

# Polynomial invariants and algebraic structures of combinatorial objects

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Théo Karaboghossian. Polynomial invariants and algebraic structures of combinatorial objects. Algebraic Topology [math.AT]. Université de Bordeaux, 2020. English. NNT: 2020BORD0123. tel-03019148

### HAL Id: tel-03019148 https://theses.hal.science/tel-03019148

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## **THÈSE**

PRÉSENTÉE À

## L'UNIVERSITÉ DE BORDEAUX

ÉCOLE DOCTORALE DE MATHÉMATIQUES ET D'INFORMATIQUE

par Théo Karaboghossian

POUR OBTENIR LE GRADE DE

### **DOCTEUR**

SPÉCIALITÉ : INFORMATIQUE

# Polynomial invariants and algebraic structures of combinatorial objects

Date de soutenance : 05 Octobre 2020

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Titre: Invariants polynomiaux et structures algébriques d'objets combinatoires

Résumé: Dans la première moitié de ce mémoire, nous étudions les invariants polynomiaux définis par Aguiar et Ardila dans arXiv:1709.07504 dans le contexte des monoïdes de Hopf. Nous donnons d'abord une interprétation combinatoire de ces polynômes pour les monoïdes de Hopf des permutaèdres généralisés et des hypergraphes, sur les entiers naturels et négatifs. Nous en déduisons ensuite des interprétations similaires sur d'autres objets combinatoires (graphes, complexes simpliciaux, building sets, etc). Dans la seconde moitié de ce mémoire, nous proposons une nouvelle façon de définir et d'étudier des opérades de multigraphes et d'objets similaires. Nous étudions en particulier deux opérades obtenues avec cette méthode. La première est une généralisation directe de l'opérade Kontsevich-Willwacher, qui peut être considérée comme une opérade canonique sur les multigraphes et possède de nombreuses sous-opérades intéressantes. La seconde est une extension naturelle de l'opérade pré-Lie et a aussi un lien avec l'opérade précédente. Nous présentons également divers résultats sur certaines sous-opérades finiment enegendrées et établissons des liens entre elles et les opérades commutative et commutative magmatique.

Mots clefs: Combinatoire algébrique, Espèces, Monoïdes de Hopf, Hypergraphes, Invariants polynomiaux, Opérades, Multigraphes, Graphes, Pré-Lie, Koszulité.

Title: Polynomial invariants and algebraic structures of combinatorial objects

Abstract: In the first half of this dissertation, we study the polynomial invariants defined by Aguiar and Ardila in arXiv:1709.07504 in the context of Hopf monoids. We first give a combinatorial interpretation of these polynomials over the Hopf monoids of generalized permutahedra and hypergraphs in both non negative and negative integers. We then use them to deduce similar interpretation on other combinatorial objects (graphs, simplicial complexes, building sets, etc). In the second half of this dissertation, we propose a new way of defining and studying operads on multigraphs and similar objects. We study in particular two operads obtained with our method. The former is a direct generalization of the Kontsevich-Willwacher operad. This operad can be seen as a canonical operad on multigraphs, and has many interesting sub-operads. The latter operad is a natural extension of the pre-Lie operad in a sense developed here and it is related to the multigraph operad. We also present various results on some of the finitely generated sub-operads of the multigraph operad and establish links between them and the commutative operad and the commutative magmatic operad.

**Keywords:** Algebraic combinatorics, Species, Hopf monoids, Hypergraphs, Polynomial invariants, Operads, Multigraphs, Graphs, Pre-Lie, Koszulity.

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#### Résumé

Le sujet de cette thèse est l'étude d'invariants et de structures algébriques d'objets combinatoires. Nos contributions principales se divisent en deux parties : une étude des invariants polynomiaux définis par Aguiar et Ardila sur les monoïdes de Hopf et la définition et l'étude d'opérades de graphes.

En combinatoire, les structures de Hopf sont un cadre algébrique idéal pour travailler avec des opérations de fusion (produit) et de division (co-produit) d'objets combinatoires. La notion d'algèbre de Hopf est bien connue et utilisée en combinatoire depuis plus de 30 ans, elle a prouvé sa grande force en répondant à diverses questions (voir par exemple [26]). En particulier, elle permet de définir et calculer des invariants polynomiaux sur différents objets combinatoires (voir [3], [9], [21] ou [33] pour divers exemples). Plus récemment, Aguiar et Mahajan ont défini une notion de monoïde de Hopf [4], [5] apparentée à la notion d'algèbre de Hopf et fondée sur la théorie des espèces de Joyal [31]. Comme dans le cas des algèbres de Hopf, c'est une notion utile pour travailler avec des invariants combinatoires. Ceci a été particulièrement mis en lumière par le récent et vaste article d'Aguiar et Ardila [2] où ils donnent notamment un théorème permettant de générer divers invariants polynomiaux. Ils retrouvent ainsi le polynôme chromatique sur les graphes, le polynôme de Billera-Jia-Reiner sur les matroïdes et le polynôme d'ordre strict des posets. En outre, ils fournissent également les outils nécessaires pour calculer ces invariants sur les entiers négatifs, et récupérer ainsi différents théorèmes de réciprocité. Dans la première moitié de ce manuscrit, nous appliquons les théorèmes d'Aguiar et Ardila au monoïde de Hopf des permutaè dres généralisés et au monoïde de Hopf des hypergraphes définis dans [2]. Nos résultats sont en extension directe avec ceux d'Aguiar et d'Ardila. Dans [2], après avoir donné une bonne expression pour l'antipode des permutaèdres généralisés, ils l'utilisent pour déduire des expressions similaires d'antipodes d'autres monoïdes de Hopf. Nous suivons le même processus avec leurs invariants polynomiaux  $\chi^{\zeta}$ . Nous obtenors une description combinatoire de tous les invariants  $\chi^{\zeta}$  aussi bien sur les entiers positifs que négatifs. De plus, notre description ne se limite pas au cas où  $\zeta$  est un caractère dit "basique", c'est-àdire reconnaissant les objets triviaux, et nos formules généralisent de nombreux résultats existants dans la littérature.

Dans la deuxième partie de ce mémoire nous étudions les opérades. Les opérades sont des structures mathématiques d'abord apparues en topologie et qui ont ensuite connu un essor en algèbre [36] mais aussi en combinatoire [16] —voir par exemple [40, 25] pour des références générales sur les opérades symétriques et non symétriques, les opérades ensembliste et linéaire etc au travers de la théorie des espèces. Au cours des dernières décennies, plusieurs opérades sur les arbres ont été définies, parmi elles, les plus étudiées sont l'opérade pré-Lie PLie [17] et l'opérade permutative non associative NAP [35]. Il semble alors naturel de se demander s'il est aussi possible de définir des opérades intéressantes sur les graphes et quelles sont leurs propriétés. La nécessité de définir des opérades de graphe appropriées vient de la combinatoire, où les graphes sont tout comme les arbres, des objets naturels à étudier. Elle vient aussi de la physique, où il a été récemment proposé d'utiliser des opérades de graphes afin d'encoder la combinatoire de la renormalisation des graphes

de Feynman en théorie quantique des champs [34]. Des opérades de graphes ont déjà été définies, par exemple dans [32, 45, 40, 24, 38]. Dans la seconde moitié de ce manuscrit, nous allons plus loin dans cette direction et définissons une nouvelle classe d'opérades de graphes. Nous étudions deux opérades de cette classe en particulier : nous établissons un lien avec l'opérade pré-Lie mentionnée ci-dessus, et nous étudions quelques sous-opérades finiment engendrées d'intérêt.

Ce manuscrit s'organise comme suit. Dans la section 2 nous présentons les préliminaires nécessaires aux sections suivantes. Ceux-ci consistent en une brève introduction à la théorie des espèces et une présentation des divers objets combinatoires considérés ici. Dans la section 3, nous donnons nos résultats sur les monoïdes de Hopf et dans la Section 4 ceux sur les opérades. Nous concluons avec la section 5 où nous mentionnons certains résultats qui non présentés ici ainsi que diverses pistes de recherche dans la continuité des travaux menés durant ces trois années de thèse.

#### Espèces

Les espèces ont été introduites par Joyal dans [31] et sont le cadre idéal pour travailler avec des objets étiquetés. Une espèce linéaire S est la donnée de :

- un espace vectoriel S[V] pour chaque ensemble fini V,
- un isomorphisme  $S[\sigma]:S[V]\to S[W]$  pour chaque bijection  $\sigma:V\to W.$

Ces bijections doivent de plus être compatibles avec la composition:  $S[\sigma \circ \tau] = S[\sigma] \circ S[\tau]$  et S[Id] = Id.

Un point fort de la théorie des espèces sont les multiples opérations permettant de construire de nouvelles espèces à partir d'espèce déjà existante. Étant données deux espèces ensemblistes R et S on définit ainsi les espèces suivantes:

$$Somme \quad (R+S)[V] = R[V] \oplus S[V], \qquad Produit \quad R \cdot S[V] = \bigoplus_{V_1 \sqcup V_2 = V} R[V_1] \otimes S[V_2],$$

Produit de Hadamard 
$$(R \times S)[V] = R[V] \otimes S[V]$$

$$D\acute{e}riv\acute{e}e \quad S'[V] = S[V + \{*\}] \ \text{où} \ * \not\in V, \qquad Point\acute{e}e \quad S^{\bullet}[V] = S[V] \cdot V.$$

Si de plus S est positive (i.e.  $S[\emptyset] = \{0\}$ ) on peut aussi définir la composition

$$R(S)[V] = \bigoplus_{P \text{ partition de } V} R[P] \bigotimes_{P_i \in P} S[P_i].$$

#### Monoïdes de Hopf et invariants polynomiaux

Un monoïde de Hopf M est une espèce linéaire telle que  $M[\emptyset] = \mathbb{K}$  munie d'un produit et d'un co-produit

$$\mu_{V_1,V_2}: M[V_1] \otimes M[V_2] \to M[V_1 \sqcup V_2], \qquad \Delta_{V_1,V_2}: M[V_1 \sqcup V_2] \to M[V_1] \otimes M[V_2],$$
$$x \otimes y \mapsto x \cdot y \qquad \qquad z \mapsto \sum z_1 \otimes z_2.$$

Ces deux morphismes sont sujets à des axiomes de naturalité, d'unitarité, d'associativité et de compatibilité. Tout monoïde de Hopf M est muni d'un antipode  $S: M \to M$  qui est une application qui joue un rôle d'inverse dans la théorie. Un caractère d'un monoïde de Hopf M, est une collection de formes linéaires  $\zeta_V: M[V] \to \mathbb{K}$  naturelle et compatible avec le produit.

Les invariants polynomiaux qui nous intéressent dans cette partie sont ceux définis dans le théorème suivant :

**Théorème 0.1** (Proposition 16.1 et Proposition 16.2 dans [2]). Soit M un monoïde de Hopf et  $\zeta$  un caractère de M. Alors pour tout  $x \in M[V]$ , il existe un polynôme  $\chi(x)$  tel que

- 1.  $\chi(x)(1) = \zeta(x)$ ,
- 2.  $\chi(x \cdot y) = \chi(x)\chi(y)$ ,
- 3.  $\chi(x)(-n) = \chi(S(x))(n)$  pour tout entier naturel n.

Nous fournissons d'abord une interprétation combinatoire, pour les entiers positifs et négatifs, de ces polynômes sur le monoïde de Hopf des permutaèdres généralisés. Les permutaèdres généralisés sont une famille de polytopes vérifiant certaines contraintes et jouant un rôle majeur dans la théorie des monoïdes de Hopf. Étant donné un polytope  $P \subset \mathbb{R}V$ , Q l'une de ses faces et n un entier naturel, on définit les cônes ouvert et fermé :

$$\mathcal{N}_{P}^{o}(Q)_{n} = \left\{ c \in [n]^{V} \mid P_{c} = Q \right\}$$
  
$$\mathcal{N}_{P}(Q)_{n} = \left\{ c \in [n]^{V} \mid Q \text{ est une face de } P_{c} \right\},$$

où  $P_c = \{p \in P \mid c(p) \geq c(q) \text{ pour tout } q \in P\}$ . Les éléments de  $\mathcal{N}_P^o(Q)_n$  et  $\mathcal{N}_P(Q)_n$  sont respectivement appelés les colorations (avec [n]) strictement compatibles avec Q et les colorations (avec [n]) compatibles avec Q.

Notre premier résultat s'exprime alors ainsi, où  $\mathbb{K}GP$  est l'espèce des permutaèdres généralisés :

**Théorème 0.2.** Soit  $\zeta$  un caractère de  $\mathbb{K}GP,\ V$  un ensemble fini et P un permutaèdre généralisé. Alors

$$\chi_V^{\zeta}(P)(n) = \sum_{Q \le P} \zeta(Q) |\mathcal{N}_P^o(Q)_n|,$$
  
$$\chi_V^{\zeta}(h)(-n) = \sum_{P < Q} (-1)^{|V| - \dim Q} \zeta(Q) |\mathcal{N}_P(Q)_n|.$$

De plus, si  $\zeta$  prend des valeurs dans  $\{0,1\}$ ,  $\chi_V^{\zeta}(P)(n)$  est le nombre de paires strictement compatibles (Q,c) où Q est une face de P non annulée par  $\zeta$  et c une coloration avec [n]. De même,  $\chi_V^{\zeta}(P)(-n)$  est le nombre de telles paires compatibles. En particulier,  $(-1)^{|V|}\chi^{\zeta}(P)(-1)$  est le nombre de faces de P non annulées par  $\zeta$ .

Ce résultat s'obtient assez directement en utilisant les outils développés par Ardila et Aguiar dans [2].

Nous nous intéressons ensuite au monoïde de Hopf  $\mathbb{K}HG$  des hypergraphes. Un hypergraphe sur V est un multi-ensemble de parties de V. On définit une notion d'orientation acyclique sur ces objets ainsi qu'une notion de (stricte) compatibilité entre les orientations acycliques et les colorations. Pour h un hypergraphe,  $f \in \mathcal{A}_h$  une orientation acyclique de h et n un entier naturel, on note  $C_{h,f,n}$  et  $\overline{C}_{h,f,n}$  les ensembles de colorations strictement compatibles et compatibles avec f.

**Théorème 0.3.** Soit  $\zeta$  un caractère de  $\mathbb{K}HG$ , V un ensemble fini et h un hypergraphe. Alors

$$\chi_V^{\zeta}(h)(n) = \sum_{f \in \mathcal{A}_h} \zeta(f(h))|C_{h,f,n}|,$$
  
$$\chi_V^{\zeta}(h)(-n) = \sum_{f \in \mathcal{A}_h} (-1)^{\operatorname{cc}(f(h))} \zeta(f(h))|\overline{C}_{h,f,n}|.$$

De plus, si  $\zeta$  prend des valeurs dans  $\{0,1\}$ ,  $\chi_V^{\zeta}(h)(n)$  est le nombre de paires strictement compatibles (f,c) où f est une orientation acyclique de h telle que f(h) ne soit pas annulé par  $\zeta$  et c une coloration avec [n]. De même,  $\chi_V^{\zeta}(h)(-n)$  est le nombre de telles paires compatibles. En particulier,  $(-1)^{|V|}\chi^{\zeta}(h)(-1)$  est le nombre d'orientation acycliques telles que  $\zeta(f(h)) \neq 0$ .

Nous démontrons ce résultat de deux façons différentes. Une première approche est directe ; elle consiste à d'abord exprimer les polynômes  $|C_{h,f,n}|$  et  $|\overline{C}_{h,f,n}|$  en terme de polynômes de Faulhaber généralisés —que l'on introduit dans ce mémoire— puis d'exploiter le bon comportement de ces polynômes sur les entiers négatifs à l'aide d'un lemme technique sur des sommes alternées. La deuxième approche repose sur le Théorème 0.2: il y a une bijection entre les hypergraphes et les polytopes hypergraphiques, qui forment un sous monoïde de Hopf de  $\mathbb{K}GP$ . Il s'agit ensuite de montrer que sous cette bijection les orientations acycliques d'un hypergraphe sont équivalentes aux faces d'un polytope hypergraphique.

Le reste de cette partie s'appuie sur une propriété intéressante des polynômes  $\chi$  :

**Proposition 0.4.** Soit M et N deux monoïdes de Hopf,  $\zeta^M$  et  $\zeta^N$  des caractères de ces monoïdes de Hopf et  $fM \to N$  un morphisme de monoïdes de Hopf tel que  $\zeta^N \circ f = \zeta^M$ . Alors  $\chi^{N,\zeta^N} \circ f = \chi^M$ .

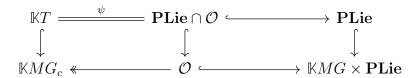
En exploitant cette proposition ainsi que le Théorème 0.3 on obtient des résultats analogues aux Théorèmes 0.2 et 0.3 sur les monoïdes de Hopf des hypergraphes simples, des graphes, des complexes simpliciaux, des building sets, des graphes simples, des partitions et des ensembles de chemins.

#### **Opérades**

Une opérade est une espèce linéaire positive  $\mathcal{O}$  munie d'une composition partielle  $\circ_* : \mathcal{O}' \cdot \mathcal{O} \to \mathcal{O}$  vérifiant des axiomes de naturalité, d'associativité, de commutativité et d'unitarité. Le premier résultat de cette section est la définition d'une structure d'opérade sur  $\mathbb{K}MG$ , l'espèce des multigraphes (*i.e.* graphes avec répétition d'arêtes et boucles). Pour  $g_1$  et  $g_2$  deux multigraphes, on définit  $g_1 \circ_* g_2$  comme la somme de tous les graphes obtenus de la façon suivante.

- Prendre l'union disjointe de  $g_1$  et  $g_2$ .
- Enlever le sommet \* de  $g_1$ . On a alors des bouts d'arêtes libres.
- Recoller chaque bout d'arête libre sur n'importe quel sommet de  $g_2$ .

On montre ensuite qu'il existe une lien non trivial entre cette opérade et l'opérade pré-Lie sur les arbres enracinés. Soit  $\psi : \mathbb{K}MG \to \mathbb{K}MG^{\bullet}$  le morphisme qui envoie un multigraphe sur la somme de toutes les façons de le pointer. Il existe alors une opérade  $\mathcal{O}$  telle que le diagramme suivant commute:



Dans la deuxième partie de cette section, on s'intéresse à quatre sous opérades finiment engendrées de  $\mathbb{K}MG$ :

$$\{a \ b\}, \{a - b\}, \{a \ b, a - b\} \text{ et } \left\{ \begin{array}{c} O \\ O \end{array}, a \ b \right\}.$$

On les note respectivement  $G_{\emptyset}$ , Seg, SP et LP. On montre que  $G_{\emptyset}$  est isomorphe à l'opérade commutative Com et que Seg est isomorphe à l'opérade commutative magmatique ComMag. Pour ce deuxième résultat, on utilise notamment la fonction  $\psi$  définie précédemment et le résultat [14]. On montre ensuite que SP est binaire quadratique et Koszul et on donne son dual de Koszul. Afin de montrer la Koszulité, on se réfère aux travaux [20] de Dotsenko et Khoroshkin sur les bases de Gröbner pour les opérades. On finit cette section en montrant que LP est une sous opérade stricte de  $\mathbb{K}MG$  en utilisant des outils de calcul formel pour montrer que le multigraphe



n'est pas dans LP.

## Contents

1	Intr	oducti	ion	10
2	Spe	cies		12
	2.1		theory of species	12
		2.1.1	Set species	12
		2.1.2	Linear species	14
		2.1.3	Constructions over species	15
		2.1.4	Enriched Schröder trees	16
	2.2	Combi	inatorial objects	17
		2.2.1	Multisets	17
		2.2.2	Graphs and related objects	18
		2.2.3	Decomposition and compositions	21
3	Pol	vnomia	al invariants over Hopf monoids	23
_	3.1		monoids	23
	9	3.1.1	Definitions	23
		3.1.2	Aguiar and Ardila polynomial invariant	25
		3.1.3	The Hopf monoid of generalized permutahedra	27
	3.2		omial invariants and reciprocity theorems on the Hopf monoid of gen-	
			ed permutahedra	30
	3.3		omial invariants and reciprocity theorems on the Hopf monoid of hy-	
			iphs	33
		3.3.1	Generalized Faulhaber's polynomials	34
		3.3.2	Chromatic polynomials of hypergraphs	36
		3.3.3	Reciprocity theorem	43
		3.3.4	Alternative proof	48
	3.4	Other	Hopf monoids	49
		3.4.1	Simple hypergraphs	50
		3.4.2	Graphs	51
		3.4.3	Simplicial complexes	53
		3.4.4	Building sets	55
		3.4.5	Graphs, ripping and sewing	58
		3.4.6	Partitions	60
		3.4.7	Set of paths	61
4	One	erads o	on graphs	63
_	4.1		ds	63
	_,_	4.1.1	Definitions and examples	63
		4.1.2	Free operad, generators and relations	66
		4.1.3	Koszul duality	67
		4.1.4	Koszul operads	68

	Graph insertion operads
4.4	Applications
	4.4.1 The $\mathbb{K}MG$ operad
	4.4.2 Finitely generated sub-operads

#### 1 Introduction

The topic of this thesis is the study of invariants and algebraic structures of combinatorial objects. Our main contributions can be separated in two parts: a study of polynomial invariants over Hopf monoids, and a study of operad structures over graphs and related objects.

In combinatorics, Hopf structures give an algebraic framework to deal with operations of merging (product) and splitting (co-product) combinatorial objects. The notion of Hopf algebra is well known and used in combinatorics for over 30 years, and has proved its great strength in answering various questions (see for example [26]). In particular, they are useful to define and compute polynomial invariants (see [3], [9], [21] or [33] for various examples). More recently, Aguiar and Mahajan defined a notion of Hopf monoid [4],[5] akin to the notion of Hopf algebra and built on Joyal's theory of species [31]. Such as in the case of Hopf algebras, they are useful when working with polynomial invariants, as was showed by the seminal paper of Aguiar and Ardila [2]. In particular they give a theorem to generate various polynomial invariants and use it to recover the chromatic polynomial of graphs, the Billera-Jia-Reiner polynomial of matroids and the strict order polynomial of posets. Furthermore, Aguiar and Ardila also give a way to compute these polynomial invariants on negative integers hence also recovering the different reciprocity theorems associated to these combinatorial objects.

In the first half of this dissertation, we apply Aguiar and Ardila's theorem to the Hopf monoid of generalized permutahedra and the Hopf monoid of hypergraphs defined in [2]. Our results are a direct extension to Aguiar and Ardila's results: from their expression of the antipode for the generalized permutahedra they deduced formulas for the antipode of many different Hopf monoids. We follow the same process but with their polynomial invariant  $\chi^{\zeta}$  instead. We obtain a combinatorial description for the all the invariants  $\chi^{\zeta}$  for both the non negative and negative integers. We do not restrict ourselves to the basic characters for  $\zeta$  and our results generalize many existing results in the literature.

In the second part of this dissertation, we study operads. Operads are mathematical structures which have been intensively studied in the context of topology, algebra [36] but also of combinatorics [16] —see for example [40, 25] for general references on symmetric and non-symmetric operads, set operads through species, etc. In the last decades, several interesting operads on trees have been defined. Amongst these tree operads, maybe the most studied are the pre-Lie operad PLie [17] and the nonassociative permutative operad NAP [35]. It seems natural to ask what kind of operads can be defined on graphs and what are their properties? The need for defining appropriate graph operads comes from combinatorics, where graphs are, just like trees, natural objects to study. It comes also from physics, where it was recently proposed to use graph operads in order to encode the combinatorics of the renormalization of Feynman graphs in quantum field theory [34]. Other graph operads have been defined for example in [32, 45, 40, 24, 38]. In this dissertation, we go further in this direction and we define, using the combinatorial species setting [12], new graph operads. Moreover, we investigate several properties of these operads: we describe an explicit link with the pre-Lie operad mentioned above, and we study interesting (finitely

generated) sub-operads.

This dissertation is organized as follow. In Section 2 we give some preliminaries to the following sections. These consist in a brief introduction to the theory of species and a presentation of diverse combinatorial objects used in this dissertation. In Section 3 we present our results on Hopf monoids and in Section 4 those on operads. We conclude with Section 5 where we mention some results which were not presented it in this dissertation as well as some future directions naturally arising from the research we conducted during these three years of thesis.

### 2 Species

In this first section we present the notion of species, which will be the framework of the next two sections, along with some examples of species of particular interest in this dissertation.

In all this dissertation, V will always denote a finite set and  $V_1$  and  $V_2$  two disjoint sets such that  $V = V_1 \sqcup V_2$ . The letter n always denotes a non negative integer and we denote by [n] the set  $\{1, \ldots, n\}$  and by  $\mathfrak{S}_n$  the group of permutations over [n]. All vector spaces appearing in this dissertation are defined over a field of characteristic 0 denoted by  $\mathbb{K}$ .

#### 2.1 Basic theory of species

Species were first introduced by Joyal in [31] and are a very useful tool to manipulate labelled structures. We present here a few basic definitions and properties which will be of use to define Hopf monoids and operads in sections 3 and 4. We refer the reader to [12] for a more involved approach to the theory of species.

#### 2.1.1 Set species

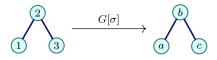
A set species S consists of the following data:

- for each finite set V, a set S[V],
- for each bijection of finite sets  $\sigma: V \to V'$ , a bijection  $S[\sigma]: S[V] \to S[V']$ . These maps should be such that  $S[\sigma_1 \circ \sigma_2] = S[\sigma_1] \circ S[\sigma_2]$  and S[Id] = Id.

Furthermore if  $|S[\emptyset]| = 0$ , S is said to be *positive*. Beware that with our definition, S[V] is not necessarily finite unlike the usual convention.

One should think of S[V] as a set of combinatorial objects labelled with V and of  $S[\sigma]$  as a relabelling operation. For example, for G the set species of graphs (whatever is a graph for now), G[V] is the set of graphs with vertex set V and  $G[\sigma]$  is the relabelling of vertices.

**Example 2.1.** For  $\sigma: \{1,2,3\} \to \{a,b,c\}$  the bijection which sends 1 to a, 2 to b and 3 to c,  $G[\sigma]$  acts as follow:



As shown in this example, in practice the maps  $S[\sigma]$  are often very natural and we do not need to explicitly give them when describing the species S.

We now give a list of example of species that we use through all this dissertation.

**Example 2.2.** 1. We denote by X the set species defined by X[V] = V if V is a singleton and  $X[V] = \emptyset$  else.

- 2. The singleton set species E defined by  $E[V] = \{V\}$  is not a positive species but the identity set species Id defined by Id[V] = V is one.
- 3. A decomposition of V is a finite sequence of pairwise disjoint sets  $(V_1, \ldots, V_n)$  such that  $\sqcup_i V_i = V$ . We denote by  $l(V_1, \ldots, V_n) = n$  the length of a decomposition. A composition of V is a decomposition of V where all elements are non empty. We denote this by  $(V_1, \ldots, V_n) \vDash V$ . A partition of V is a set  $\{P_1, \ldots, P_k\}$  of disjoint non empty sets such that  $\sqcup_i P_i = V$ . We respectively denote by Dcomp, Comp and  $\Pi$  the set species of decompositions, compositions and partitions.
- 4. We denote by  $Pol_+$  the positive set species of polynomials with null constant coefficient in  $\mathbb{K}$ , i.e.  $Pol_+[V]$  is the *infinite set* (not the vector space) of polynomials with variables in V and null constant coefficient when  $V \neq \emptyset$  and  $Pol_+[V] = \emptyset$  else.

As with any algebraic structure, set species also have notions of set sub-species and morphisms. Let R and S be two set species. The set species R is a set sub-species of S if  $R[V] \subseteq S[V]$  for every finite set V and  $R[\sigma] = S[\sigma]$  for every bijection of finite sets  $\sigma$ . A morphism of set species from R to S is a collection of maps  $f_V : R[V] \to S[V]$  such that for each bijection  $\sigma : V \to V'$ , we have  $f_{V'} \circ R[\sigma] = S[\sigma] \circ f_V$ . For the sake of reducing the notations, we will often forget the index V and only write f for any of the maps  $f_V$ .

- **Example 2.3.** 1. The set species of compositions is a set sub-species of the set species of decompositions and X is a set sub-species of Id.
  - 2. For a set species S and an integer n, we denote by  $S_{n+}$  the set sub-species of S defined by  $S_{n+}[V] = S[V]$  if  $|V| \ge n$  and  $S_{n+}[V] = \emptyset$  else. We also denote by  $S_{+} = S_{1+}$ .
  - 3. The collection of maps  $f_V: Id[V] \to Pol_+[V]$  which maps the element v onto the polynomial of degree one v is a morphism of set species  $Id \to Pol_+$ .
  - 4. We have two natural morphisms from  $E_+$  to  $Pol_+$ : one which sends  $\{V\}$  onto the monomial  $\prod V = \prod_{v \in V} v$  and one which sends V onto  $\bigoplus V = \bigoplus_{v \in V} v$ . We prefer to use the symbol  $\bigoplus$  for the addition of polynomials instead of the usual + which we keep for the addition of vectors in vector spaces (see Example 2.4).

In combinatorics, we are usually interested in counting the objects we use and this is often done through the notion of generating series. In the context of species we use the name of Hilbert series: if S is a set species such that S[V] is always a finite set, the *Hilbert series* of S is the formal power series  $\mathcal{H}_S$  defined by:  $\mathcal{H}_S(x) = \sum_{n\geq 0} \frac{|S[[n]]|}{n!} x^n$ . Note that since we are working on labelled sets, we have a  $\frac{1}{n!}$  coefficient which comes from the action of the symmetric group. The set species E, Id and X defined in Examples 2.2 and 2.3 have simple Hilbert series:  $\mathcal{H}_E(x) = \exp(x)$ ,  $\mathcal{H}_{Id}(x) = x \exp(x)$ , and  $\mathcal{H}_X(x) = x$ .

#### 2.1.2 Linear species

Informally, linear species are identical to set species but within the context of linear algebra. A linear species S consists of the following data:

- For each finite set V, a vector space S[V],
- For each bijection of finite sets  $\sigma: V \to V'$ , a linear map  $S[\sigma]: S[V] \to S[V']$ . These maps should be such that  $S[\sigma_1 \circ \sigma_2] = S[\sigma_1] \circ S[\sigma_2]$  and S[Id] = Id.

Furthermore if dim  $S[\emptyset] = 0$ , S is said to be positive.

Let R and S be two linear species. The linear species R is a linear sub-species of S if R[V] is a sub-space of S[V] for every finite set V and  $R[\sigma] = S[\sigma]$  for every bijection of finite sets  $\sigma$ . A morphism of linear species from R to S is a collection of linear maps  $f_V : R[V] \to S[V]$  such that for each bijection  $\sigma : V \to V'$ , we have  $f_{V'} \circ R[\sigma] = S[\sigma] \circ f_V$ . As with set species, we will often forget the index V. We denote by  $S_{n+}$  the linear sub-species of S which is equal to S on  $|V| \ge n$  and equal to S else.

The linearization functor

$$\mathcal{L}:\mathsf{Set}\to\mathsf{Vec}$$

is the functor from the category of sets and functions to the category of vector spaces which sends a set to the vector space with basis the given set. Composing a set species S with this functor gives us a linear species  $\mathcal{L} \circ S$  which we denote by  $\mathbb{K}S$ . This procedure enables us to see any set species as a linear species. We call such linear species linearized species. In this dissertation all linear species will be linearized species and we will often refer to 'species' without specifying whether we consider set species or linearized species which will be clear from the context. We also do not make any difference between a morphism of set species and its linearization.

- **Example 2.4.** 1. When considering  $\mathbb{K}Pol_+$  one has to take into consideration the fact that we need to differentiate the plus of polynomials and the addition of vectors. We will thus denote by  $\oplus$  the former and keep + for the latter and we will denote by  $0_V \in Pol_+[V]$  the polynomial constant to 0 and keep the notation 0 for the null vector. For example,  $ab \oplus c$  is an element of  $Pol_+[\{a,b,c\}]$ , but  $a \oplus b + c$  is a vector in  $\mathbb{K}Pol_+[\{a,b,c\}]$ .
  - 2. There is a natural morphism of linear species from  $\mathbb{K}E_+$  to  $\mathbb{K}Pol_+$  which sends the singleton  $\{V\}$  onto  $\sum V = \sum_{v \in V} v$ . Note that this map is not linearized.
  - 3. In the same way we have a morphism from  $\Pi$  to Comp which sends a partition onto the sum over all the ways of ordering it.

We have the same definition of *Hilbert series* on linear species by replacing cardinalities by dimension: for S a linear species such that S[V] is of finite dimension for every finite set V, we have  $\mathcal{H}_S(x) = \sum_{n \geq 0} \frac{\dim S[[n]]}{n!} x^n$ .

#### 2.1.3 Constructions over species

One strong point of set species and linear species is the different operations on them which enable to construct new set/linear species from existing ones. Let R and S be two set species. We can then construct new set species which are defined as follows:

$$Sum \quad (R+S)[V] = R[V] \sqcup S[V], \qquad Product \quad R \cdot S[V] = \bigsqcup_{V_1 \sqcup V_2 = V} R[V_1] \times S[V_2],$$

$$Hadamard\ product\ (R\times S)[V]=R[V]\times S[V]$$

Derivative  $S'[V] = S[V + \{*\}]$  where  $* \notin V$ , Pointing  $S^{\bullet}[V] = S[V] \times V$ .

Furthermore if S is positive we can also define the *composition* of R and S by:

$$R(S)[V] = \bigsqcup_{P \in \Pi[V]} R[P] \prod_{P_i \in P} S[P_i],$$

where  $\prod_{P_i \in P} S[P_i] = (S[P_1] \times \cdots \times S(P_k))_{\mathfrak{S}_k}$  should be seen as an unordered product. We also have the same definitions on linear species by replacing unions by sums and Cartesian products by tensor products. Note that these constructions are compatible with both the linearization functor:  $\mathcal{L} \circ (R+S) = \mathcal{L} \circ R + \mathcal{L} \circ S$ ,  $\mathcal{L} \circ (R \cdot S) = \mathcal{L} \circ R \cdot \mathcal{L} \circ S$  etc, and, when defined, the Hilbert series:  $\mathcal{H}_{S'} = \mathcal{H}'_S$ ,  $\mathcal{H}_{R(S)} = \mathcal{H}_R(\mathcal{H}_S)$  etc.

**Example 2.5.** • The elements of the pointing of a species S should be interpreted as elements of S with a distinguished vertex. For example, with S = G the species of graphs and  $V = \{a, b, c\}$ , the element  $(\{\{a, c\}, \{c, b\}\}, c) \in G[\{a, b, c\}] \times \{a, b, c\}$  will be represented by changing the shape of the vertex c:

- While most of these constructions are quite straightforward, the operation of composition is more involved. The species R(S) must be thought as elements of R labelled with elements of S. We provide some examples. The set species  $\Pi$  is isomorphic to the set species  $E_+(E_+)$ . The elements of  $G(E_+)[V]$  are graphs for which the vertices are subsets of V forming a partition of V. The elements of  $Pol_+(G_+)$  are polynomials with graphs on distinct vertex sets as variables. The set species X acts as a unit for the composition:  $S_+(X) \cong S_+ \cong X(S_+)$ .
- We already observed the compatibility of the product with the Hilbert series in section 2.1.1:  $\mathcal{H}_X(x)\mathcal{H}_E(x) = x \exp(x) = \mathcal{H}_{Id}(x)$  and, when V is not empty, we indeed have the isomorphism

$$\bigsqcup_{V_1 \sqcup V_2 = V} X[V_1] \times E \cong \bigsqcup_{v \in V} \{v\} \times \{V \setminus \{v\}\} \cong V. \tag{2}$$

Remark 1. In the definition of the derivative we introduce an element \* which should not appear in V. This notation is not enough when multiple derivatives appear in the same species, for example in  $S^{(2)} = S''$  or  $R' \cdot S'$ . Our convention when considering such species is given by the general following notation:

$$R^{(r)} \cdot S^{(s)}[V] = \bigsqcup_{V_1 \sqcup V_2 = V} R[V_1 + \{*_1, \dots, *_r\}] \times S[V_2 + \{*_{r+1}, \dots, *_{r+s}\}]$$
(3)

The elements  $*_1, \ldots, *_{r+s}$  are called *ghost vertices*.

#### 2.1.4 Enriched Schröder trees

A particularly interesting species we can construct using the composition of positive species is the species of Schröder trees enriched with another species. We define enriched Schröder trees for set species as in [40]. Let S be a positive species such that  $S = X + S_{2^+}$ . The species of Schröder trees enriched with S is the set species  $\mathscr{S}_S$  satisfying the following equation:

$$\mathscr{S}_S = X + S_{2^+}(\mathscr{S}_S). \tag{4}$$

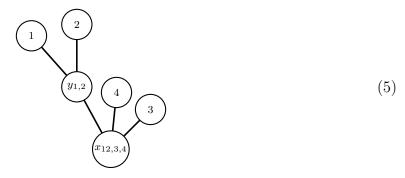
If  $V = \{v\}$  then  $\mathscr{S}_S[V] = X[V] = \{v\}$ . Else, the elements of  $\mathscr{S}_S[V]$  are the trees decorated with elements of S. More formally, these trees can be defined as follows.

- Each element of V is the label of exactly one leaf. For  $v \in V$  a leaf, we denote by  $B_v$  the singleton  $\{v\}$
- To each internal node u associate the set  $B_u$  of the labels of the leaves that are descendent of u.
- An internal node w is then labelled with an element of  $S_{2^+}[\pi_w]$ , where  $\pi_w$  is the partition  $\{B_u \mid u \text{ is a child of } w\}$  of  $B_w$ .

In this context, the elements of S are identified with the corollas of  $\mathscr{S}_S$ .

We obtain the definition of enriched Schröder trees over linear species by replacing X by  $\mathbb{K}X$  in equation (4). The description of the elements of  $\mathscr{S}_S[V]$  is then the same as above by replacing elements by vectors. In particular, we have that  $\mathscr{S}_{\mathbb{K}S} = \mathbb{K}\mathscr{S}_S$ .

**Example 2.6.** Here is an example of an element in  $\mathscr{S}_S[[4]]$  where S is a set species with an element x of size 3 and an element y of size 2.



#### 2.2 Combinatorial objects

In this subsection we present in more details some species mentioned previously as well as other species of interest in this dissertation. The reader may treat this section as a short glossary and skip it to come back to it when necessary.

#### 2.2.1 Multisets

While multisets are not objects in which we are particularly interested in, we need to give some formalism on multisets in order to properly introduce the different notions of graph in the next subsubsection. We chose to define multisets as equivalence classes of tuples.

A multiset m of V is an equivalence class of  $V^n$  under the natural action of  $\mathfrak{S}_n^1$  where n is called the *cardinal* or *size* of m. For m a multiset of V, we call the *multiplicity of* v in m and denote by m(v) the cardinality of  $\{i \mid \pi_i(\underline{m}) = v\}$  where  $\underline{m}$  is any representative element of m and  $\pi_i$  is the projection on the i-th coordinate. For  $V = \{v_1, \ldots, v_k\}$ ,

in 
$$m$$
 and denote by  $m(v)$  the cardinality of  $\{i \mid \pi_i(\underline{m}) = v\}$  where  $\underline{m}$  is any representative element of  $m$  and  $\pi_i$  is the projection on the  $i$ -th coordinate. For  $V = \{v_1, \ldots, v_k\}$ , we denote by  $\{\overbrace{v_1, \ldots, v_1}^{n_1 \text{ times}}, \ldots, \overbrace{v_k, \ldots, v_k}^{n_k \text{ times}}\}$  the multiset which is the equivalence class of  $(v_1, \ldots, v_1, \ldots, v_k, \ldots, v_k)$ .

As this notation suggests, many notions and operations on sets generalize to multisets. Let us describe them along with other notions proper to multisets. Let m and m' be two multisets of V.

- We call domain of m and denote by D(m) the set  $\{v \in V \mid m(v) > 0\}$ .
- We write that an element v is in the multiset m and denote by  $v \in m$  if  $v \in D(m)$ .
- We write that m' is a sub-multiset of m and denote by  $m' \subseteq m$  if  $m'(v) \leq m(v)$  for all  $v \in V$ .
- We call *empty* multiset and denote by  $\emptyset$  the unique multiset of size 0.
- The disjoint union of m and m' is the multiset  $m \sqcup m'$  with domain  $D(m) \cup D(m')$  defined by  $(m \sqcup m')(v) = m(v) + m'(v)$ .
- The intersection of m and m' is the multiset  $m \cap m'$  with domain  $D(m) \cap D(m')$  defined by  $(m \cap m')(v) = \min(m(v), m'(v))$ .
- If m' is a sub-multiset of m, the *complement* of m' in m is the multiset  $m \setminus m'$  defined by  $(m \setminus m')(v) = m(v) m'(v)$ .
- The intersection of m with  $W \subseteq V$  is the multiset  $m|_W$  defined by  $(m|_W)(v) = m(v)$  if  $v \in W$  and  $(m|_W)(v) = 0$  else. Remark that it is not equal to the intersection of m with W while considering W a multiset instead of a set.

 $<sup>{}^{1}\</sup>sigma\cdot(v_{1},\ldots,v_{n})=(v_{\sigma(1)},\ldots,v_{\sigma(n)})$ 

A map  $f: m \to m'$  between two multisets m and m' of V is the data of a multiset  $f_v \subseteq m'$  of size m(v) for each  $v \in m$ . We will use the notation f(v) to designate any of the elements in  $f_v$ .

We denote by  $\mathcal{M}$  the set species of multisets. We denote by  $\mathcal{M}(V)$  the set of multisets of V, preferring parentheses to the brackets of the definition of species. We also denote by  $\mathcal{M}_k(V)$  the set of multisets of size k of V and by  $\mathcal{M}(V)^+$  the set of non empty multisets of V.

#### 2.2.2 Graphs and related objects

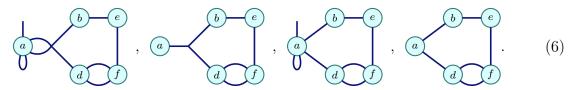
Let  $\mathcal{P}(V)$  denote the set of parts of V,  $\mathcal{P}_k(V)$  the set of parts of V of size k and  $\mathcal{P}(V)^+$  the set of non empty parts of V.

**Definition 2.7.** Let V be a finite set.

- A simple graph over V is a subset of  $\mathcal{P}_2(V)$ .
- A simple hypergraph over V is a subset of  $\mathcal{P}(V)^+$ .
- A simple multigraph over V is a subset of  $\mathcal{M}_2(V)$ .
- A simple multi-hypergraph over V is a subset of  $\mathcal{M}(V)^+$ .
- A graph over V is a multiset with domain in  $\mathcal{P}_2(V)$ .
- A hypergraph over V is a multiset with domain in  $\mathcal{P}(V)^+$ .
- A multigraph over V is a multiset with domain in  $\mathcal{M}_2(V)$ .
- A multi-hypergraph over V is a multiset with domain in  $\mathcal{M}(V)^+$ .

We respectively denote by SG, SHG, SMG, SMHG, G, HG, MG and MHG the set species associated to these objects.

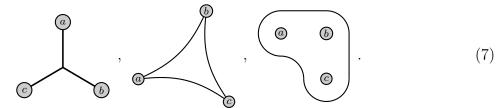
**Example 2.8.** We respectively represented a multi-hypergraph, a hypergraph, a multi-graph and a graph over the same set of vertices:



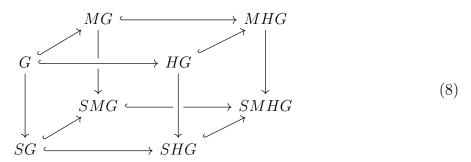
The multi-hypergraph represented here corresponds to the multi-hypergraph with domain composed of the edges  $\{a\}$ ,  $\{a,a\}$ ,  $\{a,a,b,d\}$ ,  $\{d,f\}$ ,  $\{b,e\}$  and  $\{e,f\}$ . All the edges are of multiplicity 1 except  $\{d,f\}$  which is of multiplicity 2.

One can obtain the simple counterparts of these objects by forgetting one of the edges between d and f.

Remark 2. When working only with hypergraphs, we will prefer different ways of drawing the edges depending on the context. The same edge  $\{a, b, c\}$  can thus be drawn in the three following ways:



These set species are related by the following commutative diagram:



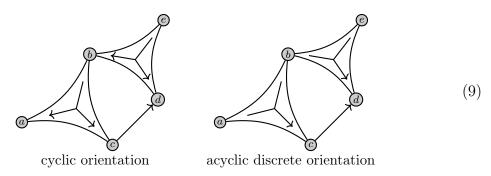
where the downward arrows are given by the domain map  $D: g \mapsto D(g)$  and the arrows from species defined over multisets to species over sets are the maps  $\{e_1, \ldots, e_k\} \mapsto [(e_1, \ldots, e_k)]$ . The remaining arrows are inclusions.

We now give the usual definitions over graphs. In all that follows, S is any species defined as above and g an element of S.

- Edges, vertices and ends. We call edges the elements of g and we call V the set of vertices of g, which we also denote by V(g). We call ends of e the elements of an edge e. Any vertex which is not an end is said to be an isolated vertex. We denote by I(g) the set of isolated vertices of g and by  $NI(g) = V(g) \setminus I(g) = \bigcup_{e \in g} e$  the set of vertices of g which belong to an edge. Note that with this definition, a vertex which does not share an edge with any other vertex is not necessarily isolated.
- Paths, connectedness and cycles. A path of g is a sequence  $e_1, \ldots, e_k$  of distinct edges satisfying  $e_i \cap e_{i+1} \neq \emptyset$  for  $1 \leq i < k$ . A path is cycle if furthermore  $e_k \cap e_1 \neq \emptyset$ . A connected component of g is either an isolated vertex or a maximal (multi) subset of edges such that for every two vertices v, v' in it, their exists a path  $e_1, \ldots, e_k$  such that  $v \in e_1$  and  $v' \in e_k$ . We say that g is connected if it has only one connected component and we denote by  $S_c$  the set sub-species of connected elements of S.
- Forests and trees. A forest is an element of SG with no cycle. We denote by F the species of forest. A connected forest is called a tree and we denote by T the species of tree. We call rooted trees the elements of  $T^{\bullet}$  and for  $(t, v) \in T^{\bullet}[V]$ , we call v the root of t.

- Orientations. An orientation of g is any map f on g such that  $f(e) \subseteq e$  for every edge  $e \in g$ . We call f(e) the targets or exits of e for the orientation f, and we call sources or entries of e for the orientation f its complement in e. We denote by  $f_s(e)$  the entries of e for f. An orientation is said to be admissible if  $f(e) \neq \emptyset$  for every edge e and discrete if |f(e)| = 1 for every edge e. By a slight abuse of notation, we consider discrete orientations as maps from g to g. For g an admissible orientation of g, we denote by g0 the object in the same species and with same vertices than g defined by g1.
- Directed paths and cycles. A directed path in an orientation f is a sequence of distinct edges  $e_1, \ldots, e_k$  such that for each  $1 \leq i < k$  either  $f(e_i) \cap f_s(e_{i+1}) \neq \emptyset$  or  $\emptyset \subsetneq f(e_i) \cap e_{i+1} \subsetneq f(e_{i+1})$ . That is to say we can enter in an edge e' from an edge e either if an exit of e is also an entry of e' or if e' share an exit with e but not all of them. In the particular case of discrete orientation this is reduced to  $f(e_i) \in f_s(e_{i+1})$  and to  $f(e_i) = f_s(e_{i+1})$  when working with graphs. A directed cycle is a directed path with  $f(e_k) \cap f_s(e_1) \neq \emptyset$ . We only impose this condition here and not the second one: we want a directed cycle to at least have one entry. An acyclic orientation is an admissible orientation with no cycles. We denote by  $\mathcal{A}_g$  the set of acyclic orientations of g.

**Example 2.9.** We represent here a hypergraph with two different orientations. One is cyclic and the other is discrete and acyclic.



• Oriented objects We define the set species  $S_{or}$  as the set species of oriented elements of S, i.e. its elements are pairs of an element in S and an orientation of it. This pair is said to be a directed element if the orientation is discrete orientation. It is furthermore acyclic if the orientation is. On the particular case of graphs, these definitions coincide with the standard definitions of same name and a directed acyclic graph defined as such is indeed the classical notion of DAG in the literature. We also consider direct graph as sets of ordered pairs of vertices.

Let us finish this presentation of graphs and related objects by mentioning that there is an isomorphism between the set species MHG and  $Pol_+$ . It is defined as follows:

• the empty graph  $\emptyset_V \in MHG[V]$  is sent on the null polynomial  $0_V$ ,

- an edge e is sent on the monomial  $\prod_{v \in e} v^{e(v)}$ ,
- an element  $h \in MHG[V]$  is sent on the polynomial  $\bigoplus_{e \in h} e$ .

This identification will be very useful in subsection 4.3 to do computations on multihypergraphs since it is easier to formally write operations on polynomials than on graphs. With this identification, hypergraphs can be seen as polynomials where each variable appears at most once in each monomial and multigraphs as homogeneous polynomials of degree 2.

**Example 2.10.** With this identification, the multi-hypergraph in Example 2.8 writes  $a \oplus a^2 \oplus a^2 bd \oplus be \oplus ef \oplus df \oplus df$ .

#### 2.2.3 Decomposition and compositions

We briefly presented the species of decompositions and compositions in Example 2.2. We give here more details on these objects.

Canonical bijection. Let V be a finite set. A coloring of V with [n] is a map from V to [n] and a part ordering of V is a surjective map with domain V and a co-domain of the form [n].

A first and very important observation, is that there exists a canonical bijection between decompositions and colorings. In section 3 we want to seamlessly pass from one notion to the other, so we give a few explanations on this bijection. Given an integer n, the canonical bijection between decompositions of V of size n and colorings of V with [n] is given by:

$$b_{V,n}: \{f: V \to [n]\} \to \{P \in Dcomp[V] \mid l(P) = n\}$$
$$f \mapsto (f^{-1}(1), \dots, f^{-1}(n)).$$
(10)

If it is clear from the context what are V and n, we will write b instead of  $b_{V,n}$ . If P is a partition we will also refer to  $b^{-1}(P)$  by P so that instead of writing "i such that  $v \in P_i$ " and "i and j such that  $v \in P_i$ ,  $v' \in P_j$  and i < j" we can just write P(v) and P(v) < P(v'). Similarly, if P is a function we will refer to b(P) by P so that  $P_i = P^{-1}(i)$ . Remark that  $b_{V,n}$  induces a bijection between compositions and part orderings.

Usual operations. Let us now give some usual operations and definitions over decompositions and compositions.

Let V and W be two disjoint sets and  $P=(P_1,\ldots,P_l)\vDash V$  and  $Q=(Q_1,\ldots,Q_k)\vDash W$  be two compositions. We call product of P and Q and we denote by  $P\cdot Q$  the composition  $(P_1,\ldots,P_l,Q_1,\ldots Q_k)$ . We call  $shuffle\ product$  of P and Q the set sh(P,Q) defined by  $sh(P,Q)=\left\{R\mid (b^{-1}(R))_{|V}=b^{-1}(P) \text{ and } (b^{-1}(R))_{|V'}=b^{-1}(P')\right\}$ , where for f a map with domain V and  $W\subseteq V$ , the map  $f_{|W}$  is defined by  $f_{|W}(v)=f(v)$  for all  $v\in W$ .

Let  $P' = (P_{1,1}, \ldots, P_{1,k_1}, P_{2,1}, \ldots, P_{2,k_2}, \ldots, P_{l,k_l})$  be another composition of V. We say that P' refines P and write  $P' \prec P$  if  $P_i = \bigcup_{j=1}^{k_i} P_{i,j}$  for  $1 \leq i \leq l$ .

**Example 2.11.** On the set [6] we have  $(16, 4, 3, 5, 2) \prec (146, 35, 2)$ .

Over integers. There are similar notions of decomposition, composition and partition over integers. Let us briefly present them.

Let n be a non negative integer. Then a decomposition of n is a finite sequence of positive integers summing to n and composition of n is a finite sequence of non negative integers summing to n. A partition of n is a decreasing sequence of non negative integers summing to n. We denote by  $\mathbf{Dcomp}_n$ ,  $\mathbf{Comp}_n$  and  $\mathbf{Part}_n$  the sets of decompositions, compositions and partitions of n and we denote by  $p \models n$  for p a composition of n. In fact these sets are the set of isomorphism classes of the set Dcomp[[n]], Comp[[n]] and  $\Pi[[n]]$  under the natural action of  $\mathfrak{S}_n$ .

We do not need much more than just these definition in this section, and we will just introduce the notion of refinement of composition. We say that a composition q refine a composition p and denote by  $q \prec p$  if the elements of p are sums of consecutive elements of q:  $p = (p_1, \ldots, p_l), q = (q_{1,1}, \ldots, q_{1,k_1}, q_{2,1}, \ldots, q_{2,k_2}, \ldots, q_{l,k_l})$  and  $p_i = \sum_{1 \leq j \leq k_i} q_{i,j}$ .

### 3 Polynomial invariants over Hopf monoids

The notion of Hopf monoid was defined by Aguiar and Mahajan in [4],[5] and is akin to the notion of Hopf algebra and built on species theory. As in the case of Hopf algebras, a useful application of Hopf monoids is to define and compute polynomial invariants, as was shown by the recent and extensive paper of Aguiar and Ardila [2]. We use their results in order and provide combinatorial interpretations to many polynomial invariants. In particular, we generalize in this section the results from [8] to all Hopf monoids characters.

This section is organized as follow. In Subsection 3.1 we provide general definitions on Hopf monoids as well as the main results from [2] which interest us. In Subsection 3.2 and Subsection 3.3, we give a combinatorial interpretation to the polynomial invariants of the Hopf monoid of generalized permutahedra and the Hopf monoid of hypergraphs. Finally we use our results in Subsection 3.4 to derive similar expressions for the polynomial invariants of other Hopf monoids.

#### 3.1 Hopf monoids

The general goal of this subsection is to give a presentation of Hopf monoids as well as to introduce the necessary tools for the rest of this section. Part 3.1.1 contains standard definitions on Hopf monoids. In part 3.1.2 we present the main theorems on polynomial invariants from [2] and finally in part 3.1.3, following [2], we introduce the Hopf monoid of generalized permutahedra from [2].

#### 3.1.1 Definitions

We give here basic definitions on Hopf monoids. The interested reader may refer to [5] for more information on this topic. Readers familiar with Hopf algebras will notice a strong resemblance with these objects. We refer them to [4] for a better understanding of these similarities.

While reading the following definition, the reader must keep in mind that in the same way that Hopf algebras formalize the notion of merging and splitting non labeled objects, Hopf monoids do the same for labeled objects.

A connected Hopf monoid in linear species is a linear species M where  $M[\emptyset] = \mathbb{K}$  and which is equipped with a product and a co-product:

$$\mu_{V_1,V_2}: M[V_1] \otimes M[V_2] \to M[V_1 \sqcup V_2], \quad \Delta_{V_1,V_2}: M[V_1 \sqcup V_2] \to M[V_1] \otimes M[V_2], \quad (11)$$

$$x \otimes y \mapsto x \cdot y \qquad \qquad z \mapsto \sum z|_{V_1} \otimes z/_{V_1}$$

with  $V_1$  and  $V_2$  disjoint sets. The notation  $\sum z|_{V_1} \otimes z/_{V_1}$  is used to indicate an element in  $M[V_1] \otimes M[V_2]$  and  $z|_{V_1}$  and  $z|_{V_1}$  may not be individually defined. However  $\Delta_{V_1,V_2}$  is often a pure tensor  $z|_{V_1} \otimes z/_{V_1}$  in which case  $z|_{V_1}$  and  $z/_{V_1}$  do define some elements in  $M[V_1]$  and  $M[V_2]$  and we call  $z|_{V_1}$  the restriction of z to  $V_1$  and  $z/_{V_1}$  the contraction of  $V_1$  from z.

The product and the co-product satisfy the following axioms.

- Naturality. The structure maps  $\mu: M \cdot M \to M$  and  $\Delta: M \to M \cdot M$  are morphisms of linear species.
- Unitality. For  $x \in M[V]$ :

$$x \cdot 1_{\mathbb{K}} = x = 1_{\mathbb{K}} \cdot x \tag{12}$$

*i.e.* merging with the unit does not change our objects.

• Co-unity.

$$\Delta_{V,\emptyset} = Id \otimes 1_{\mathbb{K}} \qquad \Delta_{\emptyset,V} = 1_{\mathbb{K}} \otimes Id \tag{13}$$

*i.e.* splitting on the empty set does not change our objects. This axiom may also be stated as saying that  $\Delta_{V,\emptyset}$  and  $\Delta_{\emptyset,V}$  are always pure tensors and  $x|_V = x = x/\emptyset$ , *i.e.* restricting on the whole set or contracting the empty set does not change our objects.

• Associativity. For  $x \in M[V_1], y \in M[V_2], z \in M[V_3]$ :

$$x \cdot (y \cdot z) = (x \cdot y) \cdot z. \tag{14}$$

*i.e.* the results of merging three objects does not depend on the order in which we merge them.

• Co-associativity.

$$\Delta_{V_1, V_2} \otimes Id \circ \Delta_{V_1 \sqcup V_2, V_3} = Id \otimes \Delta_{V_2, V_3} \circ \Delta_{V_1, V_2 \sqcup V_3}. \tag{15}$$

*i.e.* the result of splitting an object in three does not depend in the order in which we split it. In the case were the co-product is a pure tensor, this axiom can also be written as, for  $x \in M[V_1, V_2, V_3]$ :

$$(x|_{V_1 \sqcup V_2})|_{V_1} = x|_{V_1} \quad (x|_{V_1 \sqcup V_2})/_{V_1} = (x/_{V_1})|_{V_2} \quad (x/_{V_1 \sqcup V_2})/_{V_1} = (x/_{V_1})/_{V_2}. \tag{16}$$

• Compatibility. Let  $V = V_1 \sqcup V_2 = V_3 \sqcup V_4$  and for  $i \in \{1, 2\}$  and  $j \in \{3, 4\}$  denote by  $V_{ij}$  the set  $V_i \cap V_j$ . Then we have the following commutative diagram:

$$M[V_{1}] \otimes M[V_{2}] \xrightarrow{\mu_{V_{1},V_{2}}} M[V] \xrightarrow{\Delta_{V_{3},V_{4}}} M[V_{3}] \otimes M[V_{4}]$$

$$\Delta_{V_{13},V_{14}} \otimes \Delta_{V_{23},V_{24}} \downarrow \qquad \qquad \mu_{V_{13},V_{23}} \otimes \mu_{V_{14},V_{24}} \uparrow$$

$$M[V_{13}] \otimes M[V_{14}] \otimes M[V_{23}] \otimes M[V_{24}] \xrightarrow{\tau} M[V_{13}] \otimes M[V_{23}] \otimes M[V_{14}] \otimes M[V_{24}]$$

$$(17)$$

i.e. merging and splitting is the same than splitting and merging. In the case where the co-product is a pure tensor, this axiom can also be written as, for  $x \in M[V_1]$  and  $y \in M[V_2]$ :

$$(x \cdot y)|_{V_3} = x|_{V_{13}} \cdot y|_{V_{23}} \qquad (x \cdot y)/_{V_3} = x/_{V_{13}} \cdot y/_{V_{23}}. \tag{18}$$

We use the term *Hopf monoid* to refer to a connected Hopf monoid in linear species.

- **Example 3.1.** Let L be the set species of lists, that is L[V] is the set of total orders over V. Then  $\mathbb{K}L$  has a Hopf monoid structure with  $l_1 \cdot l_2$  the concatenation of  $l_1$  and  $l_2$  and  $l \mapsto l|_{V_1} \otimes l|_{V_2}$  where  $l|_{V_i}$  is the restriction of the total order to  $V_i$ .
  - For any of the species S from Definition 2.7, the product  $\mu: g_1 \otimes g_2 \mapsto g_1 \sqcup g_2$  and the co-product  $\Delta: g \mapsto g_{V_1} \otimes g_{V_2}$ , with  $g_{V_1} = \{e \in g \mid e \subset V_1\}$  gives  $\mathbb{K}S$  a Hopf monoid structure. For example, with S = G we have:

Furthermore all the maps and inclusions of species of the commutative diagram (8) are compatible with these structures and hence are also morphisms and inclusions of Hopf monoids.

Remark 3. A straightforward but important observation one can make from these definitions, is that axioms of associativity (14) and co-associativity (15) make it so that we can naturally extend the definitions of the structure maps over any decomposition of V. For  $V_1, \ldots, V_n$  a decomposition of V:

$$\mu_{V_1,\dots,V_n}: M[V_1] \otimes \dots \otimes M[V_n] \to M[V] \qquad \Delta_{V_1,\dots,V_n}: M[V] \to M[V_1] \otimes \dots \otimes M[V_n],$$
 (21)

are respectively defined by iterating any kind of maps of the form  $Id^{\otimes k} \otimes \mu_{V_i,V_{i+1}} \otimes Id^{\otimes l}$  and of the form  $Id^{\otimes k} \otimes \Delta_{V_i,V_{i+1}} \otimes Id^{\otimes l}$ , as long as the domains and co-domains coincide.

As was the case with species, we also have natural notions of Hopf sub-monoid and morphism. A Hopf sub-monoid of a Hopf monoid M is a sub-species of M stable under the product and co-product maps. A morphism of Hopf monoids is a morphism of linear species which preserves the products, co-products and unit  $1_{\mathbb{K}}$ .

Let us end this subsubsection with the definition of co-opposite Hopf monoid. The co-opposite Hopf monoid of a Hopf monoid M is the Hopf monoid  $M^{cop}$  over the same species than M and with the product and co-product defined by:  $\mu_{V_1,V_2}^{M^{cop}} = \mu_{V_1,V_2}^{M}$  and  $\Delta_{V_1,V_2}^{M^{cop}} = \Delta_{V_2,V_1}^{M}$ .

#### 3.1.2 Aguiar and Ardila polynomial invariant

We give in this subsubsection some central results from [2] on polynomial invariants over Hopf monoids on which relies most of the work done in subsection 3.2 and subsection 3.3. Before stating these results we first need to recall the definitions of characters and antipode of a Hopf monoid.

A character  $\zeta$  of a Hopf monoid M is a collection of linear maps  $\{\zeta_V : M[V] \to \mathbb{K}\}_V$  compatible with the product and sending the unit on the unit:

- $\zeta_W \circ M[\sigma] = \zeta_V$  for any bijection  $\sigma: V \to W$
- $\zeta_V(x \cdot y) = \zeta_{V_1}(x)\zeta_{V_2}(y)$  and
- $\zeta_{\emptyset} = Id_{\mathbb{K}}$ .

We say that a character is a characteristic function if it takes values in the set  $\{0,1\}$ . A discrete element of a Hopf monoid M is an element which can be obtained as a product of elements of size 1. i.e.  $x \in M[V]$  is discrete if  $V = \{v_1, \ldots, v_n\}$  and there exists  $x_1 \in M[\{v_1\}], \ldots, x_n \in M[\{v_n\}]$  such that  $x = \mu_{\{v_1\}, \ldots, \{v_n\}} x_1 \otimes \cdots \otimes x_n$ . The basic character of any Hopf monoid M is then the characteristic function of discrete elements of M. We will denote it by  $\zeta_1$ .

**Example 3.2.** The objects defined in Definition 2.7 are *discrete* if all their edges are of size at most one. This corresponds to the notion of discrete defined above for any Hopf monoid structure over these objects where the product is the disjoint union, as in Example 3.1. The basic character  $\zeta_1$  is then defined by  $\zeta_1(g) = 1$  if g is discrete and  $\zeta_1(g) = 0$  else.

**Definition 3.3.** The antipode of a Hopf monoid M is the species morphism  $S: M \to M$  defined by  $S_{\emptyset} = Id$  and for  $V \neq \emptyset$ ,

$$S_V(x) = \sum_{V_1, \dots, V_n \models V} (-1)^n \mu_{V_1, \dots, V_n} \circ \Delta_{V_1, \dots, V_n}(x).$$
 (22)

Formula (22) is known as *Takeuchi's formula*. This formula contains a lot of canceling and grouping terms and the search for a canceling-free grouping-free formula is a major question of the theory which was solved for a major family of Hopf monoids by Aguiar and Ardila in [2].

**Definition 3.4.** Let M be a Hopf monoid and  $\zeta$  a character on M. For  $x \in M[V]$  define the map

$$\chi_V^{(M,\zeta)}(x)(n) = \sum_{V=V_1 \sqcup \dots \sqcup V_n} \zeta_V \circ \mu_{V_1,\dots,V_n} \circ \Delta_{V_1,\dots,V_n}(x). \tag{23}$$

Depending on how clear it is from the context, we will not specify  $\zeta$  and/or M and use the notations  $\chi^M$ ,  $\chi^{\zeta}$  or  $\chi$  to designate the map thus defined. These maps have very interesting properties as shown in the following theorem and proposition.

**Theorem 3.5** (Proposition 16.1 and Proposition 16.2 in [2]). Let M be a Hopf monoid,  $\zeta$  a character on M and  $\chi^{(M,\zeta)}$  be the collection of maps of Definition 3.4. Then  $\chi_V^{(M,\zeta)}(x)$  is a polynomial invariant in n such that:

1. 
$$\chi_V^{(M,\zeta)}(x)(1) = \zeta(x)$$
,

2. 
$$\chi_{\emptyset}^{(M,\zeta)} = 1$$
 and  $\chi_{V_1 \cup V_2}^{(M,\zeta)}(x \cdot y) = \chi_{V_1}^{(M,\zeta)}(x) \chi_{V_2}^{(M,\zeta)}(y)$ ,

3. 
$$\chi_V^{(M,\zeta)}(x)(-n) = \chi_V^{(M,\zeta)}(S_V(x))(n)$$
.

**Example 3.6.** Let  $\zeta_1$  be the basic character of  $\mathbb{K}SG$  as defined in Example 3.2. Then  $\chi(g)$  is the chromatic polynomial of g.

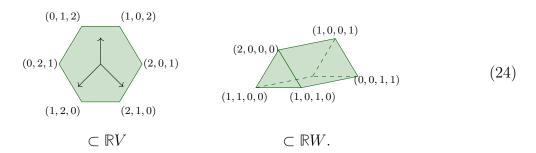
**Proposition 3.7** (Proposition 16.3 in [2]). Let M and N be two Hopf monoids,  $\zeta^M$  and  $\zeta^N$  be two character on these Hopf monoids and  $\phi: M \to N$  be a morphism of Hopf monoids compatible with the characters:  $\zeta^N \circ \phi = \zeta^M$ . Then  $\chi^N \circ \phi = \chi^M$ .

#### 3.1.3 The Hopf monoid of generalized permutahedra

We finish this subsection with the particularly important example of the Hopf monoid of generalized permutahedra as was put to light in [2]. We refer the reader interested in the general theory of polytopes to [37], for example, for more extended literature.

**Polytopes.** Let us begin with some basic definitions over polytopes. For V a set we denote by  $\mathbb{R}V$  the free  $\mathbb{R}$ -vector space over V and for A a subset of  $\mathbb{R}V$  we denote by  $\operatorname{conv}(A)$  the convex hull of A. A  $(\operatorname{convex})$  polytope in  $\mathbb{R}V$  is a subset P of  $\mathbb{R}V$  of the form  $P = \operatorname{conv}(A)$ . The dimension  $\dim P$  of a polytope is the dimension of the smallest sub-space of  $\mathbb{R}V$  containing P.

**Example 3.8.** Let V be the set  $\{e_1, e_2, e_3\}$  such that the vectors  $e_1$ ,  $e_2$  and  $e_3$  form the canonical orthonormal basis of  $\mathbb{R}^3 \cong \mathbb{R}V$  and let W be the set  $\{e_1, e_2, e_3, e_4\}$  such that the vectors  $e_1$ ,  $e_2$ ,  $e_3$  and  $e_4$  form the canonical orthonormal basis of  $\mathbb{R}^4 \cong \mathbb{R}W$ . We represent here a polytope over V and a polytope over W.



Remark that while these polytopes are respectively of dimension 2 and 3, they respectively live in the hyperplane  $x_1 + x_2 + x_3 = 3$  of  $\mathbb{R}^3$  and in the hyperplane  $x_1 + x_2 + x_3 + x_4 = 4$  of  $\mathbb{R}^4$ .

We call the elements of the dual  $(\mathbb{R}V)^* = \mathbb{R}^V$  the directions (of  $\mathbb{R}^V$ ). For P a polytope of  $\mathbb{R}V$  and y a direction in  $\mathbb{R}^V$ , we call maximum face of P in the direction y or y-maximum face of P the polytope  $P_y = \{p \in P \mid y(p) \geq y(q) \text{ for all } q \in P\}$ . In particular, the faces of dimension 1 are the edges of P.

**Example 3.9.** Let V be the set  $\{e_1, e_2, e_3\}$  and denote by  $\mathbf{e_i^*}$  the dual of  $e_i$  in  $(\mathbb{R}^3)^*$ . Let  $y_1 = 4\mathbf{e_1^*} + 2\mathbf{e_2^*} + 2\mathbf{e_3^*}$  and  $y_2 = 4\mathbf{e_1^*} + 2\mathbf{e_2^*} + 1.5\mathbf{e_3^*}$  be two directions in  $(\mathbb{R}V)^*$ .

Then with P the polytope in  $\mathbb{R}V$  defined in Example 3.8 we have:

$$P = (0,2,1) \xrightarrow{(1,0,2)} (2,0,1) \qquad P_{y_1} = \begin{pmatrix} (2,0,1) \\ (2,1,0) \end{pmatrix} \qquad P_{y_2} = \{(2,1,0)\}. \tag{25}$$

To see this remember that P is in the hyperplane  $x_1 + x_2 + x_3 = 3$ , hence maximizing  $y_1(x)$  or  $y_2(x)$ , is done by distributing a charge of 3 between  $x_1$ ,  $x_2$  and  $x_3$ . Since  $x_1$  has the greatest coefficient in both  $y_1(x) = 4x_1 + 2(x_2 + x_3)$  and  $y_2(x) = 4x_1 + 2x_2 + 1.5x_3$ , we first search to maximize  $x_1$ . This is done on the edge with ends (2, 1, 0) and (2, 0, 1) where  $x_1$  is constant equal to 2. Since  $x_1$  is constant equal to 2 on this edge, we are left with a charge of 1 to distribute between  $x_2$  and  $x_3$ . This means that  $x_2 + x_3$  is constant equal to 1 on this edge and  $y_1$  is constant and maximal on this edge. In order to maximize  $y_2$ , since  $x_2$  has a greater coefficient that  $x_3$  we must put all the remaining charge on  $x_2$  and hence we are left with the point (2, 1, 0).

We denote by  $Q \leq P$  for Q a face of P and Q < P if additionally  $Q \neq P$ . We denote by L(P) the face lattice of P, which is the poset of faces of P ordered with the previously defined order. We denote by [Q; P] the interval  $\{P' \mid Q \leq P' \leq P\}$  and by [Q; P] the same interval but with strict inequality on the right side.

For each face Q of P define the normal cones as:

$$\mathcal{N}_{P}^{o}(Q) = \left\{ y \in \mathbb{R}^{V} \mid P_{y} = Q \right\}$$

$$\mathcal{N}_{P}(Q) = \left\{ y \in \mathbb{R}^{V} \mid Q \text{ is a face of } P_{y} \right\}.$$
(26)

**Example 3.10.** Let V be the set  $\{e_1, e_2, e_3\}$  and P,  $Q_1$ ,  $Q_2$  be the polytopes over V of Example 3.9:

$$P = (0,2,1) \qquad (1,0,2) \qquad (2,0,1) \qquad Q_1 = \begin{pmatrix} (2,0,1) & Q_2 = \{(2,1,0)\} \\ (2,1,0) & (2,1,0) \end{pmatrix}$$
 (27)

With the same kind of reasoning that in Example 3.9, we can find that the cones of P on  $Q_1$  are  $\mathcal{N}_P^o(Q_1) = \{a\mathbf{e_1}^* + b\mathbf{e_2}^* + c\mathbf{e_3}^* \mid a > b = c\}$  and  $\mathcal{N}_P(Q_1) = \{a\mathbf{e_1}^* + b\mathbf{e_2}^* + c\mathbf{e_3}^* \mid a \geq b = c\}$  and the cones of P on  $Q_2$  are  $\mathcal{N}_P^o(Q_2) = \{a\mathbf{e_1}^* + b\mathbf{e_2}^* + c\mathbf{e_3}^* \mid b > c > a\}$  and  $\mathcal{N}_P(Q_2) = \{a\mathbf{e_1}^* + b\mathbf{e_2}^* + c\mathbf{e_3}^* \mid b \geq c \geq a\}$ .

We finish this short introduction with the definition of Minkowski sum. The Minkowski sum of two polytopes P and Q is the polytope P + Q defined by

$$P + Q = \{ p + q \mid p \in P, q \in Q \}.$$
 (28)

**Example 3.11.** A Minkowski sum of two simple polytopes.

Generalized Permutahedra. We are interested in the Hopf monoid structure of generalized permutahedra and we will not present more than what we need on this notion. The interested reader is referred to the vast literature on the subject (see for example [41], [23], [37]).

A generalized permutahedron in  $\mathbb{R}V$  is a polytope in  $\mathbb{R}V$  whose edges are parallel to the vectors v - v' for  $v, v' \in V$ . We denote by GP the set species of generalized permutahedra.

**Example 3.12.** The two polytopes of Example 3.8 are a generalized permutahedra. Indeed, the difference of the coordinates of the vertices of an edge is always a vector with one coordinate equal to 1, one equal to -1 and the rest equal to 0. Hence, it is parallel to one of the vectors  $e_i - e_j$  with  $1 \le i \ne j \le 4$ .

**Proposition 3.13** (Theorem 3.15 in [23]). Let V be a finite set,  $W \subseteq V$  and P be a generalized permutahedra in  $\mathbb{R}V$ . Denote by  $\mathbb{1}_W$  the direction defined by  $\mathbb{1}_W(v) = 1$  if  $v \in W$  and  $\mathbb{1}_W(v) = 0$  if  $v \in V \setminus W$ . Then there exists two generalized permutahedra  $P|_W$  in  $\mathbb{R}W$  and  $P|_W$  in  $\mathbb{R}V \setminus W$  such that  $P_{\mathbb{1}_W} = P|_W + P|_W$ .

**Theorem 3.14** (Theorem 5.3 in [2]). The set species  $\mathbb{K}GP$  as a Hopf monoid structure given by

$$\mu_{V_1,V_2}: GP[V_1] \otimes GP[V_2] \to GP[V] \qquad \Delta_{V_1,V_2}: GP[V] \to GP[V_1] \otimes GP[V_2] \qquad (30)$$

$$P \otimes Q \mapsto P + Q \qquad P \mapsto P|_{V_1} \otimes P/_{V_1}.$$

Remark that colorings of V as defined in subsubsection 2.2.3 are direction of  $\mathbb{R}V$  as defined here. Also recall from 2.2.3 that decompositions of V can be seen as colorings of V. One has:

**Proposition 3.15** (Proposition 5.4 in [2]). Let V be a finite set, P a generalized permutahedron in  $\mathbb{R}V$  and  $D = D_1, \ldots, D_n$  be a decomposition of V. Then the D-maximum face of P is given by  $P_D = \mu_D \circ \Delta_D(P)$ .

The Hopf monoid  $\mathbb{K}GP$  has the following formula for the antipode:

**Theorem 3.16** (Theorem 7.1 in [2]). The antipode of GP is given by the cancellation-free and grouping-free formula:

$$S_V(P) = \sum_{Q \le P} (-1)^{|V| - \dim Q} Q. \tag{31}$$

A very useful application of this formula is lemma 17.2 of [2].

**Lemma 3.17** (Lemma 17.2.1 in [2]). Let V be finite set, P be a generalized permutahedra in  $\mathbb{R}V$  and y be a direction of  $\mathbb{R}V$ . We then have

$$\sum_{Q \le P} (-1)^{\dim Q} Q_y = \sum_{Q \le P_{-y}} (-1)^{\dim Q} Q. \tag{32}$$

**Hypergraphic polytopes.** Let us end this subsubsection by presenting a Hopf submonoid of  $\mathbb{K}GP$ . For V a set denote by  $\Delta_V = \operatorname{conv}(v \mid v \in V)$  the *standard simplex* of  $\mathbb{R}V$ . A *hypergraphic polytope* is a Minkowski sum of standard simplices. We denote by HGP the set species of hypergraphic polytopes.

**Example 3.18.** The two polytopes of Example 3.8 are hypergraphic. The first one is equal to the sum  $\Delta_{e_1,e_2} + \Delta_{e_2,e_3} + \Delta_{e_1,e_3}$  and the second one to the sum  $\Delta_{e_1,e_2,e_3} + \Delta_{e_1,e_4}$ .

**Proposition 3.19** (Proposition 19.5 in [2]). The species  $\mathbb{K}HGP$  is a Hopf sub-monoid of  $\mathbb{K}GP$ .

An important property of hypergraphic polytopes is that they are in bijection with hypergraphs. Indeed for  $h \in HG[V]$  a hypergraph, denote by  $\Delta_h$  the Minkowski sum  $\sum_{e \in h} \Delta_e$ . Then the map  $\Delta : h \mapsto \Delta_h$  clearly is a species isomorphism from HG to HGP.

## 3.2 Polynomial invariants and reciprocity theorems on the Hopf monoid of generalized permutahedra

Using Aguiar and Ardila's results in [2], we give here an explicit combinatorial interpretation of the polynomial invariant in Definition 3.4 and its reciprocity theorem over the Hopf monoid of generalized permutahedra. The two theorems of this subsection are direct generalizations of Proposition 17.3 and 17.4 [2].

Let us begin with the interpretation of  $\chi$  over non negative integers. Most definitions necessary to state our theorem were given in subsubsection 3.1.3, but we still need to introduce two simple notions. Let  $P \in GP[V]$  be a generalized permutahedron.

- For  $\zeta$  a character of  $\mathbb{K}GP$ , P is a  $\zeta$ -face if  $\zeta(P) \neq 0$ .
- For Q a face of P and c a coloring of V, Q and c are said to be *strictly compatible* if  $P_c = Q$ . They are said to be *compatible* if  $Q \leq P_c$ . We respectively denote by  $\mathcal{N}_P^o(Q)_n = [n]^V \cap \mathcal{N}_P^o(Q)$  and  $\mathcal{N}_P(Q)_n = [n]^V \cap \mathcal{N}_P(Q)$  the set of colorings with [n] strictly compatible with Q and compatible with Q.

**Theorem 3.20.** Let  $\zeta$  be a character of  $\mathbb{K}GP$ , V be a finite set and  $P \in GP[V]$  a generalized permutahedra. Then

$$\chi_V^{\zeta}(P)(n) = \sum_{Q \le P} \zeta(Q) |\mathcal{N}_P^o(Q)_n|. \tag{33}$$

In particular, if  $\zeta$  is a characteristic function, then  $\chi_V^{\zeta}(P)(n)$  is the number of strictly compatible pairs of  $\zeta$ -faces of P and colorings with [n].

*Proof.* This theorem is an application of Proposition 3.15. We have:

$$\chi_{V}^{\zeta}(P)(n) = \sum_{V=V_{1} \sqcup \cdots \sqcup V_{n}} \zeta_{V} \circ \mu_{V_{1}, \dots, V_{n}} \circ \Delta_{V_{1}, \dots, V_{n}}(P)$$

$$= \sum_{D \text{ coloring of } V \text{ with } [n]} \zeta_{V} \circ \mu_{D} \circ \Delta_{D}(P)$$

$$= \sum_{D \text{ coloring of } V \text{ with } [n]} \zeta_{V}(P_{D})$$

$$= \sum_{Q \leq P} \sum_{D \text{ coloring of } V \text{ with } [n]} \zeta_{V}(Q)$$

$$= \sum_{Q \leq P} \zeta_{V}(Q) |\mathcal{N}_{P}^{o}(Q)_{n}|.$$
(34)

**Example 3.21.** Let  $\zeta$  be the characteristic function of *graphic polytopes i.e.* polytopes which can be written as a Minkowski sum of standard simplices of dimension 1. Let  $P = \Delta_{e_1,e_2,e_3} + \Delta_{e_1,e_4}$  be second polytope of Example 3.8:

$$P = (2,0,0,0) (1,0,0,1), (35)$$

$$(1,1,0,0) (1,0,1,0)$$

where the hidden point is of coordinate (0,1,0,1). From Theorem 3.20 we know that  $\chi^{\zeta}(P)(3)$  is the number of strictly compatible pairs of  $\zeta$ -faces of P and colorings with [2]. The  $\zeta$ -faces of P are its three rectangular faces which correspond to the sums  $\Delta_{e_1,e_2} + \Delta_{e_1,e_4}$ ,  $\Delta_{e_1,e_3} + \Delta_{e_1,e_4}$  and  $\Delta_{e_2,e_3} + \Delta_{e_1,e_4}$ . Each of these faces is strictly compatible with exactly one coloring with [2]. These colorings are respectively  $2\mathbf{e}_1^* + 2\mathbf{e}_2^* + \mathbf{e}_3^* + 2\mathbf{e}_4^*$ ,  $2\mathbf{e}_1^* + \mathbf{e}_2^* + 2\mathbf{e}_3^* + 2\mathbf{e}_4^*$  and  $\mathbf{e}_1^* + 2\mathbf{e}_2^* + 2\mathbf{e}_3^* + \mathbf{e}_4^*$ . Hence we have  $\chi^{\zeta}(P)(2) = 3$ .

The basic character  $\zeta_1$  of GP is equal to 1 on points and 0 elsewhere. There is a particular interpretation for this character which is presented in [2]. For  $P \in GP[V]$  a generalized permutahedra and y a direction in  $\mathbb{R}V$ , y is said to be P-generic if  $P_y$  is a point.

Corollary 3.22 (Theorem 9.2 (v) in [30] and Proposition 17.3 in [2]). Let V be a finite set and  $P \in GP[V]$  a generalized permutahedra. Then  $\chi^{\zeta_1}(P)(n)$  is the number of P-generic colorings of V with [n].

*Proof.* By definition the  $\zeta_1$ -faces are the points and a coloring c is strictly compatible with a face Q if  $P_c = Q$ .  $\chi^{\zeta_1}(P)$  is then counting the number of colorings c such that  $P_c$  is a point *i.e.* the number of P-generic colorings.

We now give the reciprocity theorem associated with these polynomials. A character  $\zeta$  of GP is said to be *even* if the  $\zeta$ -faces are of even dimension.

**Theorem 3.23.** Let  $\zeta$  be a character of GP, V be a finite set and  $P \in GP[V]$  a generalized permutahedra then

$$\chi_V^{\zeta}(h)(-n) = \sum_{Q < P} (-1)^{|V| - \dim Q} \zeta(Q) |\mathcal{N}_P(Q)_n|.$$
 (36)

Furthermore if  $\zeta$  is an even characteristic function then  $(-1)^{|V|}\chi^{\zeta}(P)(-n)$  is the number of compatible pairs of  $\zeta$ -faces of P and colorings with [n]. In particular,  $(-1)^{|V|}\chi^{\zeta}(P)(-1)$  is the number of  $\zeta$ -faces.

*Proof.* First remark from Lemma 3.17 that for any direction y we have:

$$\sum_{Q \le P} (-1)^{\dim Q} \zeta(Q_y) = \sum_{Q \le P_{-y}} (-1)^{\dim Q} \zeta(Q). \tag{37}$$

Beginning with Theorem 3.16 and Theorem 3.5.3 we have:

$$\chi(P)(-n) = \chi(S(P))(n) = \chi(\sum_{Q \le P} (-1)^{|V| - \dim Q} Q)(n) 
= \sum_{Q \le P} (-1)^{|V| - \dim Q} \chi(Q)(n) 
= \sum_{Q \le P} (-1)^{|V| - \dim Q} \sum_{R \le Q} \zeta(R) |\mathcal{N}_{Q}^{o}(R)_{n}| 
= \sum_{Q \le P} (-1)^{|V| - \dim Q} \sum_{R \le Q} \zeta(R) \sum_{\substack{y: V \to [n] \\ Q_{y} = R}} 1 
= \sum_{Q \le P} (-1)^{|V| - \dim Q} \sum_{y: V \to [n]} \zeta(Q_{y}) 
= \sum_{y: V \to [n]} (-1)^{|V|} \sum_{Q \le P} (-1)^{\dim Q} \zeta(Q_{y}) 
= \sum_{y: V \to [n]} (-1)^{|V|} \sum_{Q \le P_{-y}} (-1)^{\dim Q} \zeta(Q) 
= \sum_{Q \le P} (-1)^{|V| - \dim Q} \zeta(Q) \sum_{y: V \to [n] \atop Q \le P_{-y}} 1 
= \sum_{Q \le P} (-1)^{|V| - \dim Q} \zeta(Q) |\mathcal{N}_{P}(Q)_{n}|,$$
(38)

where the last equality comes from the fact that  $P_{-y} = P_{n+1-y}$  and n+1-y as co-domain [n] is and only if y has co-domain [n].

Example 3.24. The character  $\zeta$  of Example 3.21 is not even but the  $\zeta$ -faces of the polytope P of Example 3.21 are of even dimension hence  $(-1)^4 \chi^{\zeta}(P)(-2)$  is equal to the number of compatible pairs of  $\zeta$ -faces of P and colorings with [2]. For each rectangular face of P, its compatible colorings with [2] are the one given in Example 3.21 along with the colorings  $\mathbf{e}_1^* + \mathbf{e}_2^* + \mathbf{e}_3^* + \mathbf{e}_4^*$  and  $2\mathbf{e}_1^* + 2\mathbf{e}_2^* + 2\mathbf{e}_3^* + 2\mathbf{e}_4^*$ . Hence  $\chi^{\zeta}(P)(-2) = 9$ .

Corollary 3.25 (Theorem 6.3 and Theorem 9.2 (v) in [30] and Proposition 17.4 in [2]). Let V be a finite set and  $P \in GP[V]$  a generalized permutahedra. Then, we have:

$$(-1)^{|V|} \chi^{\zeta_1}(P)(-n) = \sum_{c:V \to [n]} |vertices \ of \ P_c|.$$

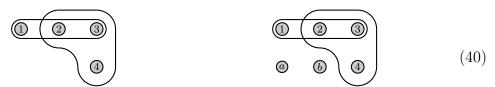
$$(39)$$

*Proof.* From Theorem 3.23 we have that  $(-1)^{|V|}\chi^{\zeta_1}(P)(-n)$  is the number of compatible pairs of points and coloring with [n]. Since the points compatible with a coloring c are by definition the points in  $P_c$ , formula (39) follows.

## 3.3 Polynomial invariants and reciprocity theorems on the Hopf monoid of hypergraphs

As in the previous section, we give here an explicit combinatorial interpretation of the polynomial invariant and its reciprocity theorem over the Hopf monoid of hypergraphs defined in [2]. We expand more on this Hopf monoid and give two proofs of both the combinatorial interpretation of  $\chi$  over positive and non negative integers. One of these proofs is self-contained and the other one uses the results of the previous subsection.

Recall from Definition 2.7 that a hypergraph over V is a multiset h of non empty parts of V called edges; and that in this context the elements of V are called vertices of h. The set species of hypergraphs is denoted by HG. Note that two hypergraphs over different sets can never be equal, e.g  $\{\{1,2,3\},\{2,3,4\}\}\in HG[[4]]$  is not the same as  $\{\{1,2,3\},\{2,3,4\}\}\in HG[[4]\cup\{a,b\}]$ . This is illustrated in the following figure.



Two hypergraphs with same edges but over different sets.

The Hopf monoid structure on  $\mathbb{K}HG$  studied here is different from the one given in Example 3.1. While the product is still the disjoint union and the co-product is still a pure tensor, the restriction of h to V and the contraction of V from h are now given by:

$$h|_{V} = \{e \in h \mid e \subseteq V\} \qquad \text{and} \qquad h/_{V} = \{e \cap V^{c} \mid e \nsubseteq V\}.$$
 (41)

**Example 3.26.** For V = [5],  $V_1 = \{1, 2, 5\}$  and  $V_2 = \{3, 4\}$ , we have the following coproduct:

The Hopf structure defined here is also different from the one defined and studied in [10] but there are similar results in both this dissertation and [10]. This is due to the fact that the notion of acyclic orientations plays a huge role when working on hypergraphs. Up to some minor subtleties, our notion of acyclic orientations is the same as the one in [10]: we trade the notion of flats for acyclic orientations where every vertex of an edge can be a target, as defined in Subsection 2.2.2. We preferred to define them as maps over hypergraphs with certain properties while they are defined as compositions of edges which induce directed acyclic graphs. We will point out the common results when they appear.

While the proofs using results of the previous section are rather short, the self contained proofs are more involved. Subsubsection 3.3.1 presents some preliminary results. The combinatorial interpretations of  $\chi(n)$  and  $\chi(-n)$  and their self contained proofs are in subsubsection 3.3.2 and subsubsection 3.3.3. The proof using the previous section is presented in subsubsection 3.3.4.

#### 3.3.1 Generalized Faulhaber's polynomials

As stated in Theorem 3.5, for any character  $\zeta$  and any hypergraph h,  $\chi^{\zeta}(h)(n)$  is a polynomial in n. The objects introduced here are useful tools to show and exploit this polynomial dependency.

Let  $p = (p_1, p_2, ..., p_t)$  be a finite sequence of positive integers. We define the *generalized Faulhaber polynomial over* p,  $F_p$ , the function over the integers given by, for  $n \in \mathbb{N}$ :

$$F_p(n) = \sum_{0 \le k_1 \le \dots \le k_t \le n-1} k_1^{p_1} \cdots k_t^{p_t}. \tag{43}$$

Note that if t > n, then  $F_p(n) = \sum_{\emptyset} \cdots = 0$ .

As their names suggest, these functions are polynomials.

**Proposition 3.27.** Let  $p_1, p_2, \ldots, p_t$  be integers and define  $d_k = \sum_{i=1}^k p_i + k$  for  $1 \le k \le t$ . Then  $F_{p_1,\ldots,p_t}$  is a polynomial of degree  $d_t$  whose constant coefficient is null and whose  $(d_t - i)$ -th (for  $i < d_t$ ) coefficient is given by

$$\sum_{j_{t-1}=0}^{\min(j_t,d_{t-1}-1)} \sum_{j_{t-2}}^{\min(j_{t-1},d_{t-2}-1)} \cdots \sum_{j_1=0}^{\min(j_2,d_1-1)} \prod_{k=1}^t \binom{d_k-j_{k-1}}{j_k-j_{k-1}} \frac{B_{j_k-j_{k-1}}}{d_k-j_{k-1}}, \tag{44}$$

where  $j_t = i$  and  $j_0 = 0$ , and the  $B_j$  numbers are the Bernoulli numbers with the convention  $B_1 = -1/2$ .

*Proof.* We show this by induction on t. For t=1 the expression of the coefficients gives us the well-known Faulhaber's formula  $F_p(n) = \sum_{i=0}^p {p+1 \choose i} \frac{B_i}{p+1} n^{p+1-i}$ . Hence the result is true for t=1. Suppose now the result is true for  $t\geq 1$  and let  $p_1, p_2, \ldots, p_{t+1}$  be t+1 integers. Denote by  $a_i$  the  $(d_t-i)$ -th coefficient of  $F_{p_1,\ldots,p_t}(n)$ . We then have:

$$F_{p_1,\dots,p_{t+1}}(n) = \sum_{0 \le k_1 < \dots < k_{t+1} \le n-1} k_1^{p_1} \dots k_{t+1}^{p_{t+1}} = \sum_{k_{t+1}=0}^{n-1} k_{t+1}^{p_{t+1}} \sum_{0 \le k_1 < \dots < k_t \le k_{t+1}-1} k_1^{p_1} \dots k_t^{p_t}$$

$$= \sum_{k=0}^{n-1} k^{p_{t+1}} F_{p_1,\dots,p_t}(k)$$

$$= \sum_{k=0}^{n-1} k^{p_{t+1}} \sum_{j=0}^{d_{t-1}} a_j k^{d_t - j}$$

$$= \sum_{j=0}^{d_{t-1}} a_j \sum_{k=0}^{n-1} k^{p_{t+1} + d_t - j} = \sum_{j=0}^{d_{t-1}} a_j \sum_{k=0}^{n-1} k^{d_{t+1} - 1 - j}$$

$$= \sum_{j=0}^{d_{t-1}} a_j F_{d_{t+1} - 1 - j}(n)$$

$$= \sum_{j=0}^{d_{t-1}} a_j \sum_{i=0}^{d_{t+1} - 1 - j} \left( \frac{d_{t+1} - j}{i} \right) \frac{B_i}{d_{t+1} - j} n^{d_{t+1} - j - i}$$

$$= \sum_{j=0}^{d_{t-1}} \sum_{i=0}^{d_{t+1} - 1 - j} a_j \left( \frac{d_{t+1} - j}{i - j} \right) \frac{B_{i-j}}{d_{t+1} - j} n^{d_{t+1} - i}$$

$$= \sum_{j=0}^{d_{t+1} - 1} \left( \sum_{j=0}^{\min(i, d_t - 1)} a_j \left( \frac{d_{t+1} - j}{i - j} \right) \frac{B_{i-j}}{d_{t+1} - j} \right) n^{d_{t+1} - i}.$$

$$= \sum_{i=0}^{d_{t+1} - 1} \left( \sum_{j=0}^{\min(i, d_t - 1)} a_j \left( \frac{d_{t+1} - j}{i - j} \right) \frac{B_{i-j}}{d_{t+1} - j} \right) n^{d_{t+1} - i}.$$

This concludes this proof.

Remark 4. These polynomials also generalize Stirling numbers of the first kind: denote by  $F_{1^k}(n)$  the generalized Faulhaber polynomial associated to the sequence of size k with all elements equal to 1.  $F_{1^k}(n) = \sum_{0 \le k_1 < \dots < k_t \le n-1} \prod k_i$  is indeed the absolute value of the coefficient of  $x^{n-k}$  in  $x(x-1)\cdots(x-n+1)$  and hence  $F_{1^k}(n) = s(n,k)$ .

**Lemma 3.28.** Let p be a sequence of positive integers of length t. We then have

$$F_p(-n) = (-1)^{d_t} \sum_{p \prec q} F_q(n+1), \tag{46}$$

where  $d_t$  is defined in the same way as in Proposition 3.27.

*Proof.* Remark that  $\sum_{p \prec q} F_q(n+1)$  can also be written as  $\sum_{0 \leq k_1 \leq \cdots \leq k_t \leq n} k_1^{p_1} \cdots k_t^{p_t}$ . We now proceed by induction on t. For t=1, we have

$$F_{p}(-n) = \sum_{i=0}^{p} {p+1 \choose i} \frac{B_{i}}{p+1} (-n)^{p+1-i}$$

$$= \frac{(-1)^{p+1}}{p+1} n^{p+1} - \frac{1}{2} (-1)^{p} n^{p} + (-1)^{p+1} \sum_{i=2}^{p} {p+1 \choose i} \frac{B_{i}}{p+1} n^{p+1-i}$$

$$= (-1)^{p+1} \left( \frac{1}{p+1} n^{p+1} + \frac{1}{2} n^{p} + \sum_{i=2}^{p} {p+1 \choose i} \frac{B_{i}}{p+1} n^{p+1-i} \right)$$

$$= (-1)^{p+1} (F_{p}(n) + n^{p}) = (-1)^{p+1} F_{p}(n+1),$$

$$(47)$$

where the second equality comes from the fact that  $B_i = 0$  when i is an odd number different from 1. Suppose now our proposition is true up to t. In the proof of Proposition 2 we showed that  $F_{p_1,\dots,p_{t+1}}(n) = \sum_{j=0}^{d_t-1} a_j F_{d_{t+1}-1-j}(n)$  where  $a_j$  is the  $d_t - j$  coefficient of  $F_{p_1,\dots,p_t}(n)$ . This gives

$$F_{p_1,\dots,p_{t+1}}(-n) = \sum_{j=0}^{d_t-1} a_j (-1)^{d_{t+1}-j} \sum_{k=0}^n k^{d_{t+1}-1-j} = -\sum_{j=0}^{d_t-1} a_j \sum_{k=0}^n (-k)^{p_{t+1}+d_t-j}$$

$$= -\sum_{k=0}^n (-k)^{p_{t+1}} \sum_{j=0}^{d_t-1} a_j (-k)^{d_t-j} = (-1)^{p_{t+1}+1} \sum_{k=0}^n k^{p_{t+1}} F_{p_1,\dots,p_t}(-k)$$

$$= (-1)^{p_{t+1}+1} \sum_{k=0}^n k^{p_{t+1}}_{t+1} (-1)^{d_t} \sum_{0 \le k_1 \le \dots \le k_t \le k_{t+1}} k^{p_1}_1 \dots k^{p_t}_t$$

$$= (-1)^{d_{t+1}} \sum_{0 \le k_1 \le \dots \le k_{t+1} \le n} k^{p_1}_1 \dots k^{p_{t+1}}_{t+1}$$

$$= (-1)^{d_{t+1}} \sum_{p \prec q} F_q(n+1),$$

$$(48)$$

where the fifth equality is our induction hypothesis.

### 3.3.2 Chromatic polynomials of hypergraphs

Before stating our results on  $\chi$  in Theorem 3.35, recall from subsubsection 2.2.3 that a coloring of V with [n] is a map from V to [n] and that there is a canonical bijection between decompositions and colorings.

**Definition 3.29.** Let h be a hypergraph over V and c be a coloring. For  $v \in e \in h$ , we say that v is a maximal vertex of e (for c) if v is of maximal color in e and we call the maximal color of e (for e) the color of a maximal vertex of e. We say that a vertex v is a maximal vertex (for e) if it is a maximal vertex of an edge and that a color is a maximal color (for e) if it is the maximal color of an edge.

If  $W \subseteq V$  is a subset of vertices, the order of appearance of W (for V) is the composition  $\operatorname{forget}_{\emptyset}(c \cap W)$  where  $c \cap W = (c_1 \cap W, \ldots, c_{l(c)} \cap W)$  and the map  $\operatorname{forget}_{\emptyset}$  sends any decomposition to the composition obtained by dropping the empty parts.

Remark 5. Since the set of colorings of V with [n] is  $[n]^V \subset \mathbb{R}^V$ , colorings can be seen as particular directions of  $\mathbb{R}^V$  as defined in 3.1.3.

When working with colorings, by a slight abuse of notation, for W a set of vertices of the same color for c, we will denote by c(W) their color. This extends c to a map from monochromatic sets of vertices to [n].

**Example 3.30.** We represent a hypergraph along a coloring on  $V = \{a, b, c, d, e, f\}$  with  $\{1, 2, 3, 4\}$ :

$$e_1 \underbrace{ \begin{array}{c} \bullet \\ \bullet \\ \bullet \\ e_4 \end{array}} e_3 \tag{49}$$

The maximal vertex of  $e_1$  is a and the maximal vertices of  $e_3$  are c and d. The maximal color of  $e_2$  is 3. The order of appearance of  $\{a, c, d, e\}$  is  $(\{e\}, \{c, d\}, \{a\})$ .

Recall now from 2.2.2 that an admissible orientation f of h is a map from h to  $\mathcal{P}(V)^+$  such that  $f(e) \subseteq e$  for every edge e. It is an acyclic orientation if there is no sequence of distinct edges  $e_1, \ldots, e_k$  such that:  $f(e_i) \cap f_s(e_{i+1}) \neq \emptyset$  or  $\emptyset \subsetneq f(e_i) \cap e_{i+1} \subsetneq f(e_{i+1})$  for  $1 \leq i < k$  and  $f(e_k) \cap f_s(e_1) \neq \emptyset$ , where  $f_s(e) = f(e) \setminus f(e)$ . Given a hypergraph h and f an admissible orientation of h, the image of h by f, f(h) is also a hypergraph:  $f(h) = \{f(e) | e \in h\}$ .

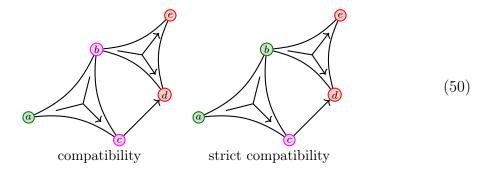
**Definition 3.31.** Let h be a hypergraph over V and f an admissible orientation of h.

- For c coloring of V, c and f are said to be *compatible* if for every edge e the elements of f(e) are maximal in e for c. They are said to be *strictly compatible* if f(e) is exactly the set of maximal elements of e for c. We denote by  $\overline{C}_{h,f,n}$  the set of colorings of V with [n] compatible with f and by  $C_{h,f,n}$  the set of those with strict compatibility.
- For  $\zeta$  a character of  $\mathbb{K}HG$ , f is said to be a  $\zeta$ -orientation of h if  $\zeta(f(h)) \neq 0$ .

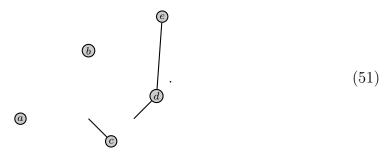
**Example 3.32.** • The coloring given in Example 3.30 has three compatible acyclic orientations: both send  $e_1$  on a,  $e_2$  on c and  $e_4$  on b, but  $e_3$  can be either sent over c, d or  $\{c, d\}$ . Among these three only the last one is strictly compatible.

Here is an example of an acyclic orientation of a hypergraph with a compatible

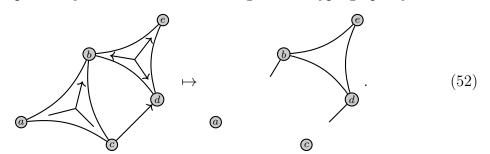
coloring and a strictly compatible coloring with  $\{1, 2, 3\}$ :



• Let  $\zeta$  be the characteristic function of hypergraphs which connected components are either of size 3 or an isolated vertex. The preceding orientation is not a  $\zeta$ -orientation since the image of the hypergraph by this orientation is the hypergraph



Here is an example of a  $\zeta$ -orientation and the image of the hypergraph by it:



Remark that with these definitions, given a coloring c and a hypergraph h, there is a unique orientation of h strictly compatible with c, which is defined by  $f(e) = \{v \in e \mid c(v) = \max(c(e))\}$ . Furthermore, this orientation is necessarily acyclic. Indeed, suppose  $e_1, \ldots, e_k$  is a directed cycle in f. then  $f(e_k) \cap f_s(e_1) \neq \emptyset$  implies that  $c(f(e_k)) < c(f(e_1))$  and for  $1 \leq i < k$  either  $f(e_i) \cap f_s(e_{i+1})$ , which would imply  $c(f(e_i)) < c(f(e_{i+1}))$  or  $f(e_i) \cap f(e_{i+1}) \neq \emptyset$  which would imply  $c(f(e_i)) = c(f(e_{i+1}))$ . This then gives us  $c(f(e_i)) < c(f(e_1))$  which is absurd. We will denote by  $\max_c$  this orientation.

With the same kind of reasoning, any coloring compatible with a cyclic orientation must be monochromatic on directed cycles. The study of  $C_{h,f,n}$  and  $\overline{C}_{h,f,n}$  is hence more interesting when f is acyclic and we have an expression of  $C_{f,h,n}$  in terms of generalized Faulhaber polynomials. Recall that for every hypergraph h over V, we have a decomposition of V in the set of isolated vertices and vertices in an edge:  $V = I(h) \sqcup NI(h)$ . **Proposition 3.33.** Let h be a hypergraph over V, f be an acyclic orientation of h. Define  $P_{h,f}$  and  $P'_{h,f}$  as the set of compositions  $P \vDash f(h)$  such that for e and e' two edges of h,

- if  $f(e) \cap f(e') \neq \emptyset$  then P(f(e)) = P(f(e')),
- else if  $f(e) \cap f_s(e') \neq \emptyset$  then P(f(e)) < P(f(e')) for  $P \in P_{h,f}$  and  $P(f(e)) \leq P(f(e'))$  for  $P \in P'_{h,f}$ .

We then have

$$|C_{h,f,n}| = n^{|I(h)|} \sum_{P \in P_{h,f}} F_{p_1,\dots,p_{l(P)}}(n) \text{ and}$$

$$|\overline{C}_{h,f,n}| = n^{|I(h)|} \sum_{P \in P'_{h,f}} F_{p_1,\dots,p_{l(P)}}(n+1),$$
(53)

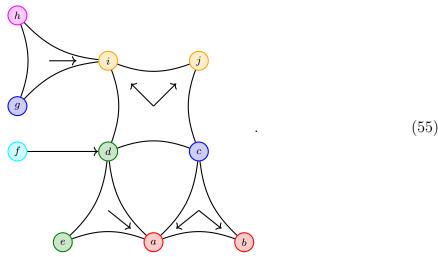
where for every composition P,  $p_i = |\widetilde{P}_i|$  and  $\widetilde{P}_i = NI(f(h))^c \cap \left(\bigcup_{e \in f^{-1}(P_i)} e\right) \bigcap_{j < i} \widetilde{P}_j^c$ .

**Example 3.34.** To prove the formula for  $|C_{h,f,n}|$  we will show that there is a bijection between the set of strictly compatible colorings and the set

$$\bigsqcup_{P \in P_{h,f}} \bigsqcup_{0 \le k_1 < k_2 < \dots < k_{l(P)} \le n-1} \prod_{1 \le i \le l(P)} [k_i]^{\widetilde{P_i}}.$$

$$(54)$$

We give here an example of how this bijection will work. Let H, F and C be the hypergraph, the acyclic orientation and the strictly compatible coloring with  $\{1, 2, 3, 4, 5, 6\}$  represented here:



The image of C is obtained in the following way:

- $P = (d, ij, ab) \in P_{H,F}$  is the relative order of the maximal vertices for C,
- $k_1 = 1$ ,  $k_2 = 4$  and  $k_3 = 5$  are the colors of the vertices in P shifted by -1, the vertices in  $P_i$  being of color  $k_i + 1$ ,

• we then have  $\widetilde{P_1} = \{f\}$ ,  $\widetilde{P_2} = \{c, g, h\}$  and  $\widetilde{P_3} = \{e\}$  and the image of C is the triplet  $(f_1, f_2, f_3)$  defined by

$$f_{1}: \{f\} \to \{1\}$$

$$f \mapsto 1$$

$$f_{2}: \{c, g, h\} \to \{1, 2, 3, 4\}$$

$$c \mapsto 3$$

$$g \mapsto 3$$

$$h \mapsto 4$$

$$f_{3}: \{e\} \to \{1, 2, 3, 4, 5\}$$

$$e \mapsto 2.$$

$$(56)$$

*Proof.* We first prove the formula for  $|C_{h,f,n}|$ . The term  $n^{|I(h)|}$  in the formula is trivially obtained and we hence consider that h has no isolated vertices.

Informally, the formula can be obtained by the following reasoning. To choose a coloring strictly compatible with f, one can proceed in the following way:

- 1. choose a part ordering of the sets of maximal vertices:  $P \in P_{h,f}$ ,
- 2. choose the color of these vertices:  $k_1 + 1, \ldots, k_{l(P)} + 1$ ,
- 3. choose the colors of the yet uncolored vertices which are in the same edge than vertices of minimal color in f(h):  $k_1^{|\widetilde{P}_1|}$ ; then those in the same edge than a vertices of second minimal color in f(h):  $k_2^{|\widetilde{P}_2|}$ ), etc.

More formally, we show that there exists a bijection between the set of strictly compatible colorings and the set

$$\bigsqcup_{P \in P_{h,f}} \bigsqcup_{0 \le k_1 < k_2 < \dots < k_{l(P)} \le n-1} \prod_{1 \le i \le l(P)} [k_i]^{\widetilde{P_i}}, \tag{59}$$

where  $[k_i]^{\widetilde{P_i}}$  is the set of maps from  $\widetilde{P_i}$  to  $[k_i]$ .

For any subset A of  $\mathbb{N}$ , we denote by  $\operatorname{bij}_A$  the unique increasing bijection from A to [|A|]. Let c be a strictly compatible coloring, that is to say,  $f = \max_c$ . We begin by constructing its image by the announced bijection. Recall that c extends to a map with domain monochromatic set of vertices and hence c(f(h)) is the set of maximal colors of c. Define:

- the part ordering of the set f(h) of maximal vertices:  $P = \text{bij}_{c(f(h))} \circ c$ . Here again we consider c as a map from monochromatic set of vertices to [n].
- The colors of the maximal vertices:  $k_i = c(P_i) 1$  for  $1 \le i \le l(P)$ .
- The remaining vertices:  $\widetilde{P}_i = NI(f(h))^c \cap \left(\bigcup_{e \in f^{-1}(P_i)} e\right) \bigcap_{j < i} \widetilde{P}_j^c$  for  $1 \le i \le l(P)$ .

The part ordering P is in  $P_{h,f}$  because the strict compatibility of c with f implies that if  $f(e) \cap f(e') \neq \emptyset$  then  $c(f(e)) = c(f(e) \cap f(e')) = c(f(e'))$  and else if  $f(e) \cap f_s(e') \neq \emptyset$  then c(f(e)) < c(f(e')) and bij $_{c(f(h))}$  is increasing by definition. The sequence  $k_1, \ldots, k_{l(P)}$  is increasing since  $c(P_i) = c(\text{bij}_{c(f(h))} \circ c)^{-1}(i) = \text{bij}_{c(f(h))}^{-1}(i)$  and  $\text{bij}_{c(f(h))}^{-1}$  is increasing by definition. The vertices in  $\widetilde{P}_i$  are the vertices which share an edge with a set of vertices in  $P_i$  ( $\bigcup_{e \in f^{-1}(P_i)} e$ ) but which are not maximal  $(NI(f(h))^c)$ . Since the set of vertices in  $P_i$  are of color  $c(P_i) = k_i + 1$ , the colors of the vertices in  $\widetilde{P}_i$  are necessarily in  $[k_i]$ . Hence the map  $c_{|\widetilde{P}_i|}$ , that is to say c restricted to  $\widetilde{P}_i$  is indeed of co-domain  $[k_i]$ . We then define the image of c as the tuple  $(c_{|\widetilde{P}_1}, \ldots, c_{|\widetilde{P}_{I(P)}})$ .

Let us now consider the other direction of the bijection. Let be a partition  $P \in P_{h,f}$ , a sequence of integers  $1 \leq k_1 < \cdots < k_{l(P)}$  and  $(c_1, \ldots c_{l(P)}) \in \prod_{1 \leq i \leq l(P)} [k_i]^{\widetilde{P_i}}$ . Define  $c: V \to [n]$  by  $c_{|\widetilde{P_i}} = c_i$  and  $c_{|f(h)}(v) = \text{bij}_{\{k_1+1,\ldots,k_{l(P)}+1\}}^{-1}(P(f(e)))$  for  $v \in f(e)$ ; this is well defined since if  $v \in f(e) \cap f(e')$  then  $f(e) \cap f(e') \neq \emptyset \Rightarrow P(f(e)) = P(f(e'))$ . This map c has indeed domain V since  $(\widetilde{P_1}, \ldots, \widetilde{P_{l(P)}}, NI(f(h)))$  is a partition of V.

Let us show that c is a coloring strictly compatible with f. If v, v' are two vertices in f(e) then by definition c(v) = c(v'). Let now be  $v \in e \setminus f(e)$ .

- If  $v \in f(e')$  then necessarily  $f(e) \cap f(e') = \emptyset$  because otherwise e', e, e' would be a directed cycle. Indeed, v is an exit of e' and an entry of e and  $f(e) \cap f(e') \neq \emptyset$  would imply that e' share an exit with e, but not all (not v). Hence, by definition of  $P_{h,f}$ , P(f(e')) < P(f(e)) and so c(v) < c(f(e)).
- If  $v \notin f(h)$  then  $v \in \widetilde{P}_i$  with  $i \leq P(f(e))$  and we do have the desired inequality:  $c(v) = c_i(v) \leq k_i < k_i + 1 \leq k_{P(f(e))} + 1 = c(f(e))$ .

We conclude this first part of the proof by remarking that the two previous constructions are inverse functions.

The proof for the formula of  $|\overline{C}_{h,f,n}|$  is the same except that we now show a bijection with

$$\bigsqcup_{P \in P'_{h,f}} \bigsqcup_{0 \le k_1 \le k_2 \le \dots \le k_{l(P)} \le n} \prod_{1 \le i \le l(P)} [k_i]^{\widetilde{P_i}}, \tag{60}$$

and that to do so the only change with what precedes is choosing  $k_i = c(P_i)$  instead of  $k_i = c(P_i) - 1$ .

We now state the first theorem of this subsection:

**Theorem 3.35.** Let  $\zeta$  be a character of  $\mathbb{K}HG$ , V be a finite set and  $h \in HG[V]$  a hypergraph. Then

$$\chi_V^{\zeta}(h)(n) = \sum_{f \in \mathcal{A}_h} \zeta(f(h))|C_{h,f,n}|. \tag{61}$$

In particular, if  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(h)(n)$  is the number of strictly compatible pairs of acyclic  $\zeta$ -orientations of h and colorings with [n]. In this case we call  $\chi^{\zeta}$  the  $\zeta$ -chromatic polynomial of h.

*Proof.* Recall the definition of  $\chi^{\zeta}$  from (3.4):

$$\chi_V^{\zeta}(h)(n) = \sum_{D \in Dcomp[V], l(D) = n} \zeta_V \circ \mu_D \circ \Delta_D(h). \tag{62}$$

The bijection b defined at (10) provides a bijection between the decomposition of size n of V and the colorings of V with [n]. To prove our theorem, we just need to show that for D a coloring of V,  $\max_D(h) = \mu_D \circ \Delta_D$  since we would then have

$$\chi_{V}^{\zeta}(h)(n) = \sum_{D \in Dcomp[V], l(D) = n} \zeta_{V} \circ \mu_{D} \circ \Delta_{D}(h)$$

$$= \sum_{D \text{ coloring of } f \text{ with } [n]} \zeta_{V}(\max_{D}(h))$$

$$= \sum_{f \in \mathcal{A}_{h}} \zeta_{V}(f(h)) |C_{h,f,n}|.$$
(63)

We prove this by induction over n. Let  $D = (D_1, D_2)$  be a decomposition of V of size 2. Then  $\mu_D \circ \Delta_D(h) = h|_{D_1} \sqcup h/_{D_2} = \{e \in h \mid e \subseteq D_1\} \sqcup \{e \cap D_2 \mid e \subsetneq D_1\}$ . We then need to show that  $\max_D(e) = e$  when  $e \subseteq D_1$  and  $\max_D(e) = e \cap D_2$  else. If  $e \subseteq D_1$ , then that means that all the vertices in e are maximal in e of color 1, and hence  $\max_D(e) = e$ . If  $e \subsetneq D_1$ , then the maximal vertices of e are of the one of color 2 i.e.  $\max_D(e) = e \cap D_2$ . This concludes the case n = 2.

Suppose now that this statement is true for n-1 and let D be a decomposition of V of size n. Denote by W the set  $V \setminus D_n$  and by  $D_{|W} = (D_1, \ldots, D_{n-1})$  the restriction of D to W (as a map). By induction we have that

$$\mu_{D} \circ \Delta_{D}(h) = \mu_{W,D_{n}} \circ \mu_{D_{|W}} \otimes Id \circ \Delta_{D_{|W}} \otimes Id \circ \Delta_{W,D_{n}}(h)$$

$$= \mu_{W,D_{n}} \circ \max_{D_{|W}} \otimes Id \circ \Delta_{W,D_{n}}(h)$$

$$= \mu_{W,D_{n}} \circ \max_{D_{|W}} \otimes Id \circ h|_{W} \otimes h/_{W}$$

$$= \max_{D_{|W}} (h|_{W}) \sqcup h/_{W},$$
(64)

and hence we must show that  $\max_{D(e)} = \max_{D|W}(e)$  when  $e \subseteq W$  and  $\max_{D(e)} = e \cap D_n$  otherwise. The first assertion is straightforward by definition of the restriction and the second assertion is proven in an analogous way that the case n = 2. This concludes this proof.

It is clear that connected hypergraphs play the role of prime elements in HG. This means that every hypergraph can be uniquely written as a product of connected elements, up to the order. When defining a character, we hence only need to define it on the connected hypergraphs. In particular, we only define characteristic functions by specifying the connected hypergraphs with value 1.

**Example 3.36.** Let  $\zeta_{e3}$  be the characteristic function of edges of size three and isolated vertices. Then  $\chi^{\zeta_{e3}}$  counts the colorings such that there is exactly three maximal vertices by edge and edges do not share maximal vertices.

Let now  $\zeta_3$  be the characteristic function of connected hypergraphs over three vertices and isolated vertices. Then  $\chi^{\zeta_3}$  counts the number of colorings such that reducing each edge to its maximal vertices gives us a hypergraph where connected components are either either of size 3 or an isolated vertex.

Of the three following colorings with  $\{1, 2, 3\}$ , the first two are counted by  $\chi^{\zeta_{e3}}$  but not the third. None of them are counted by  $\chi^{\zeta_3}$ .

Recall that the basic character  $\zeta_1$  is the characteristic function of discrete hypergraphs. We have a particular interpretation of  $\chi^{\zeta_1}$ .

Corollary 3.37 (Theorem 18 in [8]). Let V be a finite set and  $h \in HG[V]$  a hypergraph. Then  $\chi^{\zeta_1}(h)(n)$  is the number of colorings of V such that every edge of h has only one maximal vertex.

*Proof.* This proof is straightforward: the  $\zeta_1$ -orientations are exactly the discrete orientations and the colorings compatible with such orientations are colorings where each edge has exactly one maximal vertex.

**Example 3.38.** The coloring given in Example 3.30 is not counted in  $\chi_V^{\zeta_1}(h)(4)$  since  $e_3$  has two maximal vertices. However by changing the color of d to 2 we do obtain a coloring where every edge has only one maximal vertex.

Let g be the hypergraph  $\{\{1,2,3\},\{2,3,4\}\}\in HG[[4]]$  represented in Figure 40. We then have  $\chi^{\zeta_1}_{[4]}(h)(n)=n^4-\frac{8}{3}n^3+\frac{5}{2}n^2-\frac{5}{6}n$  and we verify that, for example,  $\chi_{[4]}(h)(2)=3$ .

## 3.3.3 Reciprocity theorem

We now give the reciprocity theorem which gives us an expression of  $\chi^{\zeta}$  over negative integers as well as a combinatorial interpretation when possible. A character  $\zeta$  of HG is odd if  $\zeta(h)=0$  for every h with a connected component with an even number of vertices. This can also be expressed by stating that the only connected hypergraphs on which  $\zeta$  is not null have odd number of vertices.

Denote by cc(h) the number of connected components of h.

**Theorem 3.39.** Let  $\zeta$  be a character of  $\mathbb{K}HG$ , V be a finite set and  $h \in HG[V]$  a hypergraph then

$$\chi_V^{\zeta}(h)(-n) = \sum_{f \in \mathcal{A}_h} (-1)^{\operatorname{cc}(f(h))} \zeta(f(h)) |\overline{C}_{h,f,n}|.$$
(66)

Furthermore, if  $\zeta$  is an odd characteristic function then  $(-1)^{|V|}\chi^{\zeta}(h)(-n)$  is the number of compatible pairs of acyclic  $\zeta$ -orientations of h and colorings with [n]. In particular we have in this case that  $(-1)^{|V|}\chi^{\zeta}(h)(-1)$  is the number of acyclic  $\zeta$ -orientations of h.

Corollary 3.40 (Theorem 24 in [8]). Let V be a finite set and  $h \in HG[V]$  a hypergraph. Then  $(-1)^{|V|}\chi^{\zeta_1}(h)(-n)$  is the number of compatible discrete acyclic orientation of h and colorings with [n]. In particular, we have now that  $(-1)^{|V|}\chi^{\zeta_1}(h)(-1)$  is the number of discrete acyclic orientations of h.

**Example 3.41.** For any any hypergraph h over V and any odd character  $\zeta$  of HG, we have  $\chi_V(h)(n) \leq (-1)^{|V|} \chi_V(h)(-n)$ . This comes from the fact that any strictly compatible pair is a compatible pair. This is observed for  $\zeta = \zeta_1$  and  $h = \{\{1, 2, 3\}, \{2, 3, 4\}\} \in HG[[4]]$ :

$$\chi_{[4]}(h)(n) = n^4 - \frac{8}{3}n^3 + \frac{5}{2}n^2 - \frac{5}{6}n < n^4 + \frac{8}{3}n^3 + \frac{5}{2}n^2 + \frac{5}{6}n = (-1)^4\chi_{[4]}(h)(-n). \tag{67}$$

We also verify that h does have  $\chi_{[4]}(h)(-1) = 7$  acyclic discrete orientations (3 × 3 orientations minus the two cyclic orientations).

As announced at the beginning of this section, we give here a self-contained proof which uses our previous results on generalized Faulhaber's polynomials and on compatible colorings. To give this proof, we first need some preliminary lemmas. We begin by recalling two classical combinatorial results.

**Proposition 3.42.** Let m and n be two integers. Then the number of surjections  $S_{m,n}$  from [m] to [n] is given by:

$$S_{m,n} = \sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} k^{m}.$$
 (68)

*Proof.* This formula can be obtained by the inclusion-exclusion principle.  $\Box$ 

Corollary 3.43. For m and n two integers such that m < n and P a polynomial of degree at most m, we have:

$$\sum_{k=0}^{n} (-1)^{n-k} \binom{n}{k} P(k) = 0.$$
 (69)

*Proof.* The statement above is a direct consequence of the fact that  $S_{m,n} = 0$  for m < n.  $\square$ 

We will use these two results to prove Lemma 3.44 which is the central point of this proof. Recall from subsubsection 2.2.3 the classical definitions over compositions: product, shuffle product and refinement.

**Lemma 3.44.** Let V be a set and  $P \models V$  a composition of V. We have the identity:

$$\sum_{Q \prec P} (-1)^{l(Q)} = (-1)^{|V|}. \tag{70}$$

Furthermore, let g be a directed acyclic graph on V and consider the constrained set  $C(g, P) = \{Q \prec P \mid \forall (v, v') \in g, Q(v) < Q(v')\}$ . We have the more general identity:

$$\sum_{Q \in C(g,P)} (-1)^{l(Q)} = \begin{cases} 0 & \text{if there exists } (v,v') \in g \text{ such that } P(v') < P(v), \\ (-1)^{|V|} & \text{if not.} \end{cases}$$
 (71)

*Proof.* Since  $\sum_{Q \prec P} (-1)^{l(Q)} = \prod_{i=1}^{l(P)} \sum_{Q \models P_i} (-1)^{l(Q)}$  we only need to show that  $\sum_{Q \models V} (-1)^{l(Q)} = (-1)^{|V|}$  to prove the first identity. Since the compositions of V of size n and the surjections from V to [n] are in bijection, we have that:

$$\sum_{Q \models I} (-1)^{l(Q)} = \sum_{n=1}^{|V|} (-1)^n S_{|V|,n} = \sum_{n=1}^{|V|} (-1)^n \sum_{k=1}^n (-1)^{n-k} \binom{n}{k} k^{|V|} 
= \sum_{k=1}^{|V|} (-1)^k \left( \sum_{n=k}^{|V|} \binom{n}{k} \right) k^{|V|} = \sum_{k=1}^{|V|} (-1)^k \binom{|V|+1}{k+1} k^{|V|} 
= (-1)^{|V|} \sum_{k=0}^{|V|-1} (-1)^k \binom{|V|+1}{k} (|V|-k)^{|V|} 
= (-1)^{|V|} (1 + \sum_{k=0}^{|V|+1} (-1)^k \binom{|V|+1}{k} (|V|-k)^{|V|}) 
= (-1)^{|V|}.$$
(72)

Note that the last equality is a direct consequence of Corollary 3.43.

To show the second identity first remark that the case where the sum is null is straightforward: if there exists  $(v,v') \in g$  such that P(v') < P(v), then  $C(g,P) = \emptyset$  and so the sum is null. From now on we only consider non empty summation sets. In this case we have that  $\sum_{Q \in C(g,P)} (-1)^{l(Q)} = \prod_{i=1}^{l(P)} \sum_{Q \in C(g \cap P_i^2,(P_i))} (-1)^{l(Q)}$  and we only need to show that  $\sum_{P \in C(g)} (-1)^{l(P)} = (-1)^{|V|}$  where C(g) = C(g,V). We denote by S(g) the sum  $\sum_{P \in C(g)} (-1)^{l(P)}$  from now on.

If g is not connected let  $V = V_1 \sqcup V_2$  and  $g = g_1 \sqcup g_2$  where  $V(g_i) = V_i$ . Let  $P \in C(g_1)$  and  $Q \in C(g_2)$  and suppose without loss of generality that m = l(Q) < l(P) = M. To choose R in sh(P,Q) we can first choose its length; then which indices are going to have a part of Q; and finally which indices among them are also going to have a part of P. This

leads to:

$$\sum_{R \in sh(P,Q)} (-1)^{l(R)} = \sum_{k=M}^{m+M} (-1)^k \binom{k}{m} \binom{m}{M - (k-m)}$$

$$= \sum_{k=0}^{m} (-1)^{k+M} \binom{M+k}{m} \binom{m}{k-m}$$

$$= (-1)^M \sum_{k=0}^{m} (-1)^{m-k} \binom{M+m-k}{m} \binom{m}{k}$$

$$= \frac{(-1)^M}{m!} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} \frac{(m+M-k)!}{(M-k)!}$$

$$= \frac{(-1)^M}{m!} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} (-k)^m$$

$$= \frac{(-1)^{m+M}}{m!} \sum_{k=0}^{m} (-1)^{m-k} \binom{m}{k} k^m$$

$$= \frac{(-1)^{m+M}}{m!} S_{m,m} = (-1)^{m+M} = (-1)^{l(P)+l(Q)},$$
(73)

where the fifth equality follows from Corollary 3.43. This shows that S(g) is multiplicative (with the product being the disjoint union) and so we can restrict ourselves to showing that  $S(g) = (-1)^{|V|}$ , for g a connected graph. We will prove this by induction on the number of edges of g.

Suppose now that g is connected. If g has no edge then g is reduced to a single vertex and the result is trivial. Thus let be (v,v') be an edge of g. We say that the edge (v,v') is superfluous if there exists a sequence of vertices  $v_0, v_1, ..., v_{k+1} \in V$  such that  $v=v_0, v'=v_{k+1}$  and  $(v_i,v_{i+1}) \in g$  for all  $i \in [k]$ . If (v,v') is superfluous then  $C(g) = C(g \setminus (v,v'))$  and so  $S(g) = S(g \setminus (v,v')) = (-1)^{|V|}$  by induction. Otherwise we have  $C(g \setminus (v,v')) = C(g) + C(t_{(v,v')}(g)) + C(g \setminus (v,v')) \cap \{P \models V \mid P(v) = P(v')\}$ , where  $t_{(v,v')}$  sends g on  $g \setminus (v,v') \cup (v',v)$ . By induction, we know that  $S(g \setminus (v,v')) = (-1)^{|V|}$  and since  $C(g \setminus (v,v')) \cap \{P \models V \mid P(v) = P(v')\} = C\left(g \cap (V/v')^2 \cup \bigcup_{(w,v') \in g \setminus (v,v')} (w,v) \cup \bigcup_{(v',w) \in g} (v,w)\right)$ , we also have by induction that  $\sum_{P \in C(g \setminus (v,v')) \cap \{P \models V \mid P(v) = P(v')\}} (-1)^{l(P)} = (-1)^{|V|-1}$ . Hence, we have the equality  $S(g) = S(t_{(v,v')}(g))$ .

Let  $e_1, \ldots, e_k$  be a sequence of edges such that for every  $i, g_i = t_{e_i} \circ \cdots \circ t_{e_1}(g)$  does not have a directed cycle. If g has a cycle, we can choose this sequence such that  $g_k$  has a superfluous edge and hence  $S(g) = S(g_k) = (-1)^{|V|}$ . If g does not have any cycle then any sequence  $e_1, \ldots, e_l$  of edges satisfies the conditions " $g_i$  does not have a directed cycle" and so  $S(g) = (-1)^{|V|}$  as long as there exists a directed graph g' with the same underlying non-oriented graph than g such that  $S(g') = (-1)^{|V|}$ . Given a non-oriented connected graph g', we can always find a directed graph g on it with only one vertex g such that for every g every

leads to: 
$$S(g) = -S(g \cap (V(G) - v)^2) = (-1)^{|V(g)|}$$
. This concludes the proof.

While we interpreted Lemma 3.44 as a result on graphs and partitions, it can also be seen as a result on posets and linear extensions.

We can now give our first proof to Theorem 3.39.

*Proof of Theorem 3.39.* From Theorem 3.35, Proposition 3.33 and Lemma 3.28, we have that:

$$\chi_V^{\zeta}(h)(-n) = (-n)^{|I(h)|} \sum_{f \in \mathcal{A}_h} \zeta(f(h)) \sum_{P \in P_{h,f}} (-1)^{\sum_{i=1}^{l(P)} p_i + l(P)} \sum_{(p_1, \dots, p_{l(P)}) \prec q} F_q(n+1). \tag{74}$$

Let P be a composition. We then have:

- $\sum_{i=1}^{l(P)} p_i = |NI(h)| |NI(f(h))|$ , since  $(\widetilde{P_1}, \dots \widetilde{P_{l(P)}}, NI(f(h)))$  is a partition of NI(h).
- The map

$$\phi: \{Q \vDash f(h) \mid P \prec Q\} \rightarrow \{q \vDash (|NI(h)| - |NI(f(h))|) \mid (p_1, \dots, p_{l(P)}) \prec q\}$$

$$Q \mapsto (|\widetilde{Q_1}|, \dots, |\widetilde{Q_{l(Q)}}|)$$

$$(75)$$

is a bijection  $(\widetilde{Q}_i)$  is defined in the same way that  $\widetilde{P}_i$  in Proposition 3.33). Indeed, the two sets have same cardinality  $\sum_{k=0}^{l(P)-1} \binom{l(P)}{k}$ : in both cases we choose the number k+1 of elements of the composition and then which consecutive elements of the composition to merge:  $\binom{l(P)}{k}$ . Furthermore the map  $\phi$  is a surjection, since the composition  $(q_1,\ldots,q_k)$  with  $q_i=\sum_{j=j_i}^{k_i}p_j$  is the image of the composition  $Q_1,\ldots,Q_k$  with  $Q_i=\sqcup_{j=j_i}^{k_i}P_j$ . This comes from the fact that for any two disjoint sets of sets A,B we have  $\bigcup_{e\in A\sqcup B}e=\bigcup_{e\in A}e\cup\bigcup_{e\in B}e=\bigcup_{e\in A}e\sqcup(\bigcup_{e\in B}e)\cap(\bigcup_{e\in A}e)^c$  and that the sets  $f^{-1}(P_i)$  are pairwise disjoint.

These two remarks lead to:

$$\chi_{V}^{\zeta}(h)(-n) = n^{|I(h)|} \sum_{f \in \mathcal{A}_{h}} (-1)^{|V| - |NI(f(h))|} \zeta(f(h)) \sum_{P \in P_{h,f}} (-1)^{l(P)} \sum_{P \prec Q} F_{\phi(Q)}(n+1)$$

$$= n^{|I(h)|} \sum_{f \in \mathcal{A}_{h}} (-1)^{|V| - |NI(f(h))|} \zeta(f(h)) \sum_{Q \vDash f(h)} \left( \sum_{P \prec Q \atop P \in P_{h,f}} (-1)^{l(P)} \right) F_{\phi(Q)}(n+1).$$
(76)

Let g be the graph with vertices the connected components of f(h) and with an oriented edge from a connected component  $h_1$  to another connected component  $h_2$  if there is  $e_1 \in h_1$  and  $e_2 \in h_2$  such that  $f(e_1) \cap f_s(e_2) \neq \emptyset$ . Since f is acyclic, g is a directed acyclic graph. We can see the compositions in  $P_{h,f}$  and  $P'_{h,f}$  (Proposition 3.33) as compositions over

connected components of f(h) since for such compositions, two edges of f(h) with a non empty intersection must be in the same part by definition. Remarking then that with this point of view  $\{P \prec Q \mid P \in P_{h,f}\} = C(g,Q)$ , Lemma 3.44 leads to:

$$\chi_{V}(h)(-n) = n^{|I(h)|} \sum_{f \in \mathcal{A}_{h}} (-1)^{|V| - |NI(f(h))|} \zeta(f(h)) \sum_{\substack{P \models f(h) \\ P(v) \le P(v') \forall (v,v') \in g}} (-1)^{\operatorname{cc}(f(h)) - |I(f(h))|} F_{\phi(P)}(n+1)$$

$$= n^{|I(h)|} \sum_{f \in \mathcal{A}_{h}} (-1)^{|V| - |NI(f(h))| - |I(f(h))| + \operatorname{cc}(f(h))} \zeta(f(h)) \sum_{P \in P'_{h,f}} F_{p_{1},\dots,p_{l(P)}}(n+1)$$

$$= n^{|I(h)|} \sum_{f \in \mathcal{A}_{h}} (-1)^{\operatorname{cc}(f(h))} |\overline{C}_{f,h,n}|, \tag{77}$$

where the last equality is Proposition 3.33.

To complete this proof, note that when  $\zeta$  is odd,  $\zeta(f(h)) \neq 0$  implies that  $|V| - \operatorname{cc}(f(h))$  is even since each connected component h' of f(h) participate for V(h') - 1 which is even.

## 3.3.4 Alternative proof

Let us now give the second proof. As announced this proof is shorter and we will prove both Theorem 3.35 and Theorem 3.39 at the same time. Recall from subsection 3.1.3 that there is a bijection  $\Delta: h \mapsto \Delta_h$  between hypergraphs and hypergraphic polytopes. We further extend the similarities of hypergraphs and hypergraphic polytopes with the following lemma.

**Lemma 3.45.** Let V be a finite set and h a hypergraph over V. Then the faces of  $\Delta_h$  are exactly the hypergraphic polytopes  $\Delta_{f(h)}$  for  $f \in \mathcal{A}_h$ . Furthermore, for f an acyclic orientation of h,  $C_{h,f,n} = \mathcal{N}_{\Delta_h}^o(\Delta_{f(h)})_n$  and  $\overline{C}_{h,f,n} = \mathcal{N}_{\Delta_h}(\Delta_{f(h)})_n$ .

Remark 6. This lemma is equivalent to Theorem 2.18 of [10]. Our approach and notations being different than in [10], we preferred to give an alternative proof of this lemma.

Proof. Let be  $f \in \mathcal{A}_h$ . We first show that  $\Delta_{f(h)}$  is indeed a face of  $\Delta_h$ . Let c be a coloring strictly compatible with f i.e.  $f = \max_c$ . We show that  $\Delta_{f(h)}$  is the c-maximum face of  $\Delta_h$ . Let p be a point in  $\Delta_h$ . Then by definition of  $\Delta_h$ , p can be written as  $\sum_{e \in h} \sum_{v \in e} a_{e,v} v$  where for each edge e the  $a_{e,v}$  are positive real numbers summing to one:  $\sum_{v \in e} a_{e,v} = 1$ . We then have that,

$$c(p) = \sum_{e \in h} \sum_{v \in e} a_{e,v} c(v)$$

$$= \sum_{e \in h} \left( c(f(e)) \sum_{v \in f(e)} a_{e,v} + \sum_{v \in f_s(e)} a_{e,v} c(v) \right),$$
(78)

which is maximum when  $a_{e,v} = 0$  for every edge e and every  $v \in f_s(e)$ . This implies that the c-maximum face of  $\Delta_h$  is the set of points of the form  $\sum_{e \in h} \sum_{v \in f(e)} a_{e,v} v$  with  $\sum_{v \in f(e)} a_{e,v} = 1$ . This is exactly  $\Delta_{f(h)}$ .

Let now Q be a face of  $\Delta_h$ . For P a polytope and y a direction, the y-maximum face  $P_y$  does not depend on the exact values of y but only on the induced order v < v' if y(v) < y(v'). Let hence be c a coloring with value in [n] such that  $Q = P_c$ . Then by what precedes,  $Q = \Delta_{\max_c(h)}$ .

The equalities between the sets of compatible colorings and the cones directly follow from the preceding.  $\Box$ 

This lemma together with Proposition 3.7 is enough to give the desired proof.

Proof of Theorem 3.39. Let  $\zeta$  be a character of  $\mathbb{K}HG$  and define  $\zeta'$  the character of GP defined by  $\zeta'(P) = \zeta(h)$  if  $P = \Delta_h$  is a hypergraphic polytope and  $\zeta'(P) = 0$  else. Let h be a hypergraph over V. Then, applying Proposition 3.7, Theorem 3.20 and finally Lemma 3.45, we have:

$$\chi_{V}^{\mathbb{K}HG,\zeta}(h)(n) = \chi_{V}^{\mathbb{K}GP,\zeta'}(\Delta_{h})(n) = \sum_{Q \leq \Delta_{h}} \zeta'(Q) |\mathcal{N}_{\Delta_{h}}^{o}(Q)_{n}|$$

$$= \sum_{f \in \mathcal{A}_{h}} \zeta(f(h)) |\mathcal{N}_{\Delta_{h}}^{o}(\Delta_{f(h)})_{n}|$$

$$= \sum_{f \in \mathcal{A}_{h}} \zeta(f(h)) |C_{h,f,n}|.$$
(79)

The formula over non positive integers is obtained analogously.

Remark 7. As a corollary from Lemma 3.45 and Theorem 3.16, we have that the antipode of  $\mathbb{K}HG$  is given by the cancellation-free and grouping-free expression

$$S_V(h) = \sum_{f \in A_h} (-1)^{\operatorname{cc}(f(h))} f(h). \tag{80}$$

While this expression express the antipode only in term of acyclic orientations, faces of polytopes have much more apparent structure than acyclic orientations and are easier and more intuitive to work with.

# 3.4 Other Hopf monoids

In this subsection we use Theorem 3.35 and Theorem 3.39 to obtain similar results on other Hopf monoids, more precisely the Hopf monoids from sections 19 to 25 of [2]. The general method used here is to use the fact that these Hopf monoids can be seen as sub-monoids of (most of the times) the Hopf monoid of simple hypergraphs, and then present an interpretation of what is an acyclic orientation on these particular Hopf monoids. More precisely, Proposition 3.7 tells us that if we have a morphism  $\phi: M \to SHG$ 

then  $\chi^{M,\zeta\circ\phi}=\chi^{\mathbb{K}SHG,\zeta}\circ\phi$  for  $\zeta$  any character of SHG. Since  $\phi$  will be injective in our cases, restricting its co-domain to is image makes it an isomorphism. We then have  $\chi^{M,\zeta}=\chi^{\mathbb{K}SHG,\zeta\circ\phi^{-1}}\circ\phi$  for  $\zeta$  any character of M. What remains is to find a combinatorial interpretation of acyclic orientations on the objects of M.

Remark 8. Note that this is exactly how we obtained our second proof of the combinatorial interpretation of  $\chi^{\mathbb{K}HG}$ . Here, since we are only working on purely combinatorial objects, the morphism  $\phi$  is simpler than in the case of  $\Delta: HG \to HGP$ .

Not only the results of this subsection generalize a lot of other results, but they are also obtained with a uniform approach. We provide details at the beginning of each subsubsection on the links between our results and already existing ones.

# 3.4.1 Simple hypergraphs

Recall from Definition 2.7 that a *simple hypergraph over* V is a set h of non empty parts of V.  $\mathbb{K}SHG$  admits a similar Hopf monoid structure to  $\mathbb{K}HG$ . In fact its structure maps can be defined in the same way

$$\mu_{V_1,V_2}: SHG[V_1] \otimes SHG[V_2] \to SHG[V] \quad \Delta_{V_1,V_2}: SHG[V] \to SHG[V_1] \otimes SHG[V_2] \quad (81)$$

$$h_1 \otimes h_2 \mapsto h_1 \sqcup h_2 \qquad \qquad h \mapsto h|_{V_1} \otimes h/_S V_2,$$

where we also have  $h|_V = \{e \in h \mid e \subseteq V\}$  and  $h/_V = \{e \cap V^c \mid e \not\subseteq V\}$ . The difference with HG is that here we are working with sets instead of multisets. So even if two edges  $e_1$  and  $e_1$  are such that  $e_1 \cap V = e_2 \cap V = e$ , there will only be one edge e in  $h/_V$ .

As this structure is very similar to the one over hypergraphs, it is of no surprise that the polynomial invariants also have similar expression.

**Proposition 3.46.** Let  $\zeta$  be a character of  $\mathbb{K}SHG$ , V be a finite set and  $h \in SHG[V]$  a simple hypergraph. We then have:

$$\chi_V^{\zeta}(h)(n) = \sum_{f \in \mathcal{A}_h} \zeta(f(h))|C_{h,f,n}|,$$
  
$$\chi_V^{\zeta}(h)(-n) = \sum_{f \in \mathcal{A}_h} (-1)^{\operatorname{cc}(f(h))} \zeta(f(h))|\overline{C}_{h,f,n}|.$$

If  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(h)(n)$  is the number of strictly compatible pairs of acyclic  $\zeta$ -orientations of h and colorings with [n]. Furthermore, if  $\zeta$  is odd  $(-1)^{|V|}\chi^{\zeta}_{V}(h)(-n)$  is the number of compatible ones. In particular,  $(-1)^{|V|}\chi^{\zeta}_{V}(h)(-1)$  is the number of acyclic  $\zeta$ -orientations of h.

*Proof.* Let mult be the species morphism from SHG to HG which sends a simple hypergraph on the same hypergraph. It is the right inverse of D which sends a hypergraph to its domain. Let  $\zeta$  be a character of SHG, and remark that D is a morphism of Hopf monoids

so  $\zeta \circ D$  is a character of  $\mathbb{K}HG$ . Then Proposition 3.7 with  $\phi = D$  gives us, for h a simple hypergraph

$$\chi^{\mathbb{K}HG,\zeta\circ\mathcal{D}}(\mathrm{mult}(h))(n) = \chi^{\mathbb{K}SHG,\zeta}(\mathcal{D}(\mathrm{mult}(h)))(n) = \chi^{\mathbb{K}SHG,\zeta}(h)(n). \tag{82}$$

The result follows, since  $\mathcal{A}_{\text{mult}(h)} = \mathcal{A}_h$ . Moreover, the same goes with (strictly) compatible colorings.

Corollary 3.47. Let V be a finite set and  $h \in SHG[V]$  a hypergraph. Then  $\chi^{\zeta_1}(h)(n)$  is the number of colorings of V such that every edge of h has only one maximal vertex and  $(-1)^{|V|}\chi^{\zeta_1}(h)(-n)$  is the number of compatible discrete acyclic orientation of h and colorings with [n]. In particular,  $(-1)^{|V|}\chi^{\zeta_1}(h)(-1)$  is the number of discrete acyclic orientations of h.

# **3.4.2** Graphs

Recall from Definition 2.7 that a graph over V is a hypergraph whose edges are all of cardinality 2. The species  $\mathbb{K}G$  is not stable under the restriction in  $\mathbb{K}HG$  but it still admits a close Hopf monoid structure which was given in Example 3.1. The structure maps are given by

$$\mu_{V_1,V_2}: G[V_1] \otimes G[V_2] \to G[V] \qquad \Delta_{V_1,V_2}: G[V] \to G[V_1] \otimes G[V_2] \qquad (83)$$

$$g_1 \otimes g_2 \mapsto g_1 \sqcup g_2 \qquad g \mapsto g|_{V_1} \otimes g/_{V_2},$$

where  $g/V_2$  is defined in the same way as in  $\mathbb{K}HG$  and  $g|_{V_1} = \{e \in g \mid e \subseteq V_1\}$  is the contraction of  $V_2$  to g as a hypergraph *i.e.*  $g|_{V_1} = g/V_2$ .

Usually an orientation of a graph is what we call here a discrete orientation. We hence introduce the notion of partial orientation of a graph which we think is more intuitive than the notion of admissible orientation in the case of graphs. A partial orientation of a graph g is a discrete orientation of a sub-graph h of g. The partial orientations of g are in bijection with the admissible orientations of g by the map  $\kappa$  which sends a partial orientation f on the admissible orientation  $\kappa_f$  defined by  $\kappa_f(e) = f(e)$ , if f(e) is defined, and  $\kappa_f(e) = e$  else. For f a partial orientation of g, we denote by f(g) the sub-graph of g formed of the non-oriented edges. One can think of it as if we followed the oriented edges while erasing them behind us. This is the same than the graph obtained by leaving aside the edges of size 1 in  $\kappa_f(e)$ . A partial orientation is acyclic if it is trivial (no edge is oriented) or it is not possible to complete it in order to obtain a cycle. It is equivalent to say that its image by  $\kappa$  is acyclic and we will consider  $\mathcal{A}_g$  as the set of acyclic partial orientations on g in the rest of this subsubsection.

A coloring c of V is strictly compatible (resp compatible) with a partial orientation f of g if  $f(e) = \max_c(e)$  (resp  $f(e) \subseteq \max_c(e)$ ) when f(e) is defined and the rest of the edges are monochromatic,  $\max_c(e) = e$ .

**Example 3.48.** We represent here a cyclic partial orientation and a coloring with  $\{1, 2\}$  along its strictly compatible partial orientation.



A cyclic partial orientation A coloring and its strictly compatible partial orientation

For  $\zeta$  a character of KG, a  $\zeta$ -partial orientation of g is a partial orientation f such that  $\zeta(f(g)) \neq 0$ . A character  $\zeta$  is odd if the connected graphs on which it is not null have an odd number of vertices.

Remark 9. In the literature, the preferred notion is that of pairs of flats F and discrete acyclic orientations of the quotient graph g/F. A flat F of a graph g is a sub-graph of g of the form  $\mu_D \circ \Delta_D(g) = g|_{D_1} \sqcup \cdots \sqcup g|_{D_n}$  for  $D \vDash g$ . The quotient g/F is then the graph obtained by deleting the edges in F and merging all the vertices which shared a connected component in F. The bijection with acyclic orientations of g is again easy to see: send a pair (F,a) of a flat and a discrete acyclic orientation of g/F on the acyclic orientation f defined by f(e) = a(e) if  $e \not\in F$  and f(e) = e else.

We preferred the notion of acyclic partial orientation which is more coherent in our context. All our results over hypergraphs were expressed in terms of acyclic orientations and not pairs of flat and acyclic orientation, as is done in [10]. Still, we also give our result in term of flats for the sake of completeness. For  $\zeta$  a character of  $\mathbb{K}G$ , a  $\zeta$ -flat of g is a flat on which  $\zeta$  is not null.

**Proposition 3.49.** Let  $\zeta$  be a character of  $\mathbb{K}G$ , V be a finite set and  $g \in G[V]$  a graph. We then have:

$$\chi_{V}^{\zeta}(g)(n) = \sum_{f \in \mathcal{A}_{g}} \zeta(f(g))|C_{g,f,n}| = \sum_{F \in \text{Flats}(g)} \sum_{a \in \mathcal{A}_{g/F}} \zeta(F)|C_{g/F,a,n}|,$$

$$\chi_{V}^{\zeta}(g)(-n) = \sum_{f \in \mathcal{A}_{g}} (-1)^{\text{cc}(f(g))} \zeta(f(g))|\overline{C}_{g,f,n}| = \sum_{F \in \text{Flats}(g)} \sum_{a \in \mathcal{A}_{g/F}} \zeta(F)|\overline{C}_{g/F,a,n}|.$$
(85)

If  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(g)(n)$  is the number of strictly compatible pairs of acyclic  $\zeta$ -partial orientations of g and colorings with [n]. Furthermore, if  $\zeta$  is odd  $(-1)^{|V|}\chi^{\zeta}_{V}(g)(-n)$  the number of compatible ones. In particular,  $(-1)^{|V|}\chi^{\zeta}_{V}(g)(-1)$  is the number of acyclic  $\zeta$ -partial orientations of g.

*Proof.* Let  $HG_{\leq 2}$  be the set sub-species of HG of hypergraphs with edges of size at most 2. The species  $\mathbb{K}HG_{\leq 2}$  is stable under product and co-product and is hence a Hopf sub-monoid. Let  $s: HG_{\leq 2} \to G$  be the set species morphism which forget edges of size 1. Then  $s: \mathbb{K}HG_{\leq 2} \to G$  is a morphism of Hopf monoid. Let  $\zeta$  be a character of G. Proposition 3.7 gives us, for g a graph,

$$\chi^{\mathbb{K}HG_{\leq 2},\zeta \circ s}(g)(n) = \chi^{\mathbb{K}G,\zeta}(s(g))(n) = \chi^{\mathbb{K}G,\zeta}(g). \tag{86}$$

This concludes the proof.

A proper coloring of a graph is a coloring such that no edge has its two vertices of the same color. The chromatic polynomial of a graph g is the polynomial  $T_g$  such that  $T_g(n)$  is the number of proper colorings with n colors.

Corollary 3.50 (Proposition 18.1 in [2]). Let g be a graph. Then  $\chi^{\mathbb{K}G,\zeta_1}(g)(n)=T_g(n)$ .

*Proof.* From Corollary 3.37 we know that  $\chi^{\mathbb{K}G,\zeta_1}(g)(n)$  is the number of colorings with [n] such that each edge has a unique maximal vertex. In the case of a graph, this is equivalent to saying that no edge has its two vertices of the same color, *i.e.* it is a proper coloring.  $\square$ 

In particular, by evaluating  $\chi^{\mathbb{K}G,\zeta_1}$  on non positive integers, we recover the classical reciprocity theorem of Stanley [44].

Remark 10. As was the case for simple hypergraphs and hypergraphs, the polynomial invariants of the Hopf sub-monoid of simple graphs  $\mathbb{K}SG$  of  $\mathbb{K}SHG$  admit the same formulas than the polynomial invariants defined there.

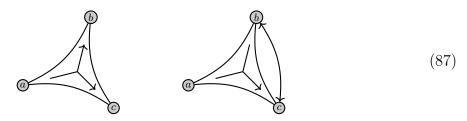
# 3.4.3 Simplicial complexes

In [11] Benedetti, Hallam, and Machacek constructed a combinatorial Hopf algebra of simplicial complexes. In particular they obtained results over some polynomial invariant which we generalize in this subsubsection.

An abstract simplicial complex, or simplicial complex, on V is a collection C of subsets of V, called faces, such that any non empty subset of a face is a face i.e.  $I \in C$  and  $\emptyset \subsetneq J \subset I$  implies  $J \in C$ . We denote by SC the set species of simplicial complexes. Proposition 21.1 of [2], states that the linear species  $\mathbb{K}SC$  of simplicial complexes is a sub-monoid of  $\mathbb{K}SHG$ .

Let us now give a simple lemma which will be useful in this subsubsection and the next one, see Figure 87 for an example of what this lemma is about.

**Lemma 3.51.** Let V be finite set,  $h \in SHG[V]$  be a simple hypergraph and f an acyclic orientation of h. Let and e and e' two edges of h of size at least 2 such that  $e' \subset e$ . Then if  $f(e) \cap e' \neq \emptyset$ , necessarily  $f(e) \cap e' = f(e')$ .



Two counter examples of Lemma 3.51. We see that we have a cycle in both cases.

Proof. Let e and e' be two such edges. Suppose there exists  $v \in f(e')$  such that  $v \notin f(e) \cap e'$ . Then  $f(e') \cap f_s(e) \neq \emptyset$  and since  $f(e) \cap e' \neq \emptyset$ , we have either  $f(e) \cap f_s(e') \neq \emptyset$  or the strict inclusions  $\emptyset \subsetneq f(e) \cap f(e') \subsetneq f(e')$ . This makes the sequence e', e a cycle. Hence  $f(e') \subseteq f(e) \cap e'$ . Suppose now there exists  $v \in f(e) \cap e'$  such that  $v \notin f(e')$ . Then similarly to the previous case,  $f(e) \cap f_s(e') \neq \emptyset$  and either  $f(e') \cap f_s(e)$  or  $\emptyset \subsetneq f(e') \cap f(e) \subsetneq f(e)$ . Hence  $f(e) \cap e' \subseteq f(e')$  and so  $f(e') = f(e) \cap e'$ .

The 1-skeleton of a simplicial complex is the simple graph formed by its faces of cardinality 2.

**Lemma 3.52.** Let be V a finite set,  $C \in SC[V]$  and g the 1-skeleton of C. Then  $\mathcal{A}_C \cong \mathcal{A}_g$ .

*Proof.* The fact that every acyclic orientation of C gives rise to an acyclic orientation of g is clear: if  $f \in \mathcal{A}_C$  then a cycle in  $f_{|g|}$  is also a cycle in f and hence it is not possible. This is a bijection because from Lemma 3.51 an orientation of a simplicial complex only needs to be defined on its faces of size 2.

For C a simplicial complex and f an acyclic orientation of its 1-skeleton, we will also denote by f the image of f by this bijection.

**Proposition 3.53.** Let  $\zeta$  be a character of  $\mathbb{K}SC$ , V be a finite set,  $C \in SC[V]$  be a simplicial complex and g be the 1-skeleton of C. We then have:

$$\chi_V^{\zeta}(C)(n) = \sum_{f \in \mathcal{A}_g} \zeta(f(C))|C_{g,f,n}|;$$

$$\chi_V^{\zeta}(C)(-n) = \sum_{f \in \mathcal{A}_g} (-1)^{\operatorname{cc}(f(g))} \zeta(f(C))|\overline{C}_{g,f,n}|.$$
(88)

If  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(C)(n)$  is the number of strictly compatible pairs of acyclic  $\zeta$ -orientations of C and colorings with [n]. Furthermore, if  $\zeta$  is odd  $(-1)^{|V|}\chi^{\zeta}_{V}(C)(-n)$  is the number of compatible ones. In particular,  $(-1)^{|V|}\chi^{\zeta}_{V}(C)(-1)$  is the number of acyclic  $\zeta$ -orientations of C.

*Proof.* This is just a direct application of Lemma 3.52. We just observe that while we do have  $C_{C,f,n} = C_{g,f,n}$ ,  $\overline{C}_{C,f,n} = \overline{C}_{g,f,n}$  and  $\operatorname{cc}(f(C)) = \operatorname{cc}(f(g))$ , we do not have f(C) = f(g), f(g) being the 1-skeleton of f(C). Hence we can not replace  $\zeta(f(C))$  and  $\zeta$ -orientation of C with  $\zeta(f(g))$  and  $\zeta$ -orientation of g.

We say that a character  $\zeta$  of  $\mathbb{K}SC$  is downward compatible if  $\zeta(C) = \zeta(g)$  for any simplicial complex C and g its 1-skeleton. The map which add to a graph all the edges of size 1 is an injective map from SG to SHG. We consider SG as a set sub-species of SHG under this map.

Corollary 3.54. Let  $\zeta$  be a downward compatible character of  $\mathbb{K}SC$ ,  $C \in SC[V]$  be a simplicial complex and g be the 1-skeleton of C. Then  $\chi_V^{\mathbb{K}SHG,\zeta}(C)(n) = \chi_V^{\mathbb{K}SG,\zeta}(g)(n)$ .

Corollary 3.55 (Corollary 28 in [8]). Let V be a finite set,  $C \in SC[V]$  be a simplicial complex and g be the 1-skeleton of C. Then  $\chi_V^{\zeta_1}(C)$  is the chromatic polynomial of g.

## 3.4.4 Building sets

Building sets and graphical building sets have been studied in a Hopf algebraic context by Grujić in [27] where he gave results in link with the one obtained here.

Building sets were independently introduced by De Concini and Procesi in [19] and by Schmitt in [42]. A building set on V is collection B of subsets of V, called connected sets, such that if  $I, J \in B$  and  $I \cap J \neq \emptyset$  then  $I \cup J \in B$  and for all  $v \in V$ ,  $\{v\} \in B$ . We denote by BS the set species of building sets. By Proposition 22.3 of [2] the linear species  $\mathbb{K}BS$  of building sets is a sub-monoid of  $\mathbb{K}SHG$ .

**Definition 3.56** ([22] [41]). Let V be a finite set and B a building set on V. Let F be a forest of rooted trees whose vertices are labelled by the elements of a partition  $\pi$  of V. We denote by  $\leq$  the relation "is a descendent of" over  $\pi$  implied by F and we denote by  $F_{\leq p} = \bigsqcup_{q \leq p} q$  for  $p \in \pi$ . The forest F is then a B-forest if it satisfies the three following conditions.

- 1. If r is a root of F, then  $F_{\leq r}$  is the set of vertices of the connected component containing r.
- 2. For any node  $p, F_{\leq p} \in B$ .
- 3. For any  $k \geq 2$  and pairwise incomparable nodes  $p_1, \ldots, p_k, \bigcup F_{p_i} \notin B$ .

We denote by B- $\mathcal{F}$  the set of B-forest of B and call B-trees the B-forests of B when B is a connected.

**Lemma 3.57.** Let V be a finite set and B a connected building set on V. Then the B-trees also admit the following inductive definition.

- The unique B-tree of the building set on a singleton  $\{v\}$  is the rooted tree with only its root  $\{v\}$ .
- If V is not a singleton, let r be a subset of V and denote by  $V_1, \ldots, V_k$  the maximal connected component of B which does not intersect with r. For  $1 \le i \le k$  let  $B_i$  be the connected building set associated to  $V_i$ , which is defined by  $B_i = \{e \in B \mid e \subset V_i\}$  and let  $T_i$  be a  $B_i$ -tree. Then the tree rooted on r obtained by doing the disjoint union of the  $T_i$  and adding an edge between r and the roots of the  $T_i$  is a B-tree.

Remark 11. This lemma is in a way the same as saying that there is a bijection between B-forest and nested sets of B ([22], [41]). The formulation given here is more adapted to what we need in the sequel.

*Proof.* We begin by showing that the tree defined in such a way are indeed B-trees. We do this by induction over |V|. If V is a singleton then it is obvious. Suppose now V is not a singleton and let  $r, V_1, \ldots, V_k$  and  $B_1, \ldots, B_k$  be as defined in the lemma.

1. To show the first item, we prove that  $V_1, \ldots, V_k$  is a partition of  $V \setminus r$  because then, by denoting by  $r_i$  the root of  $T_i$ ,

$$T_{\leq r} = \sqcup_{p \leq r} p = r \sqcup_{p \leq r} p = r \sqcup_i \sqcup_{p \leq r_i} = r \sqcup_i T_{i, \leq r_i} = r \sqcup V_i = V,$$
 (89)

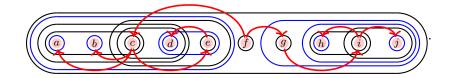
where the fourth equality is obtained by induction. Suppose  $V_i \cap V_j \neq \emptyset$ . Then since B is a building set,  $V_i \cup V_j \in B$ , and since neither  $V_i$  nor  $V_j$  intersect with r, their union does not either. This contradicts the maximality of  $V_i$  and  $V_j$  and it is hence not possible. Let now be  $v \in V \setminus r$  then since  $\{V\} \in V$ , there exists a maximal edge connected component not intersecting V which contains v.

- 2. We already showed the second case in the case of r. Let  $p \neq r$  be a node of T. Then there exists i such that p is a node of  $T_i$  and hence by induction  $T_{\leq p} \in B_i \subset B$ .
- 3. Let be  $l \geq 2$  and  $p_1, \ldots, p_l$  be pairwise incomparable nodes of T. Suppose that  $\bigcup p_i \in B$ . Then if there exists j such that all the  $p_i$  are in  $T_j$ , all the  $p_i$  would be subset of  $V_j$  and we would have  $\bigcup p_i \in B_j$  which is not possible by induction. So there is at least two indices i, j such that  $p_i \in T_{k_i}$  and  $p_j \in T_{k_j}$  (the  $p_i$ s can not be equal to r since r is comparable to every node). Then  $\bigcup p_i$  is in B but in no  $B_i$  and hence it intersects with r by definition. This is not possible since no  $p_i$  intersects with r. This shows that  $\bigcup p_i \notin B$

Let now T be a B-tree, r be its root,  $T_1, \ldots, T_k$  be its direct sub-trees and  $r_1, \ldots, r_k$  be their respective roots. For  $1 \leq i \leq k$ , let  $V_i = T_{\leq r_i} = T_{i, \leq r_i}$  and  $B_i$  be the connected building set associated to  $V_i$ . Then by definition of B-trees, for  $1 \leq i \leq k$ ,  $T_i$  is a  $B_i$ -tree. We only need to show that the  $V_i$  are the maximal connected sets which do not intersect r to conclude. Clearly they do not intersect r since they are union of nodes and all nodes are pairwise disjoint. Suppose W is a connected set not intersecting r and such that  $V_i \subsetneq W$  for one of the  $V_i$ s. Since  $V_1, \ldots, V_k$  forms a partition of  $V \setminus r$ , W must intersect with some  $V_{j_1}, \ldots, V_{j_i}, j_m \neq i$  for  $1 \leq i \leq k$ . Suppose without loss of generality that  $i_m = m$  and i = l + 1. Then  $i_m \in V_{i_m}$  and  $i_m \in V_{i_m}$  is a building set. But this is not possible since this is also equal to  $\bigcup_{1 \leq j \leq l+1} V_j = \bigcup_{1 \leq j \leq l+1} T_{\leq r_j}$  and the  $i_m \in V_i$  are maximal.

**Example 3.58.** We represented here an induction step of the construction of a B-tree. The set W is in red and the connected sets in blue are the maximal connected sets not intersecting W.

We also represent a B-tree obtained by beginning with the above choice:



Let V be a set, F a rooted forest on V and c a coloring of V. We say that F and c are (strictly) compatible if c is a (strictly) increasing map on F. Respectively denote by  $C_{F,n}$  and  $\overline{C}_{F,n}$  the set of colorings strictly compatible and compatible with F.

**Lemma 3.59.** Let V be a finite set and B a building set on V. Then there is a bijection  $A_B \cong B - \mathcal{F}$  which preserves (strict) compatibility with colorings.

*Proof.* First remark that for B and B' two building sets over two disjoint sets we have  $A_{B \sqcup B'} = A_B \times A_{B'}$  and  $B \sqcup B' - \mathcal{F} = B - \mathcal{F} \times B' - \mathcal{F}$ , so it is sufficient to prove this lemma on connected building sets and B-trees.

We construct a bijection b between  $\mathcal{A}_B$  and B- $\mathcal{F}$  by induction on |V|. If V is a singleton then there is a unique B-tree possible and a unique acyclic orientation possible and the bijection is trivial. Suppose now V is not a singleton. Let f be an acyclic orientation of B. Let  $V_1, \ldots V_k$  be the maximal connected sets not intersecting f(V) and  $B_1, \ldots, B_k$  their associated connected building sets. Then for  $i \in [k]$ ,  $f_{|V_i|}$  is an acyclic orientation of  $B_i$  and  $T_i = b(f_{|V_i|})$  is a  $B_i$ -tree for  $1 \le i \le k$ . Define b(f) as the rooted tree in f(V) obtained by doing the disjoint union of the  $T_i$  and adding an edge between f(V) and the roots of the  $T_i$ s. Then b(f) is a B-tree by Lemma 3.57.

Let now T be a B-tree and  $r, V_1, \ldots, V_k$  and  $B_1, \ldots, B_k$  as defined in Lemma 3.57. Let  $B_0$  be the set of edges intersecting with r and let  $b^{-1}(T)$  be the orientation defined by  $b^{-1}(T)(e) = b^{-1}(T_i)(e)$  if  $e \in B_i$  and  $b^{-1}(T)(e) = r$  if  $e \in B_0$ . Suppose there exists  $e_1, \ldots, e_k$  a cycle in  $b^{-1}(T)$ . Since  $r, V_1, \ldots, V_k$  is partition of V, this cycle must be entirely contained in one of the  $B_i$ . Since by induction this cycle can not be entirely in a  $B_i$ , it must be contained in  $B_0$ . But for every edge in  $e \in B_0$   $b^{-1}(f)(e) = r$ . Hence  $b^{-1}(f)$  is acyclic.

The fact that in the two preceding constructions the root of the B-tree is the image of the connected component along with the induction hypothesis enable us to conclude that the b and  $b^{-1}$  thus defined are indeed inverse functions. It also gives us that b preserves (strict) compatibility with colorings, since for a (strictly) compatible coloring c of f the color c(f(V)) is necessarily the maximal color:  $f(V) = \max_c(V) = \{v \in V \mid c(v) \text{ is maximal in } V\}$ .

Let B be a building set and F be a B-forest. The F-induced building set is the building set whose connected sets are obtained by taking the non empty intersection of each connected set with the maximum node possible in F. We denote it by  $B \cap F$ . For  $\zeta$  a character of  $\mathbb{K}BS$  we say that F is a  $\zeta$ -B-forest if  $\zeta(B \cap F) \neq 0$ .

**Proposition 3.60.** Let  $\zeta$  be a character of  $\mathbb{K}BS$ , V be a finite set and  $B \in BS[V]$  be a building set. We then have:

$$\chi_V^{\zeta}(B)(n) = \sum_{F \in B - \mathcal{F}} \zeta(B \cap F) |C_{F,n}|,$$

$$\chi_V^{\zeta}(B)(-n) = \sum_{F \in B - \mathcal{F}} (-1)^{\operatorname{cc}(B \cap F)} \zeta(B \cap F) |\overline{C}_{F,n}|.$$
(91)

If  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(B)(n)$  is the number of strictly compatible pairs of  $\zeta$ -B-forests and colorings with [n]. Furthermore, if  $\zeta$  is odd  $(-1)^{|V|}\chi_V^{\zeta}(B)(-n)$  is the number of compatible ones. In particular,  $(-1)^{|V|}\chi_V^{\zeta}(B)(-1)$  is the number of  $\zeta$ -B-forest.

*Proof.* Again, this is a direct application of the previous lemma. We just need to remark from the construction of the bijection of Lemma 3.59 that with our definition of  $B \cap F$  we have  $B \cap F = b^{-1}(F)(B)$ .

## 3.4.5 Graphs, ripping and sewing

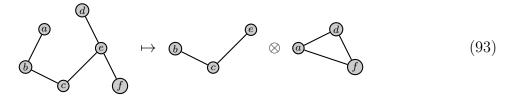
The linear species  $\mathbb{K}SG$  of simple graphs admits another Hopf monoid structure than the one given in Example 3.1 and subsubsection 3.4.2. This Hopf monoid is defined in Definition 23.2 of [2] and its structure maps are given by

$$\mu_{V_1,V_2}: SG[V_1] \otimes SG[V_2] \to SG[V] \qquad \Delta_{V_1,V_2}: SG[V] \to SG[V_1] \otimes SG[V_2] \qquad (92)$$

$$g_1 \otimes g_2 \mapsto g_1 \sqcup g_2 \qquad g \mapsto g|_{V_1} \otimes g/_{V_1},$$

where  $g|_{V_1}$  is the sub-graph of g induced by  $V_1$  and  $g/_{V_1}$  is the simple graph on  $V_2$  with an edge between v and v' if there is a path from v to v' in which all the vertices which are not ends are in  $V_1$ . These two operations are respectively called *ripping out*  $V_1$  and *sewing through*  $V_1$ .

Here is an example of co-product with the set  $V = \{a, b, c, d, e, f\}$  and  $V_1 = \{b, c, e\}$  and  $V_2 = \{a, d, f\}$ :



**Definition 3.61** (Definition 23.1 in [2]). Let be  $g \in SG[V]$ . A tube is a subset  $W \subseteq V$  such that  $g|_W$  is connected. The set of tubes of g is a building set called graphical building set of g and which we denote tubes (g).

By Proposition 23.3 of [2] we know that  $g \mapsto \text{tubes}(g)$  is a Hopf monoid morphism from  $\mathbb{K}SG$  to  $\mathbb{K}BS$ .

**Definition 3.62.** Let be V be a finite set and  $g \in SG_c[V]$  a connected simple graph. A partitioning tree of g is a rooted tree whose vertices are labelled by the elements of a partition of V and which is inductively defined by the following.

- If V is a singleton, then the unique partitioning tree is the trivial tree with V as sole vertex.
- Else choose  $W \subset V$  and a partitioning tree for each connected component of  $g_{V \setminus W}$ . The tree with root W and direct sub-trees these partitioning trees is then a partitioning tree of g.

If g is not connected anymore, a partitioning forest of g is the disjoint union of partitioning trees of each connected component of g. We denote by PF(g) the set of partitioning forest of g.

Let g be a simple graph and F be a partitioning forest of g. The graph ripped and sewed through F is the graph  $g_T$  obtained by the following process. Begin with  $g_T = \emptyset$  and iteratively repeat the following: for each leaf V of F, add  $g_V$  to  $g_F$  and sew g through V. Delete all the leaves of F and repeat the previous operation. The process terminates when F is empty. For  $\zeta$  a character of KSG, we say that F is a  $\zeta$ -partitioning forest if  $\zeta(g_F) \neq 0$ .

**Proposition 3.63.** Let  $\zeta$  be a character of  $\mathbb{K}SG$ , V be a finite set and  $g \in SG[V]$  be a simple graph. We then have:

$$\chi_V^{\zeta}(g)(n) = \sum_{F \in PF(g)} \zeta(g_F) |C_{F,n}|,$$

$$\chi_V^{\zeta}(g)(-n) = \sum_{F \in PF(g)} (-1)^{\operatorname{cc}(g_F)} \zeta(g_F) |\overline{C}_{F,n}|.$$
(94)

If  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(g)(n)$  is the number of strictly compatible pairs of  $\zeta$ -partitioning forests of g and colorings with [n]. Furthermore, if  $\zeta$  is odd  $(-1)^{|V|}\chi_V^{\zeta}(g)(-n)$  is the number of compatible ones. In particular,  $(-1)^{|V|}\chi_V^{\zeta}(g)(-1)$  is the number of  $\zeta$ -partitioning forests of g.

Proof. Since  $\chi^{\mathbb{K}SG,\zeta}(g)(n) = \chi^{\mathbb{K}BS,\zeta \text{otubes}^{-1}} \circ \text{tubes}(g)(n)$ , we only must verify that the partitioning forest of g are the tubes(g)-forest and that tubes $(g_F) = \text{tubes}(g) \cap F$ . We do this in the case where g is connected, the other case being a direct consequence from this one. This is quite straightforward: in the definition of a partitioning tree, the set W is a subset of V = tubes(g) and if  $V_1, \ldots, V_k$  are the set of vertices of the connected components of  $g_{V\setminus W}$ , then there are the maximal connected sets of tubes(g) which does not intersect with g. This and Lemma 3.57 show that the definition of partitioning trees of g is the same than that of tubes(g)-trees and hence they are the same objects.

Let us now show that  $\operatorname{tubes}(g_T) = \operatorname{tubes}(g) \cap T$ . Let  $V_1, \ldots, V_k$  be the nodes of T starting with the leaves and going the way up until the root. Denote by D the partition  $V_1, \ldots, V_k$ . Then by definition of  $g_T, g_T = \mu_D \circ \Delta_D(g)$ . Since tubes is a Hopf monoid

morphism, we have that  $\operatorname{tubes}(mu_D \circ \Delta_D(g)) = \mu_D \circ \Delta_D(\operatorname{tubes}(g)) = \max_D(\operatorname{tubes}(g)) = b(T)(\operatorname{tubes}(g)) = \operatorname{tubes}(g) \cap T$ , where  $\max_D$  is the unique strictly compatible orientation of D and b is the bijection defined in Lemma 3.59.

We have a particular interpretation of this proposition for the basic character.

Corollary 3.64 (Corollary 34 in [8]). Let V be a finite set and  $g \in SG[V]$  a simple graph. Then  $\chi_V^{\zeta_1}(g)(n)$  is the number of colorings of V with [n] such that every path in g with ends of the same color has a vertex of color strictly greater than the colors of the ends.

Proof. Again we only show this in the case of g connected. Since  $\zeta_1$  is the characteristic function of discrete elements, the  $\zeta_1$ -partitioning trees are the trees where every node is a singleton. Let T be a partitioning tree of g and c a coloring strictly compatible with T. Let  $\{v\}$  and  $\{v'\}$  be two nodes of T of the same color. Then they are incomparable by definition of strict compatibility. Let  $\{a\}$  be their lowest common ancestor and A the set of strict ancestors of a ( $a \notin A$ ). Again by definition of strict compatibility, a has a color strictly greater than v and v'. Every path from v to v' must pass by a since v and v' are in two different connected components of  $g_{V \setminus A \cup \{a\}}$  be in a same connected component of  $g_{V \setminus A}$ .

Let now c be a coloring of V such that every path in g with ends of the same color has a vertex of color strictly greater than the colors of the ends. Then there is a unique vertex in c which is of maximal color: else, since g is connected, we would have a path between two of them and hence a vertex with a color strictly greater. Let v be the unique vertex of maximal color. Then each connected component of  $g_{V\setminus v}$  must also have one vertex of maximal color. Hence we have an inductive way to construct a tree strictly compatible with c. Since this way coincides with the definition of partitioning tree whose vertices are singletons, this concludes the proof.

## 3.4.6 Partitions

Recall that a partition of V is a set  $\{P_1, \ldots, P_k\}$  of disjoint non empty sets, called parts, such that  $\sqcup_i P_i = V$ . The linear species  $\mathbb{K}\Pi$  admits a Hopf monoid structure with structure maps:

$$\mu_{V_1,V_2}: \Pi[V_1] \otimes \Pi[V_2] \to \Pi[V] \qquad \Delta_{V_1,V_2}: \Pi[V] \to \Pi[V_1] \otimes \Pi[V_2] \qquad (95)$$

$$\pi_1 \otimes \pi_2 \mapsto \pi \sqcup \pi_2 \qquad \pi \mapsto \pi|_{V_1} \otimes \pi|_{V_2},$$

where for  $\pi = \{P_1, \dots, P_k\}$ ,  $\pi|_{V_1}$  is the partition of  $V_1$  obtained by taking the intersection with  $V_1$  of each part  $P_i$  and forgetting the empty parts.

A cliquey graph is a simple graph which is the disjoint union of cliques. The species morphism which sends a partition  $\{P_1, \ldots, P_k\}$  on the cliquey graph composed of the cliques on  $P_1, \ldots, P_k$ . By Proposition 24.2 of [2], this is a Hopf monoid morphism  $\mathbb{K}\Pi \to \mathbb{K}SG^{cop}$  with the ripping and sewing Hopf structure on  $\mathbb{K}SG$ .

We say that a partition  $\tau$  refines a partition  $\pi$ , and denote  $\tau \prec \pi$  is the parts of  $\pi$  are the unions of the parts of  $\tau$ . For D a decomposition, denote by  $\pi(D)$  the partition

obtained by forgetting the order and the empty parts of D. We say that a decomposition D is induced by  $\pi$  is  $\pi(D) \prec \pi$  For  $\zeta$  a character of  $\mathbb{K}\Pi$ , we say that a decomposition D is a  $\zeta$ -decomposition if  $\zeta(\pi(D)) \neq 0$ .

**Proposition 3.65.** Let  $\zeta$  be a character of  $\mathbb{K}\Pi$ , V be a finite set and  $\pi \in \Pi[V]$  be a partition. We then have:

$$\chi_V^{\zeta}(\pi)(n) = \sum_{\tau \prec \pi} \zeta(\tau)\ell(\tau)! \binom{n}{\ell(\tau)}$$
(96)

If  $\zeta$  is a characteristic function, then  $\chi^{\zeta}(\pi)(n)$  is the number of  $\zeta$ -decomposition of size n induced by  $\pi$ .

Proof. As done in the previous section, since  $\chi$  is multiplicative we only need to look at the trivial partition  $\pi = \{V\}$ . Let g be the image of  $\pi$  by the previously defined morphism i.e. g is the cliquey graph over V. For  $W \subset V$ , it is clear that  $g_{V\setminus W}$  is the cliquey graph over  $V\setminus W$  and the partitioning trees of g are then chain trees. These are in bijection with compositions of V. By definition of  $g_T$ , for  $T = T_1, \ldots, T_k$  such a tree/decomposition,  $g_T$  is the disjoint union of the cliquey graphs over  $V_1, \ldots, V_k$ . A coloring strictly compatible with a line tree with k vertices is an increasing map from [k] to [n]. This is equal to  $\binom{n}{k}$  and is the number of decomposition of size n which reduce to the line tree when forgetting the empty parts. Hence we have  $\chi_V^{\zeta}(\{V\})(n) = \sum_{P \models V} \zeta(\pi(P))\binom{n}{\ell(P)}$  which is equal to the desired formula grouping by partitions  $\tau$  such that  $\pi(P) = \tau$ .

We do not give the formula for the negative integers here since the formula for the non negative ones is sufficiently explicit and the objects are simple enough that the notion of compatible colorings is not particularly revealing.

#### 3.4.7 Set of paths

A word on V is a total ordering of V. The paths on V are the words on V quotiented by the relation  $w_1 \dots w_{|V|} \sim w_{|V|} \dots w_1$ . A set of paths  $\alpha$  of V is a partition  $\{V_1, \dots, V_k\}$  of V with a path  $s_i$  on each part  $V_i$  and we will write  $\alpha = s_1 | \dots | s_l$ . We denote by Path the set species of set of paths. The linear species  $\mathbb{K}Path$  of sets of paths admits a Hopf monoid structure with structure maps

$$\mu_{V_1,V_2}: Path[V_1] \otimes Path[V_2] \to Path[V] \quad \Delta_{V_1,V_2}: Path[V] \to Path[V_1] \otimes Path[V_2] \quad (97)$$

$$\alpha_1 \otimes \alpha_2 \mapsto \alpha_1 \sqcup \alpha_2 \qquad \qquad \alpha \mapsto \alpha|_{V_1} \otimes \alpha/_{V_1}$$

where if  $\alpha = s_1 | \dots | s_l$ ,  $\alpha |_{V_1} = s_1 \cap S | \dots | s_l \cap S$  forgetting the empty parts and  $\alpha /_{V_1}$  is the set of paths obtained by replacing each occurrence of an element of  $V_1$  in  $\alpha$  by the separation symbol | and removing the multiplicity of |.

**Example 3.66.** For  $V = \{a, b, c, d, e, f, g\}$  and  $V_1 = \{b, c, e\}$  and  $V_2 = \{a, d, f, g\}$ , we have:

$$\Delta_{V_1,V_2}(bfcg|aed) = bc|e \otimes f|g|a|d. \tag{98}$$

For  $\alpha = s_1 | \dots | s_l$  a set of path, denote by  $l(\alpha)$  the simple graph whose connected components are the paths induced by  $s_1, \dots, s_l$ . By Proposition 25.1 of [2] we know that  $\alpha \mapsto l(\alpha)$  is a morphism of Hopf monoids from  $\mathbb{K}Path$  to  $\mathbb{K}SG^{cop}$ .

**Example 3.67.** For  $V = \{a, b, c, d, e, f, g\}$  and  $\alpha = bfcg|aed, l(\alpha)$  is the following graph:

We only give the interpretation for  $\chi^{\zeta_1}$  here.

**Proposition 3.68** (Corollary 38 in [8]). Let V be a finite set and  $\alpha \in Path[V]$  be a path on V. Then  $\chi_V^{\zeta_1}(\alpha)(n)$  is the number of strictly compatible pairs of binary trees with |V| vertices and colorings with [n] and  $\chi_V^{\zeta_1}(\alpha)(-n)$  is the number of compatible pairs of binary trees with |V| vertices and colorings with [n]. In particular  $\chi_V^{\zeta_1}(\alpha)(-1) = C_{|V|}$  where  $C_n = \frac{1}{n+1} \binom{2n}{n}$  is the n-th Catalan number.

*Proof.* First remark that by definition of  $\chi$ , we have  $\chi^{\mathbb{K}SG^{cop}} = \chi^{\mathbb{K}SG}$  and so  $\chi_V^{\mathbb{K}Path,\zeta_1}(\alpha)(n) = \chi_V^{\mathbb{K}SG,\zeta_1}(l(\alpha))(n)$ . Fix one of the two total orderings of V induced by  $\alpha$  so that we can consider the left and the right of a vertex v of  $l(\alpha)$ . Then each vertex of  $l(\alpha)$  is totally characterised by the number of vertices on its left (and on its right) and hence the partitioning trees of  $l(\alpha)$  with singletons for vertices are exactly the binary trees with |V| vertices.

# 4 Operads on graphs

In the last decades, several interesting operads on trees have been defined. Amongst these tree operads, maybe the most studied are the pre-Lie operad **PLie** [17] and the nonassociative permutative operad **NAP** [35]. We aim in this section to generalize the operadic structure of **PLie** and **NAP** to any kind of graph-like object, as defined in Definition 2.7. This section is a replica of the article [6] which is a collaboration of the author with Jean-Christophe Aval, Adrian Tanasa and Samuele Giraudo. The results presented here can also be found in [7], the extended abstract of [6] for FPSAC 2020.

This section is organized as follows. In Subsection 4.1 we give the definitions of operads as well as classical results on these objects. In Subsection 4.2 we propose new ways of constructing species and operads. We use these new constructions in Subsection 4.3 to define and study the main operads of interest of this section. Finally, in Subsection 4.4 we investigate several properties of these operads: we describe an explicit link with the pre-Lie operad mentioned above, and we study interesting (finitely generated) sub-operads.

All the species considered in this section are positive and we will just write species for positive species. For  $\mathbb{K}B$  a vector space with basis B and  $v = \sum_{b \in B} a_b b \in \mathbb{K}B$ , we call support of v the elements of  $b \in B$  such that  $a_b \neq 0$ .

# 4.1 Operads

We give here basic definitions and results of the theory as well as some classical examples. We refer the reader to [40] and [36] for a more general approach to the theory of operads. The reader may note some similarities between the definition of an operad and the monoid part of a Hopf monoid. Moreover, we refer the reader to [4] for an in depth study of monoids in monoidal categories.

# 4.1.1 Definitions and examples

In Example 2.5 we described the elements of the composition of two species R(S) as elements of R labelled with elements of S. It is thus natural to wonder if from one element of S(S), one can recover an element of S. We already provided an example with  $E_+$  by noting that  $E_+(E_+)$  is isomorphic to the species of partitions, which are indeed sets. A straightforward example is  $Pol_+(Pol_+)$ , where we can recover a polynomial by doing the classical composition of polynomials. Moreover, this polynomial composition is such that we can consider elements of the form P(Q,R) and P(Q(R)) without ambiguity, and the trivial polynomial x behaves as the unity for the composition. Operads are a general solution to this question. In the following definitions, while the composition does not appear in the axioms, the axioms do translate what we want: the elements  $*,*_1$  and  $*_2$  are to be thought as the "variables" where we compose.

A symmetric linear operad is a positive linear species  $\mathcal{O}$  equipped with an unity  $e: \mathbb{K}X \to \mathcal{O}$  and a morphism of linear species  $\circ_* *: \mathcal{O}' \cdot \mathcal{O} \to \mathcal{O}$  called partial composition, such that the following diagrams commute

$$\mathcal{O}'' \cdot \mathcal{O}^{2} \xrightarrow{\circ_{*1}} \mathcal{O}' \cdot \mathcal{O} \qquad \qquad \mathcal{O}' \cdot \mathcal{O}' \cdot \mathcal{O} \xrightarrow{\circ_{*1} \cdot Id} \mathcal{O}' \cdot \mathcal{O} \\
\downarrow \circ_{*2} \circ Id \cdot \tau \qquad \downarrow \circ_{*2} \qquad \qquad \downarrow Id \cdot \circ_{*2} \qquad \downarrow \circ_{*2} \\
\mathcal{O}' \cdot \mathcal{O} \xrightarrow{\circ_{*1}} \mathcal{O} \qquad \qquad \mathcal{O}' \cdot \mathcal{O} \xrightarrow{\circ_{*1}} \mathcal{O}$$

$$\mathcal{O}' \cdot \mathbb{K}X \xrightarrow{\mathcal{O}' \cdot e} \mathcal{O}' \cdot \mathcal{O} \xleftarrow{e' \cdot \mathcal{O}} \mathbb{K}X' \cdot \mathcal{O}$$

$$\downarrow \circ_{*} \cong \qquad \downarrow \circ_{*} \cong \qquad \downarrow$$

where  $\tau : x \otimes y \mapsto y \otimes x$  and  $p_V : x \otimes v \mapsto \mathcal{O}[\sigma](x)$  with  $\sigma$  is the bijection that sends \* on v and is the identity on  $V \setminus \{v\}$ .

We refer to symmetric linear operads as operads. Note that while we only used partial compositions over ghost vertices in our definition, we can consider them over any element  $v \in V$ .

A sub-operad of an operad  $\mathcal{O}$  is a sub-species of  $\mathcal{O}$  containing the image of e and stable under partial composition. For  $\mathcal{O}$  an operad, the sub-operad of  $\mathcal{O}$  generated by a set E of elements of  $\mathcal{O}$  is the smallest sub-operad of  $\mathcal{O}$  containing E. A morphism of operads  $f: \mathcal{O}_1 \to \mathcal{O}_2$  is a morphism of species stable under the structure maps:  $f \circ e = e$  and  $f(x \circ_* y) = f(x) \circ_* f(y)$ .

In practice the map e is often trivial and we do not mention it. Let us now give a series of examples of operads.

**Com.** The species  $KE_+$  has a natural operad structure given by the partial composition  $\{V_1 + *\} \circ_* \{V_2\} = \{V_1 + V_2\}$ . This operad is called the *commutative operad* and denoted by **Com**. For instance, we have:

In this context we denote by  $\mu_V = \{V\}$  the basis element of  $\mathbf{Com}[V]$  so that  $\mathbf{Com}[V] = \mathbb{K}\mu_V$ .

**Perm.** The species  $\mathbb{K}Id$  has a natural operad structure given by  $v \circ_* w = v|_{*\leftarrow w}$  which is equal to w if v = \* and equal to v else. This operad is called *perm operad* or *commutative diassociative operad* and denoted by **Perm**.

**Polynomials.** As announced, the species  $\mathbb{K}Pol_+$  has a natural partial composition given by the composition of polynomials: for  $p_1(v_1, \ldots, v_k, *)$  and  $p_2(v'_1, \ldots, v'_l)$  two polynomials over disjoint sets of variables,

$$(p_1 \circ_* p_2)(v_1, \dots, v_k, v_1', \dots, v_l') = p_1|_{* \leftarrow p_2} = p_1(v_1, \dots, v_k, p_2(v_1', \dots, v_l')).$$
 (101)

One can directly check that this partial composition satisfies the commutative diagrams of Definition 4.1.1. This turns  $\mathbb{K}Pol_+$  into an operad where the units are the singleton polynomials  $v \in Pol_+[\{v\}]$ .

The injective species morphism of Example 2.3.2 from Id to  $Pol_+$  defined by  $v \mapsto v$  is an operad morphism from  $\mathbb{K}Id$  to  $\mathbb{K}Pol_+$  and hence makes  $\mathbb{K}Id$  a sub-operad of  $\mathbb{K}Pol_+$ . The three morphisms of linear species from  $\mathbf{Com}$  to  $\mathbb{K}Pol_+$  respectively given by  $\mu_V \mapsto \prod_{v \in V} v$ ,  $\mu_V \mapsto \bigoplus_{v \in V} v$  and  $\mu_V \mapsto \sum_{v \in V} v$  are all operad morphisms and give three ways to see  $\mathbb{K}E_+$  as a sub-operad of  $\mathbb{K}Pol_+$ .

**NAP.** Let be  $t_1$  and  $t_2$  be two rooted trees and let  $t_1 \circ_* t_2$  be the rooted tree obtained by the following operation.

- 1. Remove the vertex \* from  $t_1$  and take the union of the resulting forest with  $t_2$ .
- 2. Add an edge between the parent of \* in  $t_1$  and the root of  $t_2$ .
- 3. Add an edge between each child of \* in  $t_1$ , and the root of  $t_2$ .

This operation is a partial composition and turns the species  $\mathbb{K}T^{\bullet}$  of rooted trees into an operad. This operad is called *non associative permutative operad* [35] (or NAP for short) and is denoted by NAP. For instance, by depicting the roots by squares, we have:

**PreLie.** Let be  $t_1$  and  $t_2$  be two rooted trees and let  $t_1 \circ_* t_2$  be the sum over all rooted trees obtained by the following operation.

- 1. Remove the vertex \* from  $t_1$  and take the union of the resulting forest with  $t_2$ .
- 2. Add an edge between the parent of \* in  $t_1$  and the root of  $t_2$ .
- 3. For each child of \* in  $t_1$ , add an edge between this vertex and any vertex of  $t_2$ .

This operation is a partial composition and turns the species  $\mathbb{K}T^{\bullet}$  into an operad. This operad is called *pre-Lie operad* [17] and is denoted by **PLie**. Remark that the partial composition of  $t_1$  and  $t_2$  as elements of **NAP** is always in the support of the partial composition of  $t_1$  and  $t_2$  as elements of **PLie**. For instance, we have:

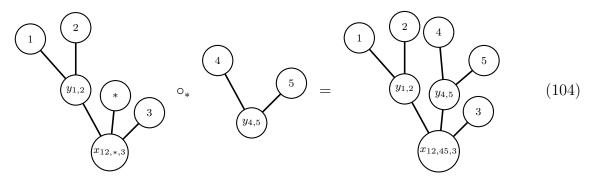
**Hadamard product.** If  $\mathcal{O}_1$  and  $\mathcal{O}_2$  are two operads, then the species  $\mathcal{O}_1 \times \mathcal{O}_2$  is also an operad with partial composition:  $(x_1 \otimes x_2) \circ_* (y_1 \otimes y_2) = (x_1 \circ_* y_1) \otimes (x_2 \circ_* y_2)$ .

## 4.1.2 Free operad, generators and relations

In all the above examples, we defined operads by explicitly describing the vector spaces  $\mathcal{O}[V]$  and the partial compositions. There is another way to present an operad which is as a quotient of a free operad.

Let S be a positive linear species such that  $S = \mathbb{K}X + S_{2^+}$ . Recall from subsubsection 2.1.4 that  $\mathscr{S}_S$  is the species whose elements are trees decorated with S. This species has a natural operad structure given by the grafting of trees. For  $t_1 \in \mathscr{S}'_S[V_1]$  and  $t_2 \in \mathscr{S}_S[V_2]$ , the partial composition  $t_1 \circ_* t_2$  is the tree obtained by grafting  $t_2$  on the leaf \* of  $t_1$  and relabeling the nodes of  $t_1$  accordingly. This operad is called *free operad over* S and we denote it by  $\mathbf{Free}_S$ .

**Example 4.1.** We give here an example of partial composition in a free operad over a species with an element x of size 3 and y of size 2.



In the case of linearized species  $\mathbb{K}S$ , we also denote by  $\mathbf{Free}_S = \mathscr{S}_S$  so that we have  $\mathbb{K}\mathbf{Free}_S = \mathbf{Free}_{\mathbb{K}S}$ .

Remark 12. In the sequel, we consider free operads over species which are sub-species of an operad  $\mathcal{O}$ . When this happens, we denote by  $\circ_*^{\xi}$  the partial composition in the free operad in order to not confuse it with the partial composition in  $\mathcal{O}$ .

**Example 4.2** (ComMag). Let  $sym_2$  be the set species over one symmetric element of size 2. More formally, it is the set species defined by  $sym_2[V] = \emptyset$  if  $|V| \neq 2$  and  $sym_2[\{a,b\}] = \{s_{ab}\}$  else. The action of the transposition (ab) is then necessarily trivial:  $s_{ba} = (ab) \cdot s_{ab} = sym_2[(ab)](s_{ab}) = s_{ab}$ . The operad  $\mathbb{K}$ Free<sub> $sym_2$ </sub> is then an operad structure over abstract binary trees. This operad is called *commutative magmatic operad* [14] and is denoted by ComMag.

An *ideal* of an operad  $\mathcal{O}$  is a sub-species  $\mathcal{I}$  such that the image of the products  $\mathcal{O}' \cdot \mathcal{I}$  and  $\mathcal{I}' \cdot \mathcal{O}$  by the partial composition maps are in  $\mathcal{I}$ . The *quotient species*  $\mathcal{O}/\mathcal{I}$  defined by  $(\mathcal{O}/\mathcal{I})[V] = \mathcal{O}[V]/\mathcal{I}[V]$  is then an operad with the natural partial composition and unit :  $[x] \circ_* [y] = [x \circ_* y]$  where [x] is the equivalence class of x. For  $\mathcal{G}$  a species, if  $\mathcal{R}$  is a sub-species of  $\mathbf{Free}_{\mathcal{G}}$ , we denote by  $(\mathcal{R})$  the smallest ideal of  $\mathbf{Free}_{\mathcal{G}}$  containing  $\mathcal{R}$  and write that  $(\mathcal{R})$  is  $\mathbf{generated}$  by  $\mathcal{R}$ .

Denote by  $\mathbf{Free}_{\mathcal{G}}^{(2)}$  the sub-species of  $\mathbf{Free}_{\mathcal{G}}$  of trees with two internal node.

**Definition 4.3.** Let  $\mathcal{G}$  be a species and  $\mathcal{R}$  be a sub-species of  $\mathbf{Free}_{\mathcal{G}}$ . We denote by  $\mathrm{Ope}(\mathcal{G},\mathcal{R}) = \mathbf{Free}_{\mathcal{G}}/(\mathcal{R})$  the operad generated by  $\mathcal{G}$  and with relation  $\mathcal{R}$ . The operad  $\mathrm{Ope}(\mathcal{G},\mathcal{R})$  is binary if the species  $\mathcal{G}$  of generators is concentrated in cardinality 2 (i.e. for all  $n \neq 2$ ,  $\mathcal{G}[[n]] = \{0\}$ ). This operad is quadratic if the species  $\mathcal{R}$  of relations is a sub-species of  $\mathbf{Free}_{\mathcal{G}}^{(2)}$ .

For S a species and E a set of elements of S, the species generated by E is the smallest sub-species of S containing E.

**Example 4.4.** The operad **Com** is the quotient of the free operad over one symmetric element of size two by the associativity relation. More formally, denote by  $\mathcal{R}$  the subspecies of **ComMag**<sup>(2)</sup> generated by the associativity relation  $s_{a*} \circ_* s_{bc} - s_{c*} \circ_* s_{ab}$ . Then **Com** = Ope( $\mathbb{K}sym_2, \mathcal{R}$ ). This operad is hence binary and quadratic.

# 4.1.3 Koszul duality

For S a linear species, we denote by  $S^*$  the dual species of S which is defined by  $S^*[V] = S[V]^*$  and  $S^*[\sigma](f) = f \circ S[\sigma^{-1}]$ . We denote by  $S^{\vee}$  a species defined by  $S^{\vee}[V] = S^*[V]$  and  $S^{\vee}[\sigma](f) = \text{sign}(\sigma)f \circ S[\sigma^{-1}]$ , where  $\text{sign}(\sigma)$  is the signature of  $\sigma$ . It is indeed a species and not the since this does not define the maps  $S[\sigma]$  when  $\sigma$  is a bijection between two different sets. This is not a problem and any of the possible species will do. For the sake of simplicity, we will specify how certain maps act when necessary (see Example 4.6).

**Definition 4.5.** Let  $\mathcal{O} = \text{Ope}(\mathcal{G}, \mathcal{R})$  be a binary quadratic operad. Define the linear form  $\langle - | - \rangle$  on  $\text{Free}_{\mathcal{G}^{\vee}}^{(2)} \times \text{Free}_{\mathcal{G}}^{(2)}$  by

$$\langle f_1 \circ_* f_2 | x_1 \circ_* x_2 \rangle = f_1(x_1) f_2(x_2),$$
 (105)

The Koszul dual of  $\mathcal{O}$  is then the operad  $\mathcal{O}^! = \operatorname{Ope}(\mathcal{G}^{\vee}, \mathcal{R}^{\perp})$  where  $\mathcal{R}^{\perp}$  is the orthogonal of  $\mathcal{R}$  for  $\langle - | - \rangle$ .

**Example 4.6.** Let  $\alpha, \beta \in \mathscr{A} = \{a, b, c \dots, z, *\}$  be two letters in the Latin alphabet plus \*, such that  $\alpha$  appears before  $\beta$  (\* appears after z). We then denote by  $s_{\alpha\beta}^{\vee} \in (\mathbb{K}sym_2)^{\vee}[\{\alpha, \beta\}]$  the dual of  $s = s_{\alpha\beta} = s_{\beta\alpha} \in sym_2[\{\alpha, \beta\}]$  and for  $\sigma$  a bijection with domain  $\{\alpha, \beta\}$  and codomain in  $\mathscr{A}$  we denote by  $s_{\sigma(\alpha)\sigma(\beta)} = (\mathbb{K}sym_2)^{\vee}[\sigma](s_{\alpha\beta})$ . In particular we have  $s_{\beta\alpha} = -s_{\alpha\beta}$ .

For this example, also denote  $[a, b] = s_{ab}^{\vee}$ . The *Lie* operad **Lie** is the quotient of the free operad over one antisymmetric generator by the Jacobi relation. More formally, let  $\mathcal{R}$  be the sub-species of  $\mathbf{Free}^{(2)}_{(\mathbb{K}sym_2)^{\vee}}$  generated by the *Jacobi relation* [a, [b, c]] + [c, [a, b]] + [b, [c, a] (one can check that this is indeed stable under the action of  $\mathfrak{S}_{a,b,c}$  and hence  $\mathcal{R}$  is indeed a species). Then  $\mathbf{Lie} = \mathrm{Ope}((\mathbb{K}sym_2)^{\vee}, \mathcal{R})$ . This operad is the Koszul dual of  $\mathbf{Com}$ . Indeed,

we have, for example:

$$\langle s_{a*}^{\lor} \circ_{*} s_{bc}^{\lor} + s_{c*}^{\lor} \circ_{*} s_{ab}^{\lor} + s_{b*}^{\lor} \circ_{*} s_{ca}^{\lor} | s_{a*} \circ_{*} s_{bc} - s_{c*} \circ_{*} s_{ab} \rangle$$

$$= \langle s_{a*}^{\lor} \circ_{*} s_{bc}^{\lor} | s_{a*} \circ_{*} s_{bc} \rangle + \langle s_{c*}^{\lor} \circ_{*} s_{ab}^{\lor} | s_{a*} \circ_{*} s_{bc} \rangle + \langle s_{b*}^{\lor} \circ_{*} s_{ca}^{\lor} | s_{a*} \circ_{*} s_{bc} \rangle$$

$$- \langle s_{a*}^{\lor} \circ_{*} s_{bc}^{\lor} | s_{c*} \circ_{*} s_{ab} \rangle - \langle s_{c*}^{\lor} \circ_{*} s_{ab}^{\lor} | s_{c*} \circ_{*} s_{ab} \rangle - \langle s_{b*}^{\lor} \circ_{*} s_{ca}^{\lor} | s_{c*} \circ_{*} s_{ab} \rangle$$

$$= s_{a*}^{\lor} (s_{a*}) s_{bc}^{\lor} (s_{bc}) + s_{c*}^{\lor} (s_{a*}) s_{ab}^{\lor} (s_{bc}) + s_{b*}^{\lor} (s_{a*}) s_{ca}^{\lor} (s_{bc})$$

$$- s_{a*}^{\lor} (s_{c*}) s_{bc}^{\lor} (s_{ab}) - s_{c*}^{\lor} (s_{c*}) s_{ab}^{\lor} (s_{ab}) - s_{b*}^{\lor} (s_{c*}) s_{ca}^{\lor} (s_{ab})$$

$$= 1 + 0 + 0 - 1 - 0 - 0 = 0.$$

$$(106)$$

## 4.1.4 Koszul operads

Koszulity is an important aspect of operad theory. In the sequel, we show that a particular operad is Koszul. Since this is our only reason for introducing Koszulity, we only give here a very quick overview of Koszulity and Gröbner bases for operads which hides a lot of the theory. We do not give the general results but only restricted versions which suffice for our use. We refer the reader to the literature; for a broader approach of the topic, see for example [36], [40], [28] and [20]. In particular, all the examples presented here come from [20].

In order to give the characterisation which interests us, we need to introduce the concepts of  $\mathcal{L}$ -species, shuffle operads and Gröbner bases. Informally, we can see these objects as the same as species and operads, except with a total order on every set of vertices.

#### $\mathscr{L}$ -species

A set (resp linear) positive  $\mathcal{L}$ -species consists of the following data:

- for each finite set V and total order l on V, a set (resp vector space) S[V, l], such that  $S[\emptyset, \emptyset] = \emptyset$  (resp  $\{0\}$ ).
- For each increasing bijection  $\sigma:(V,l)\to (V',l')$ , a (resp linear) map  $S[\sigma]:S[V,l]\to S[V',l']$ . These maps should be such that  $S[\sigma_1\circ\sigma_2]=S[\sigma_1]\circ S[\sigma_2]$  and S[Id]=Id.

In the sequel, we write order to designate a total order and  $\mathcal{L}$ -species to designate positive  $\mathcal{L}$ -species. As for species, we can compose a set  $\mathcal{L}$ -species S with the linearization functor in order to obtained a *linearized*  $\mathcal{L}$ -species  $\mathbb{K}S$ . For S an  $\mathcal{L}$ -species and l an order on V, we also denote by S[l] = S[V, l]. We can do this since the data of V is included in l.

**Example 4.7.** • We denote by X the  $\mathcal{L}$ -species defined  $X[V, l] = \emptyset$  if V is not a singleton and  $X[\{v\}, v] = v$  else.

• The  $\mathscr{L}$ -species of shuffle compositions  $Comp_{sh}$  is defined as follows: the elements  $Comp_{sh}[V,l]$  are compositions  $P=P_1,\ldots,P_k$  of V such that, for every  $1 \leq i < j \leq k$ ,  $\min_l P_i < \min_l P_j$ .

As in the case of classical species,  $\mathcal{L}$ -species also have constructions on them, but before giving them, let us give some notations on orders.

- For l an order on V and  $W \subseteq V$  a subset of V, we denote by  $l_W$  the order on W induced by l.
- For  $l = l_1 \dots l_n$  an order on a set V of size  $n, i \in [n]$  and  $* \notin V$ , we denote by  $l \stackrel{i}{\leftarrow} *$  the order  $l_1 \dots l_{i-1} * l_i \dots l_n$  on V + \*.
- For  $l^1, \ldots, l^k$  k order on pairwise disjoint sets  $V_1, \ldots, V_k$ , we denote by  $sh(l^1, \ldots, l^k)$  the set  $\{w \mid w_{V_i} = l^i\}$  of shuffles of  $l^1, \ldots, l^k$ . Note that this is an "associative operation" in the sense that for  $l^1, l^2, l^3$  three orders, the union of the shuffles of  $l^1$  with the elements of  $sh(l^2, l^3)$  is exactly  $sh(l^1, l^2, l^3)$ .

Let R and S be two linear  $\mathcal{L}$ -species and l a total order on V. Denote by n = |V| and let be  $i \in [n]$ . We define the following operations.

Product 
$$R \cdot S[V, l] = \bigoplus_{l \in sh(l', l'')} R[l'] \otimes S[l''],$$

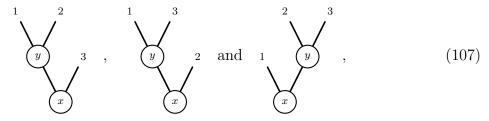
$$i\text{-th}Derivative \quad S^{i}[V,l] = S[V+*,l \stackrel{i}{\leftarrow} *],$$

Composition 
$$R(S)[V,l] = \bigoplus_{P \in Comp_{sh}[V,l]} R[\{P_1,\ldots,P_k\},P] \otimes S[P_1,l_{P_1}] \otimes \cdots \otimes S[P_k,l_{P_k}].$$

Since we have the  $\mathscr{L}$ -species  $\mathbb{K}X$  and the notion of composition, we can define Schröder tree on  $\mathscr{L}$ -species in the same way as for species. In this case, for S a set  $\mathscr{L}$ -species, the set  $\mathscr{L}_S[V]$  have the same description as for a set species except that the trees are now planar instead of abstract. This is because of the orders: instead of having a partition  $\pi_w$  for each internal node w, we have a shuffle composition  $\pi_w$ .

For S a  $\mathcal{L}$ -species and l an order on V, the fact that we have an order enables us an easier notation of the elements of  $\mathcal{S}_S[V,l]$  as operations e.g.  $\alpha(l_1,\ldots,l_n)$ .

**Example 4.8.** Let S be the set  $\mathscr{L}$ -species defined by  $S[V, l] = \emptyset$  when  $|V| \neq 2$  and S[V, l] = [n] else. Then the elements of  $\mathscr{S}_S^{sh}[[3], 123]$  are the trees



where  $1 \le x, y \le n$ . This is because the only shuffle compositions of size 2 of [3] are (12,3), (13,2) and (1,23). These trees can be denoted in a more compact way by  $\mu_x(\mu_y(1,2),3)$ ,  $\mu_x(\mu_y(1,3),2)$  and  $\mu_x(1,\mu_y(2,3))$ .

Let us end this brief presentation of  $\mathscr{L}$ -species by giving their link to classical species. Let  $\mathscr{F}$  be the forgetful functor which send a species S on the  $\mathscr{L}$ -species  $S^{\mathscr{F}}$  defined by:

- for l an order on V,  $S^{\mathscr{F}}[V,l] = S[V]$ .
- For  $\sigma:(V,l)\to (V',l')$  an increasing bijection,  $S^{\mathscr{F}}[\sigma]$  is given by

$$S^{\mathscr{F}}[V,l] = S[V] \xrightarrow{\sigma} S[W] = S^{\mathscr{F}}[W,l']. \tag{108}$$

• For  $f: S \to R$  a species morphism,  $f^{\mathscr{F}}$  is the  $\mathscr{L}$ -species morphism given by

$$f_{V,l}^{\mathscr{F}}: S^{\mathscr{F}}[V,l] = S[V] \xrightarrow{f} R[V] = R^{\mathscr{F}}[V,l].$$
 (109)

This is a forgetful functor in the sense that we forget the action  $\sigma_V$  on S[V]. We have the following fundamental proposition from [20].

**Proposition 4.9** (Proposition 3 in [20]). Let S and R be two species. Then

$$(R(S))^{\mathscr{F}} = R^{\mathscr{F}}(S^{\mathscr{F}}). \tag{110}$$

# Shuffle operads

We would like to define shuffle operads as  $\mathcal{L}$ -species satisfying the same axioms that a linear species must satisfy to be an operad. For now we can not do this because we do not have the notion of derivative of a shuffle operad  $\mathcal{O}'$ . Fortunately, there is a way to make sense of the different species appearing in the diagrams (4.1.1).

For l an order on V and  $v \in V$ , denote by  $\arg_l v$  the index of v in l:  $l_{\arg_l v} = v$ . For R and S two  $\mathscr{L}$ -species we define the  $\mathscr{L}$ -species  $R' \cdot S$  and  $R'' \cdot S^2$  as follow:

$$R' \cdot S[V, l] = \bigotimes_{l \in sh(l^1, l^2)} R^{\arg_l l_1^2}[l^1] \otimes S[l^2],$$

$$R'' \cdot S^2[V, l] = \bigotimes_{l \in sh(l^1, l^2, l^3)} R[V_1 + \{*_1, *_2\}, l^{1+}] \otimes S[V_2, l^2] \otimes S[V_3, l^3],$$
(111)

where  $l^{1+}$  is the total order obtained by replacing  $l_1^2$  by  $*_1$  and  $l_1^3$  by  $*_2$  in  $l_{V_1 + \{l_1^2, l_1^3\}}$ .

A shuffle operad is then a  $\mathscr{L}$ -species  $\mathscr{O}$  with a unity e and a partial composition  $\circ^{sh}_*$  such that the diagrams (4.1.1) commutes. For S a  $\mathscr{L}$ -species, the free shuffle operad over S is denoted by  $\mathbf{Free}^{sh}_S$  and defined in the same way as the free operad over a species. The same goes with the *ideal of a shuffle operad* and the notation  $\operatorname{Ope}_s h(\mathcal{G}, \mathcal{R})$ .

Remark 13. With the notations of elements of the free operad as operations, the partial composition of the free operad is then the composition of operation:  $\mu_x(\ldots,*,\ldots) \circ_*^{\xi}$   $\mu_y(\ldots) = \mu_x(\ldots,\mu_y(\ldots),\ldots)$ .

We have the following corollary from Proposition 4.9.

**Theorem 4.10** (Corollary 1 in [20]). Let  $\mathcal{G}$  be a linear species. The image by  $\mathscr{F}$  of the free operad generated by  $\mathcal{G}$  is isomorphic to the free shuffle operad generated by  $\mathscr{F}(\mathcal{G})$ . For  $\mathcal{R}$  a sub-species of  $\mathbf{Free}_{\mathcal{G}}$ , the image by  $\mathscr{F}$  of the operad ideal generated by  $\mathcal{R}$  is isomorphic to the shuffle operad ideal generated by  $\mathscr{F}(\mathcal{R})$ . This writes as  $\mathbf{Free}_{\mathcal{G}}^{\mathscr{F}} \cong \mathbf{Free}_{\mathcal{G}}^{sh}$  and  $(\mathcal{R})^{\mathscr{F}} = (\mathcal{R}^{\mathscr{F}})$ .

Hence  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})^{\mathscr{F}} \cong \operatorname{Ope}_{sh}(\mathcal{G}^{\mathscr{F}}, \mathcal{R}^{\mathscr{F}}).$ 

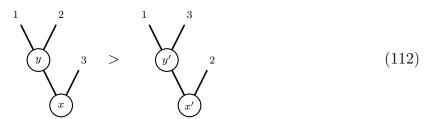
#### Admissible order

Let S be a set  $\mathscr{L}$ -species. In order to define the notion of Gröbner bases, we need to introduce an order on the trees of  $\mathbf{Free}_S[V,l]$ . Instead of giving the broader notion of admissible order defined in [20], we only give a small variation of the *path-lexicographic ordering*.

First for every order l on V, fix an order on the elements of S[l] such that for every  $x < y \in S[l]$  and  $\sigma: l \to l'$  we have  $\sigma \cdot x < \sigma \cdot y$ . That is to say, the order does not depend on the labels (but it can depend on their relative order). Given this order, we also have an order on the words on elements of S given by the lexicographic order. Let now be  $t \in \mathbf{Free}_S[l_1 \dots l_n]$ . For all  $i \in [n]$ , there is a unique path from  $l_i$  to the root of t. Denote by  $a_i$  the word composed, from left to right, of the labels of the nodes of this path, from the root to the leaf. We associate to t the sequence  $(a_1, \dots, a_i, w)$ , where w is the word obtained by reading the leaves of t from left to right.

For two trees  $t, t' \in S$ , with associated sequences  $(a_1, \ldots, a_n, w)$  and  $(b_1, \ldots, b_n, w')$  we then compare t and t' by lexicographically comparing  $a_1$  with  $b_1$  then  $a_2$  with  $b_2$  etc and reverse lexicographically comparing w with w' if  $a_i = b_i$  for all i.

**Example 4.11.** The sequences attached to the trees from Example 4.8 are respectively (xy, xy, x, 123), (xy, x, xy, 132) and (x, xy, xy, 123). We have



if x > x' or x = x' and y > y' or x = x' and y = y'.

Now that we have an order on  $\mathbf{Free}_S$ , for  $x \in \mathbb{K}\mathbf{Free}_S$  the leading term of x is the maximal element in its support and denote it by  $\mathrm{lt}(x)$ .

#### Divisibility and S-polynomials

Let S be a set  $\mathscr{L}$ -species. A tree t of  $\mathbf{Free}_S^{sh}$  is divisible by another tree t' of  $\mathbf{Free}_S^{sh}$  if t' is a sub-tree of t. Here a sub-tree must also conserve the order of the leaves. A tree u of  $\mathbf{Free}_S^{sh}$  is a small common multiple of two tree t and t' if it is divisible by both t and t' and its number of vertices is less than the total number of vertices of t and t'.

**Example 4.12.** Let S be a set  $\mathscr{L}$ -species and  $l = l_1, \ldots l_n$  an order. Then the element  $\alpha(\beta(l_1, l_3), \gamma(\beta(l_2, l_6), l_4, l_5))$  of  $\mathbf{Free}_S^{sh}$  has among its divisors  $\alpha(\beta(l_1, l_3), l_2)$  and  $\gamma(\beta(l_1, l_4), l_2, l_3)$  but not  $\gamma(\beta(l_1, l_3), l_2, l_4)$ .

If t is divisible by t', then there exists trees  $\alpha$  and  $\beta_1, \ldots, \beta_k$  such that  $t = \alpha(\ldots, t'(\beta_1, \ldots, \beta_k), \ldots)$ . We denote by  $m_{t,t'}$  the operation on any tree with same number of leaves than t' which associate to a tree u the tree  $\alpha(\ldots, u(\beta_1, \ldots, \beta_k), \ldots)$ . Let now V be a finite set, l an order on V and  $x, y \in \mathbb{K}\mathbf{Free}_S^{\mathscr{F}}[V, l]$ . Assume  $\mathrm{lt}(x)$  and  $\mathrm{lt}(y)$  have a small common multiple u. Then we have  $m_{u,\mathrm{lt}(x)}(\mathrm{lt}(x)) = u = m_{u,\mathrm{lt}(y)}(\mathrm{lt}(y))$ . We call S-polynomial of x and y (corresponding to u) the element

$$s_u(x,y) = m_{u,lt(x)}(x) - \frac{c_x}{c_y} m_{u,lt(y)}(y),$$
 (113)

where  $c_x$  and  $c_y$  are the respective coefficients of the leading terms of x and y.

#### Gröbner bases and Koszulity

We can finally give the definition of a Gröbner bases and a Koszul operad.

**Definition 4.13** (Definition 13 in [20]). Let  $\mathcal{G}$  be a set  $\mathcal{L}$ -species and  $\mathcal{R}$  be a  $\mathcal{L}$ -subspecies of  $\mathbf{Free}_{\mathcal{G}}^{sh}$ . Let  $\mathcal{B}$  be basis of  $\mathcal{R}$ . We say that  $\mathcal{B}$  is a *Gröbner bases* of  $\mathcal{R}$  if for every  $x \in (\mathcal{R})$ , the leading term of x is divisible by the leading term of one element in  $\mathcal{B}$ .

**Definition 4.14** (Corollary 3 in [20]). Let  $\mathcal{G}$  be a set  $\mathcal{L}$ -species and  $\mathcal{R}$  be a quadratic  $\mathcal{L}$ -sub-species of  $\mathbf{Free}_{\mathcal{G}}^{sh}$ . We say that  $\mathrm{Ope}_{sh}(\mathcal{G},\mathcal{R})$  is  $\mathit{Koszul}$  if  $\mathcal{R}$  admits a Gröbner bases. Let  $\mathcal{G}$  be a set species and  $\mathcal{R}$  be a quadratic sub-species of  $\mathbf{Free}_{\mathcal{G}}^{sh}$ . We say that  $\mathrm{Ope}(\mathcal{G},\mathcal{R})$  is  $\mathit{Koszul}$  if  $\mathrm{Ope}_{sh}(\mathcal{G}^{\mathcal{F}},\mathcal{R}^{\mathcal{F}})$  is  $\mathit{Koszul}$ .

When  $\mathcal{O}$  is a Koszul symmetric operad, it admits a Koszul dual  $\mathcal{O}^!$ . In this case the Hilbert series of  $\mathcal{O}$  and  $\mathcal{O}^!$  are related by the identity:

$$\mathcal{H}_{\mathcal{O}}(-\mathcal{H}_{\mathcal{O}!}(-t)) = t. \tag{114}$$

Let us finish by a characterisation of Gröbner bases.

**Proposition 4.15** (Theorem 1 in [20]). Let  $\mathcal{G}$  be a set  $\mathcal{L}$ -species and  $\mathcal{R}$  be a  $\mathcal{L}$ -subspecies of  $\mathbf{Free}_{\mathcal{G}}^{sh}$ . Let  $\mathcal{B}$  be basis of  $\mathcal{R}$ . Then  $\mathcal{B}$  is a Gröbner bases if and only if for all pair of elements in  $\mathcal{B}$ , their S-polynomials are congruent to zero modulo  $\mathcal{B}$  (*i.e.* they are in  $(\mathcal{R})$ ).

# 4.2 Some constructions on species and operads

The goal of this subsection is to define some constructions on species and operads. We define three constructions: the augmentation, the semi-direct product and the maps from a set to an operad.

**Definition 4.16.** Let A be a set and S be a set (resp linear) species. An A-augmentation of S is a set (resp linear) species A-S such that A-S[V]  $\cong$  S[A  $\times$  V] for every finite set V.

#### **Example 4.17.** Let A be a set.

- Instead of considering an A-augmented multi-hypergraph on V as a multi-hypergraph on  $V \times A$ , we consider them as multi-hypergraphs on V where the ends of the edges are labelled with elements of A. In particular, the species of oriented multi-hypergraphs  $MHG_{or}$  is in bijection with the species of  $\{s,t\}$ -augmented multi-hypergraphs  $\{s,t\}$ -MHG. For  $h \in MHG$  and f an orientation of h, the pair h, f is sent on the multi-hypergraph obtained by respectively labeling by t and s the targets f(e) and sources  $f_s(e)$  of each edge e.
- Instead of seeing the elements in A- $Pol_+[V]$  as polynomials with set of variables the couples  $(v, a) \in V \times A$ , we consider them as polynomials with set of variables  $\{v_a \mid v \in V, a \in A\}$  of elements of V indexed by elements of A.

Remark 14. For S and R any two species and  $f:R\to S$  a morphism, f extends to a morphism between any two A-augmentation of R and S by A- $R[V]\cong R[A\times V]\xrightarrow{f} S[A\times V]\cong A$ -S. In particular the bijection  $MHG\cong Pol_+$  given in subsubsection 2.2.2 extends to a bijection which sends an edge e on the monomial  $\prod_{(v,a)\in e} v_a^{e(v,a)}$ .

In the following proposition, we give an operad structure to a Hadamard product  $S \times \mathcal{O}$  where S is a species and  $\mathcal{O}$  is an operad.

**Proposition 4.18.** Let S be a linear species and  $\mathcal{O}$  an operad. Let  $\varphi$  be a morphism from  $S' \cdot (S \times \mathcal{O})$  to S and denote by  $x \circ_*^f y = \varphi(x \otimes y \otimes f)$ . Suppose  $\varphi$  satisfies the following hypotheses.

**Commutativity.** For x an element S'' and  $y \otimes f$  and  $z \otimes g$  two elements of  $S \times \mathcal{O}$ ,

$$(x \circ_{*_1}^f y) \circ_{*_2}^g z = (x \circ_{*_2}^g z) \circ_{*_1}^f y.$$
(115)

**Associativity.** For x an element of S',  $y \otimes f$  an element of  $(S \times \mathcal{O})'$  and  $z \otimes h$  an element of  $S \times \mathcal{O}$ ,

$$(x \circ_{*_1}^f y) \circ_{*_2}^g z = x \circ_{*_1}^{f \circ_{*_2} g} (y \circ_{*_2}^g z).$$
 (116)

**Unity.** There exists a map  $e: \mathbb{K}X \to S$  such that

$$x \circ_*^{e_{\mathcal{O}}(v)} e(v) = S[\sigma](x) \quad \text{and} \quad e(*) \circ_*^f x = x,$$
 (117)

where  $e_{\mathcal{O}}$  is the unit of  $\mathcal{O}$  and  $\sigma$  is the bijection which sends \* on v and is the identity on the rest of the set on which x is defined.

Then the partial composition  $\circ^{\varphi}_{*}$  defined by

$$\circ_*^{\varphi} : (S \times \mathcal{O})' \cdot S \times \mathcal{O} \to S \times \mathcal{O} 
(x \otimes f) \otimes (y \otimes g) \mapsto x \circ_*^g y \otimes f \circ_* g$$
(118)

makes  $S \times \mathcal{O}$  an operad with unit e. We call this operad the semi-direct product of S and  $\mathcal{O}$  over  $\varphi$  and we denote it by  $S \ltimes_{\varphi} \mathcal{O}$ .

*Proof.* We must verify that the three diagrams (4.1.1) commutes.

• Let  $V_1, V_2, V_3$  be three disjoint sets and  $x \otimes f \in (S \times \mathcal{O})''[V_1], y \otimes g \in S \times \mathcal{O}[V_2]$  and  $z \otimes h \in S \times \mathcal{O}[V_3]$ . We then have

$$\begin{aligned}
\left((x \otimes f) \circ_{*_{1}}^{\varphi} (y \otimes g)\right) \circ_{*_{2}}^{\varphi} (z \otimes h) &= \left((x \circ_{*_{1}}^{g} y) \circ_{*_{2}}^{h} z\right) \otimes \left((f \circ_{*_{1}} g) \circ_{*_{2}} h\right) \\
&= \left((x \circ_{*_{2}}^{h} z) \circ_{*_{1}}^{g} y\right) \otimes \left((f \circ_{*_{2}} h) \circ_{*_{1}} g\right) \\
&= \left((x \otimes f) \circ_{*_{1}}^{\varphi} (z \otimes h)\right) \circ_{*_{2}}^{\varphi} (y \otimes g),
\end{aligned} \tag{119}$$

where the second equality follows from (115) and the fact that  $\mathcal{O}$  is an operad.

• Let  $V_1, V_2, V_3$  be three disjoint sets and  $x \otimes f \in (S \times \mathcal{O})'[V_1], y \otimes g \in (S \times \mathcal{O})'[V_2]$ and  $z \otimes h \in S \times \mathcal{O}[V_3]$ . We then have

$$\begin{aligned}
\left((x \otimes f) \circ_{*_{1}}^{\varphi} (y \otimes g)\right) \circ_{*_{2}}^{\varphi} (z \otimes h) &= \left((x \circ_{*_{1}}^{g} y) \circ_{*_{2}}^{h} z\right) \otimes \left((f \circ_{*_{1}} g) \circ_{*_{2}} h\right) \\
&= \left(x \circ_{*_{1}}^{g \circ_{*_{1}} h} (y \circ_{*_{2}}^{h} z)\right) \otimes f \circ_{*_{1}} (g \circ_{*_{2}} h)\right) \\
&= (x \otimes f) \circ_{*_{1}}^{\varphi} \left((y \otimes g) \circ_{*_{2}}^{\varphi} (z \otimes h)\right),
\end{aligned} (120)$$

where the second equality follows from (116) and the fact that  $\mathcal{O}$  is an operad.

• Let be  $x \otimes f \in (S \times \mathcal{O})'[V]$  and  $v \notin V$ . We then have

$$(x \otimes f) \circ_*^{\varphi} (e(v) \otimes e_{\mathcal{O}}(v)) = x \circ_*^{e_{\mathcal{O}}(v)} e(v) \otimes f \circ_* e(v) = S[\sigma](x \otimes f)$$
(121)

where  $\sigma$  is the bijection which sends \* to v and is the identity on V. The last equality follows from the first equality from (117) and the fact that  $\mathcal{O}$  is an operad. Let now be  $x \otimes f \in S \times \mathcal{O}[V]$ . Then

$$(e(*) \otimes e_{\mathcal{O}}(*)) \circ_* (x \otimes f) = e(*) \circ_*^f x \otimes e_{\mathcal{O}}(*) \circ_* f = x \otimes f$$
(122)

where the last equality comes from second equality from (117) and the fact that  $\mathcal{O}$  is an operad.

When it is clear from the context, we do not mention  $\varphi$  and just write semi-direct product of S and  $\mathcal{O}$  and denote it by  $S \ltimes \mathcal{O}$ . In practice, the operad structure  $\mathcal{O}$  of  $S \ltimes \mathcal{O}$  is transparent and we are just interested in what happens on S, that it is to say the "pseudo partial composition"  $x \circ_*^g y$ .

74

**Example 4.19.** Let C be a finite set and also denote by C the trivial species given by C[V] = C for all set V. We would like to provide  $\mathbb{K}C$  with a trivial operad structure  $c_1 \circ_* c_2 = c_1$  but this would not satisfy the existence of a unity. Instead, we define the linear species  $C = \mathbb{K}X + \mathbb{K}C_{2+}$  which has an operad structure close to what we want. The partial composition is defined by, for  $c_1 \in C'[V_1]$  and  $c_2 \in C[V_2]$ :  $c_1 \circ_* c_2 = c_1$  if  $V_1 \neq \emptyset$  and  $* \circ_* c_2 = c_2$  when  $V_1 = \emptyset$  and  $* \in X[\{*\}]$ .

\*  $\circ_* c_2 = c_2$  when  $V_1 = \emptyset$  and  $* \in X[\{*\}]$ . Let  $\mathcal{F}^C = X + \mathcal{F}_{2+}^C$  be the set species of maps with co-domain  $C: \mathcal{F}^C[V] = \{f: V \to C\}$  for |V| > 1. We define a semi-direct product structure  $\mathbb{K}\mathcal{F}^C \ltimes_{\varphi} \mathcal{C}$ . Let  $V_1, V_2$  be two disjoint sets and suppose that  $|V_1 + \{*\}|, |V_2| > 1$ . Let be  $f \in \mathcal{F}^C[V_1 + \{*\}]$  and  $g \otimes x \in \mathcal{F}^C \times \mathcal{C}[V_2]$ .

sets and suppose that  $|V_1 + \{*\}|, |V_2| > 1$ . Let be  $f \in \mathcal{F}^C[V_1 + \{*\}]$  and  $g \otimes x \in \mathcal{F}^C \times \mathcal{C}[V_2]$ . We then have  $f \circ_*^c g = 0$  if  $f(*) \neq c$  and  $f \circ_*^c g(v) = \begin{cases} f(v) & \text{if } v \in V_1 \\ g(v) & \text{if } v \in V_2 \end{cases}$  else. When  $V_1 = \emptyset$  or  $V_2$  is a singleton, the action of  $\varphi$  is implied by the unit hypothesis.

We call this operad the C-coloration operad. When this operad is considered alone, one can see an element of  $(f,c) \in \mathbb{K}\mathcal{F}^C\mathbb{K} \ltimes C[V]$  as a corolla on V with its root colored by c and its leaves  $v \in V$  colored by f(v). The partial composition consists then in grafting two corollas if the root and the leaf on which it must be grafted share the same colors. For instance we have, by representing the elements of C with colors:

A way to define *colored operads* (see [46] for more details on the theory of colored operads) is then to define them as any Hadamard product of a C-coloration operad with another operad.

Let us now define our last construction.

**Definition 4.20.** Let A be a set and S be a species. The set species of functions from A to S is defined by  $\mathcal{F}_A^S[V] = \{f : A \to S[V]\}.$ 

The following proposition then tells us that if  $\mathcal{O}$  has an operad structure, it naturally reflects on  $\mathcal{F}_A^{\mathcal{O}}$ .

**Proposition 4.21.** If  $\mathcal{O}$  is an operad with unit e,  $\mathbb{K}\mathcal{F}_A^{\mathcal{O}}$  has an operad structure with the elements  $e_v: A \to \{e(v)\} \in \mathcal{F}_A^{\mathcal{O}}[\{v\}]$  as units and partial composition defined by  $f_1 \circ_* f_2(a) = f_1(a) \circ_* f_2(a)$ .

*Proof.* We must verify that the diagrams (4.1.1) are indeed commutative.

• Let be  $f_1 \in (\mathcal{F}_A^{\mathcal{O}})''[V_1], f_2 \in \mathcal{F}_A^{\mathcal{O}}[V_2]$  and  $f_3 \in \mathcal{F}_A^{\mathcal{O}}[V_3]$ . Then for all  $a \in A$ , we have

$$((f_1 \circ_{*_1} f_2) \circ_{*_2} f_3)(a) = (f_1 \circ_{*_1} f_2(a)) \circ_{*_2} f_3(a)$$

$$= (f_1(a) \circ_{*_1} f_2(a)) \circ_{*} f_3(a)$$

$$= f_1(a) \circ_{*_2} f_3(a) \circ_{*} f_2(a)$$

$$= (f_1 \circ_{*_2} f_3(a)) \circ_{*_1} f_2(a)$$

$$= ((f_1 \circ_{*_2} f_3) \circ_{*_1} f_2)(a),$$

$$(125)$$

where the third equality follows from the fact that  $\mathcal{O}$  is an operad. Hence, we have  $(f_1 \circ_{*_1} f_2) \circ_{*_2} f_3 = (f_1 \circ_{*_2} f_3) \circ_{*_1} f_2$ .

• Let be  $f_1 \in (\mathcal{F}_A^{\mathcal{O}})'[V_1], f_2 \in (\mathcal{F}_A^{\mathcal{O}})'[V_2]$  and  $f_3 \in \mathcal{F}_A^{\mathcal{O}}[V_3]$ . Then for all  $a \in A$ :

$$((f_1 \circ_{*_1} f_2) \circ_{*_2} f_3)(a) = (f_1 \circ_{*_1} f_2(a)) \circ_{*_2} f_3(a)$$

$$= f_1(a) \circ_{*_1} f_2(a) \circ_{*} f_3(a)$$

$$= f_1(a) \circ_{*_2} f_3(a) \circ_{*} f_2(a)$$

$$= (f_1 \circ_{*_2} f_3(a)) \circ_{*_1} f_2(a)$$

$$= ((f_1 \circ_{*_2} f_3) \circ_{*_1} f_2)(a),$$
(126)

where the third equality comes from the fact that  $\mathcal{O}$  is an operad. Hence, we have  $(f_1 \circ_{*_1} f_2) \circ_{*_2} f_3 = (f_1 \circ_{*_2} f_3) \circ_{*_1} f_2$ .

• Let be  $f \in (\mathcal{F}_A^{\mathcal{O}})'[V]$  and  $v \notin V$ . Then for all  $a \in A$ , we have the equalities  $f \circ_* e_v(a) = f(a) \circ_* e(v) = \mathcal{O}[\sigma](f(a))$  and so  $f \circ_* e_v = \mathcal{O}[\sigma](f)$ , where  $\sigma$  is the bijection which sends \* to v and is the identity over V. If now  $f \in \mathcal{F}_A^{\mathcal{O}}$ , we have for all  $a \in A$ :  $e_* \circ_* f(a) = e(*) \circ_* f(a) = f(a)$  and so  $e_* \circ_* f(a) = f(a)$ .

Note that if A is a singleton then  $\mathcal{F}_A^{\mathcal{O}} \cong \mathcal{O}$ . Let A, B, C, D four sets such that A and B are disjoint and  $f: A \to C$  and  $g: B \to D$  two maps. We denote by  $f \uplus g$  the map from  $A \sqcup B$  to  $C \cup D$  defined by  $f \uplus g(a) = f(a)$  for  $a \in A$  and  $f \uplus g(b) = g(b)$  for  $b \in B$ .

**Proposition 4.22.** Let A and B be two disjoint sets and  $\mathcal{O}_1$  and  $\mathcal{O}_2$  be two operads. Then the species  $\mathbb{K}\mathcal{F}_{A,B}^{\mathcal{O}_1,\mathcal{O}_2}$  defined by  $\mathcal{F}_{A,B}^{\mathcal{O}_1,\mathcal{O}_2}[V] = \{f \uplus g \mid f \in \mathcal{F}_A^{\mathcal{O}_1}, g \in \mathcal{F}_B^{\mathcal{O}_2}\}$  is an operad with same partial composition than in Proposition 4.21.

*Proof.* We remark that since A and B are disjoint,  $f_1 \uplus f_2 \circ_* g_1 \uplus g_2 = (f_1 \circ_* g_1) \uplus (f_2 \circ_* g_2)$ . To conclude we apply what was already shown in the proof of Proposition 4.21.

## 4.3 Graph insertion operads

We now use the construction of the previous subsection to define operad structures on graphs. The goal of this subsection is to give a general construction of operads on graphs and related objects where the partial composition of two elements  $g_1 \circ_* g_2$  is given by:

- 1. take the disjoint union of  $g_1$  and  $g_2$ ,
- 2. remove the vertex \* from  $g_1$ ,
- 3. connect independently each loose ends of  $g_1$  to  $g_2$  in a certain way.

What we mean by independently is that the way of connecting one end does not depend on how we connect the other ends. Note that the "certain way" in which an end can be connected may include duplication of edges and augmentation of the number of vertices of edges. This is done in the following theorem.

Recall from Remark 14 that there is a bijection between A-MHG and  $A\text{-}Pol_+$ . We now make use of this bijection and consider the elements of A-MHG as both multi-hypergraphs and polynomials. Let  $p \in \mathbb{K}Pol_+[V]$  be a sum of polynomials whose variables are not indexed. Then for A a set and  $a \in A$ , we denote by  $p_a \in A\text{-}Pol_+$  the sum of polynomials obtained by indexing all the variables in p by a. Let now p be any polynomial and  $x_1, \ldots, x_n$  a subset of its variables. Then for  $q_1, \ldots, q_n$  n polynomials, we denote by  $p|_{\{x_i \leftarrow q_i\}}$  the polynomial resulting from the composition  $(\ldots((p_1 \circ_{x_1} q_1) \circ_{x_2} q_2) \ldots) \circ_{x_n} q_n$ . We generalize this notation to sum of polynomials by considering that the multiplication and addition of polynomials are bilinear maps (recall from Example 2.4 that we distinguish the addition of polynomials  $\oplus$ , and the addition of vectors +). Note that the order in which we do the compositions does not matter because of the first commutative diagram in the definition of an operad: for  $\mathcal{O}$  an operad,  $V_1, V_2, V_3$  three pairwise disjoint sets and  $x \in \mathcal{O}''[V_1]$ ,  $y \in \mathcal{O}[V_2]$  and  $z \in \mathcal{O}[V_3]$  we have  $(x \circ_{*_1} y) \circ_{*_2} z = (x \circ_{*_2} z) \circ_{*_1} y$ .

**Example 4.23.** For A the singleton  $\{a\}$  and p the polynomial  $xy \oplus x^2 + zy \in Pol_+[\{x, y, z\}]$  we have  $p_a = x_a y_a \oplus x_a^2 + z_a y_a$ . Let now be  $p = x \oplus yz$ ,  $q_1 = u + v$  and  $q_2 = x_1 \oplus x_2$ . Then

$$p|_{x \leftarrow q_1, y \leftarrow q_2} = q_1 \oplus q_2 z = (u+v) \oplus (x_1 \oplus x_2) z$$
  
=  $u \oplus x_1 z \oplus x_2 z + v \oplus x_1 z \oplus x_2 z.$  (127)

**Theorem 4.24.** Let A be a set and  $\varphi$  be the morphism from  $\mathbb{K}A\text{-}MHG \cdot (A\text{-}MHG \times \mathcal{F}_A^{\mathbb{K}MHG})$  to  $\mathbb{K}A\text{-}MHG$  given by

$$h_1 \circ_*^f h_2 = h_1|_{\{*_a \leftarrow f(a)_a\}} \oplus h_2.$$
 (128)

Then  $\varphi$  satisfies the hypotheses of Proposition 4.18 and we can consider the semidirect product of  $\mathbb{K}A\text{-}MHG$  and  $\mathcal{F}_A^{\mathbb{K}MHG}$  over  $\varphi$ .

*Proof.* We need to check that  $\varphi$  satisfies the three hypotheses of Proposition 4.18. The first two are simply computations over polynomials.

**Commutativity.** Let  $h_1$  be an element of A-MHG'' and  $h_2 \otimes f$  and  $h_3 \otimes g$  two elements of A- $MHG \times \mathcal{F}_A^{\mathbb{K}MHG}$ . Then

$$(h_{1} \circ_{*_{1}}^{f} h_{2}) \circ_{*_{2}}^{g} h_{3} = (h_{1}|_{\{*_{1a} \leftarrow f(a)_{a}\}} \oplus h_{2})|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{3}$$

$$= h_{1}|_{\{*_{1a} \leftarrow f(a)_{a}\}}|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{2} \oplus h_{3}$$

$$= h_{1}|_{\{*_{2a} \leftarrow g(a)_{a}\}}|_{\{*_{1a} \leftarrow f(a)_{a}\}} \oplus h_{3} \oplus h_{2}$$

$$= (h_{1}|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{3})|_{\{*_{1a} \leftarrow f(a)_{a}\}} \oplus h_{2}$$

$$= (h_{1} \circ_{*_{2}}^{g} h_{3}) \circ_{*_{1}}^{f} h_{2}.$$

$$(129)$$

**Associativity.** Let  $h_1$  an element of A-MHG',  $y \otimes f$  an element of  $(A\text{-}MHG \times \mathcal{F}_A^{\mathbb{K}MHG})'$  and  $z \otimes h$  an element of  $A\text{-}MHG \times \mathcal{F}_A^{\mathbb{K}MHG}$ . Then

$$(h_{1} \circ_{*_{1}}^{f} h_{2}) \circ_{*_{2}}^{g} h_{3} = (h_{1}|_{\{*_{1a} \leftarrow f(a)_{a}\}} \oplus h_{2})|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{3}$$

$$= h_{1}|_{\{*_{1a} \leftarrow f(a)_{a}\}}|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{2}|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{3}$$

$$= h_{1}|_{\{*_{1a} \leftarrow f(a)_{a}|_{\{*_{2a} \leftarrow g(a)_{a}\}}\}} \oplus h_{2}|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{3}$$

$$= h_{1}|_{\{*_{1a} \leftarrow f \circ_{*_{2}} g(a)_{a}\}} \oplus h_{2}|_{\{*_{2a} \leftarrow g(a)_{a}\}} \oplus h_{3}$$

$$= h_{1} \circ_{*_{1}}^{f \circ_{*_{1}} g} (h_{2} \circ_{*_{2}}^{g} h_{3}).$$

$$(130)$$

**Unity.** Let  $e: \mathbb{K}X \to \mathbb{K}A\text{-}MHG$  be defined by  $e(v) = \emptyset_{\{v\}}$  and let  $e_{\mathcal{F}}$  the unit of  $\mathcal{F}_A^{\mathbb{K}MHG}$ . Let be  $h \in A\text{-}MHG'[V]$  and  $v \notin v$ . Then

$$h \circ_{*}^{e_{\mathcal{F}}(v)} e(v) = h|_{\{*_{a} \leftarrow e_{\mathcal{F}}(v)(a)_{a}\}} \oplus \emptyset_{\{v\}}$$
  
=  $h|_{\{*_{a} \leftarrow v_{a}\}} = A\text{-}MHG[\sigma](h),$  (131)

where  $\sigma$  is the bijection which sends \* to v and is the identity over V. If now  $h \in A\text{-}MHG$ , then

$$e(*) \circ_*^f h = \emptyset_{\{*\}}|_{\{*_a \leftarrow f(a)_a\}} \oplus h = h.$$
 (132)

In all the following we only consider this semi-direct, albeit not exactly on A-MHG and  $\mathcal{F}_A^{\mathbb{K}MG}$ , and we will hence omit the  $\varphi$  index. We call graph insertion operad any operad which can be written with this semi-direct product.

Remark 15. This notion of graph insertion operad is different than the one mentioned in [34], in the context of Feynman graph insertions in quantum field theory.

As mentioned above, this construction is supposed to encode partial compositions of the form: take the disjoint union, forget the vertex on which we compose, and independently reconnect loose edges. Let  $h_1 \otimes f_1$  and  $h_2 \otimes f_2$  be two elements of  $A\text{-}MHG \ltimes \mathcal{F}_A^{\mathbb{K}MG}$ . The ends of  $h_1$  are labelled by elements of A. When considering  $h_1 \circ_*^{f_2} h_2$ , the map  $f_2$  is there to tell us how we should connect the loose ends obtained by forgetting \*: each end labelled with a will be connected to the elements of  $f_2(a)$ .

Let us give two simple examples of operads which can be defined using this semi-direct product. Recall from Example 2.3.4 and Example 2.4.2 that we have a natural embedding of Id in  $Pol_+$ , two natural embeddings of  $E_+$  in  $Pol_+$  one natural embedding of  $\mathbb{K}E_+$  in  $\mathbb{K}Pol_+$ .

**Example 4.25.**  $\mathbb{K}G^{\bullet}$  has a natural operad structure given by  $G^{\bullet} \cong G \times Id \cong \{0\}$  - $G \ltimes \mathcal{F}^{\mathbb{K}Id}_{\{0\}}$ . For  $(g_1, v_1)$  and  $(g_2, v_2)$  two pointed graphs, the partial composition  $(g_1, v_1) \circ_* (g_2, v_2)$  is then equal to  $(g_3, v_1|_{*\leftarrow v_2})$  where  $g_3$  is the graph obtained by connecting all the ends on \* to  $v_2$ . More formally,

$$(g_1, v_1) \circ_* (g_2, v_2) = (g_1|_{*\leftarrow v_2} \oplus g_2, v_1|_{*\leftarrow v_2})$$
  
=  $(G[\sigma](g_1) \oplus g_2, v_1|_{*\leftarrow v_2}),$  (133)

where  $\sigma$  is the bijection which sends \* on  $v_2$  and which is the identity on the rest of its domain. For instance, we have:

Remark that the operad **NAP** [35] is a sub-operad of the operad above and hence is a graph insertion operad.

**Example 4.26.**  $\mathbb{K}G$  has a natural operad structure given by  $G \cong G \times E_+ \cong \{0\}$  - $G \ltimes \mathcal{F}_{\{0\}}^{\mathbb{K}E_+}$ , where we consider here the embedding  $\{V\} \mapsto \bigoplus V$ . For  $g_1$  and  $g_2$  two graphs, the partial composition  $g_1 \circ g_2$  is then the graph obtained by adding an edge between each neighbour of \* and each vertex of  $g_2$ . More formally, for  $g_1 \in G'[V_1]$  and  $g_2 \in G[V_2]$ :

$$g_{1} \circ_{*} g_{2} = g_{1}|_{* \leftarrow \bigoplus V_{2}} \oplus g_{2}$$

$$= g_{1}|_{V_{1}} \oplus \bigoplus n(*) \bigoplus V_{2} \oplus g_{2}$$

$$= g_{1}|_{V_{1}} \oplus \bigoplus n(*)V_{2} \oplus g_{2},$$

$$(135)$$

where  $g_1|_{V_1} = \{e \in g \mid e \subset V_1\}$ , n(\*) is the set of neighbours of \* and for A and B two sets, we denote by  $AB = A \cdot B$  the set of product of elements in A with elements in B:  $AB = \{ab \mid a \in A, b \in B\}$ . Let us explain how one should interpret this formula. The term  $g_1|_{V_1}$  means that we leave aside the vertex \* in  $g_1$ , the term  $\bigoplus n(*)V_2$  means that we add an edge between any element in n(\*) and any element in  $V_2$ , and finally the term  $g_2$  means that we keep all the edges of  $g_2$ . For instance, we have:

We now give two other graph insertion operads which are similar to our two examples but much more interesting. Let  $V_1$  and  $V_2$  be two disjoint sets. For any multigraphs  $g_1 \in MG'[V_1]$  and  $g_2 \in MG[V_2]$ , define a partial composition of  $g_1$  and  $g_2$  as the sum of all the multigraphs of  $MG[V_1 \sqcup V_2]$  obtained by the following:

- 1. Take the disjoint union of  $g_1$  and  $g_2$ ;
- 2. Remove the vertex \*. We then have some edges with one (or two if \* has loops) loose end(s);
- 3. Connect each loose end to any vertex in  $V_2$ .

For instance, we have:

$$a \xrightarrow{*} \circ_{*} b \xrightarrow{c} = a \xrightarrow{b} \xrightarrow{c} + 2 \xrightarrow{b} \xrightarrow{c} + 2 \xrightarrow{b} \xrightarrow{c} + 4 \xrightarrow{b} \xrightarrow{c} + 2 \xrightarrow{b} + 2 \xrightarrow{c} +$$

**Theorem 4.27.** The species  $\mathbb{K}MG$ , endowed with the preceding partial composition, is an operad.

*Proof.* This is the operad structure on  $\mathbb{K}MG$  given by  $MG \cong MG \times E_+ \cong \{0\}$  - $MG \ltimes \mathcal{F}^{\mathbb{K}E_+}_{\{0\}}$  when considering the embedding of  $\mathbb{K}E_+$  in  $\mathbb{K}Pol_+$ ,  $\{V\} \mapsto \sum V$ .

One notes that the species  $\mathbb{K}SG$  and  $\mathbb{K}MG_c$  are sub-operads of  $\mathbb{K}MG$ , that  $\mathbb{K}SG_c$  a sub-operad of  $\mathbb{K}SG$ , and that  $\mathbb{K}T$  is a sub-operad of  $\mathbb{K}SG_c$ . In particular, this structure on  $\mathbb{K}SG$  is known as the Kontsevich-Willwacher operad [38]. This partial composition can be formally written as follows. For any  $g_1 \in MG'[V_1]$  and  $g_2 \in MG[V_2]$ :

$$g_{1} \circ_{*} g_{2} = g_{1}|_{* \leftarrow \sum V_{2}} \oplus g_{2}$$

$$= g_{1}|_{V_{1}} \oplus \bigoplus n(*)(\sum V_{2}) \oplus ((\sum V_{2})^{2})^{\oplus g_{1}(**)} \oplus g_{2}$$

$$= \sum_{f:n(*) \to V_{2}} \sum_{l:[g_{1}(**)] \to V_{2}V_{2}} g_{1}|_{V_{1}} \oplus \bigoplus_{v \in n(*)} vf(v) \oplus \bigoplus_{i=1}^{g_{1}(**)} l(i) \oplus g_{2},$$
(138)

where n(\*) is the multiset of neighbours of \* in  $g_1$  and  $g_1(**)$  is the number of loops on \* in  $g_1$ . The term  $\bigoplus n(*)(\sum V_2)$  must be understood as "for all vertices in n(\*), sum over the ways of connecting it to  $g_2$ " and the term  $((\sum V_2)^2)^{\oplus g_1(**)}$  as "for each loop over \*, add an edge between any two elements of  $V_2$ ". This partial composition reformulates in a simpler way on  $\mathbb{K}SG$ . For any  $g_1 \in SG'[V_1]$  and  $g_2 \in SG[V_2]$ :

$$g_{1} \circ_{*} g_{2} = g_{1}|_{* \leftarrow \sum V_{2}} \oplus g_{2}$$

$$= g_{1}|_{V_{1}} \oplus \bigoplus n(*)(\sum V_{2}) \oplus g_{2}$$

$$= \sum_{f:n(*) \to V_{2}} g_{1}|_{V_{1}} \oplus \bigoplus_{v \in n(*)} vf(v) \oplus g_{2},$$

$$(139)$$

where n(\*) is now the set of neighbour of \* in  $g_1$ . For instance, we have:

In particular, we observe that all the graphs appearing in  $g_1 \circ_* g_2$  have 1 as coefficient.

Let us turn to the oriented case. Let  $V_1$  and  $V_2$  be two disjoint sets. For any rooted (i.e. pointed) oriented multigraphs  $(g_1, v_1) \in (MG_{or}^{\bullet})'[V_1]$  and  $(g_2, v_2) \in MG_{or}^{\bullet}[V_2]$ , define a partial composition of  $(g_1, v_1)$  and  $(g_2, v_2)$  as the sum of all the rooted multigraphs of  $MG_{or}^{\bullet}[V_1 \sqcup V_2]$  obtained by the following:

- 1. Take the disjoint union of  $g_1$  and  $g_2$ ;
- 2. Remove the vertex \*. We then have some edges with a loose end;
- 3. Connect each loose source end to  $v_2$ ;
- 4. Connect each loose target end to any vertex in  $V_2$ ;
- 5. The new root is  $v_1$  if  $v_1 \neq *$  and is  $v_2$  otherwise.

For instance, we have:

**Theorem 4.28.** The species  $\mathbb{K}MG_{orc}^{\bullet}$ , endowed with the preceding partial composition, is an operad.

*Proof.* Recall from Example 4.17 that we have a bijection  $MG_{or} \cong \{s,t\}$ -MG. The isomorphism  $MG_{or}^{\bullet} \cong \{s,t\}$ - $MG \times Id \times E_{+} \cong \{s,t\}$ - $MG \ltimes \mathcal{F}^{Id,E_{+}}_{\{s\},\{t\}}$ , give the desired operad structure on  $\mathbb{K}MG_{or}^{\bullet}$  when considering the embedding of  $\mu_{V} \mapsto \sum V$  of  $\mathbb{K}E_{+}$  in  $\mathbb{K}Pol_{+}$ .

It is straightforward to note that the subspecies of connected components  $\mathbb{K}MG_{orc}^{\bullet}$  and the species  $\mathbb{K}SG_{orc}^{\bullet}$  are sub-operads of  $\mathbb{K}MG$  and that  $\mathbb{K}SG_{orc}^{\bullet}$  is a sub-operad of  $\mathbb{K}SG_{or}^{\bullet}$ .

In a rooted tree, each edge has a parent end and a child end. Given a rooted tree t with root r, denote by  $t_r$  the oriented tree where the targets are the parent ends and the sources are the child ends. Then the monomorphism  $T^{\bullet} \hookrightarrow SG^{\bullet}_{orc}$  which sends each ordered pair (t,r), where t is a tree and r is its root, on  $(t_r,r)$  induces an operad structure on the species of rooted trees which is exactly the operad **PLie**. Hence **PLie** is a graph insertion operad.

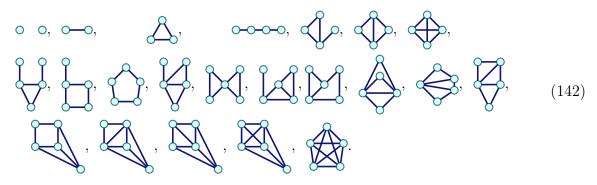
# 4.4 Applications

We now analyse in more detail the operad structure on  $\mathbb{K}MG$  given by Theorem 4.27. We first obtain results on some of its natural sub-operad ( $\mathbb{K}MG_c$ ,  $\mathbb{K}SG$ ,  $\mathbb{K}T$  etc) and then we study some of its finitely generated sub-operads.

### 4.4.1 The $\mathbb{K}MG$ operad

We study here in more detail the operad structure on  $\mathbb{K}SG$  implied by the one on  $\mathbb{K}MG$  given in Theorem 4.27. We will see that while  $\mathbb{K}SG$  itself has an involved operadic structure, it has many interesting sub-operads.

We first search for a smallest family of generators of  $\mathbb{K}SG$ , a minimal set E of elements of  $\mathbb{K}SG$  such that there is no strict sub-operad of  $\mathbb{K}SG$  containing E. The search for such a family is computationally hard. Using computer algebra, we obtain a family which generates simple graphs of arity less than 5:



Due to the symmetric group action on  $\mathbb{K}SG$ , only the knowledge of the shapes of the graphs is significant. While (142) does not provide to us any particular insight on a possible characterisation of the generators, it does suggest that any graph with "enough" edges must be a generator. This is confirmed by the following lemma. We say that a simple graph  $g \in SG$  is generated by a set E of graphs if g is in the sub-operad generated by E.

**Lemma 4.29.** Let  $\{V_i\}_{i\in I}$  be a family of non empty finite sets,  $\{g_i\}_{i\in I}$  be a family of graphs such that  $g_i \in SG[V_i]$ , and let g be a graph in SG[V] with at least  $\binom{n-1}{2} + 1$  edges, where n = |V|. Then g is generated by  $\{g_i\}_{i\in I}$  if and only if  $g = g_i$  for some  $i \in I$ .

Proof. Suppose that  $g \notin \{g_i\}_{i\in I}$ . It is sufficient to show that g cannot appear in the support of any vector of the form  $g_1 \circ_* g_2$  for any  $g_1$  and  $g_2$  different of g. Hence let  $V_1$  and  $V_2$  be two disjoint finite sets such that  $V_1 \sqcup V_2 = V$ ,  $g_1 \in SG'[V_1]$  and  $g_2 \in SG[V_2]$ , and denote by  $e_1$  the number of edges of  $g_1$  and by  $e_2$  the number of edges of  $g_2$ . Then the graphs in the support of  $g_1 \circ_* g_2$  have  $e_1 + e_2$  edges. This is maximal when  $g_1$  and  $g_2$  are both complete graphs and is then equal to  $\binom{x}{2} + \binom{n+1-x}{2} = x^2 - (n+1)x + \binom{n+1}{2}$  where  $1 \leq x = |V_1| \leq n$ .

If x=1 then necessarily  $g_1=\emptyset_*$  and  $g\in \operatorname{Supp}(g_1\circ_*g_2)=\operatorname{Supp}(g_2)$  if and only if  $g=g_2$ . This is impossible, hence  $x\neq 1$ . Similarly we have  $x\neq n$ . The expression  $x^2-(n+1)x+\binom{n+1}{2}$  is then maximal for x=2 or x=n-1 and is equal in both cases to  $\binom{n-1}{2}<\binom{n-1}{2}+1$ . This implies that g can not be in the support of  $g_1\circ_*g_2$ . This concludes the proof.

**Proposition 4.30.** The operad KSG is not free and has an infinite number of generators.

*Proof.* The fact that  $\mathbb{K}SG$  has an infinite number of generators is a direct consequence of Lemma 4.29. Moreover, the relation

shows that  $\mathbb{K}SG$  is not free.

As a consequence of Proposition 4.30, it seems particularly involved to further investigate the structure of  $\mathbb{K}SG$ . Let us then restrict further to its sub-operad  $\mathbb{K}T$  of trees. A family of generators of  $\mathbb{K}T$  with arity less than 6 is:

$$\circ$$
— $\circ$ ,  $\circ$ — $\circ$  $\circ$ ,  $\circ$ — $\circ$  $\circ$ ,  $\circ$ — $\circ$  $\circ$ . (144)

This operad KT has a non trivial link with the pre-Lie operad **PLie** [17]. This link is given by the following result.

Recall from Example 4.1.1 that **PLie** can be seen as an operad structure on  $\mathbb{K}T^{\bullet}$ .

**Proposition 4.31.** The monomorphism of species  $\psi : \mathbb{K}T \to \mathbb{K}T^{\bullet}$  defined by, for any tree  $t \in T[V]$ ,

$$\psi(t) = \sum_{r \in V} (t, r),\tag{145}$$

is a monomorphism of operads from  $\mathbb{K}T$  to **PLie**.

Before giving the proof of this proposition, we illustrate it on an example:

$$\psi\left(\begin{array}{c}b\\\end{array}\right)\circ_*\psi\left(\begin{array}{c}c\\\end{array}\right)=\left(\begin{array}{c}b\\\end{array}\right)+\left(\begin{array}{c}b\\\end{array}\right)+\left(\begin{array}{c}c\end{array}\right)+\left(\begin{array}{c}c\\\end{array}\right)+\left(\begin{array}{c}c\\\end{array}\right)+\left(\begin{array}{c}c\end{array}\right)+\left(\begin{array}{c}c\\\end{array}\right)+\left(\begin{array}{c}c\end{array}\right)+\left(\begin{array}{c}c\\\end{array}\right)+\left(\begin{array}{c}c\end{array}\right)+\left(\begin{array}{c}c\end{array}\right)+\left(\begin{array}{c}c\\\end{array}\right)+\left(\begin{array}{c}c\end{array}\right)$$

We can note that the case when \* is the root plays a particular role.

*Proof.* Let  $t \in T[V]$  be a tree and  $r, v \in V$ . Recall that  $t_r$  is the oriented tree where the targets are the parent ends and the sources are the child ends. Denote by  $n_t(v)$  the set of neighbours of v in t and denote by  $c_{t,r}(v)$  the set of children of v in  $t_r$ . If  $r \neq v$ , further denote by  $p_{t,r}(v)$  the parent of v in  $t_r$ .

Let  $V_1$  and  $V_2$  be two disjoint sets and  $t_1 \in T'[V_1]$  and  $t_2 \in T[V_2]$ . We now make full use of the correspondence between graphs and polynomials:

$$\psi_{V_{1}}(t_{1}) \circ_{*} \psi_{V_{2}}(t_{2}) = \sum_{r_{1} \in V_{1} + \{*\}} (t_{1}, r_{1}) \circ_{*} \sum_{r_{2} \in V_{2}} (t_{2}, r_{2})$$

$$= \sum_{r_{1} \in V_{1} + \{*\}} \sum_{r_{2} \in V_{2}} (t_{1}, r_{1}) \circ_{*} (t_{2}, r_{2})$$

$$= \sum_{r_{1} \in V_{1}} \sum_{r_{2} \in V_{2}} (t_{1}|_{V_{1}} \oplus p_{t_{1}, r_{1}}(*)r_{2} \oplus t_{2} \oplus \bigoplus c_{t_{1}, r_{1}}(*) \left(\sum V_{2}\right), r_{1}\right)$$

$$+ \sum_{r_{2} \in V_{2}} (t_{1}|_{V_{1}} \oplus t_{2} \oplus \bigoplus c_{t_{1}, *}(*) \left(\sum V_{2}\right), r_{2}\right)$$

$$= \sum_{r_{1} \in V_{1}} (t_{1}|_{V_{1}} \oplus p_{t_{1}, r_{1}}(*) \left(\sum V_{2}\right) \oplus t_{2} \oplus \bigoplus c_{t_{1}, r_{1}}(*) \left(\sum V_{2}\right), r_{1}\right)$$

$$+ \sum_{r_{2} \in V_{2}} (t_{1}|_{V_{1}} \oplus t_{2} \oplus \bigoplus c_{t_{1}, *}(*) \left(\sum V_{2}\right), r_{2}\right)$$

$$= \sum_{r \in V_{1} + V_{2}} (t_{1}|_{V_{1}} \oplus \bigoplus n_{t_{1}}(*) \left(\sum V_{2}\right) \oplus t_{2}, r\right)$$

$$= \sum_{r \in V_{1} + V_{2}} (t_{1}|_{* \leftarrow \sum V_{2}} \oplus t_{2}, r)$$

$$= \psi_{V_{1} + V_{2}}(t_{1} \circ_{*} t_{2})$$
(147)

A natural question to ask is how to extend this morphism to  $\mathbb{K}SG_c$  and  $\mathbb{K}MG_c$ . Let us introduce some notations in order to answer this question. For  $g \in MG_c[V]$ ,  $r \in V$ , and  $t \in T[V]$  a spanning tree of g, let  $\overrightarrow{g}^{(t,r)} \in MG_{orc} \cong \{\mathfrak{s},\mathfrak{t}\}$ - $MG_c$  be the oriented multigraph obtained by labelling the edges of g in t in the same way as the edges of  $t_r$ , and by labelling as targets all the other ends. More formally, we have  $\overrightarrow{g}^{(t,r)} = t_r \oplus \iota_G(g \setminus t)$ , where  $\iota : \mathbb{K}MG \to \mathbb{K}MG_{or}$  sends a multigraph to the oriented multigraph obtained by labelling all the ends as targets.

Define  $\mathbb{K}\mathcal{O}_2 \subset \mathbb{K}\mathcal{O}_1 \subset \mathbb{K}\mathbf{ST}$  (ST standing for "spanning tree") three subspecies of  $\mathbb{K}MG_{orc}^{\bullet}$  by

$$\mathbf{ST}[V] = \left\{ (\overrightarrow{g}^{(t,r)}, r) : g \in MG_c[V], r \in V \text{ and } t \text{ a spanning tree of } g \right\}, \tag{148}$$

$$\mathcal{O}_1[V] = \left\{ \sum_{r \in V} (\overrightarrow{g}^{(t(r),r)}, r) : g \in MG_c[V] \text{ and for each } r, t(r) \text{ a spanning tree of } g \right\},$$
(149)

$$\mathcal{O}_2[V] = \{ (\overrightarrow{g}^{(t_1,r)}, r) - (\overrightarrow{g}^{(t_2,r)}, r) : g \in MG_c[V], r \in V,$$
  
and  $t_1$  and  $t_2$  two spanning trees of  $g \}$ . (150)

**Example 4.32.** Let  $V = \{a, b, c, d\}$ . We give example of elements in  $\mathbf{ST}[V]$ ,  $\mathcal{O}_1[V]$  and  $\mathcal{O}_2[V]$ . For the sake of an easier reading, instead of representing the orientation of the edges, we just colored the spanning trees in red. The blue edges should have both ends with an arrow shape and the red edges only the end nearest the root.

$$\begin{array}{ccc}
a & b \\
\hline
a & c
\end{array} \in \mathbf{ST}[V] \tag{151}$$

$$\begin{array}{cccc}
 & b & \\
 & c & \\
 & d & \\
\end{array}$$

$$\begin{array}{cccc}
 & \in \mathcal{O}_2[V] & \\
\end{array}$$

$$(153)$$

**Lemma 4.33.** The following properties hold:

- (i)  $\mathbb{K}\mathbf{ST}$  is a sub-operad of  $\mathbb{K}MG_{orc}^{\bullet}$  isomorphic to  $\mathbb{K}MG \times \mathbf{PLie}$ ,
- (ii)  $\mathbb{K}\mathcal{O}_1$  is a sub-operad of  $\mathbb{K}\mathbf{ST}$ ,
- (iii)  $\mathbb{K}\mathcal{O}_2$  is an ideal of  $\mathbb{K}\mathcal{O}_1$ .

Proof. Before proving these three items, we first give two equalities which will help us for the two last items. Let  $U: \mathbb{K}MG_{or} \to \mathbb{K}MG$  be the forgetful functor which sends an oriented graph on the graph obtained by forgetting the orientation. Let  $V_1$  and  $V_2$  be two disjoint sets,  $g_1 \in MG'_c[V_1]$  and  $g_2 \in MG_c[V_2]$  be two connected multigraphs, t a spanning tree of  $g_1$  and for each  $v \in V_2$ , t(v) a spanning tree of  $g_2$ . When \* is the root of the spanning tree t, all the ends pointing to \* are targets. Since the target ends in an oriented graph behave the same than the normal ends in a non-oriented graph, the forgetful functor

preserves the partial composition. For example we have:

$$U \times Id \left( \begin{array}{c} & & & \\$$

More formally, for  $r \in V_2$ , we have:

$$U \times Id\left((\overrightarrow{g_1}^{(t,*)}, *) \circ_* (\overrightarrow{g_2}^{(t(r),r)}, r)\right)$$

$$= \left(g_1|_{V_1} \oplus \bigoplus n(*) \left(\sum V_2\right) \oplus \left((\sum V_2)^2\right)^{\oplus g_1(**)} \oplus g_2, r\right)$$

$$= (g_1 \circ_* g_2, r). \tag{155}$$

Let now r be a vertex in  $V_1$ . Denote by p the parent of \* in  $t_r$ , by c(\*) the children of \* in  $t_r$ , by  $n_{g_1\setminus t}(*)$  the multiset of neighbours of \* in  $g_1\setminus t$  and by n(\*) the multiset of neighbours of \* in  $g_1$ , so that  $n(*) = n_{g_1\setminus t}(*) \cup c(*) \cup \{p\}$ . We then have

$$U \times Id\left((\overrightarrow{g_{1}}^{(t,r)}, r) \circ_{*} \sum_{v \in V_{2}} (\overrightarrow{g_{2}}^{(t(v),v)}, v)\right)$$

$$= \sum_{v \in V_{2}} U \times Id\left((\overrightarrow{g_{1}}^{(t,r)}, r) \circ_{*} (\overrightarrow{g_{2}}^{(t(v),v)}, v)\right)$$

$$= \sum_{v \in V_{2}} \left(g_{1}|_{V_{1}} \oplus pv \oplus \bigoplus c(*) \left(\sum V_{2}\right) \oplus \bigoplus n_{g_{1}\setminus t}(*) \left(\sum V_{2}\right) \oplus \left((\sum V_{2})^{2}\right)^{\oplus g_{1}(**)} \oplus g_{2}, r\right)$$

$$= \left(g_{1}|_{V_{1}} \oplus p \left(\sum V_{2}\right) \oplus \bigoplus c(*) \left(\sum V_{2}\right) \oplus \bigoplus n_{g_{1}\setminus t}(*) \left(\sum V_{2}\right) \oplus \left((\sum V_{2})^{2}\right)^{\oplus g_{1}(**)} \oplus g_{2}, r\right)$$

$$= \left(g_{1}|_{V_{1}} \oplus \bigoplus n(*) \left(\sum V_{2}\right) \oplus \left((\sum V_{2})^{2}\right)^{\oplus g_{1}(**)} \oplus g_{2}, r\right)$$

$$= \left(g_{1} \circ_{*} g_{2}, r\right). \tag{156}$$

*Proof of i.* The linear species morphism from  $\mathbb{K}MG \times \mathbf{PLie}$  to  $\mathbb{K}MG^{\bullet}_{orc}$  given by  $(g,(t,r)) \mapsto (\overrightarrow{g}^{(t,r)},r)$  is an operad morphism and hence its image  $\mathbf{ST}$  is a sub-operad of  $\mathbb{K}MG^{\bullet}_{orc}$ .

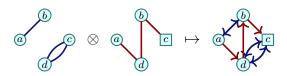


Figure 1: An example of the isomorphism of item i.

Proof of ii. Let  $V_1$  and  $V_2$  be two disjoint sets,  $g_1 \in MG'_c[V_1]$  and  $g_2 \in MG_c[V_2]$  be two connected multigraphs and for each  $v \in V_1 + \{*\}$ , t(v) a spanning tree of  $g_1$  and for each  $v \in V_2$ , t(v) a spanning tree of  $g_2$ . We have

$$\sum_{r_{1} \in V_{1} + \{*\}} \overrightarrow{g_{1}}^{(t(r_{1}), r_{1})} \circ_{*} \sum_{r_{2} \in V_{2}} \overrightarrow{g_{2}}^{(t(r_{2}), r_{2})} = \sum_{r_{1} \in V_{1} + \{*\}} \sum_{r_{2} \in V_{2}} \overrightarrow{g_{1}}^{(t(r_{1}), r_{1})} \circ_{*} \overrightarrow{g_{2}}^{(t(r_{2}), r_{2})}$$

$$= \sum_{r_{1} \in V_{1} + \{*\}} \sum_{r_{2} \in V_{2}} \left( \overrightarrow{g_{1}}^{(t(r_{1}), r_{1})} \big|_{*_{s} \leftarrow r_{2s}, *_{t} \leftarrow (\sum V_{2})_{t}} \oplus \overrightarrow{g_{2}}^{(t(r_{2}), r_{2})}, r_{1} \big|_{* \leftarrow r_{2}} \right). \tag{157}$$

Then from (155) and (156) we know that applying  $U \times Id$  to the preceding sum gives us:

$$\sum_{r \in V_1 + V_2} (g_1 \circ_* g_2, r). \tag{158}$$

To conclude note that  $\mathbb{K}\mathcal{O}_1[V]$  is the reciprocal image of  $\mathbb{K}\{\sum_{v\in V}(g,v)\,|\,g\in MG_c[V]\}$  by  $U\times Id:\mathbb{K}\mathbf{ST}\to\mathbb{K}MG^{\bullet}$ .

Proof of iii. It is easy to see that  $\mathbb{K}\mathcal{O}_2$  is a left ideal of  $\mathbb{K}\mathbf{S}\mathbf{T}$  and hence of  $\mathbb{K}\mathcal{O}_1$ . Let  $V_1$  and  $V_2$  be two disjoint finite sets,  $g_1 \in MG'_c[V_1]$  and  $g_2 \in MG_c[V_2]$ ,  $r \in V_1$ , t a spanning tree of  $g_1$  and for every  $v \in V_2$ , t(v) a spanning tree of  $g_2$ . Then from (155) and (156) we know that  $U \times Id(\overrightarrow{g_1}^{(t,r)} \circ_* \sum_{v \in V_2} \overrightarrow{g_2}^{(t(v),v))}$  is of the form  $(g_1 \circ_* g_2, r)$  if  $r \neq *$ , and of the form  $\sum_{v \in V_2} (g_1 \circ_* g_2, v)$  otherwise. In both cases it does not depend on t. This concludes this proof since  $\mathbb{K}\mathcal{O}_2[V]$  is the kernel of  $(U \times Id)_V : \mathbb{K}\mathbf{S}\mathbf{T}[V] \to \mathbb{K}G^{\bullet}_{\mathfrak{c}}[V]$ .

We can see **PLie** as a sub-operad of **ST** by the monomorphism  $(t, r) \mapsto (t_r, r)$ . The image of the operad morphism  $\psi$  of Proposition 4.31 is then  $\mathbb{K}\mathcal{O}_1 \cap \mathbf{PLie}$  and we have that  $\mathbb{K}\mathcal{O}_2 \cap \mathbf{PLie} = \{0\}$  and hence  $\mathbb{K}\mathcal{O}_1 \cap \mathbf{PLie} / \mathbb{K}\mathcal{O}_2 \cap \mathbf{PLie} = \mathbb{K}\mathcal{O}_1 \cap \mathbf{PLie}$ .

**Proposition 4.34.** The operad isomorphism  $\psi : \mathbb{K}T \to \mathbf{PLie} \cap \mathbb{K}\mathcal{O}_1$  extends into an operad isomorphism  $\psi : \mathbb{K}MG_c \to \mathbb{K}\mathcal{O}_1/\mathbb{K}\mathcal{O}_2$  satisfying, for any  $g \in MG_c[V]$ ,

$$\psi(g) = \sum_{r \in V} \overrightarrow{g}^{(t(r),r)}, \tag{159}$$

where for each  $r \in V$ , t(r) is a spanning tree of g. Furthermore, this isomorphism restricts itself to an isomorphism  $\mathbb{K}SG_c \to \mathbb{K}\mathcal{O}_1 \cap \mathbb{K}SG_{orc}^{\bullet}/\mathbb{K}\mathcal{O}_2 \cap \mathbb{K}SG_{orc}^{\bullet}$ .

*Proof.* This statement is a direct consequence of Lemma 4.33 and its proof.  $\Box$ 

The last results are summarized in the following commutative diagram of operad morphisms.

$$\mathbb{K}T \xrightarrow{\sim} \mathbf{PLie} \cap \mathbb{K}\mathcal{O}_{1}/\mathbb{K}\mathcal{O}_{2} = = \mathbf{PLie} \cap \mathbb{K}\mathcal{O}_{1} \hookrightarrow \mathbf{PLie}$$

$$\downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$$

$$\mathbb{K}SG_{c} \xrightarrow{\sim} \mathbb{K}\mathcal{O}_{1} \cap \mathbb{K}SG_{orc}^{\bullet}/\mathbb{K}\mathcal{O}_{2} \cap \mathbb{K}G_{orc}^{\bullet} \leftarrow = \mathbb{K}SG_{orc}^{\bullet} \cap \mathbb{K}\mathcal{O}_{1} \hookrightarrow \mathbb{K}SG_{orc}^{\bullet} \cap \mathbb{K}\mathbf{ST}$$

$$\downarrow \qquad \qquad \downarrow \qquad \qquad \downarrow$$

$$\mathbb{K}MG_{c} \xrightarrow{\sim} \mathbb{K}\mathcal{O}_{1}/\mathcal{O}_{2} \leftarrow = \mathbb{K}\mathcal{O}_{1} \hookrightarrow \mathbb{K}MG \times \mathbf{PLie}$$

$$(160)$$

### 4.4.2 Finitely generated sub-operads

Let us now focus on finitely generated sub-operads of  $\mathbb{K}MG$ . In particular we will study the operads generated by:

- 1.  $\{a \mid b\}$  which we denote by  $G_{\emptyset}$  and which is isomorphic to **Com**,
- 2. {a-b} which we denote by **Seg** and which is isomorphic to **ComMag**,
- 3.  $\{(a), (b), (a)-(b)\}$  which we denote by **SP**,

4. 
$$\left\{ \begin{array}{cc} & \\ & \\ \\ & \end{array} \right\}$$
 which we denote by **LP**.

First, note that the sub-operad  $G_{\emptyset}$  generated by  $\{a \in b\}$  is isomorphic to the commutative operad **Com**. Indeed, recall from Example 4.4 that **Com** is the quotient of the free operad over one symmetric element of size two,  $\mathbb{K}sym_2$  by the associativity relation. By definition  $G_{\emptyset}$  is also generated by one symmetric element of size 2, and furthermore we have:

$$(a) * \circ_* (b) (c) = (a) (b) (c) = (*) (c) \circ_* (a) (b),$$
 (161)

which is the associativity relation. Hence  $G_{\emptyset} \cong \mathbf{Com}$ . This could also be observed from the fact that we clearly have  $G_{\emptyset}[V] = \mathbb{K} \emptyset_V$  and hence the map  $\emptyset_V \mapsto \mu_V$  implies an isomorphism from  $G_{\emptyset}$  to  $\mathbf{Com}$ .

The other three cases are more involved.

**Proposition 4.35.** The sub-operad **Seg** of  $\mathbb{K}G$  generated by  $\{a-b\}$  is isomorphic to **ComMag**.

*Proof.* We know from Proposition 4.31 that **Seg** is isomorphic to the sub-operad of **PLie** generated by

Then [14] gives us that the map which sends the above element to  $s_{ab} \in sym_2[\{a,b\}]$  induces an isomorphism between the sub-operad and **ComMag**. This concludes the proof.

The isomorphisms  $\mathbf{Com} \cong \mathbb{K}G_{\emptyset}$  and  $\mathbf{ComMag} \cong \mathbf{Seg}$  allow us to see  $\mathbf{Com}$  and  $\mathbf{ComMag}$  as disjoint sub-operads of  $\mathbb{K}G$  and hence gives us a natural way to define the smallest operad containing these two as disjoint sub-operads. Denote by  $\mathcal{G}$  the set subspecies of G generated by  $\{a \mid b, a-b\}$  and  $\mathbf{SP}$  the sub-operad of  $\mathbb{K}G$  generated by these two elements. This operad has some interesting properties. Recall from Remark 12 that we use the notation  $\circ_*^{\xi}$  for the grafting of tree in a free operad and that we denote the equivalence class of x by [x].

**Proposition 4.36.** The operad SP is isomorphic to the operad  $Ope(\mathbb{K}\mathcal{G}, R)$  where R is the subspecies of  $\mathbb{K}Free_{\mathcal{G}}$  generated by

and

$$(a)$$
  $(a)$   $(a)$   $(b)$   $(b)$   $(c)$   $(c)$ 

Therefore, **SP** is binary and quadratic.

Proof. The element  $[a \ b]$  of  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$  is symmetric of size 2 and follows the associativity relation (163a). Hence the sub-operad of  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$  generated by  $[a \ b]$  is equal to  $\operatorname{\mathbf{Com}}$ . This implies that all the trees in  $\operatorname{\mathbf{Free}}_{\mathcal{G}}$  with V as leaves and whose labels are all empty graphs over two points are in the same equivalence class of  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$ . We will denote by  $\mu_V$  this equivalence class. In the same way, the element [a - b] of  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$  is symmetric of size 2 and do not follow any relation involving only itself, hence the sub-operad of  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$  generated by [a - b] is equal to  $\operatorname{\mathbf{ComMag}}$ . We denote by  $s_{ab} \in sym_2[\{a, b\}]$  the equivalence class of the segment.

There is a natural epimorphism  $\phi$  from  $\mathbb{K}\mathbf{Free}_{\mathcal{G}}$  to  $\mathbf{SP}$  which is the identity on ⓐ ⓑ and ⓐ ⓑ and which sends a partial composition  $g_1 \circ_*^{\xi} g_2$  on the partial composition  $g_1 \circ_* g_2$ . We already proved by (161) that the vector (163a) is in the kernel  $\phi$ . The case of (163b) is also straightforward:

$$(a)$$
  $\circ_*$   $(b)$   $(c)$   $(c)$ 

To conclude; we must now show that for any  $w \in \operatorname{Ope}(\mathbb{K}\mathcal{G}, \mathcal{R})[V]$ ,  $\phi(w) = 0$  implies w = 0. Because of (163b), we have that the vector  $[a \cdot \circ \circ_*^{\xi} b \cdot c]$  is equal to the vector  $[b \cdot \circ \circ_*^{\xi} a \cdot c] + [c \cdot \circ \circ_*^{\xi} a \cdot b]$  in  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$ . Hence, by iterating this process, we get that all elements of  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})$  can be written as a sum of equivalence classes of trees where no segment vertex has a points vertex as descendent. This means that  $\operatorname{Ope}(\mathcal{G}, \mathcal{R})[V]$  has the following generating family (cf Figure 166 for an example):

$$\left\{ \left[ \left( \dots \left( \left( T \circ_1^{\xi} t_1 \right) \circ_2^{\xi} t_2 \right) \dots \right) \circ_k^{\xi} t_k \right] \mid T \in A_p[[k]], t_i \in A_s[V_i] \right\}_{\{V_1, \dots, V_k\} \text{ partition of } V}, \quad (165)$$

where  $A_p[V]$  is the set of trees with set of leaves V and only points vertices and  $A_t[V]$ 

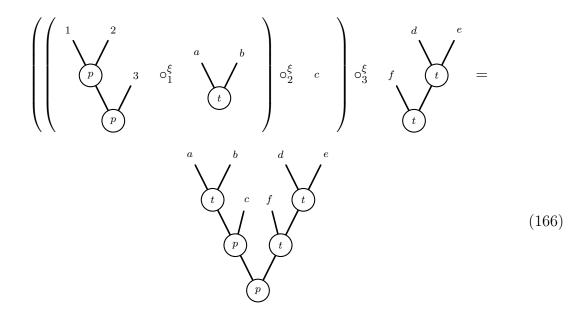


Figure 2: An element in the generating family of  $Ope(\mathcal{G}, \mathcal{R})[\{a, b, c, d, e, f\}]$ . The labels p represent the empty graph over two points and the labels s the segment graph.

those with only segment vertices. An element of this family rewrites then:

$$\left[ (\dots((T \circ_{1}^{\xi} t_{1}) \circ_{2}^{\xi} t_{2}) \dots) \circ_{k}^{\xi} t_{k} \right] = (\dots(([T] \circ_{1}^{\xi} [t_{1}]) \circ_{2}^{\xi} [t_{2}]) \dots) \circ_{k}^{\xi} [t_{k}] 
= (\dots((\mu_{[k]} \circ_{1}^{\xi} t_{1}) \circ_{2}^{\xi} t_{2}) \dots) \circ_{k}^{\xi} t_{k},$$
(167)

where in the second line the elements  $t_i$  are this time in  $\mathbf{Free}_{sym_2}[V_i]$ . Since  $\mathfrak{S}_k$  acts trivially on  $\mu_{[k]}$ , all the elements obtained by permuting the  $t_i$  in in (167) are equal. The generating family (165) can hence be reduced to

$$\left\{ \mu_{[k]} \circ^{\xi} (t_1, t_2 \dots t_k) \mid t_i \in \mathbf{Free}_{sym_2}[V_i] \right\}_{\{V_1, \dots, V_k\} \text{ partition of } V}, \tag{168}$$

where by  $\mu_{[k]} \circ^{\xi} (t_1, t_2 \dots t_k)$  we denote any of the equal trees  $(\dots (\mu_{[k]} \circ^{\xi}_1 t_{\sigma(1)}) \dots) \circ^{\xi}_k t_{\sigma(k)}$  for  $\sigma$  a permutation of [k].

Let now be w of the form  $\sum_{i=1}^{l} a_i w_i$  where for each  $1 \leq i \leq l$ ,  $a_i \in \mathbb{K}$  and there is a partition of  $P_i = \{V_{i,1}, \ldots, V_{i,k_i}\}$  of V such that  $w_i = (\ldots (\mu_{[k_i]} \circ^{\xi} (t_{i,1} \ldots t_{i,k_i}))$  with  $t_{i,j}$  in  $\mathbf{Free}_{sym_2}[V_{i,j}]$ .

For i an index in [l], the image of  $\mu_{[k_i]}$  by  $\phi$  is the empty graph over  $[k_i]$ , and so the image of  $w_i$  is equal to:

$$\bigoplus_{i=1}^{k_i} \phi(t_{i,j}) = \bigsqcup_{j=1}^{k_i} \phi(t_{i,j}).$$
 (169)

Hence, for  $i \neq j$  two indices, if  $P_i \neq P_j$  the support of  $\phi(w_i)$  and  $\phi(w_j)$  are disjoint. We can then restrict ourselves to the case where all the  $w_i$  are on the same partition of V i.e.  $P_i = \{V_1, \ldots, V_k\}$  for all indices i.

Denote by  $G[V_1, \ldots, V_k]$  the set  $\{g_1 \oplus \cdots \oplus g_k \mid g_i \in G[V_i]\}$ . Then there is an isomorphism from  $\mathbb{K}G[V_1, \ldots, V_k]$  to  $\mathbb{K}G[V_1] \otimes \cdots \otimes \mathbb{K}G[V_k]$  defined by  $g_1 \oplus \cdots \oplus g_k \mapsto g_1 \otimes \cdots \otimes g_k$ . This isomorphism sends  $\phi(w)$  on  $\sum_{i=1}^l a_i \bigotimes_{j=1}^{k_i} \phi(t_{i,j})$ . Since for all  $1 \leq i \leq k$  **Free**<sub> $sym_2$ </sub>[ $V_i$ ] is a free family in **ComMag**[ $V_i$ ]  $\subset G[V_i]$  (by definition of a basis), the family  $\{(v_1 \otimes \cdots \otimes v_k)_{\mathfrak{S}_k} \mid v_i \in \mathbf{Free}_{sym_2}[V_i]\}$  is also free and hence  $\phi(w) = 0$  implies  $a_i = 0$  for all  $1 \leq i \leq k$ . This shows that the epimorphism  $\phi$  is also a monomorphism and hence an isomorphism. This concludes the proof.

A further consequence of Proposition 4.36 is that the generating family (168) is a basis and hence the operad **SP** is isomorphic to **Com(ComMag)**.

From now on we denote by  $p_{ab} = @$  @ @ and by  $s_{ab} = @$  @ @ @ We now exhibit the Koszul dual of **SP**. We use the same convention as in Example 4.6 for the notation  $p_{\alpha\beta}^{\vee}$  and  $s_{\alpha\beta}^{\vee}$  for  $\alpha, \beta \in \mathscr{A}$ .

**Proposition 4.37.** The operad **SP** admits as Koszul dual the operad **SP**! which is isomorphic to the operad  $Ope((\mathbb{K}\mathcal{G})^{\vee}, R)$  where R is the subspecies of  $\mathbf{Free}_{\mathbb{K}\mathcal{G}^{\vee}}$  generated by

(a) 
$$(*)^{\vee} \circ_{*}^{\xi} (b) - (c)^{\vee} + (c) - (*)^{\vee} \circ_{*}^{\xi} (a) (b)^{\vee} + (b) - (*)^{\vee} \circ_{*}^{\xi} (a) (c)^{\vee},$$
 (170b)

(a) 
$$(*)^{\vee} \circ_{*}^{\xi} (b) (c)^{\vee} + (c) (*)^{\vee} \circ_{*}^{\xi} (a) (b)^{\vee} + (b) (*)^{\vee} \circ_{*}^{\xi} (c) (a)^{\vee}.$$
 (170c)

*Proof.* Let us respectively denote by  $r_1$  and  $r_2$  and  $r'_1$ ,  $r'_2$ , and  $r'_3$  the vectors (163a), (163b), (170a), (170b), and (170c). Denote by  $\mathcal{I}$  the operad ideal generated by  $r_1$  and  $r_2$ . As a vector space,  $\mathcal{I}[[\{a,b,c\}]]$  is then the linear span of the set

$$\{r_1, (ab) \cdot r_1, r_2, (abc) \cdot r_2, (acb) \cdot r_2\},$$
 (171)

where  $\cdot$  is the action of the symmetric group,  $e.g \ r_1 \cdot (ab) = \mathbf{Free}_{\mathcal{G}}[(ab)](r_1)$ . This space is a sub-space of dimension 5 of  $\mathbf{Free}_{\mathcal{G}}[\{a,b,c\}]$ , which is of dimension 12. Hence, since as a vector space we have

$$\mathbb{K}\mathbf{Free}_{\mathcal{G}^{\vee}}[\{a, b, c\}] \cong \mathbb{K}\mathbf{Free}_{\mathcal{G}^{*}}[\{a, b, c\}] \cong \mathbb{K}\mathbf{Free}_{\mathcal{G}}[\{a, b, c\}], \tag{172}$$

we conclude that  $\mathcal{I}^{\perp}[\{a,b,c\}]$  must be of dimension 7.

Denote by  $\mathcal{J}$  the ideal generated by  $r'_1$ ,  $r'_2$  and  $r'_3$ . As a vector space  $\mathcal{J}[\{a,b,c\}]$  is then the linear span of the set

$$\{r'_1, (ab) \cdot r'_1, (ac) \cdot r'_1, r'_2, (abc) \cdot r'_2, (acb) \cdot r'_2, r'_3\}.$$
 (173)

This vector space is of dimension 7. To conclude, we need to show that for any elements f of  $\mathcal{J}[\{a,b,c\}]$  and x of  $\mathcal{I}[\{a,b,c\}]$  we have  $\langle f | x \rangle = 0$ . Among the 21 cases to check, we have for example:

$$\langle r'_{1} | r_{1} \rangle = \langle s_{a*}^{\vee} \circ_{*}^{\xi} s_{bc}^{\vee} | p_{*,c} \circ_{*}^{\xi} p_{ab} - p_{a*} \circ_{*}^{\xi} p_{bc} \rangle$$

$$= \langle s_{a*}^{\vee} \circ_{*}^{\xi} s_{bc}^{\vee} | p_{*,c} \circ_{*}^{\xi} p_{ab} \rangle - \langle s_{a*}^{\vee} \circ_{*}^{\xi} s_{bc}^{\vee} | p_{a*} \circ_{*}^{\xi} p_{bc} \rangle$$

$$= s_{a*}^{\vee} (p_{*,c}) s_{bc}^{\vee} (p_{ab}) - s_{a*}^{\vee} (p_{a*}) s_{bc}^{\vee} (p_{bc}) = 0,$$
(174)

and

$$\langle (abc) \cdot r_{2}' \rangle | r_{2} \rangle =$$

$$\langle p_{b*}^{\vee} \circ_{*}^{\xi} s_{ca}^{\vee} + s_{a*}^{\vee} \circ_{*}^{\xi} p_{bc}^{\vee} + s_{c*}^{\vee} \circ_{*}^{\xi} p_{ab}^{\vee} | s_{a*} \circ_{*} p_{bc} - p_{c*} \circ_{*} s_{ab} - p_{b*} \circ_{*} s_{ca} \rangle$$

$$= p_{b*}^{\vee} (s_{a*}) s_{ca}^{\vee} (p_{bc}) - p_{b*}^{\vee} (p_{c*}) s_{ca}^{\vee} (s_{ab}) - p_{b*}^{\vee} (p_{b*}) s_{ca}^{\vee} (s_{ca})$$

$$+ s_{a*}^{\vee} (s_{a*}) p_{bc}^{\vee} (p_{bc}) - s_{a*}^{\vee} (p_{c*}) p_{bc}^{\vee} (s_{ab}) - s_{a*}^{\vee} (p_{b*}) p_{bc}^{\vee} (s_{ca})$$

$$+ s_{c*}^{\vee} (s_{a*}) p_{ab}^{\vee} (p_{bc}) - s_{c*}^{\vee} (p_{c*}) p_{ab}^{\vee} (s_{ab}) - s_{c*}^{\vee} (p_{b*}) p_{ab}^{\vee} (s_{ca})$$

$$= -1 + 1 = 0.$$

$$(175)$$

We leave the verification of the 19 remaining cases as an exercise to the interested reader.

In order to compute the Hilbert series of  $SP^!$  we need to use identity (114) and hence to prove that the operad SP is Koszul.

## Proposition 4.38. The operad SP is Koszul.

*Proof.* Let  $\mathcal{R}$  be the species defined as in Proposition 4.36 so that  $\mathbf{SP} \cong \mathrm{Ope}(\mathbb{K}\mathcal{G}, \mathcal{R})$ . Denote by  $\mathfrak{p}(a,b)$  and  $\mathfrak{s}(a,b)$  the elements of  $\mathcal{G}^{\mathscr{F}}[\{a,b\},ab]$ . Then the following vectors form a basis  $\mathcal{B}$  of  $\mathcal{R}^{\mathscr{F}}[\{a,b,c\},abc]$ :

$$\mathfrak{v}_1 = \mathfrak{p}(\mathfrak{p}(a,b),c) - \mathfrak{p}(a,\mathfrak{p}(b,c)) , \quad \mathfrak{v}_2 = \mathfrak{p}(\mathfrak{p}(a,c),b) - \mathfrak{p}(a,\mathfrak{p}(b,c))$$
 (176)

$$\mathfrak{v}'_1 = \mathfrak{s}(\mathfrak{p}(a,b),c) - \mathfrak{p}(\mathfrak{s}(a,c),b) - \mathfrak{p}(a,\mathfrak{s}(b,c)) \tag{177}$$

$$\mathfrak{v}'_2 = \mathfrak{s}(\mathfrak{p}(a,c),b) - \mathfrak{p}(\mathfrak{s}(a,b),c) - \mathfrak{p}(a,\mathfrak{s}(b,c))$$
(178)

$$\mathfrak{v}'_3 = \mathfrak{s}(a, \mathfrak{p}(b, c)) - \mathfrak{p}(\mathfrak{s}(a, b), c) - \mathfrak{p}(\mathfrak{s}(a, c), b). \tag{179}$$

We need to show that it is a Gröbner bases of  $(\mathcal{R}^{\mathscr{F}})$ . Let now consider the path-lexicographic ordering presented in subsubsection 4.1.4 with s > p. Then the leading terms of  $\mathfrak{v}_1$ ,  $\mathfrak{v}_2$ ,  $\mathfrak{v}'_1$ ,  $\mathfrak{v}'_2$  and  $\mathfrak{v}'_3$  are respectively  $\mathfrak{p}(\mathfrak{p}(a,b),c)$ ,  $\mathfrak{p}(\mathfrak{p}(a,c),b)$ ,  $\mathfrak{s}(\mathfrak{p}(a,b),c)$ ,  $\mathfrak{s}(\mathfrak{p}(a,c),b)$  and  $\mathfrak{s}(a,p(b,c))$ . We conclude with Proposition 4.15. Indeed, it is shown in [20] that the S-polynomials of pairs of elements in  $\{\mathfrak{v}_1,\mathfrak{v}_2\}$  are congruent to zero modulo  $\mathcal{B}$ . We show for example that the S-polynomial of  $\mathfrak{v}_1$  and  $\mathfrak{v}'_1$  corresponding to  $\mathfrak{c} = \mathfrak{s}(\mathfrak{p}(\mathfrak{p}(a,b),c),d) \in \mathbf{Free}^{sh}_{\mathcal{G}}[\{a,b,c,d\},abcd]$  is congruent to zero. We have

$$m_{\mathfrak{c},\operatorname{lt}(\mathfrak{v}_1)}(\mathfrak{v}_1) = \mathfrak{c} - \mathfrak{s}(\mathfrak{p}(a,\mathfrak{p}(b,c)),d)$$

$$m_{\mathfrak{c},\operatorname{lt}(\mathfrak{v}'_1)}(\mathfrak{v}'_1) = \mathfrak{c} - \mathfrak{p}(\mathfrak{s}(\mathfrak{p}(a,b),d),c) - \mathfrak{p}(\mathfrak{p}(a,b),\mathfrak{s}(c,d)),$$
(180)

which gives us

$$s_{\mathfrak{c}}(\mathfrak{v}_1,\mathfrak{v}'_1) = \mathfrak{p}(\mathfrak{s}(\mathfrak{p}(a,b),d),c) + \mathfrak{p}(\mathfrak{p}(a,b),\mathfrak{s}(c,d)) - \mathfrak{s}(\mathfrak{p}(a,\mathfrak{p}(b,c)),d). \tag{181}$$

Let us look how each of the terms of  $s_{\mathfrak{c}}(\mathfrak{v}_1,\mathfrak{v}'_1)$  reduces modulo  $\mathcal{B}$ :

$$\mathfrak{p}(\mathfrak{s}(\mathfrak{p}(a,b),d),c) \equiv_{\mathfrak{v}_1} \mathfrak{p}(\mathfrak{p}(\mathfrak{s}(a,d),b),c) + \mathfrak{p}(\mathfrak{p}(a,\mathfrak{s}(b,d)),c)$$

$$\equiv_{\mathfrak{v}_1} \mathfrak{p}(\mathfrak{s}(a,d),\mathfrak{p}(b,c)) + \mathfrak{p}(a,\mathfrak{p}(\mathfrak{s}(b,d),c),$$

$$\mathfrak{p}(\mathfrak{p}(a,b),\mathfrak{s}(c,d)) \equiv_{\mathfrak{v}_1} \mathfrak{p}(a,\mathfrak{p}(b,\mathfrak{s}(c,d)), \tag{182}$$

$$\mathfrak{s}(\mathfrak{p}(a,\mathfrak{p}(b,c)),d) \equiv_{\mathfrak{p}_1'} \mathfrak{p}(\mathfrak{s}(a,d),\mathfrak{p}(b,c)) + \mathfrak{p}(a,\mathfrak{s}(\mathfrak{p}(b,c),d))$$
$$\equiv_{\mathfrak{p}_1'} \mathfrak{p}(\mathfrak{s}(a,d),\mathfrak{p}(b,c)) + \mathfrak{p}(a,\mathfrak{p}(\mathfrak{s}(b,d),c)) + \mathfrak{p}(a,\mathfrak{p}(b,\mathfrak{s}(c,d))).$$

Putting this together in (181) gives us that  $s_{\mathfrak{c}}(\mathfrak{v}_1,\mathfrak{v}'_1)$  reduces to 0 modulo  $\mathcal{B}$ . We leave the verification of the other cases to the interested reader.

**Proposition 4.39.** The Hilbert series of  $SP^{!}$  is given

$$\mathcal{H}_{\mathbf{SP}^!}(x) = \frac{(1 - \log(1 - x))^2 - 1}{2}.$$
 (183)

*Proof.* The Hilbert series of **ComMag** is  $\mathcal{H}_{\mathbf{ComMag}}(x) = 1 - \sqrt{1 - 2x}$  hence the Hilbert series of  $\mathbf{SP} \cong \mathbf{Com}(\mathbf{ComMag})$  is  $\mathcal{H}_{\mathbf{SP}}(x) = e^{1 - \sqrt{1 - 2x}} - 1$ , where the -1 comes from the fact that we consider positive species. We deduce the Hilbert series of  $\mathbf{SP}^!$  from  $\mathcal{H}_{\mathbf{SP}}$  and the identity (114).

The first dimensions dim  $\mathbf{SP}^![[n]]$  for  $n \geq 1$  are

$$1, 2, 5, 17, 74, 394, 2484, 18108, 149904.$$
 (184)

This is sequence **A000774** of [43]. This sequence is in particular linked to some pattern avoiding signed permutations and mesh patterns.

Before ending this section let us mention the sub-operad LP of  $\mathbb{K}MG$  generated by

$$\left\{ \bigcirc, \bigcirc, \bigcirc, \bigcirc \bigcirc \right\}. \tag{185}$$

This operad seems particularly interesting to us since its two generators can be considered as minimal elements in the sense that a partial composition with the two isolated vertices adds exactly one vertex and no edge, while a partial composition with the loop adds exactly one edge and no vertex. A natural question to ask at this point concerns the description of the multigraphs generated by these two minimal elements.

**Proposition 4.40.** The following properties hold:

• the operad SP is a sub-operad of LP;

• the operad LP is a strict sub-operad of  $\mathbb{K}MG$ . In particular, the multigraph

is in  $\mathbb{K}MG$  but is not in **LP**.

*Proof.* • The following identity shows that ⓐ-ⓑ is in  $\mathbf{LP}[\{a,b\}]$  and hence that  $\mathbf{SP}$  is a sub-operad of  $\mathbf{LP}$ :

$$\bigcirc \bullet_* \quad \boxed{a} \quad \boxed{b} - \quad \bigcirc \bigcirc \qquad \boxed{b} = 2 \quad \boxed{a} - \boxed{b}.$$
(187)

• Using computer algebra, one generates all vectors in  $\mathbf{LP}[\{a,b,c\}]$  with three edges and shows that the announced multigraph is not a linear combination of these.

## 5 Conclusion and perspectives

We presented in this dissertation the main results obtained during our three years of PhD. Our contribution to Hopf monoid theory is a natural continuation of Aguiar and Ardila's paper [2] and brings together a lot of similar results thorough the literature. Our contribution to operad theory is a combinatorial approach to the study of operads on graphs and related objects. Many other results obtained during this PhD were not presented in this dissertation, either because they were not advanced enough or because they were in great part covered by already existing literature. Let us cite them here along with some research direction naturally arising from this dissertation.

The study of the coefficient of the polynomial invariant of [2]. Let M be a Hopf monoid,  $\zeta$  be a character of M and  $x \in M[V]$  and element of M. What can we say on the coefficients of  $\chi_V^{M,\zeta}(x)(n)$ ? More precisely, if this polynomial writes  $\sum a_k n^k$ , is the sequence  $a_1, \ldots, a_{|V|}$  alternating, unimodular and log-concave? The sequence being alternating is not a too difficult question and we managed to prove it for  $\chi^{\mathbb{K}HG,\zeta_1}$  and hence for any  $\chi^{M,\zeta_1}$  where M is any of the Hopf monoid we studied except GP. We do not think the more general study of  $\chi^{\mathbb{K}GP,\zeta}$ , for any  $\zeta$ , to be more complicated. On the other hand, the question about unimodularity and log-concavity are much more involved. The paper [29] provides a general answer for matroids and hence for graphs (since graphs can be seen as graphic matroids, a particular type of matroids).

The Duchamp et. al. construction of polynomial invariants. In [21], the authors provide a way to construct polynomial invariant over Hopf algebra. They apply it to the Hopf algebra of multigraphs with a contraction deletion co-product and recover the Tutte polynomial. We applied their method to other Hopf algebras but the obtained polynomials were too simple to be of interest. It seems their method is interesting in the particular case were the Hopf algebra have two primitive elements of size 1.

Terminal element of the category of combinatorial Hopf monoids. A combinatorial Hopf monoid is a pair  $(M, \zeta)$  of a Hopf monoid and a character on this Hopf monoid. There is a Hopf monoid structure over the species Comp of compositions such that  $(Comp, \zeta_1)$  is a terminal element in the category of Hopf monoid. While we proved this fact, this was already proven in the case of co-commutative Hopf monoid and  $\Pi$  in [39]. The proof are nearly identical.

Weighted graphs and chromatic function. We studied the chromatic function of weighted variations of graphs, oriented graphs and posets. Our results are in great part covered by [18] and [1]. Nevertheless, our approach to the link between weighted object and contraction-deletion is more general and our research on this subject is still ongoing.

Generalizing species. As is put to light with  $\mathcal{L}$ -species in subsubsection 4.1.4, changing the domain category of a species can lead to very interesting objects. An important

- project of ours, is to generalize species this way. One of our main lead is the definition of a notion of co-monoidal category. It was planned to discuss the feasibility and interest of this project with François Bergeron but this was canceled because of the covid19 epidemic. Our research on this topic is however still ongoing.
- Link with the universal Tutte polynomial. In [15], O.Bernardi et al. give a generalization of the Tutte polynomial to hypergraphs. As they asked in [15], is it possible to see the  $\zeta_1$  chromatic polynomial of hypergraphs defined here as a specialization of their universal Tutte polynomial?
- Various questions about graph insertion operads. Are their other interesting graph insertion operads than the one studied here? Is there a characterisation of the generators the operads  $\mathbb{K}MG$  and its sub-operads? How to describe  $\mathbf{LP}[V]$ ? And does any of  $\mathbf{SP}, \mathbf{SP}^!, \mathbf{LP}$  provide an interesting type of algebra?
- A sub-species of LP. Denote by p the operation which adds a vertex to a graph, and by l the operation which sends a graph on the sum of graphs obtained by adding an edge between two vertices of g. The vectors obtained by consecutively composing l and p form a sub-species of LP. We studied this sub-species which have some interesting links with paths with steps (1,1) and (1,-1). Unfortunately, this study did not help in the comprehension of LP.
- The SP! operad. Does the operad SP! translate in a natural operad structure over the families counted by the sequence A000774 of [43]?
- Factorizing PLie. Do the morphisms ComMag  $\hookrightarrow \mathbb{K}T \hookrightarrow \mathbf{PLie}$  provide some insight in the search of an operad  $\mathcal{O}$  such that  $\mathbf{PLie} = \mathcal{O}(\mathbf{ComMag})$  as conjectured in [13]?

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