting on points of sort X. The exponents n and k are called *degree* of M in X and T. The cycle index series of a two-sort molecular species $M(X,T) = X^nT^k/H$ is given by the expression

$$Z_M(x_1, x_2, \ldots; t_1, t_2, \ldots) = \frac{1}{|H|} \sum_{h \in H} x_1^{c_1(h)} x_2^{c_2(h)} \cdots t_1^{d_1(h)} t_2^{d_2(h)} \cdots ,$$

where $c_i(h)$ (respectively $d_i(h)$), for $i \geq 1$, denotes the number of cycles of length i of the permutation on points of sort X (respectively T) induced by the element $h \in H$ and $|H|$ is the cardinality of H. Note that $\mathbb{S}_n^X \times \mathbb{S}_k^T$ is isomorphic to the Young subgroup $\mathbb{S}_{n,k} \leq \mathbb{S}_{n+k}$ permuting independently $\{1, 2, \ldots, n\}$ and $\{n+1, n+2, \ldots, n+k\}$.

It is important to notice that in the series Z_M above, the monomials in the x_i's always appear before the ones in the t_i's.

In this paper, we use the following graphical conventions:

1) for any species $F = F(X)$, we find appropriate to represent a F-structure by a drawing of the form of Figure 3 a) where black dots stand for the distinct elements (of sort X) of the underlying set;
2) for two-sort species $\Omega = \Omega(X,T)$, Figure 3 b) shows a convention used to represent an Ω-structure, where black dots (respectively black squares) are elements of sort X (respectively of sort T);
3) setting $T := 1$ in a species $\Omega(X,T)$, we obtain the species $\Omega(X,1)$ where points of sort T are unlabelled. Notice that white squares represent indistinguishable unlabelled elements of sort T; see Figure 3 c) and the substitution is possible if $\Omega(X,T)$ is "finitary in T". This means that for every finite set U of points of sort X there is no Ω-structure on the pair of sets (U,V) for every sufficiently large finite set V of points of sort T. The cycle index series $Z_{\Omega(X,1)}$ of $\Omega(X,1)$ is computed as follows:

$$Z_{\Omega(X,1)}(x_1,x_2,\ldots) = Z_{\Omega(X,T)}(x_1,x_2,\ldots;t_1,t_2,\ldots)\big|_{t_i:=1} = Z_{\Omega(X,T)}(x_1,x_2,\ldots;1,1,\ldots). \tag{5}$$

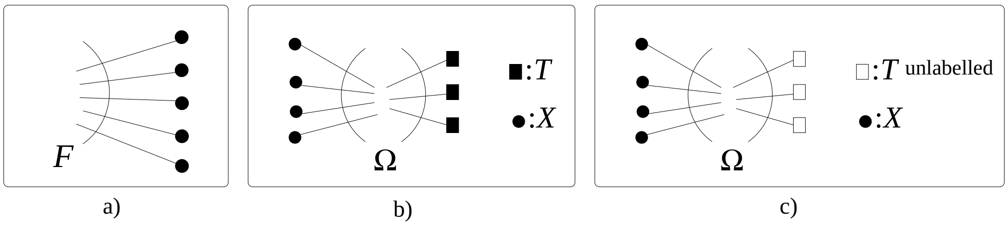


FIGURE 3. a) $F(X)$-structure; b) $\Omega(X,T)$-structure; c) $\Omega(X,1)$-structure

Using these kinds of graphical conventions, the structures belonging, for example, to the cartesian product $\Omega_1(X,T) \times \Omega_2(X,T)$ of two-sort species can be represented by Figure 4 a) and a structure belonging ot the species $F'(X)$ can be represented by Figure 4 b).

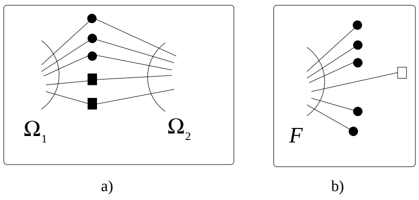


FIGURE 4. a) $\Omega_1(X,T) \times \Omega_2(X,T)$-structure; b) $F'(X)$-structure

Finally, we will make an extensive use in this paper of the so-called *partial cartesian product* according to a sort. Considering two-sort species $\Omega_1(X,T)$ and $\Omega_2(X,T)$, the *partial cartesian product* with respect to the sort T of Ω_1 and Ω_2 is denoted by

$$\Omega_1(X,T) \times_T \Omega_2(X,T) \tag{6}$$

and is illustrated by Figure 5. Formally, a $\Omega_1(X,T) \times_T \Omega_2(X,T)$-structure s on a pair (U,V) of sets of sort X and T, respectively, is a pair $s=(s_1,s_2)$ where $s_1 \in \Omega_1[U_1,V]$ and $s_2 \in \Omega_2[U_2,V]$ where $U_1 \cup U_2 = U$ and $U_1 \cap U_2 = \emptyset$. This operation had been first introduced by Gessel and Labelle in [7] in the context of Lagrange inversion.

The cycle index series $Z_{\Omega_1 \times_T \Omega_2}$ is computed in the following way

$$Z_{\Omega_1 \times_T \Omega_2}(x_1,x_2,\ldots;t_1,t_2,\ldots) = \sum_{n_1,n_2,\ldots} \omega_{1,n_1,n_2,\ldots}(x_1,x_2,\ldots)\omega_{2,n_1,n_2,\ldots}(x_1,x_2,\ldots)\frac{t_1^{n_1}t_2^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots}, \quad (7)$$

where $\omega_{1,n_1,n_2,\ldots}(x_1,x_2,\ldots)$ and $\omega_{2,n_1,n_2,\ldots}(x_1,x_2,\ldots)$ are defined by

$$Z_{\Omega_i}(x_1,x_2,\ldots;t_1,t_2) = \sum_{n_1,n_2,\ldots} \omega_{i,n_1,n_2,\ldots}(x_1,x_2,\ldots)\frac{t_1^{n_1}t_2^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots}, \qquad \text{for} \quad i=1,2. \quad (8)$$

The right-hand side of (7) is denoted by $Z_{\Omega_1} \times_{\mathbf{t}} Z_{\Omega_2}$ and is called the *Hadamard product* of Z_{Ω_1} and Z_{Ω_2} relative to $\mathbf{t}=(t_1,t_2,\ldots)$

It can be checked that $\times_T$ can be written in terms of the ordinary cartesian product as $\Omega_1(X,T)E(Y) \times \Omega_2(Y,T)E(X)\big|_{Y:=X}$, where E denotes the species of finite sets.

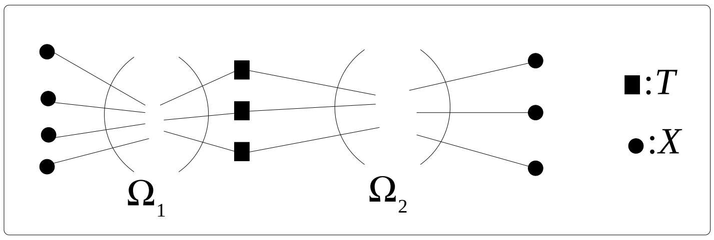


FIGURE 5. Representation of an $\Omega_1(X,T) \times_T \Omega_2(X,T)$-structure

2. General combinatorial differential operators

2.1. **Basic definitions.** We are now ready to state our main definition.

Definition 1 (General combinatorial differential operators). *Let $\Omega(X,T)$ be a two-sort species and $F(X)$ be a species. If $\Omega(X,T)$ is finitary in T or $F(X)$ is of finite degree in X, then $\Omega(X,D)F(X)$ is the species defined by*

$$\Omega(X,D)F(X) := \Omega(X,T) \times_T F(X+T)|_{T:=1}. \quad (9)$$

□

Figure 6 a) describes a typical $\Omega(X,D)F(X)$-structure on a set of 9 elements of sort X. For example, let $\Omega(X,T)=A(X,T)$ be the species of rooted trees with internal nodes of sort X and leaves of sort T and $F(X)=C_{10}(X)$ be the species of oriented cycles of length 10, then Figure 6 b) shows a typical $A(X,D)C_{10}(X)$-structure. Taking $\Omega(X,D)=E(L_{\geq 2}(X)D)$ where E and $L_{\geq 2}$ are the species of sets and of lists of length ≥ 2, respectively, then the species of octopuses (see Figure 6 c)) can be written as $\mathrm{Oct}(X)=E(L_{\geq 2}(X)D)C(X)$ where $C(X)$ is the species of oriented cycles.

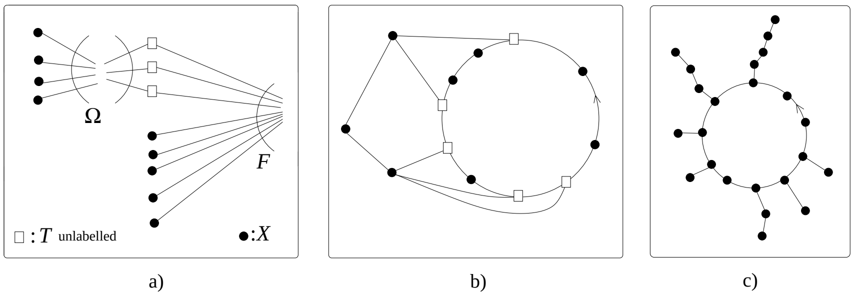


FIGURE 6. a) $\Omega(X,D)F(X)$-structure, b) $A(X,D)C_{10}(X)$-structure and c) an octopus

Another example is given by taking $\Omega(X,D) = E(\mathcal{P}_{\geq 2}(X)D)$, where $\mathcal{P}(X)$ is any species of the form $\mathcal{P}(X) = X + \mathcal{P}_{\geq 2}(X)$. Then, it is easily seen that

$$E(\mathcal{P}_{\geq 2}(X)D)F(X) = F(\mathcal{P}(X))$$

and formula (13) of Proposition 1 below reduces to the plethystic substitution $Z_{F\circ\mathcal{P}} = Z_F \circ Z_{\mathcal{P}}$ as the reader can check. The operator $\mathcal{P}_{\geq 2}(X)D$ is similar to an "eclosion" operator in the terminology of [10].

Note that the restrictions on Ω or F in Definition 1 are necessary in order that (9) defines a species. For example, for the species $C(X)$ of oriented cycles (of arbitrary lengths), $A(X,D)C(X)$ is not a species since the number of structures would be infinite on any non-empty finite set U. From now, we will always assume that the restrictions in Definition 1 are satisfied.

Since every two-sort species $\Omega(X,T)$ can be written as a linear combination $\sum \omega_K \frac{X^nT^k}{K}$ of molecular species, every differential operator $\Omega(X,D)$ is a linear combination of the corresponding *molecular* linear operators of the form $X^nD^k/K,\ K \leq S_{n,k}$. We will denote the action of these operators on species $F(X)$ by

$$\left(\frac{X^nD^k}{K}\right)F(X) = \frac{X^nF^{(k)}(X)}{K}$$

in conformity with the classical notation $X^nD^kF(X) = X^nF^{(k)}(X)$ corresponding to the degenerate case where $K = \{\mathrm{id}\}$. With these notations, we have

Theorem 1 (GENERALIZED LEIBNIZ RULE). *Let $F(X)$ and $G(X)$ be two species. Then,*

$$\frac{X^nD^k}{K}F(X)G(X) = \sum_{i+j=k}\sum_{L:S_{n,i,j}} \binom{K}{L}\frac{X^nF^{(i)}(X)G^{(j)}(X)}{L}, \tag{10}$$

where $L : S_{n,i,j}$ means that L runs through a complete system of representatives of the conjugacy classes of subgroups of $S_{n,i,j}$ and the coefficients $\binom{K}{L}$ are defined by the "addition formula" [1],

$$X^n(T_1+T_2)^k/K = \sum_{i+j=k}\sum_{L:S_{n,i,j}} \binom{K}{L} X^nT_1^iT_2^j/L. \tag{11}$$

Proof. By definition of X^nD^k/K, we have (see Figure 7)

$$\frac{X^nD^k}{K}F(X)\cdot G(X) = \frac{X^nT^k}{K} \times_T (F(X+T)\cdot G(X+T))\Big|_{T:=1}. \qquad (12)$$

The result then follows immediately from (11) by interpreting the white squares in

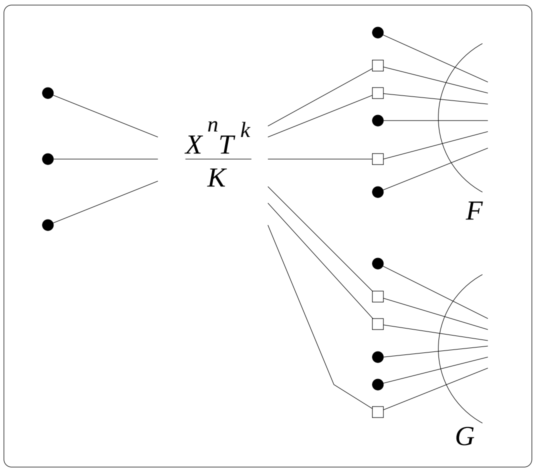


FIGURE 7. Overview of a $[X^nD^k/K]F(X)G(X)$-structure

the F-structure (respectively in the G-structure) as unlabelled singletons of sort T_1 (respectively T_2) and using linearity. □

For example, $n = 0$ and $K = \{\mathrm{id}\}$ corresponds to the classical Leibniz rule

$$D^kF(X)G(X) = \sum_{i+j=k} \binom{k}{i} F^{(i)}(X)G^{(j)}(X),$$

while, the molecular operator $E_2(XD)$, where E_2 is the species of 2-sets, corresponds to the formula

$$E_2(XD)(F\cdot G) = (E_2(XD)F)\cdot G + X^2F^{'}\cdot G^{'} + F\cdot(E_2(XD)G)\,.$$

In the context of cycle index series, the combinatorial differential operators behave as follows.

Proposition 1. *Let $G(X) = \Omega(X,D)F(X)$, then we have*

$$Z_G(x_1,x_2,x_3,\ldots) = Z_\Omega(x_1,x_2,x_3,\ldots;\frac{\partial}{\partial x_1},2\frac{\partial}{\partial x_2},3\frac{\partial}{\partial x_3},\ldots)Z_F(x_1,x_2,x_3,\ldots). \qquad (13)$$

Proof. Writing $Z_{\Omega(X,T)}$ in the form

$$Z_{\Omega(X,T)}(x_1,x_2,\ldots;t_1,t_2,\ldots) = \sum_{n_1,n_2,\ldots} \omega_{n_1,n_2,\ldots}(x_1,x_2,\ldots)\frac{t_1^{n_1}t_2^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots},$$

we have successively, using (7),

$$\begin{aligned}
Z_G(x_1,x_2,\ldots) &= Z_\Omega(x_1,x_2,\ldots;t_1,t_2,\ldots)\times_{\mathbf{t}} Z_F(x_1+t_1,x_2+t_2,\ldots)\big|_{t_i:=1}\\
&= Z_\Omega(x_1,x_2,\ldots;t_1,t_2,\ldots)\times_{\mathbf{t}} \mathrm{e}^{t_1(\frac{\partial}{\partial x_1})+t_2(\frac{\partial}{\partial x_2})+\cdots} Z_F(x_1,x_2,\ldots)\big|_{t_i:=1}\\
&= \sum_{n_1,n_2,\ldots}\omega_{n_1,n_2,\ldots}(x_1,x_2,\ldots)\left(\frac{\partial}{\partial x_1}\right)^{n_1}\left(2\frac{\partial}{\partial x_2}\right)^{n_2}\cdots\\
&\qquad\qquad \cdot Z_F(x_1,x_2,\ldots)\frac{t_1^{n_1}t_2^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots}\bigg|_{t_i:=1}\\
&= Z_\Omega(x_1,x_2,\ldots;\frac{\partial}{\partial x_1},2\frac{\partial}{\partial x_2},\ldots)Z_F(x_1,x_2,\ldots).
\end{aligned}$$

□

In Proposition 1, the convention of writing all the t_j's to the right of all the x_i's in $Z_\Omega(x_1,x_2,\ldots,t_1,t_2,\ldots)$ must be applied. For example, taking $\Omega(X,D)=E(XD)$, where E is the species sets, we have $E(XD)F(X)=F(2X)$. In this case, we must take

$$Z_{E(XD)}(x_1,x_2,\ldots,\frac{\partial}{\partial x_1},2\frac{\partial}{\partial x_2},\ldots)=\sum\frac{x_1^{n_1}x_2^{n_2}\cdots(\frac{\partial}{\partial x_1})^{n_1}(\frac{\partial}{\partial x_2})^{n_2}\cdots}{n_1!n_2!\cdots},$$

not

$$\sum\frac{(x_1\frac{\partial}{\partial x_1})^{n_1}(x_2\frac{\partial}{\partial x_2})^{n_2}\cdots}{n_1!n_2!\cdots}.$$

Corollary 1. *Let $G(X)=\Omega(X,D)F(X)$. Then, the exponential generating series $G(x)$ for labelled G-structures and the tilde generating series $\widetilde{G}(x)$ for unlabelled G-structures are given by*

$$G(x)=\sum_{n_1,n_2,\ldots}\omega_{n_1,n_2,\ldots}(x,0,0,\ldots)\left[\frac{\left(\frac{\partial}{\partial x_1}\right)^{n_1}\left(\frac{\partial}{\partial x_2}\right)^{n_2}\cdots}{n_1!n_2!\cdots}Z_F\right](x,0,0,\ldots), \tag{14}$$

$$\widetilde{G}(x)=\sum_{n_1,n_2,\ldots}\omega_{n_1,n_2,\ldots}(x,x^2,x^3,\ldots)\left[\frac{\left(\frac{\partial}{\partial x_1}\right)^{n_1}\left(\frac{\partial}{\partial x_2}\right)^{n_2}\cdots}{n_1!n_2!\cdots}Z_F\right](x,x^2,x^3,\ldots), \tag{15}$$

where $\omega_{n_1,n_2,\ldots}(x_1,x_2,x_3,\ldots)$ are defined by

$$Z_\Omega(x_1,x_2,\ldots;t_1,t_2,\ldots)=\sum_{n_1,n_2,\ldots}\omega_{n_1,n_2,\ldots}(x_1,x_2,x_3,\ldots)\frac{t_1^{n_1}t_2^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots}. \tag{16}$$

Proof. Immediate from the proof of Proposition 1 and the fact that $G(x)=Z_G(x,0,0,\ldots)$ and $\widetilde{G}(x)=Z_G(x,x^2,x^3,\ldots)$. □

Note that, in the particular case $\Omega(X,D)=D$, formulas (14) and (15) reduce to the classical formulas

$$(DF)(x)=\frac{\partial}{\partial x}F(x),\qquad \widetilde{F'}(x)=\left[\frac{\partial}{\partial x_1}Z_F\right](x,x^2,x^3,\ldots).$$

However, for a general differential operator $\Omega(X,D)$, the computation of $[\Omega(X,D)F](x)$ and $[\widetilde{\Omega(X,D)}F](x)$ depends on Z_Ω and the mixed derivations $\left(\frac{\partial}{\partial x_1}\right)^{n_1}\left(\frac{\partial}{\partial x_2}\right)^{n_2}\cdots Z_F$.

Definition 2 (Composition of differential operators). *Let $\Omega_1(X,T)$ and $\Omega_2(X,T)$ be two-sort species. Then, we define the composition of $\Omega_1(X,T)$ by $\Omega_2(X,T)$ by*

$$\Omega_2(X,T)\odot\Omega_1(X,T)=\Omega_3(X,T), \tag{17}$$

where

$$\Omega_3(X,T)=\Omega_2(X,T+T_0)\times_{T_0}\Omega_1(X+T_0,T)|_{T_0:=1}, \tag{18}$$

and T_0 is an auxiliary extra sort. The differential operator corresponding to $\Omega_3(X,T)$ is denoted $\Omega_2(X,D)\odot\Omega_1(X,D)$ and is called the composition of $\Omega_1(X,D)$ by $\Omega_2(X,D)$.

Figure 8 illustrates an $\Omega_3(X,T)$-structure.

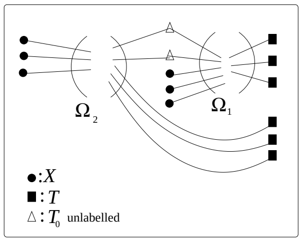


Figure 8. $\Omega_2(X,T+T_0)\times_{T_0}\Omega_1(X+T_0,T)|_{T_0:=1}$-structure

The operation $\odot$ is noncommutative and associative. For example, $(XD)\odot(X^2D)=2X^2D+X^3D^2$ while $(X^2D)\odot(XD)=X^2D+X^3D^2$. The proof of associativity is left to the reader. The next proposition states that the composition $\Omega_2(X,D)\odot\Omega_1(X,D)$ corresponds to the application of $\Omega_1(X,D)$ followed by $\Omega_2(X,D)$.

Proposition 2. *For any species $F=F(X)$,*

$$\left(\Omega_2(X,D)\odot\Omega_1(X,D)\right)F(X)=\Omega_2(X,D)\left[\Omega_1(X,D)F(X)\right].$$

Proof. We first write

$$\begin{aligned}\Omega_2(X,D)\left[\Omega_1(X,D)F(X)\right]&=\Omega_2(X,D)\left[\Omega_1(X,T_1)\times_{T_1}F(X+T_1)|_{T_1:=1}\right]\\&=\left\{\Omega_2(X,T_2)\times_{T_2}\left[\left[\Omega_1(X,T_1)\times_{T_1}F(X+T_1)\big|_{T_1:=1}\right]\right]\Big|_{X:=X+T_2}\right\}\Big|_{T_2:=1}.\end{aligned}$$

The proof is then established by examining Figure 9. □

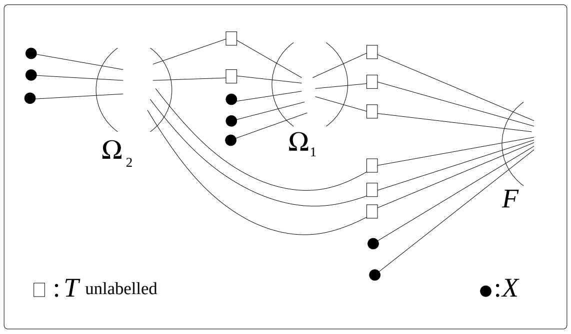
For cycle index series, the operation $\odot$ has the following counterpart.

Theorem 2. *Let $\Omega_2(X,T)$ and $\Omega_1(X,T)$ be any two-sort species. Then, we have*

$$Z_{\Omega_2\odot\Omega_1}=\sum_{n_1,n_2,\ldots}\frac{\left((\frac{\partial}{\partial t_1})^{n_1}(2\frac{\partial}{\partial t_2})^{n_2}\cdots Z_{\Omega_1}\right)\left((\frac{\partial}{\partial x_1})^{n_1}(2\frac{\partial}{\partial x_2})^{n_2}\cdots Z_{\Omega_2}\right)}{1^{n_1}n_1!2^{n_2}n_2!\cdots}. \tag{19}$$

Proof. We have

$$\begin{aligned}Z_{\Omega_2(X,T_0+T)}&=\mathrm{e}^{t_{01}\frac{\partial}{\partial t_1}+\frac{t_{02}}{2}\frac{2\partial}{\partial t_2}+\frac{t_{03}}{3}\frac{3\partial}{\partial t_3}+\cdots}Z_{\Omega_2(X,T)}(x_1,x_2,\ldots;t_1,t_2,\ldots) &(20)\\&=\sum_{n_1,n_2,\ldots}\frac{t_{01}^{n_1}t_{02}^{n_2}\cdots(\frac{\partial}{\partial t_1})^{n_1}(2\frac{\partial}{\partial t_2})^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots}Z_{\Omega_2(X,T)}(x_1,x_2,\ldots;t_1,t_2,\ldots) &(21)\end{aligned}$$



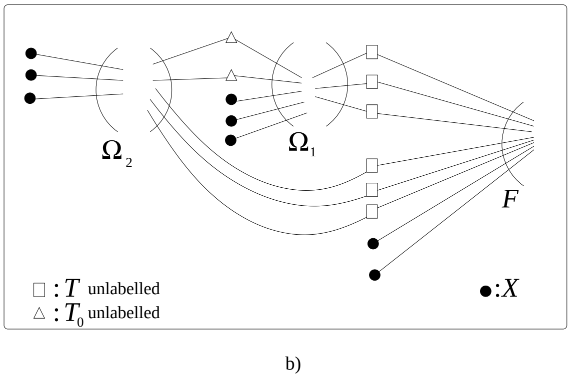


FIGURE 9. a) $\Omega_2(X,D)\,[\Omega_1(X,D)F(X)]$ and b) $[\Omega_2(X,D)\odot\Omega_1(X,D)]\,F(X)$

In a similar way,

$$Z_{\Omega_1(X+T_0,T)} = \sum_{n_1,n_2,\ldots} \frac{t_{01}^{n_1}t_{02}^{n_2}\cdots(\frac{\partial}{\partial x_1})^{n_1}(2\frac{\partial}{\partial x_2})^{n_2}\cdots}{1^{n_1}n_1!2^{n_2}n_2!\cdots} Z_{\Omega_1(X,T)}(x_1,x_2,\ldots;t_1,t_2,\ldots). \quad (22)$$

The result follows using the Hadamard product according to the sort T_0 and letting $t_{0i} := 1$, $i = 1,2,3,\ldots$. □

The following example exhibits a curious hidden symmetry involving combinatorial differential operators. Let $F = F(X)$ be a species and consider the combinatorial operator $F(X + XD)$ associated to the two-sort species $F(X + XT)$. For any species $G(X)$, we have the combinatorial equality

$$F(X + XD)G(X) = G(X + XD)F(X) \quad (23)$$

as Figure 10 shows. In this equality, F and G play symmetric roles. We denote the common value in (23) by $F\dot{\times}G$ and call it the "*kiss product*" of the species F and G for obvious reasons. The two classical products $F \cdot G$ and $F \times G$ are subspecies of $F\dot{\times}G$ since they can be respectively interpreted as the "empty kiss product" and the "full kiss product" of the species F and G :

$$F \cdot G \subset F\dot{\times}G \qquad \text{and} \qquad F \times G \subset F\dot{\times}G \quad (24)$$

The computations of the associated series $Z_{F\dot{\times}G}(x_1,x_2,\ldots)$, $(F\dot{\times}G)(x)$ and $\widetilde{F\dot{\times}G}(x)$

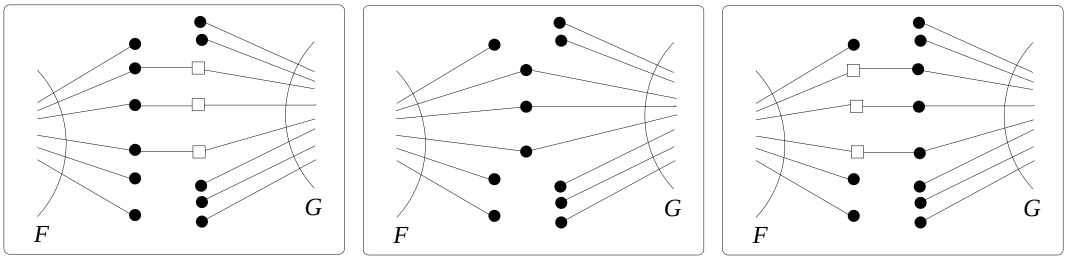


FIGURE 10. $F(X + XD)G = F\dot{\times}G = G(X + XD)F$

are left to the reader.

Figure 11 shows a $C\dot{\times}C$-structure, where C is the species of oriented cycles.

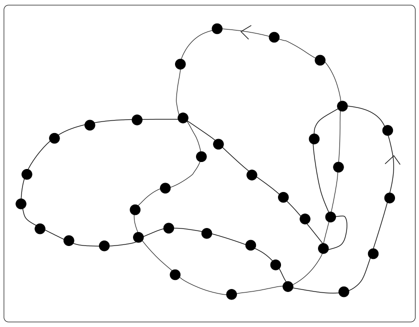


FIGURE 11. A $C\dot{\times}C$-structure

2.2. **Bilinear form and adjoint operators.** In [8], Joyal introduced a bilinear form, denoted $\langle\ ,\ \rangle$, in the realm of species in the following way: given two species $F = F(X)$ and $G = G(X)$, $\langle F(X), G(X) \rangle$ is defined by

$$\langle F(X), G(X) \rangle \;=\; F(X) \times_X G(X)|_{X:=1} \;=\; \text{number of unlabelled } F \times G-\text{structures}, \tag{25}$$

provided it is finite (see Figure 12 a)). He showed that, for any species $H(X)$,

$$\langle H(D)F(X), G(X) \rangle \;=\; \langle F(X), H(X)G(X) \rangle, \tag{26}$$

which means that multiplication by $H(X)$ is a right adjoint to $H(D)$.

We have the following more general result:

Proposition 3. *Let $\Omega(X,T)$ be a two-sort species. Then,*

$$\langle \Omega(X,D)F(X), G(X) \rangle \;=\; \langle F(X), \Omega(D,X)G(X) \rangle. \tag{27}$$

That is $(\Omega(X,D))^* := \Omega(D,X)$ is the adjoint *operator of $\Omega(X,D)$.*

Proof. See Figure 12 b). □

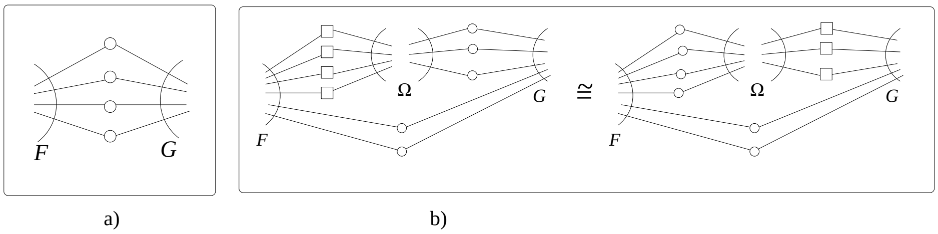


FIGURE 12. a) $\langle F(X), G(X) \rangle$ and b) $\langle \Omega(X,D)F(X)), G(X) \rangle = \langle F(X), \Omega(D,X)G(X) \rangle$

Proposition 4. *Let $\Omega_1(X,D)$ and $\Omega_2(X,D)$ be two sort-species. Then, we have*

$$(\Omega_2(X,D) \odot \Omega_1(X,D))^* = \Omega_1^*(X,D) \odot \Omega_2^*(X,D) = \Omega_1(D,X) \odot \Omega_2(D,X). \tag{28}$$

□

3. Special cases

3.1. **Combinatorial Hammond differential operators.** The special case $\Omega(X,T) = \Theta(T)$ corresponds to the classical Hammond combinatorial differential operator defined by (see [6, 9])

$$\Theta(D)F(X) = (E(X)\Theta(T)) \times (F(X+T))\Big|_{T:=1} := \Theta(T) \times_T F(X+T)\Big|_{T:=1}. \quad (29)$$

Figure 13 shows a typical $\Theta(D)F(X)$-structure. Note that, contrarily to the general

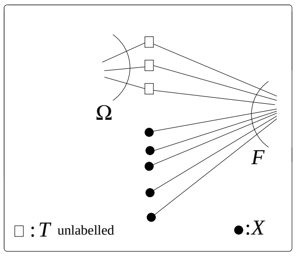


Figure 13. A typical $\Omega(D)F(X)$-structure

case, the composition $\Theta(D) \odot \Psi(D)$ of Hammond operators is commutative since it corresponds to ordinary multiplication:

$$\Theta(D) \odot \Psi(D) = (\Theta \cdot \Psi)(D). \quad (30)$$

Example 1. The following relations can be easily established by appropriate drawings and details are left to the reader.

(1) For $\Theta(T) = E_2(T)$, the species of two-element sets, we have

$$E_2(D)(F \cdot G) = (E_2(D)F) \cdot G + F^{'}G^{'} + (E_2(D)G) \cdot F, \quad (31)$$

$$E_2(D)(E \circ F) = (E \circ F) \cdot (E_2(D)F + E_2(F^{'})). \quad (32)$$

In particular, for the species $F = C$ of oriented cycles and $E \circ C = S$ of permutations, the previous equation takes the form

$$E_2(D)S = S \cdot (E_2(D)F + E_2(L)).$$

(2) *Translation operators.* Taking $\Theta(X) = E(X)$, the species of sets, we obtain the translation operator denoted $E(D)$, whose action is described by

$$E(D)F(X) = F(X+1), \qquad E^n(D)F(X) = F(X+n).$$

(3) When $\Theta(T) = T^n$, $n \geq 0$, then we recover the usual n-th derivatives

$$\Theta(D)F(X) = D^nF(X) = \frac{d^nF(X)}{dX^n}.$$

(4) *Catalan derivative.* Let $\Theta(T) = B(T)$ be the species of binary trees. It is well known that this species satisfies the functional equation $B = 1 + TB^2$. Since $1/B(T) = 1 - TB(T)$ we deduce that

$$B(D)F(X) = G(X) \quad \Longleftrightarrow \quad F(X) = (1 - DB(D))\, G(X).$$

It is important to notice that the species $1 - TB(T)$ is virtual, in this case.

(5) We can generalize the preceding example by taking any species $\mathcal{B} = \mathcal{B}(T)$ with constant term equal to 1 since such a species is invertible under product (in the context of virtual species; see [2, 9]), we have

$$\mathcal{B}(D)F(X) = G(X) \Longleftrightarrow F(X) = \frac{1}{\mathcal{B}(D)}G(X).$$

□

3.2. **Self-adjoint and pointing operators.** Since the adjoint of an operator $\Omega(X, D)$ is $\Omega(D, X)$, self-adjoint operators correspond to symmetric species $\Omega(X, T) = \Omega(T, X)$. For example, the operator X^3D^3/K, where $K = \langle\, (123)(456)\,\rangle \leq S_{3,3}$ is self-adjoint and $\Phi(X + D)$ is self-adjoint for any species $\Phi(X)$.

An important class of self-adjoint operators is the Λ-pointing operators defined by $\Lambda(XD)$, where $\Lambda = \Lambda(T)$ is an arbitrary species. Figure 14 a) shows a typical $\Lambda(XD)F(X)$-structure. The special case $\Lambda(T) = T$ corresponds to the classical one-element pointing. The composition of pointing operators is commutative and is given by

$$\Lambda_2(XD) \odot \Lambda_1(XD) = (\Lambda_2 \dot{\times} \Lambda_1)(XD),$$

where $\dot{\times}$ denotes the kiss product operation.

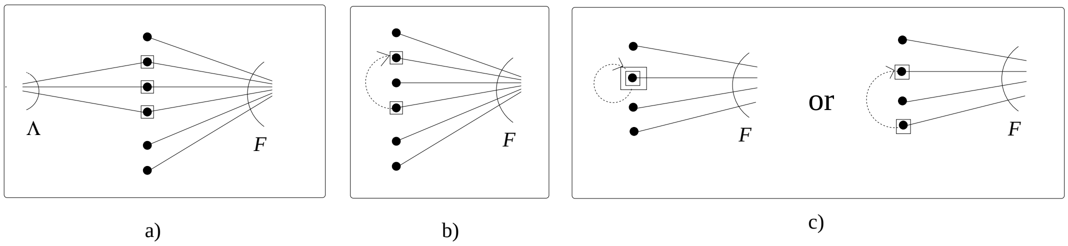


FIGURE 14. a) Λ-pointed F-structure, b) $(XD)^2F$-structure and c) $(XD \odot XD)F$-structure

Taking $\Lambda(T) = T^2$, we obtain the operator $(XD)^2$ which corresponds to point an ordered pair of *distinct* elements in structures (see Figure 14 b)). Note that

$$(XD) \odot (XD) = XD + X^2D^2 \neq (XD)^2 = X^2D^2$$

since we can point the *same* element in two successive pointings (see Figure 14 c)).

Taking $\Lambda(T) = C(T)$, the species of oriented cycles, we obtain the operator $C(XD)$ of cyclic-pointing. An interesting subspecies of $C(XD)F(X)$ has recently been introduced by Bodirsky et al. [3]. It consists of all *unbiased* cyclically pointed F-structures. In such structures, the pointed cycle must be one of the cycles of an automorphism of the F-structure. They applied this unbiased pointing to the uniform random generation of classes of unlabelled structures.

3.3. **Finite differences operators.** We saw in Section 3.1, that $E(D)$ is the translation operator on species (of finite degree): $E(D)F(X) = F(X + 1)$. Hence, we can define the difference operator Δ by the equation

$$\Delta = E_+(D),$$

where $E_+ = E - 1$ is the species of non-empty finite sets. We obviously have

$$\Delta F(X) = F(X+1) - F(X). \tag{33}$$

Note that the right-hand side of (33) is not a virtual species since $F(X)$ is always a subspecies of $F(X+1)$. Conversely, we can write $D = E_+^{<-1>}(\Delta)$, where $E_+^{<-1>}$ is the inverse under substitution of the species E_+ (see [2] for a description of $E_+^{<-1>}$). This opens the way to a completely new theory of general combinatorial difference operators of the form $\Phi(X, \Delta) = \Phi(X, E_+(D))$ where $\Phi(X, T)$ is an arbitrary species.

3.4. **Handle operators.** Let K be a subgroup of $\mathbb{S}_{n,k}$. By definition, the number k is called the *degree* of the molecular differential operator $X^n D^k/K$. More generally, the degree of the differential operator $\Omega(X, D)$, is the supremum (possibly infinite) of the degrees occurring in its molecular expansion $\Omega(X, D) = \sum_K \omega_K X^n D^k/K$. If all the degrees involved are k, the operator is said to be *homogeneous of degree* k. Degree 0 operator are simply the multiplication operators $H(X)$ which are adjoint, as we saw before, to the Hammond operators $H(D)$. Homogeneous operators of degree 1 are easily classified. They are of the form $H(X)D$, since every species $\Omega(X, T)$, homogeneous of degree 1 in T is of the form $H(X)T$. Homogeneous operator of degree 2 are a little more involved. We call them *handle operators* for obvious reasons (see Figure 15). The molecular handle operators $X^n D^2/K$ fall into two classes:

a) the oriented ones, for which the second projection $\pi_2(K)$ is trivial in $\mathbb{S}_2$;
b) the unoriented ones, for which $\pi_2(K) \simeq \mathbb{S}_2$.

For example, $C_3(X)D^2$ is oriented and $E_2(XD)$ is unoriented.

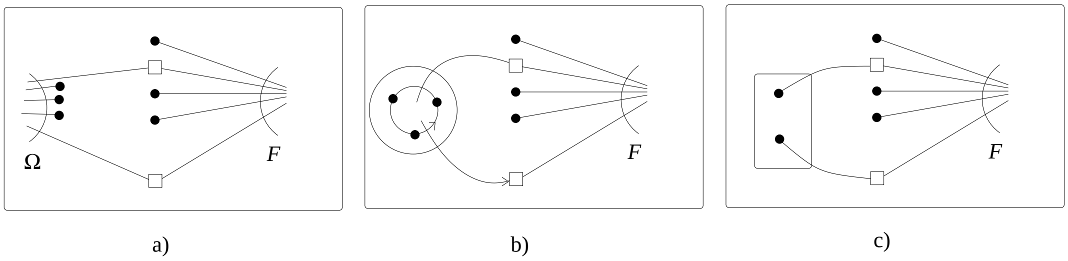


FIGURE 15. a) Handle, b) oriented handle and c) unoriented handle

3.5. **Splittable and classical operators.** Let us say that a molecular operator $X^n D^k/K$ is *splittable* if it can be written in the form of a product

$$\frac{X^n D^k}{K} = \frac{X^n}{K_1} \cdot \frac{D^k}{K_2}$$

where $K_1 \leq \mathbb{S}_n$ and $K_2 \leq \mathbb{S}_k$. More generally, any linear combination of splittable operators is called splittable. For example, $X^3 D^2$ and $C(X)E_2(D) + E(D)$ are splittable but $E(XD)$ and the operator $X^3 D^3/K$ where $K = \langle\, (123)(456)\, \rangle \leq \mathbb{S}_{3,3}$ are not splittable. Of course, the adjoint of a splittable operator is always splittable. In particular, every Hammond operator $H(D)$ is splittable as well as every multiplication $H(X)$. However, splittable operators are not closed under composition $\odot$. To see this, consider the composition of the splittable operators $C_4(D)$ and $C_4(X)$. Some computations gives

$$C_4(D) \odot C_4(X) = C_4(X)C_4(D) + X^3 D^3 + 4X^2 D^2 + E_2(XD) + 6XD + 3,$$

which is not splittable since

$$E_2(XD) = \frac{X^2D^2}{\langle\,(12)(34)\,\rangle}$$

is not.

An important subclass of splittable combinatorial operators are those for which $K_2 = \{\mathrm{id}\}$. These operators are closed under $\odot$ and form an algebra:

$$(A(X)D^k) \odot (B(X)D^\ell) = \sum_{i=0}^{k} \binom{k}{i} A(X)B^{(i)}(X)D^{k+\ell-i}.$$

Such operators have been used by Mishna to define a notion of holonomic species [11]. When both subgroups K_1 and K_2 are trivial, the corresponding operators are said to be *classical*. They also form an algebra (using complex coefficients in molecular expansions) under $+$ and $\odot$ which is isomorphic to the classical Weyl $\mathbb{C}$-algebra generated by X and D.

3.6. **Computations with molecular and atomic differential operators.** Recall that every species $F(X)$ can be written (uniquely, up to isomorphism [2]) as a $\mathbb{N}$-linear combination of molecular species X^n/H,

$$F(X) = \sum_{H,n} f_H \frac{X^n}{H}, \tag{34}$$

where, for each $n \geq 0$, H runs through a system of representatives of the conjugacy classes of subgroups of $\mathbb{S}_n$ (written $H : \mathbb{S}_n$), and, similarly

$$\Omega(X,T) = \sum_{K,m,k} \omega_K \frac{X^mT^k}{K}, \tag{35}$$

where $K : \mathbb{S}_{m,k} \simeq \mathbb{S}_m \times \mathbb{S}_k$. Hence, the computation of $\Omega(X,D)F(X)$ can be reduced, by linearity, to the computation of

$$\frac{X^mD^k}{K}\frac{X^n}{H}. \tag{36}$$

We have the following general reduction formulas from which the computation of (36) can be achieved, using, for example, the GAP software [5].

Theorem 3. *For any subgroups $H \leq \mathbb{S}_n$ and $K \leq \mathbb{S}_{m,k}$, we have*

i) $\displaystyle \frac{X^mD^k}{K}\frac{X^n}{H} = \frac{X^mT^k}{K} \times_T \frac{(X+T)^n}{H}\Big|_{T:=1},$

ii) $\displaystyle \frac{(X+T)^n}{H} = \sum_{k=0}^{n} \sum_{\omega \in \mathbb{S}_{n-k,k}\backslash \mathbb{S}_n/H} \frac{X^{n-k}T^k}{\omega H \omega^{-1} \cap \mathbb{S}_{n-k,k}},$

iii) $\displaystyle \frac{X^aT^k}{A} \times_T \frac{X^bT^k}{B} = \sum_{\tau \in (\pi_2 A)\backslash \mathbb{S}_k/(\pi_2 B)} \frac{X^{a+b}T^k}{A} \times_{\mathbb{S}_k} B^\tau,$

iv) $\displaystyle \left[\frac{X^aT^k}{A}\right]_{T:=1} = \frac{X^a}{\pi_1 A},$

where, $\omega \underline{\in} H_1\backslash\mathbb{S}_p/H_2$ means that ω runs through a system of representatives of the bilateral cosets $H_1\sigma H_2$, $\sigma \in \mathbb{S}_p$; $\pi_i G = \{g_i \in \mathbb{S}_{n_i} \mid (g_1, g_2) \in G\}$, $G \leq \mathbb{S}_{n_1,n_2}$; $B^\tau = (\mathrm{id}_{[b]}, \tau)B(\mathrm{id}_{[b]}, \tau^{-1})$; $A \times_{\mathbb{S}_k} B$ is the fibered product (pullback) of A by B over $\mathbb{S}_k$.

Proof (Sketch). Formula (i) is immediate by definition. Formula (ii) is a classical addition formula (for more details see [2])). Formula (iii) essentially follows form the fact that the stabilizer of a $(X^aT^k/A) \times_T (X^bT^k/B)$-structure $s = (s_1, s_2)$ on $[a, b, k]$, where $s_1 \in (X^aT^k/A)[a, k]$ and $s_2 \in (X^bT^k/B)[b, k]$ is of the form

$$\begin{aligned}\mathrm{stab}(s_1, s_2) &= \{(\sigma_1, \sigma_2, \tau) \mid (\sigma_1, \tau) \in \mathrm{stab}(s_1)\,,\, (\sigma_2, \tau) \in \mathrm{stab}(s_2)\} \\ &= \mathrm{stab}(s_1) \times_{\mathbb{S}_k} \mathrm{stab}(s_2).\end{aligned}$$

Finally, formula (iv) is a consequence of the fact that if $A = \mathrm{stab}(s)$, where s is a X^nT^k/A-structure, then $\pi_1 A$ is the stabilizer of s_1 where s_1 is the $(X^nT^k/A)\big|_{T:=1}$-structure associated to s by unlabelling all its underlying elements of sort T. ☐

A molecular species X^mT^k/K is said to be an *atomic* species if it is irreducible under the ordinary (Cauchy) product of species. Atomic species behave as prime numbers since Y. N. Yeh [12] has proved that every molecular species can be written in a unique way (up to isomorphism and order) as a product of atomic species. By convention, the degenerate molecular species 1 is not considered as atomic (to preserve unicity as in the case of prime numbers). The notion of atomicity is extended to combinatorial differential operators in the obvious way :

$$X^mD^k/K \quad \text{is atomic} \quad \text{if and only if} \quad X^mT^k/K \quad \text{is atomic.} \tag{37}$$

Hence, to generate all combinatorial differential operators, it is sufficient to consider only the atomic ones and to use products and linear combinations.

Using the GAP software [5], we computed in Table 1 below, all "small" atomic differential operators X^mD^k/K satisfying $m + k \leq 7$. In this table, the subgroups $K \leq \mathbb{S}_{m,k} \simeq \mathbb{S}_m \times \mathbb{S}_k$ are given in terms of generators. For better readability, these generators are permutations of the set $\underbrace{1, 2, 3, \ldots}_{m}; \underbrace{A, B, C, \ldots}_{k}$ written in cyclic notation. Our table extends the one given by Chiricota in [4] in which he expresses every molecular species of the form X^m/K ($K \leq \mathbb{S}_m$, $m \leq 7$) in terms of quotients of simpler species E_ν, C_ν, ...

3.7. **Further extensions of the theory.** Allowing coefficients ω_K in molecular expansions

$$\Omega(X, D) = \sum \omega_K X^mD^k/K \tag{38}$$

to be a real or complex numbers, new very curious identities arise. For example, it can be shown that for any real or complex numbers a, b, we have

$$E(aXD) \odot B(bXD) = E((a + b + ab)XD). \tag{39}$$

In particular, $E(-XD)$ is $\odot$-idempotent,

$$E(-XD) \odot E(-XD) = E(-XD), \tag{40}$$

and $E(-2XD)$ is a $\odot$-square root of the identity operator 1,

$$E(-2XD) \odot E(-2XD) = 1. \tag{41}$$

Furthermore, $E(-\frac{1}{2}XD)$ has no effect on $E(-XD)$! Indeed,

$$E(-\tfrac{1}{2}XD) \odot E(-XD) = E(-XD). \tag{42}$$

More generally, making use of multisort species, it is easy to further extend the preceding theory to combinatorial partial differential operators as follows. Consider p sorts of singletons $X_1, X_2, \ldots, X_p$ and denote by $\partial_1, \partial_2, \ldots, \partial_p$ the usual combinatorial partial differential operators

$$\partial_i = \frac{\partial}{\partial X_i}, \qquad i = 1, 2, \ldots, p.$$

Given p extra sorts $T_1, T_2, \ldots, T_p$ and a multisort species

$$\Omega(X_1, X_2, \ldots, X_p; T_1, T_2, \ldots, T_p),$$

we define a corresponding combinatorial partial differential operator

$$\Omega(X_1, X_2, \ldots, X_p; \partial_1, \partial_2, \ldots, \partial_p)$$

acting on species $F(X_1, X_2, \ldots, X_p)$ in the obvious manner:

$$\begin{aligned}
&\Omega(X_1, X_2, \ldots, X_p; \partial_1, \partial_2, \ldots, \partial_p) F(X_1, X_2, \ldots, X_p) \\
&\qquad := \Omega(X_1, X_2, \ldots, X_p; T_1, T_2, \ldots, T_p) \\
&\qquad\qquad \times_{T_1, T_2, \ldots, T_p} F(X_1 + T_1, X_2 + T_2, \ldots, X_p + T_p)\big|_{T_i := 1,\ i = 1, 2, \ldots, p},
\end{aligned}$$

where the partial cartesian product $\times_{T_1, T_2, \ldots, T_p}$ is defined "componentwise". The composition operator $\odot$ is extended by the formula

$$\begin{aligned}
&\Omega_2(X_1, X_2, \ldots, X_p; T_1, T_2, \ldots, T_p) \odot \Omega_1(X_1, X_2, \ldots, X_p; T_1, T_2, \ldots, T_p) \\
&\qquad = \Omega_2(X_1, \ldots, X_p; T_1 + T_{10}, \ldots, T_p + T_{p0}) \\
&\qquad\qquad \times_{T_{10}, \ldots, T_{p0}} \Omega_1(X_1 + T_{10}, \ldots, X_p + T_{p0}; T_1, \ldots, T_p)\big|_{T_{i0} := 1, i = 1, \ldots, p},
\end{aligned}$$

where $T_{10}, T_{20}, \ldots, T_{p0}$ are auxiliary extra sorts of singletons. In this multisort context, molecular and atomic differential operators are of the form

$$\frac{X_1^{m_1} X_2^{m_2} \cdots X_p^{m_p} \partial_1^{k_1} \partial_2^{k_2} \cdots \partial_p^{k_p}}{K},$$

where $K \leq \mathbb{S}_{m_1, m_2, \ldots, m_p; k_1, k_2, \ldots, k_p} \simeq \mathbb{S}_{m_1} \times \mathbb{S}_{m_2} \times \cdots \times \mathbb{S}_{m_p} \times \mathbb{S}_{k_1} \times \mathbb{S}_{k_2} \cdots \times \mathbb{S}_{k_p}$. Hence, every combinatorial partial differential operator $\Omega(X_1, X_2, \ldots, X_p; \partial_1, \partial_2, \ldots, \partial_p)$ can be written in the form

$$\Omega(X_1, X_2, \ldots, X_p; \partial_1, \partial_2, \ldots, \partial_p) = \sum \omega_K \frac{X_1^{m_1} X_2^{m_2} \cdots X_p^{m_p} \partial_1^{k_1} \partial_2^{k_2} \cdots \partial_p^{k_p}}{K},$$

where the summation is taken over $m_1 \geq 0, m_2 \geq 0, \ldots, m_p \geq 0, k_1 \geq 0, k_2 \geq 0, \ldots, k_p \geq 0$, $K : \mathbb{S}_{m_1, m_2, \ldots, m_p; k_1, k_2, \ldots, k_p}$ and the coefficients ω_K are arbitrary complex numbers.

Moreover, allowing weight variables $t, u, v, \ldots$ acting multiplicatively on structures, the coefficients ω_K can be taken in the ring $\mathbb{C}[[t, u, v, \ldots]]$. This means that these combinatorial differential operators form a ring (under "+" and the ordinary product "·") isomorphic to

$$\mathbb{C}[[t, u, v, \ldots, \mathcal{A}\mathrm{tomic}]],$$

where $\mathcal{A}$tomic is the set of all atomic combinatorial partial differential operators. This ring is very rich and is equipped with a multitude of extra operations, $\odot, \times, \dot{\times}, \ldots$ Not only classical differential operators (*e.g.* Laplacians $\partial_1^2 + \partial_2^2 + \cdots + \partial_p^2$ or symmetric Laplacians $E_2(\partial_1) + E_2(\partial_2) + \cdots + E_2(\partial_p)$) belong to this ring but also entirely new ones. For example,

$$C((\pi + iu)E_2(X_1\partial_2) - \frac{3}{4}tE(tX_2 + \partial_4)) \in \mathbb{C}[[t, u, v, \ldots, \mathcal{A}\text{tomic}]]$$

where C is the species of oriented cycles. This ring contains a great variety of extra tools for a better understanding, generation, enumeration and classification of structures that appear in algebraic combinatorics.

Table 1. The atomic combinatorial differential operators $X^m D^k/K$, for $K : \mathbb{S}_{m,k}$, $m+k \leq 7$.

$m=0, k=0$
Empty, since 1 is non atomic.

$m=1, k=0$
X

$m=0, k=1$
D
This is the adjoint of X.

$m=2, k=0$
$X^2/\langle\,(1,2)\,\rangle$

$m=1, k=1$
Empty, since XD factorizes.

$m=0, k=2$
$D^2/\langle\,(A,B)\,\rangle$
This is the adjoint of $X^2/\langle\,(1,2)\,\rangle$.

$m=3, k=0$
$X^3/\langle\,(123)\,\rangle$
$X^3/\langle\,(132),(12)\,\rangle$

$m=2, k=1$
Empty, since D is a factor of every molecular species X^2D/K.

$m=1, k=2$
Empty, since X is a factor of every molecular species XD^2/K.

$m=0, k=3$
$D^3/\langle\,(ABC)\,\rangle$
$D^3/\langle\,(ACB),(AB)\,\rangle$
These are the adjoints of the case $m=3, k=0$.

$m=4, k=0$
$X^4/\langle\,(13)(24)\,\rangle$
$X^4/\langle\,(14)(23),(13)(24)\,\rangle$
$X^4/\langle\,(12)(34),(1324)\,\rangle$
$X^4/\langle\,(13)(24),(14)(23),(12)\,\rangle$

$X^4/\langle\,(13)(24),(14)(23),(243)\,\rangle$
$X^4/\langle\,(13)(24),(14)(23),(243),(12)\,\rangle$

$m=3,k=1$
Empty, since D is a factor of every molecular species X^3D/K.

$m=2,k=2$
$X^2D^2/\langle\,(12)(AB)\,\rangle$ (self-adjoint)

$m=1,k=3$
Empty, since X is a factor of every molecular species XD^3/K.

$m=0,k=4$
Take the adjoints of the case $m=4,k=0$.

$m=5,k=0$
$X^5/\langle\,(12345)\,\rangle$
$X^5/\langle\,(345),(12)(45)\,\rangle$
$X^5/\langle\,(12345),(25)(34)\,\rangle$
$X^5/\langle\,(12345),(25)(34),(2354)\,\rangle$
$X^5/\langle\,(12345),(345)\,\rangle$
$X^5/\langle\,(12345),(12)\,\rangle$

$m=4,k=1$
Empty, since D is a factor of every molecular species X^4D/K.

$m=3,k=2$
$X^3D^2/\langle\,(132),(12)(AB)\,\rangle$

$m=2,k=3$
$X^2D^3/\langle\,(ACB),(AB)(12)\,\rangle$
This is the adjoint of the case $m=3,k=2$.

$m=1,k=4$
Empty, since X is a factor of every molecular species XD^4/K.

$m=0,k=5$
Take the adjoints of the case $m=5,k=0$.

$m=6,k=0$
$X^6/\langle\,(12)(34)(56)\,\rangle$
$X^6/\langle\,(123)(456)\,\rangle$
$X^6/\langle\,(34)(56),(12)(56)\,\rangle$
$X^6/\langle\,(34)(56),(12)(3546)\,\rangle$
$X^6/\langle\,(34)(56),(12)(35)(46)\,\rangle$
$X^6/\langle\,(123)(456),(14)(26)(35)\,\rangle$
$X^6/\langle\,(123)(456),(23)(56)\,\rangle$
$X^6/\langle\,(12)(34)(56),(135)(246)\,\rangle$
$X^6/\langle\,(56),(34),(12)(35)(46)\,\rangle$
$X^6/\langle\,(34)(56),(35)(46),(12)(56)\,\rangle$
$X^6/\langle\,(34)(56),(3546),(12)(56)\,\rangle$
$X^6/\langle\,(34)(56),(12)(56),(135)(246)\,\rangle$
$X^6/\langle\,(12)(34)(56),(135)(246),(35)(46)\,\rangle$
$X^6/\langle\,(456),(123),(23)(56)\,\rangle$
$X^6/\langle\,(456),(123),(14)(25)(36)\,\rangle$

$X^6/\langle\,(56),(34),(12),(135)(246)\,\rangle$
$X^6/\langle\,(34)(56),(35)(46),(456),(12)(56)\,\rangle$
$X^6/\langle\,(34)(56),(12)(56),(135)(246),(35)(46)\,\rangle$
$X^6/\langle\,(34)(56),(12)(56),(135)(246),(3546)\,\rangle$
$X^6/\langle\,(456),(123),(23)(56),(14)(25)(36)\,\rangle$
$X^6/\langle\,(456),(123),(23)(56),(14)(2536)\,\rangle$
$X^6/\langle\,(56),(34),(12),(145)(236),(35)(46)\,\rangle$
$X^6/\langle\,(12346),(14)(56)\,\rangle$
$X^6/\langle\,(456),(46),(123),(23),(14)(25)(36)\,\rangle$
$X^6/\langle\,(15364),(16)(24),(3465)\,\rangle$
$X^6/\langle\,(12345),(456)\,\rangle$
$X^6/\langle\,(123456),(12)\,\rangle$

$m=5, k=1$
Empty, since D is a factor of every molecular species X^5D/K.

$m=4, k=2$
$X^4D^2/\langle\,(13)(24)(AB)\,\rangle$
$X^4D^2/\langle\,(13)(24),(14)(23)(AB)\,\rangle$
$X^4D^2/\langle\,(12)(34),(34)(AB)\,\rangle$
$X^4D^2/\langle\,(12)(34),(1324)(AB)\,\rangle$
$X^4D^2/\langle\,(13)(24),(14)(23),(12)(AB)\,\rangle$
$X^4D^2/\langle\,(12)(34),(13)(24)(AB),(1324)\,\rangle$
$X^4D^2/\langle\,(12)(34),(13)(24)(AB),(34)\,\rangle$
$X^4D^2/\langle\,(13)(24),(14)(23),(243),(12)(AB)\,\rangle$

$m=3, k=3$
$X^3D^3/\langle\,(132)(ACB)\,\rangle$ (self-adjoint)
$X^3D^3/\langle\,(132)(ACB),(23)(BC)\,\rangle$ (self-adjoint)
$X^3D^3/\langle\,(132),(ACB),(12)(AB)\,\rangle$ (self-adjoint)

$m=2, k=4$
Take the adjoints of the case $m=4, k=2$.

$m=1, k=5$
Empty, since X is a factor of every molecular species XD^5/K.

$m=0, k=6$
Take the adjoints of the case $m=6, k=0$.

$m=7, k=0$
$X^7/\langle\,(567),(12)(34)(67)\,\rangle$
$X^7/\langle\,(1234567)\,\rangle$
$X^7/\langle\,(34567),(12)(47)(56)\,\rangle$
$X^7/\langle\,(45)(67),(46)(57),(123)(567)\,\rangle$
$X^7/\langle\,(567),(34)(67),(12)(67)\,\rangle$
$X^7/\langle\,(567),(12)(34),(13)(24)(67)\,\rangle$
$X^7/\langle\,(567),(12)(34),(1324)(67)\,\rangle$
$X^7/\langle\,(1234567),(27)(36)(45)\,\rangle$
$X^7/\langle\,(34567),(47)(56),(12)(4576)\,\rangle$
$X^7/\langle\,(1234567),(235)(476)\,\rangle$

$X^7/\langle\,(567),(34)(67),(12)(67),(13)(24)(67)\,\rangle$
$X^7/\langle\,(67),(45),(123),(23)(46)(57)\,\rangle$
$X^7/\langle\,(567),(34)(67),(12)(67),(13)(24)\,\rangle$
$X^7/\langle\,(45)(67),(46)(57),(123)(567),(23)(67)\,\rangle$
$X^7/\langle\,(1234567),(235)(476),(27)(36)(45)\,\rangle$
$X^7/\langle\,(567),(14)(23),(12)(34),(234),(34)(67)\,\rangle$
$X^7/\langle\,(12345),(345),(45)(67)\,\rangle$
$X^7/\langle\,(1234567),(12)(36)\,\rangle$
$X^7/\langle\,(1234567),(567)\,\rangle$
$X^7/\langle\,(1234567),(12)\,\rangle$

$m=6,k=1$
Empty, since D is a factor of every molecular species X^6D/K.

$m=5,k=2$
$X^5D^2/\langle\,(345),(12)(45)(AB)\,\rangle$
$X^5D^2/\langle\,(12345),(25)(34)(AB)\,\rangle$
$X^5D^2/\langle\,(45)(AB),(123),(23)(AB)\,\rangle$
$X^5D^2/\langle\,(12345),(25)(34),(2354)(AB)\,\rangle$
$X^5D^2/\langle\,(125),(142),(234),(45)(AB)\,\rangle$

$m=4,k=3$
$X^4D^3/\langle\,(13)(24)(BC),(ABC)\,\rangle$
$X^4D^3/\langle\,(14)(23),(13)(24)(BC),(ABC)\,\rangle$
$X^4D^3/\langle\,(13)(24),(14)(23),(243)(ACB)\,\rangle$
$X^4D^3/\langle\,(12)(34),(1324)(BC),(ABC)\,\rangle$
$X^4D^3/\langle\,(12)(34),(34)(BC),(ABC)\,\rangle$
$X^4D^3/\langle\,(13)(24),(14)(23),(12)(BC),(243)(ACB)\,\rangle$
$X^4D^3/\langle\,(13)(24),(14)(23),(12)(BC),(ACB)\,\rangle$
$X^4D^3/\langle\,(12)(34),(13)(24)(BC),(ABC),(34)\,\rangle$
$X^4D^3/\langle\,(12)(34),(13)(24)(BC),(ABC),(1324)\,\rangle$
$X^4D^3/\langle\,(13)(24),(14)(23),(ABC),(243),(12)(BC)\,\rangle$

$m=3,k=4$
Take the adjoints of the case $m=4,k=3$.

$m=2,k=5$
Take the adjoints of the case $m=5,k=2$.

$m=1,k=6$
Empty, since X is a factor of every molecular species XD^6/K.

$m=0,k=7$
Take the adjoints of the case $m=4,k=3$.

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