GROUPOIDS AND FAÀ DI BRUNO FORMULAE FOR GREEN FUNCTIONS IN BIALGEBRAS OF TREES

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ABSTRACT. We prove a Faà di Bruno formula for the Green function in the bialgebra of P-trees, for any polynomial endofunctor P. The formula appears as relative homotopy cardinality of an equivalence of groupoids. For suitable choices of P, the result implies also formulae for Green functions in bialgebras of graphs.

CONTENTS

INTRODUCTION

This paper is a contribution to the combinatorial understanding of renormalisation in perturbative quantum field theory. It can be seen as part of the general programme, pioneered by Joyal, Baez–Dolan (and in a sense already by Grothendieck), of gaining insight into combinatorics, especially regarding symmetries, by upgrading from finite sets to suitably finite groupoids. We derive Faà di Bruno formulae in bialgebras of trees by realising them as relative homotopy cardinalities of equivalences of groupoids. An attractive aspect of this approach is that all issues with symmetries are handled completely transparently

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by the groupoid formalism, and take care of themselves throughout the equivalences without appearing in the calculations. In fact the general philosophy is that sum weighted by inverses of symmetry factors always arise as groupoid cardinalities. It is our hope that these kinds of techniques can be useful more generally in perturbative quantum field theory, and related areas.

Our starting point is the seminal work of van Suijlekom on Hopf algebras and renormalisation of gauge field theories [38], [39], [40]. Among several more important results in his work, the following caught our attention: for each interaction label v of a quantum field theory, the Connes–Kreimer Hopf algebra of Feynman graphs contains a formal series Y_v satisfying the multi-variate 'Faà di Bruno' formula

$$(1) \qquad \Delta(Y_v) = \sum_{n_1 \cdots n_k} Y_v Y_{v_1}^{n_1} \cdots Y_{v_k}^{n_k} \otimes p_{n_1 \cdots n_k}(Y_v),$$

where $p_{n_1 \cdots n_k}$ is the projection onto graphs containing n_i vertices of type v_i. The series Y_v is the renormalised (combinatorial) 1PI Green function

$$Y_v = \frac{G_v}{\prod_{e \in v} \sqrt{G_e}},$$

where

$$G_v = 1 + \sum_{\mathrm{res}\,\Gamma = v} \frac{\Gamma}{|\mathrm{Aut}\,\Gamma|}$$

is the bare Green function of all connected 1PI graphs Γ with residue v, the product is over the lines of the one-vertex graph v, and where the denominators

$$G_e = 1 - \sum_{\mathrm{res}\,\Gamma = e} \frac{\Gamma}{|\mathrm{Aut}\,\Gamma|}$$

constitute a renormalisation factor, cf. the Dyson formula (see [21, Ch. 8]) or [24, Ch. 7]).

The importance of Green functions in the Hopf algebra of graphs is of course that, unlike the individual graphs, the Green functions actually have a physical interpretation. The proof of the formula is a matter of expanding everything, keeping track of several different combinatorial factors associated to graphs, and comparing them with the help of the orbit-stabiliser theorem. (The formula is Proposition 12 of [40], but the bulk of the proof is contained in various lemmas in [38] where the involved combinatorial factors are computed.)

The Faà di Bruno Hopf algebra plays an important role in Hopf algebra approach to renormalisation, and many different relationships between it and the Hopf algebras of graphs or trees have been uncovered. One reason for the importance of the Faà di Bruno Hopf algebra is the general idea, expressed for example by Delamotte [13], that in the end renormalisation should be a matter of reparametrisation, i.e. substitution of power series.

Already Connes and Kreimer [11] constructed a Hopf algebra homomorphism from the Faà di Bruno Hopf algebra (or rather the Connes–Moscovici Hopf algebra) to the Hopf algebra of Feynman graphs in the case of ϕ^3 in six space-time dimensions. Bellon and Schaposnik [4] were perhaps the first to explicitly write down the Faà di Bruno formula, in a form

$$\Delta(a) = \sum_n a^n \otimes a_n,$$

very pertinent to the formula we establish in the present paper. Recently the Faà di Bruno formula has been exploited by Ebrahimi-Fard and Patras [15] in the development of exponential renormalisation. Their paper contains also valuable information on the relationship with the Dyson formula.

It seems unlikely that a formula like this can exist for the Green functions in the Hopf algebra of *trees* — indeed, the symmetry factors of the involved trees are not related to the combinatorics of grafting in the same way as symmetry factors of graphs are related to insertion of graphs (except in very special cases, such as considering only iterated one-loop self-energies in massless Yukawa theory in four dimensions, an example considered by many authors, e.g. [12], [6], [32]).

In the present paper we work with *operadic trees* instead of the combinatorial trees of the usual (Butcher)–Connes–Kreimer Hopf algebra — this is an essential point: operadic trees are more closely related to Feynman graphs, and have meaningful symmetry factors in this respect, cf. [28] and Section 9 below.

Our main theorem (7.3) at the algebraic level establishes the Faà di Bruno formula

(2) $$\Delta(G) = \sum_n G^n \otimes p_n(G)$$

for the Green function $G = \sum_T T/\left|\operatorname{Aut}(T)\right|$ in the bialgebra of P-trees, for any polynomial endofunctor P.

The proof we give is very conceptual: the equation appears as an equivalence of groupoids, and all the symmetry factors are hidden and take care of themselves. Precisely, at the groupoid level, our main theorem (5.5) states the following equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$:

$$\int^{T\in\mathbf{T}} \operatorname{cut}(T) \simeq \int^{n\in\widetilde{I}} \mathbf{F}_n \times {}_n\mathbf{T},$$

which is essentially a double-counting formula. Here the integral signs are integration over groupoids (which corresponds to sums with symmetry factors), $\mathbf{F}$ is the groupoid of P-forests, $\mathbf{T}$ is the groupoid of P-trees, $\operatorname{cut}(T)$ is the discrete groupoid of cuts of a tree T, n is an (I-coloured) finite set, and ${}_n\mathbf{T}$ is the homotopy fibre over n of the leaf map, i.e. the groupoid of trees with leaf profile n, and similarly, $\mathbf{F}_n$ is the homotopy fibre over n of the root map, i.e. the groupoid of forests

with root profile n. The algebraic Faà di Bruno formula (2) is obtained just by taking homotopy cardinality (relative to $\mathbf{F} \times \mathbf{T}$) on both sides of the equivalence.

Depending on the choice of polynomial endofunctor P, the formula specialises to many formulae of independent interest. Most notably, we show in Section 9 that for P a suitable functor defined in terms of interaction labels and 1PI graphs (for any quantum field theory), a Faà di Bruno formula for the Green function in a version of the bialgebra of graphs is obtained.

In order to arrive at a level of abstraction where the arguments become pleasant and the essential features are in focus, we have moved away quite a bit from the starting point mentioned above, and at the moment we have not completely succeeded in deriving van Suijlekom's formula from ours (or conversely). We do come pretty close though, and discuss these issues in Section 9. The problem resides in the renormalisation factor, which can be seen to account for substitution of graphs into internal lines, an operation we do not know how to capture operadically. Nevertheless, the combinatorial clarity obtained is of independent mathematical interest, and we hope that the conceptual insight provided can also be useful for quantum field theory in particular.

Outline of the paper. Section 1 and 2 are mostly motivational. We begin in Section 1 by revisiting the classical Faà di Bruno Hopf algebra, gradually recasting it in more categorical language, starting with composition of formal power series, then the incidence algebra viewpoint (cf. [14]), then finally the category of surjections (cf. [22]). We work with the non-reduced *bi*algebra rather than with the reduced *Hopf* algebra. This is an important point. In order to motivate the groupoid machinery, we outline a groupoid-equivalence proof of the classical Faà di Bruno formula. In Section 2 we briefly revisit the (Butcher)–Connes–Kreimer Hopf algebra of trees, introduce an operadic version of it that we need, and state one version of the main theorem for the bialgebra of operadic trees and the corresponding Green function.

The theory of groupoids is at the same time our main technical tool and the most important conceptual ingredient in our approach. Section 3 recalls the most important notions, such as homotopy pullbacks, homotopy fibres, homotopy quotients and slice categories, in the hope of rendering the paper accessible to readers without a substantial background in category theory. In Section 4 we set up the formalism of operadic trees and forests, in terms of polynomial endofunctors, following [25]. This formalism is needed in particular to be able to talk about decorated trees — P-trees for a polynomial endofunctor P — at the level of generality needed to cover the examples envisaged.

In Section 5 we establish our main result, the equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$:

$$\int^{T \in \mathbf{T}} \mathrm{cut}(T) \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T}$$

already mentioned. Most of the arguments are formal consequences of general properties of groupoids; the only thing we need to prove by hand is the equivalence

$$\mathbf{C} \simeq \mathbf{F} \times_{\widetilde{I}} \mathbf{T}.$$

(Lemma 5.3) between trees with a cut and pairs consisting of a forest and a tree such that the roots of the forest 'coincide' with the leaves of the tree. In a precise sense, this is the essence of the Hopf algebra of trees.

Section 6 reviews and extends appropriate notions of groupoid cardinality, following Baez–Dolan [2] and Baez–Hoffnung–Walker [3]. In particular, we consider relative cardinality with respect to a morphism of groupoids and describe its formal properties. In Section 7 we finally prove the Faà di Bruno formula in the bialgebra of trees by taking the cardinality of the groupoid equivalence of Section 5. Examples of polynomial endofunctors giving rise to several kinds of trees are given in Section 8. In particular we relate our Faà di Bruno formulae with the classical one. Finally, in Section 9 we comment further on the relationship with van Suijlekom's Faà di Bruno formula, and outline in particular how our formula, for a suitable choice of polynomial endofunctor P yields a Faà di Bruno formula in a certain bialgebra of Feynman graphs. The appendix contains an explicit calculation with trees, relating to the our comparison of the classical Faà di Bruno bialgebra and those of trees in Section 8.

0.1. Acknowledgments. We are indebted to Kurusch Ebrahimi-Fard for many illuminating discussions on quantum field theory.

1. THE FAÀ DI BRUNO FORMULA REVISITED

In this section we briefly review the classical Faà di Bruno bialgebra, starting from power series representations and partitions, and leading to a groupoid version in terms of surjections.

1.1. Power series and the classical Faà di Bruno formula. Consider formal power series in one variable without constant term and with linear term equal to z:

$$f(z) = \sum_{n=0}^{\infty} \frac{A_n(f) \, z^n}{n!} \qquad A_0 = 0, \ A_1 = 1.$$

These form a group under substitution of power series, sometimes denoted $\mathrm{Diff}(\mathbb{C}, 0)$, as the series can be regarded as germs of smooth

functions tangent to the identity at 0. The classical Faà di Bruno Hopf algebra $\mathcal{H}$ is the polynomial algebra on the symbols

$$a_n := A_n/n!, \quad n \geq 2,$$

viewed as linear forms on $\mathrm{Diff}(\mathbb{C}, 0)$,

$$\langle a_n, f \rangle = a_n(f) = A_n(f)/n!, \qquad a_n \in \mathbb{C}[[z]]^*.$$

The comultiplication is defined by

$$\langle \Delta(a_n), f \otimes g \rangle = \langle a_n, g \circ f \rangle,$$

and the counit by $\varepsilon(a_n) = \langle a_n, \mathbf{1} \rangle$. An explicit formula for Δ can be obtained by expanding

$$(3) \qquad (g \circ f)(z) = \sum_{n=1}^{\infty} a_n(g) \left(\sum_{m=1}^{\infty} a_m(f)\, z^m \right)^n,$$

and involves the Bell polynomials. So far $\mathcal{H}$ is a bialgebra; it acquires an antipode by general principles by observing that it is a connected graded bialgebra: the grading is given by

$$\deg(a_k) = k - 1.$$

We refer to Figueroa and Gracia-Bondía [16] for details on this classical object and its relevance in quantum field theory.

The formula for Δ can be packaged into a single equation, by considering the formal series

$$A = 1 + \sum_{k \geq 2} \frac{A_k}{k!} = 1 + \sum_{k \geq 2} a_k \quad \in \mathbb{C}[[a_2, a_3, \ldots]].$$

The comultiplication now takes the following form:

$$\Delta(A) = A \otimes 1 + \sum_{k \geq 2} A^k \otimes a_k.$$

The values of Δ on the individual generators a_k can be extracted from this formula.

1.2. The (non-reduced) Faà di Bruno bialgebra. For our purposes it is important to give up the condition $a_1 = 1$. In this case, substitution of power series does not form a group but only a monoid, and the algebra is just a bialgebra rather than a Hopf algebra. We denote it by $\mathcal{F} = \mathbb{C}[a_1, a_2, a_3, \ldots]$. The definition of the comultiplication is still the same, and again it can be encoded in a single equation, involving now the formal series

$$A = \sum_{k \geq 1} \frac{A_k}{k!} = \sum_{k \geq 1} a_k \quad \in \mathbb{C}[[a_1, a_2, a_3, \ldots]].$$

The resulting form of the Faà di Bruno formula is the Leitmotiv of the present work:

Proposition. 1.3 (Classical Faà di Bruno identity)**.** *The formal series* A *satisfies*

$$\Delta(A) = \sum_{k \geq 1} A^k \otimes a_k.$$

We stress that the bialgebra $\mathcal{F}$ (with grading $\deg(a_k) = k - 1$) is not connected: $\mathcal{F}_0$ is spanned by the powers of a_1, all of which are group-like. One can obtain the classical Hopf algebra $\mathcal{H}$ by imposing the relation $a_1 = 1$, which is easily seen to generate a bi-ideal.

1.4. Note on grading convention. Since $\deg(a_k) = k - 1$, it is common in the literature to employ a different indexing, shifting the index so that it agrees with the degree. With the shifted index convention, the Faà di Bruno formula then reads

$$\Delta(A) = \sum_{n \geq 1} A^{n+1} \otimes a_n.$$

This is the convention used by van Suijlekom and many others, and explains the extra factor Y_v in the formula (1) quoted above. Beware that this convention means that certain indices are allowed to start at -1 and when it is said that $p_n(G)$ is the part of the Green function corresponding to graphs with n vertices, it is actually means $n + 1$ vertices.

While the shifted indexing convention can have its advantages, it is important for us to keep the indexing as above, so that the exponent in A^k matches the index in a_k. As we pass to more involved Faà di Bruno formulae, this will always express a type match: the outputs of one operation (the exponent) matching the input of the following (the subscript).

1.5. Faà di Bruno Hopf algebra in terms of partitions. The coefficients — the Bell polynomials which we did not make explicit — count partitions. In fact, it is classical (Doubilet [14], 1975) that the Hopf algebra $\mathcal{H}$ can be realised as the reduced incidence bialgebra of the family of posets given by partitions of finite sets. We give only a brief outline here.

The partitions of a finite set S form a lattice, in which $\sigma \leq \tau$ when σ is a refinement of τ. Any such two partitions define an interval $[\sigma, \tau] := \{\rho \mid \sigma \leq \rho \leq \tau\}$. Consider the family of all intervals in partition lattices of finite sets, and declare two intervals equivalent if they are isomorphic as abstract posets. This is an order-compatible equivalence relation, meaning that the comultiplication formula

$$\Delta([\sigma, \tau]) = \sum_{\rho \in [\sigma, \tau]} [\sigma, \rho] \otimes [\rho, \tau]$$

is well-defined on equivalence classes. Disjoint union of finite sets defines furthermore a multiplication on these equivalence classes. Any

interval is equivalent to a finite product of nontrivial maximal intervals (i.e. full partition lattices of some finite sets of cardinality at least 2), and this product expression is unique up to isomorphism of the sets involved. Denote by a_k, $k \geq 2$, the equivalence class of the partition lattice of a k-element set. The reduced incidence coalgebra on the vector space spanned by all equivalence classes (that is, the polynomial ring on the classes a_k, $k \geq 2$) is naturally isomorphic to the Faà di Bruno Hopf algebra $\mathcal{H}$.

In order to get the 'nonreduced' bialgebra $\mathcal{F}$, one has to consider a finer equivalence relation: define an interval $[\sigma, \tau]$ to have *type* $1^{\lambda_1} 2^{\lambda_2} \cdots$ if λ_k is the number of blocks of τ that consist of exactly k blocks of σ, and declare two intervals equivalent if they have the same type. Every interval is isomorphic as a poset to a type-equivalent product of (possibly trivial) maximal intervals, yielding a 'nonreduced' incidence algebra isomorphic to $\mathcal{F}$.

The technicalities involved here can be avoided by considering surjections instead of partitions.

1.6. Faà di Bruno in terms of surjections. A surjection $E \twoheadrightarrow B$ clearly induces a partition of the set E, and conversely, a partition of E induces a surjection to the set of blocks. This correspondence provides a groupoid equivalence between the groupoid of sets-with-a-partition and their isomorphisms, and the groupoid $\mathbf{S}$ of surjections. The arrows in the groupoid $\mathbf{S}$ are pairs of isomorphisms forming a diagram

$$
\begin{array}{ccc}
E & \xrightarrow{\;\cong\;} & E' \\
\downarrow & & \downarrow \\
\twoheaddownarrow & & \twoheaddownarrow \\
B & \xrightarrow{\;\cong\;} & B'.
\end{array}
$$

From the groupoid of surjections, one can get a bialgebra $\mathcal{F}$ directly. As a vector space it has as basis the isomorphism classes of surjections, the multiplicative structure comes from the monoidal structure on $\mathbf{S}$ given by disjoint union, and the formula for comultiplication is

$$
\Delta(E \twoheadrightarrow B) = \sum_{E \twoheadrightarrow S \twoheadrightarrow B} (E \twoheadrightarrow S) \otimes (S \twoheadrightarrow B).
$$

Here the sum is over isomorphism classes of factorisations $E \twoheadrightarrow S \twoheadrightarrow B$. In detail, consider the *factorisation groupoid* $\mathrm{Fact}(E \twoheadrightarrow B)$, whose objects are factorisations of $E \twoheadrightarrow B$ into two surjections $E \twoheadrightarrow S \twoheadrightarrow B$, and whose morphisms are bijections $S \simeq S'$ making the two triangles commute:

$$
\begin{array}{ccc}
 & S & \\
\nearrow & \downarrow \simeq & \searrow \\
E & & B \, . \\
\searrow & \uparrow & \nearrow \\
 & S' & \\
\end{array}
$$

Then the above sum is over $\pi_0(\mathrm{Fact}(E \twoheadrightarrow B))$, the set of connected components of the factorisation groupoid.

Observe that any surjection is the disjoint union of *connected* surjections $a_k = (\{1, \ldots, k\} \twoheadrightarrow \{1\})$, and hence is a product of such in $\mathcal{F}$. This gives

$$\mathrm{Fact}(E \twoheadrightarrow B) = \mathrm{Fact}\big(\sum_{b \in B}(E_b \twoheadrightarrow \{b\})\big) = \prod_{b \in B} \mathrm{Fact}(E_b \twoheadrightarrow \{b\}).$$

It follows that $\mathcal{F}$ indeed coincides with the classical Faà di Bruno bialgebra.

The Faà di Bruno *Hopf* algebra is also easily obtained from the groupoid of surjections, but instead of identifying just isomorphic surjections, we identify surjections with equivalent factorisation groupoids. Thus invertible surjections are all equivalent, as they have trivial factorisation groupoids. This relation is clearly generated by the equation $(1 \twoheadrightarrow 1) = (\emptyset \twoheadrightarrow \emptyset)$, that is, $a_1 = 1$.

The construction of the Faà di Bruno bialgebra in terms of the groupoids of surjections seems to be due to Joyal [22]. It is in the spirit of incidence algebras of Möbius categories introduced by Leroux [34], and studied recently by Lawvere and Menni [33]. However, the category of surjections is not a Möbius category, since it contains non-trivial isomorphisms. The theory of *homotopy Möbius categories* that we develop in [18] extends the classical theory to cover the category of surjections, and also the category of trees in Section 4 below.

1.7. Towards a groupoid proof. The viewpoint of the Faà di Bruno bialgebra in terms of the groupoid of surjections is what leads to analogous formulae for bialgebras of trees. We anticipate this by giving here the corresponding proof for the classical Faà di Bruno formula. Here we make use of basic constructions with groupoids, explained Section 3.

The idea is simple: the series

$$A = \sum_{n \geq 1} A_n/n!$$

is the *relative groupoid cardinality* (7.1) of the groupoid of *connected* surjections, which is just the groupoid $\mathbf{B}$ of non-empty finite sets, relative to the groupoid of all surjections $\mathbf{S}$. This series A, of connected objects divided by their symmetry factors, is analogous to the Green function in the bialgebra of graphs, and to the Green function in the bialgebra of trees, to be introduced shortly. Taking the relative cardinality of an equivalence of groupoids, obtained by looking at the groupoid $\mathbf{S}$ of surjections in two different ways, will give the classical Faà di Bruno formula.

1.8. Double counting of surjections. The groupoid of surjections **S** has two projections to **B**,

$$
\left(n \xrightarrow{\;\cong\;} n' \right) \longleftarrow\!\shortmid
\left(
\begin{array}{ccc}
n & \xrightarrow{\;\cong\;} & n' \\
\downarrow & & \downarrow \\
k & \xrightarrow[\cong]{} & k'
\end{array}
\right)
\longmapsto
\left(k \xrightarrow{\;\cong\;} k' \right).
$$

Now the double-counting lemma 3.11 gives equivalences of groupoids

$$
\int^{n\in\mathbf{B}} {}_n\mathbf{S} \;\simeq\; \mathbf{S} \;\simeq\; \int^{k\in\mathbf{B}} \mathbf{S}_k,
$$

where ${}_n\mathbf{S}$ denotes the (homotopy) fibre over n for the left-hand projection, and $\mathbf{S}_k$ denotes the (homotopy) fibre for the right-hand projection.

To calculate the right-hand side, we have the 'key lemma'

$$
(4) \qquad\qquad \mathbf{S}_k \simeq \boldsymbol{Grpd}(k, \mathbf{B}) = \mathbf{B}^k
$$

which encodes a surjection onto k in terms of its k nonempty fibres.

For the left-hand side, the fibre ${}_n\mathbf{S}$ is the groupoid of surjections out of n. There is at most one isomorphism between two such surjections, which is to say that the groupoid ${}_n\mathbf{S}$ is a discrete groupoid, and it is clearly equivalent to the set of partitions of n:

$$
(5) \qquad\qquad {}_n\mathbf{S} \simeq \mathcal{P}(n).
$$

Combining the previous formulae, we get the following result.

Proposition. 1.9. *We have natural equivalences of groupoids*

$$
\int^{n\in\mathbf{B}} \mathcal{P}(n) \simeq \mathbf{S} \simeq \int^{k\in\mathbf{B}} \mathbf{B}^k.
$$

This is essentially the Faà di Bruno formula. It remains to take groupoid cardinality. As **S** has infinitely many components, this has to be relative cardinality (6.6), which amounts to introducing a formal symbol for each component. The natural choice would be relative cardinality with respect to **S** itself, but to obtain the Faà di Bruno formula as in 1.3, we have to take relative cardinality with respect to $\mathbf{S} \times \mathbf{B}$, via the projection $\mathbf{S} \to \mathbf{B}$ sending $n \twoheadrightarrow k$ to k. So for each component of $\mathbf{S} \times \mathbf{B}$, introduce a label: for $k \in \mathbf{B}$ we use the label A_k, and for $p \in \mathbf{S}$ we use as label the corresponding monomial in the A_i under the equivalence (4). The image in $\mathbf{S} \times \mathbf{B}$ of the singleton integrand 1 in

$$
\int^{n\in\mathbf{B}} \mathcal{P}(n) = \int^{n\in\mathbf{B}} \int^{p\in\mathcal{P}(n)} 1
$$

is

$$
(p, k)
$$

when $p : n \twoheadrightarrow k$ is a surjection with codomain k. On the right-hand side, the cardinality of $\mathbf{B}^k$ over $\mathbf{S}$ is precisely A^k, whereas the second factor clearly is $\{k\}$. Altogether we get

$$\sum_n \left(\sum_{p:n \twoheadrightarrow k} \{p\} \times \{k\} \right) /n! = \sum_k A^k \otimes A_k/k!$$

But here the left-hand side is precisely $\Delta(A)$, by linearity.

## 2. THE BIALGEBRA OF TREES, AND THE MAIN THEOREM

2.1. The bialgebra of rooted trees of Connes and Kreimer [30], which in essence was studied already by Butcher [7] in the early 70s, is the free algebra $\mathcal{H}$ on the set of isomorphism classes of *combinatorial trees* (defined for example as finite connected graphs without loops or cycles, and with a designated root vertex). The comultiplication is given on generators by

$$\begin{aligned} \Delta : \mathcal{H} &\longrightarrow \mathcal{H} \otimes \mathcal{H} \\ T &\longmapsto \sum_c P_c \otimes S_c, \end{aligned}$$

where the sum is over all admissible cuts of T; the left-hand factor P_c is the forest (interpreted as a monomial) found above the cut, and S_c is the subtree found below the cut (or the empty forest, in case the cut is below the root). Admissible cut means: either a subtree containing the root, or the empty set. $\mathcal{H}$ is a connected bialgebra: the grading is by the number of nodes, and $\mathcal{H}_0$ is spanned by the unit. Therefore, by general principles (see for example [16]), it acquires an antipode and becomes a Hopf algebra.

2.2. Operadic trees. For the present purposes it is crucial to work with *operadic trees* instead of combinatorial trees; this amounts to allowing loose ends (leaves). A formal definition is given in 4.1. For the moment, the following drawings should suffice to exemplify operadic trees — as usual the planar aspect inherent in a drawing should be disregarded:
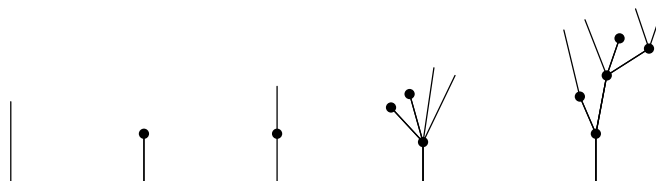
Note that certain edges (the *leaves*) do not start in a node, and that one edge (the obligatory *root edge*) does not end in a node. A node without incoming edges is not the same thing as a leaf; it is a nullary operation (i.e. a constant), in the sense of operads. In operad theory, the nodes represent operations, and trees are formal combinations of operations. The small incoming edges drawn at every node serve to keep track of

the arities of the operations. Furthermore, for coloured operads, the operations have type constraints on their inputs and output, encoded as attributes of the edges.

The trees appearing in BPHZ renormalisation are naturally operadic, cf. [28]. With the appropriate decorations, these trees even acquire meaningful symmetry factors, so that the Green function of operadic trees faithfully reflects the Green function of Feynman graphs. This is explained in Section 9 below.

2.3. The bialgebra of operadic trees (cf. [26]). A *cut* of an operadic tree is defined to be a subtree containing the root — note that the arrows in the category of operadic trees are arity preserving (4.3), meaning that if a node is in the subtree, then so are all the incident edges of that node.

If $c : S \subset T$ is a subtree containing the root, then each leaf e of S determines an ideal subtree of T (4.3), namely consisting of e (which becomes the new root) and all the edges and nodes above it. This is still true when e is also a leaf of T: in this case, the ideal tree is the trivial tree consisting solely of e. Figuratively, this means that for operadic trees cuts are not allowed to go above the leaves, and that cutting an edge does not remove it, but really cuts it(!). Note also that the root edge is a subtree; the ideal tree of the root edge is of course the tree itself. This is the analogue of the cut-below-the-root in the combinatorial case. For a cut $c : S \subset T$, define P_c to be the forest consisting of all the ideal trees generated by the leaves of S.

Let $\mathcal{B}$ be the free algebra on the set of isomorphism classes of operadic trees. With comultiplication defined on the generators by

$$\begin{aligned} \Delta : \mathcal{B} &\longrightarrow \quad \mathcal{B} \otimes \mathcal{B} \\ T &\longmapsto \quad \sum_{c:S \subset T} P_c \otimes S, \end{aligned}$$

as for combinatorial trees, $\mathcal{B}$ becomes a graded bialgebra. It is not connected: $\mathcal{B}_0$ is spanned by the trivial tree $\vert$ and all its powers (the empty power is the algebra unit 1). These are all grouplike, so one could obtain a connected bialgebra by imposing the equation $\vert = 1$.

2.4. The Green function. In the completion of $\mathcal{B}$, the power series ring, the series

$$G := \sum_T \delta_T / |\mathrm{Aut}(T)|$$

is called the *Green function*, in analogy with the (combinatorial) Green function of Feynman graphs. The sum is over all isomorphism classes of (operadic) trees, and there is a formal symbol δ_T for each isomorphism class of trees. We shall soon consider decorated trees, in which case there is one Green function for each possible decoration of the root

edge, in analogy with the situation in QFT, where there is one Green function for each possible residue (interaction label) in the theory.

The following Faà di Bruno formula for the Green function in the bialgebra of (operadic) trees is a special case of our main theorem (7.3).

Theorem. 2.5. *Write $G = \sum_{n \in \mathbb{N}} g_n$, where g_n is the summand in the Green function corresponding to trees with n leaves. Then*

$$\Delta(G) = \sum_{n \in \mathbb{N}} G^n \otimes g_n.$$

The more general formula we prove is valid for P-trees for any polynomial endofunctor P. In addition to the naked trees considered so far, this covers many examples (Section 8 such as planar trees, binary trees, cyclic trees, as well as the trees decorated by connected 1PI graphs of a quantum field theory (Section 9). The latter allows to transfer the Faà di Bruno formula to a bialgebra of graphs.

It is essential that we use operadic trees. There seems to be no reasonable Green function for combinatorial trees, since their symmetry factors are not related to the combinatorics of grafting.

We now first need to review some standard groupoid theory, then introduce more formally the trees and P-trees we treat, before coming to the proofs.

3. Groupoids

We recall some basic facts about groupoids; although this is well known material in category theory, we do not know of a suitable reference. It is essential to use the correct *homotopy* notions of the basic constructions such as pullback, fibre, and quotient. The correct notions can all be deduced from the beautiful simplicial machinery developed by Joyal [23] to generalise the theory of categories to quasi-categories (called ∞-categories by Lurie [35]).

3.1. Basics. A *groupoid* is a category in which every arrow is invertible. A *morphism* of groupoids is a functor, and we shall also need their natural transformations. While category theory language is the main technical tool to deal with groupoids, the intuition is rather that groupoids are 'fat sets with symmetries': instead of having just a few isolated points (elements in a set) we now have large chunks of points which are equivalent, with specific arrows linking them up. More than one arrow can exist between two given objects, and indeed a single object can have more than one arrow to itself — these are its symmetries.

A set is considered a groupoid in which the only arrows are the identity arrows. This defines a functor

$$D : \mathbf{Set} \to \mathbf{Grpd}.$$

Conversely, a groupoid X gives rise to a set by taking its set of connected components, i.e. the set of isomorphism classes in X, denoted $\pi_0(X)$; this defines a functor in the other direction (the left adjoint of D)

$$\pi_0 : \mathbf{Grpd} \to \mathbf{Set}.$$

Many sets arising in combinatorics and physics are actually π_0 of a groupoid, like when we say 'the set of all trees' to mean the set of isomorphism classes of trees.

A group can be considered as a groupoid with only one object. Conversely, for each object x in a groupoid X there is associated a group, the *vertex group*, denoted $\pi_1(x)$ or $\mathrm{Aut}(x)$, which consists of all the arrows from x to itself.

The homotopy notations π_0 and π_1 from topology are not a whim: groupoids are in a precise sense a model for certain topological spaces, namely the homotopy 1-types. To a topological space one associates the fundamental groupoid, whose objects are the points of the space and whose arrows are the (homotopy classes of) paths between points. Conversely, from a groupoid X one can build a CW complex, the classifying space BX, whose fundamental groupoid is X and which has vanishing higher homotopy groups ($\pi_k = 0$ for $k \geq 2$): these spaces are called homotopy 1-types.

The homotopy viewpoint on groupoids is a very important aspect, as all the good notions to deal with them are homotopy notions (e.g. homotopy pullback, homotopy fibres, homotopy quotients, etc.), as we proceed to recall.

3.2. Equivalences of groupoids; discreteness and contractibility. An *equivalence* of groupoids is just an equivalence of categories, i.e. a functor admitting a pseudo-inverse. Pseudo-inverse means that the two composites are not necessarily exactly the identity functors, but are only required to be isomorphic to the identity functors. This is the analogue of a homotopy equivalence in topology. Like in category theory, equivalences of groupoids can also be characterised as functors which are fully faithful and essentially surjective. Just as sets are often only interesting up to bijection, the appropriate notion of sameness for groupoids is equivalence. Equivalent groupoids have the same properties, for example the same π_0, π_1, and the same cardinality (cf. Section 6 below).

A groupoid X is called *discrete* if it is equivalent to a set considered as a groupoid; this set can then be taken to be $\pi_0(X)$. Another way of saying the same is that all vertex groups are trivial: $\pi_1(x) = 1$ for all objects $x \in X$, so all the information is stored in π_0. (There is a potential risk of confusion with the word 'discrete': in settings where one considers Lie groupoids (as in [8]), the word discrete ususally designates groupoids whose underlying topological space is discrete.)

A groupoid is called *contractible* if it is equivalent to a singleton set.

3.3. Fibrations of groupoids. A morphism of groupoids $p : X \to Y$ is a *fibration* if it has the path lifting property: for each object x of X and arrow $g : y' \to px$ of Y there exists an arrow $f : x' \to x$ such that $pf = g$. Fibrations are really just a technical notion to simplify some constructions. We will see below that any morphism may be replaced by a fibration if necessary.

3.4. Pullbacks and fibres. The naïve notions of pullback and fibres are not very useful for groupoids, as these notions are not stable under equivalence. The appropriate notions are homotopy pullbacks and homotopy fibres. Given a diagram of groupoids X, Y, S indicated by the solid arrows,

$$
\begin{array}{ccc}
X \times_S Y & \overset{q}{-\,-\,\to} & Y \\
{\scriptstyle p}\downarrow & \lrcorner & \downarrow {\scriptstyle g} \\
X & \underset{f}{\longrightarrow} & S
\end{array}
$$

the *homotopy pullback* is the groupoid $X \times_S Y$ whose objects are triples (x, y, ϕ) with $x \in X$, $y \in Y$ and $\phi : fx \to gy$ an arrow of S, and whose arrows are pairs $(\alpha, \beta) : (x, y, \phi) \to (x', y', \phi')$ consisting of $\alpha : x \to x'$ an arrow in X and $\beta : y \to y'$ an arrrow in Y such that the following diagram commutes in S

$$
\begin{array}{ccc}
fx & \overset{\phi}{\longrightarrow} & gy \\
{\scriptstyle f(\alpha)}\downarrow & & \downarrow {\scriptstyle g(\beta)} \\
fx' & \underset{\phi'}{\longrightarrow} & gy'.
\end{array}
$$

The morphisms p and q are the projections.

The homotopy pullback can be characterised up to canonical equivalence by a universal property: it is the 2-terminal object in a certain 2-category of solid diagrams of the shape in question. 2-terminal means that the comparison map is not unique but rather that the comparison maps form a contractible groupoid.

If f is a fibration then so is q, and in this case the homotopy pullback is equivalent to the naïve (strict) pullback. The *fibrant replacement* of a morphism $p : E \to B$ is an equivalent fibration $\bar{p} : \bar{E} \to B$, which can be obtained by performing the above explicit (homotopy) pullback construction of p along the identity morphism $B \to B$. Indeed, for any object $(b', e, b' \overset{\phi}{\longrightarrow} pe)$ of $\bar{E}$, any arrow $g : b \to b'$ may be lifted to an

arrow in $\bar{E}$,

$$
\begin{array}{ccc}
b & \xrightarrow{\phi g} & pe \\
{\scriptstyle g}\downarrow & & \| \\
b' & \xrightarrow{\phi} & pe.
\end{array}
$$

The notion of fibre is a special case of pullback, and again we need the homotopy version. If b in an object of B, we denote the inclusion morphism

$$
1 \xrightarrow{\ulcorner b \urcorner} B.
$$

The *(homotopy) fibre* E_b of a morphism $p : E \to B$ over an object b in B is the (homotopy) pullback of p along $\ulcorner b \urcorner$:

$$
\begin{array}{ccc}
E_b & \longrightarrow & E \\
\downarrow_{\lrcorner} & & \downarrow{\scriptstyle p} \\
1 & \xrightarrow{\ulcorner b \urcorner} & B.
\end{array}
$$

Again, if p is a fibration then the homotopy fibre is equivalent to the strict fibre. Henceforth the words pullback and fibre will always mean the homotopy pullback and homotopy fibre, since these notions are invariant under equivalence (unlike the strict notions).

The *slice* $X_{/x}$ over an object x of X is the fibre X_x of the identity functor $X \to X$, so the functor $X_{/x} \to X$ is always a fibration. In general, the fibre E_b will rarely be equivalent to the strict pullback of $p : E \to B$ and $\ulcorner b \urcorner : 1 \to B$ unless p is a fibration, but we may replace the functor $\ulcorner b \urcorner$ by the fibration $B_{/b} \to B$ and take the strict pullback.

We shall need the fact that for a (homotopy) fibre product of groupoids $X \times_J Y$, the (homotopy) fibre $(X \times_J Y)_j$ is naturally equivalent to the ordinary product $X_j \times Y_j$. (There are actually two ways of defining the fibre $(X \times_J Y)_j$, since there are two distinct but homotopic ways to go around the square to J, but the two fibres are naturally equivalent.)

3.5. Homotopy quotient. Whenever a group acts on a set or a groupoid X, say $X \times G \to X$, the *homotopy quotient* X/G is the groupoid obtained by gluing in a path (i.e. an arrow) between x and y for each $g \in G$ such that $xg = y$. (The homotopy quotient is often denoted $X//G$ to distinguish it from the naïve quotient. Since naïve quotients are badly behaved in many respects, and since we shall never need them, we reserve the single-slash notation for the homotopy quotient.) If G acts on a point 1, then the homotopy quotient $1/G$ is the groupoid with one object and vertex group G.

3.6. Skeletal groupoids. A groupoid X splits into connected components. Recall that the set of connected components is denoted $\pi_0 X$. Any arrow between two objects within a connected component induces,

by conjugation, an isomorphism between the vertex groups. A connected groupoid is equivalent to the one-object groupoid formed by any one of its objects and all its automorphisms, i.e. the full subgroupoid consisting of one object x. This groupoid is denoted $1/\operatorname{Aut}(x)$, in accordance with the quotient notation.

It is now clear that for every groupoid X we have an equivalent skeleton:
$$X \simeq \sum_{x \in \pi_0 X} \{x\}/\operatorname{Aut}(x) \simeq \sum_{x \in \pi_0 X} 1/\operatorname{Aut}(x).$$

Here the sum sign denotes disjoint union of groupoids. We stress that although formally we sum over all elements x in the set $\pi_0 X$, when we write $\operatorname{Aut}(x)$ we are referring to x as an object of the groupoid X. As mentioned, for different representatives of the same connected component, these automorphism groups are isomorphic.

Lemma. 3.7. *Two groupoids are equivalent if and only if their skeleta are isomorphic.*

3.8. Integration and 'Fubini'. More generally if $p : X \to B$ is a morphism of groupoids, we can look at the fibre over b for each $b \in \pi_0 B$. The 'inclusion' of the fibre $X_b \to X$ is faithful but not full in general. But $\operatorname{Aut}(b)$ acts on it canonically, and the homotopy quotient
$$X_b/\operatorname{Aut}(b)$$

provides exactly the missing arrows, so as to make the natural morphism $X_b/\operatorname{Aut}(b) \to X$ fully faithful. Since every object $x \in X$ must map to some connected component of B, we find the equivalence

(6) $$X \simeq \sum_{b \in \pi_0 B} X_b/\operatorname{Aut}(b).$$

We shall adopt an integral notation, writing
$$\int^{b \in B} X_b := \sum_{b \in \pi_0 B} X_b/\operatorname{Aut}(b)$$

for such sums. Another useful view of right hand side of (6) is as the Grothendieck construction of the functor

(7) $$\begin{aligned} p' : \pi_0 B &\longrightarrow \boldsymbol{Grpd} \\ x &\longmapsto X_b/\operatorname{Aut}(b). \end{aligned}$$

We shall need the following general Fubini formula (integration along the fibres):

Lemma. 3.9. *Given morphisms of groupoids $X \xrightarrow{f} B \xrightarrow{t} I$, we have*
$$\sum_{b \in \pi_0 B} X_b/\operatorname{Aut}(b) \simeq \sum_{i \in \pi_0 I} \left(\sum_{b \in \pi_0 B_i} X_b/\operatorname{Aut}_i(b) \right)/\operatorname{Aut}(i)$$

In integral notation,

$$\int^{b \in B} X_b \simeq \int^{i \in I} \left(\int^{b \in B_i} X_b \right).$$

Note that $\mathrm{Aut}_i(b)$ denotes the automorphism group of b inside the fibre B_i, not the full automorphism group $\mathrm{Aut}(b)$ in all of B. (Note also that $\pi_0 B_i$ denotes the set of connected components of B_i which is typically different from the set of connected components of B that intersect the fibre: objects in the fibre might be connected only via arrows in B which are not in the fibre.) The proof of the lemma is easy; yet the lemma contains, and automatically takes care of, a lot of automorphism yoga, which without the setting of groupoids tends to become messy.

3.10. Double counting. Applying the integration formula (6) twice we get the following useful double-counting lemma. It can be seen as the groupoid analogue of the double counting in a bipartite graph, held by Aigner [1] as one of the most important principles in enumerative combinatorics.

Lemma. 3.11. *Let A, B, U be groupoids, together with morphisms*

$$B \longleftarrow U \longrightarrow A$$

and write $U_S, {}_T U \subseteq U$ for the (homotopy) fibres over $S \in A$ and $T \in B$ respectively. Then there are equivalences of groupoids

$$\int^{T \in B} {}_T U \;\; \simeq \;\; U \;\; \simeq \;\; \int^{S \in A} U_S.$$

3.12. Slices. We shall need homotopy slices, sometimes called weak slices. First recall the usual notion of slice category: If $\mathscr{C}$ is a category, and $I \in \mathscr{C}$, then the usual slice category $\mathscr{C}_{/I}$ is the category whose objects are morphisms $X \to I$ in $\mathscr{C}$ and whose arrows are commutative triangles

$$
\begin{array}{ccc}
X & \longrightarrow & X' \\
& \searrow \quad \swarrow & \\
& I. &
\end{array}
$$

We are concerned instead with groupoid-enriched categories $\mathscr{C}$, i.e. categories such that for each pair of objects X, Y, the arrows $\mathrm{Hom}(X, Y)$ form a groupoid instead of just a set, and such that composition are functors instead of just functions. This means that between two parallel arrows $X \rightrightarrows Y$ there may be (invertible) 2-cells. The slice category $\mathscr{C}_{/I}$ then has as objects the morphisms $X \to I$; its arrows are triangles

with a 2-cell

(8)

$$X \longrightarrow X'$$

$$\Downarrow$$

$$I.$$

Two such arrows can be composed by pasting the triangles, and altogether the slice is a category (in fat again a groupoid-enriched category, but this will not be important here). If $\mathscr{C}$ is a groupoid then $\mathscr{C}_{/I}$ is again a groupoid.

The basic example is the groupoid-enriched category **Grpd** of all groupoids: the objects are groupoids, the morphisms are functors, and the 2-cells are natural transformations: since we are talking groupoids, the natural transformations are automatically invertible.

3.13. Basic adjoints between slices. Taking homotopy pullback along a morphism of groupoids $f : B' \to B$ defines a functor between the slice categories

$$f^* : \mathbf{Grpd}_{/B} \to \mathbf{Grpd}_{/B'}.$$

This has a homotopy left adjoint

$$f_! : \mathbf{Grpd}_{/B'} \to \mathbf{Grpd}_{/B}$$

and a homotopy right adjoint

$$f_* : \mathbf{Grpd}_{/B'} \to \mathbf{Grpd}_{/B}.$$

The homotopy adjoint properties are expressed by natural equivalences of mapping groupoids

(9) $$\mathbf{Grpd}_{/B}(f_! E', E) \simeq \mathbf{Grpd}_{/B'}(E', f^* E),$$

(10) $$\mathbf{Grpd}_{/B'}(f^* E', E) \simeq \mathbf{Grpd}_{/B}(E', f_* E),$$

which will be invoked at a few occasions.

3.14. I-coloured finite sets, or families of objects in I. Let **Bij** denote the groupoid of finite sets and bijections. We shall need also coloured finite sets, the colours being objects in a groupoid I. We put

$$\widetilde{I} := \mathbf{Bij}_{/I}$$

Hence the objects of $\widetilde{I}$ are groupoid maps $X \to I$, where X is a finite set considered as a groupoid, and the arrows of $\widetilde{I}$ are triangles with a 2-cell as in 8. The groupoid $\widetilde{I}$ can be interpreted as the groupoid of I-coloured finite sets: the map $X \to I$ then associates a 'colour' to each element in X. Note that maps of I-coloured sets are required to be bijective and respect the colour, but only up to specified isomorphism of colours (that's the content of the 2-cell triangle). If $I = 1$ is the

one-point trivial groupoid, we recover $\widetilde{1} \simeq \mathbf{Bij}$ (the case of only one colour).

The groupoid $\widetilde{I}$ can be considered also as the groupoid of families of objects in I. In this case, the finite set X plays a secondary role, it is merely an indexing set for the family. We use this viewpoint for example when we say that a forest is a family of trees. Formally, if $\mathbf{T}$ is the groupoid of trees (cf. below), then the groupoid of forests is

$$\mathbf{F} = \widetilde{\mathbf{T}}.$$

As another important exampe, note that a surjection of sets is just a disjoint union of connected surjections, and a connected surjection is determined by a single non-empty set (mapping to a point), so the groupoid of surjections can be considered as the groupoid of families of non-empty sets and bijections,

$$\mathbf{S} = \widetilde{\mathbf{B}}.$$

It should be mentioned, although we will not need this fact, that $\widetilde{I}$ is the free symmetric monoidal category on I.

4. Trees and forests

4.1. Trees. It was observed in [25] that operadic trees can be conveniently encoded by diagrams of the same shape as polynomial functors. By definition, a *finite rooted tree* is a diagram of finite sets

$$(11) \qquad\qquad A \xleftarrow{\ s\ } M \xrightarrow{\ p\ } N \xrightarrow{\ t\ } A$$

satisfying the following three conditions:

(1) t is injective

(2) s is injective with singleton complement (called the *root* and denoted 1).

With $A = 1 + M$, define the walk-to-the-root function $\sigma : A \to A$ by $1 \mapsto 1$ and $e \mapsto t(p(e))$ for $e \in M$.

(3) $\forall x \in A : \exists k \in \mathbb{N} : \sigma^k(x) = 1$.

The elements of A are called *edges*. The elements of N are called *nodes*. For $b \in N$, the edge $t(b)$ is called the *output edge* of the node. That t is injective is just to say that each edge is the output edge of at most one node. For $b \in N$, the elements of the fibre $M_b := p^{-1}(b)$ are called *input edges* of b. Hence the whole set $M = \sum_{b \in N} M_b$ can be thought of as the set of nodes-with-a-marked-input-edge, i.e. pairs (b, e) where b is a node and e is an input edge of b. The map s returns the marked edge. Condition (2) says that every edge is the input edge of a unique node, except the root edge. Condition (3) says that if you walk towards the root, in a finite number of steps you arrive there. The edges not in the image of t are called *leaves*.

From now on we just say *tree* for 'operadic tree'.

The tree

$$1 \leftarrow 0 \rightarrow 0 \rightarrow 1$$

is the *trivial tree* $\big|$.

4.2. Polynomial functors. The importance of the above tree formalism is that diagrams of shape (11) are precisely what define polynomial endofunctors. The theory of polynomial functors (for which we refer to [19]) is very useful to encode combinatorial structures, types and operations, and covers notions such as species and operads. A diagram of sets or groupoids

$$I \xleftarrow{s} E \xrightarrow{p} B \xrightarrow{t} I$$

defines a polynomial functor

$$\boldsymbol{Grpd}_{/I} \xrightarrow{s^*} \boldsymbol{Grpd}_{/E} \xrightarrow{p_*} \boldsymbol{Grpd}_{/B} \xrightarrow{t_!} \boldsymbol{Grpd}_{/I}.$$

(Here of course we are talking about homotopy slices, and upperstar, lowerstar and lowershriek refer to the adjunctions in 3.13.) In this work we do not need the actual functors, only their representing diagrams. The intuition is that B is a collection of operations, the arity of an operation $b \in B$ is the size of the fibre E_b, and that each operation is typed: the output type of b is $t(b)$, and the input types are the $s(e)$ for $e \in E_b$. We shall see examples of polynomial functors in Sections 8 and 9.

4.3. Morphisms of trees (cf. [25]). A *tree embedding* is by definition a diagram

(12)
$$\begin{array}{ccccccc}
A' & \longleftarrow & M' & \longrightarrow & N' & \longrightarrow & A' \\
{\scriptstyle\alpha}\downarrow & & \downarrow & & \downarrow & & \downarrow{\scriptstyle\alpha} \\
A & \longleftarrow & M & \longrightarrow & N & \longrightarrow & A,
\end{array}$$

where the rows are trees. This is just the notion of cartesian morphism in the category of polynomial endofunctors [19]. The terminology is justified by the fact that each of the components of such a map is necessarily injective; this follows from the tree axioms [25]. Hence the category of trees and tree embeddings, denoted **TEmb**, is mostly concerned with subtrees, but note that it also contains automorphisms of trees.

The fact that the middle square is cartesian means that there is specified, for each node b of the first tree, a bijection between the incoming edges of b and the incoming edges of the image of b. In other words, a tree embedding is arity preserving.

A tree embedding is *root-preserving* when it sends the root to the root. In formal terms, these are diagrams (12) such that also the left-hand square is cartesian.

An *ideal embedding* (or an *ideal subtree*) is a subtree S in which for every edge e, all the edges and nodes above e are also in S. There is one

ideal subtree generated by each edge in the tree. The ideal embeddings are characterised as having also the right-hand square of (12) cartesian.

Ideal embeddings and root-preserving embeddings admit pushouts along each other in the category **TEmb** [25]. The most interesting case is pushout over a trivial tree: this is then the root of one tree and a leaf of another tree, and the pushout is the grafting onto that leaf.

4.4. Decorated trees: P-trees. A very efficient way of encoding and manipulating decorations of trees is in terms of polynomial functors [25] (see also [26, 27, 28, 29]). We fix a polynomial endofunctor P given by a diagram

$$I \leftarrow E \xrightarrow{p} B \rightarrow I,$$

which we keep fixed throughout, until in Sections 8 and 9 where we consider differente choices for P. By definition, a P-tree is a diagram

$$
\begin{array}{ccccccc}
A & \longleftarrow & M & \longrightarrow & N & \longrightarrow & A \\
\downarrow & & \downarrow{\lrcorner} & & \downarrow & & \downarrow \\
I & \longleftarrow & E & \longrightarrow & B & \longrightarrow & I,
\end{array}
$$

where the top row is a tree. The squares are commutative up to isomorphism, and it is important that the isos be specified as part of the structure. Unfolding the definition, we see that a P-tree is a tree whose edges are decorated in I, whose nodes are decorated in B, and with the additional structure of a bijection for each node $n \in N$ (with decoration $b \in B$) between the set of input edges of n and the fibre E_b, subject to the compatibility condition that such an edge $e \in E_b$ has decoration $s(e)$, and the output edge of n has decoration isomorphic to $t(b)$.

Standard examples of P-trees are given in Section 8, and in Section 9 we consider groupoid-polynomial decorated trees arising naturally in quantum field theory, where in order to account for symmetries it is crucial that the representing diagram $I \leftarrow E \rightarrow B \rightarrow I$ be of groupoids, not just sets.

The category of P-trees is the slice category **TEmb**$_{/P}$. The notions of root-preserving and ideal embeddings work the same in this category as in **TEmb**, and again these two classes of maps allow pushouts along each other. Observe that P-trees can have more automorphisms than the underlying tree. For example, if P is given by $I \leftarrow 1 \rightarrow 1 \rightarrow I$, where the groupoid I has one object and vertex group G, then the trivial P-tree $\vert$ has also automorphism group G. This follows easily from the observation that the I-family $1 \rightarrow I$ has autormorphism group G.

4.5. The bialgebra of P-trees. This is precisely the same prescription as for naked trees in 2.3.

4.6. Forests. A forest can be defined as a family of trees, or equivalently as a finite sum of trees in the category of polynomial endofunctors. It is convenient to have also an elementary definition, similar to that of trees.

By definition, a *(finite rooted) forest* is a diagram of finite sets

$$A \xleftarrow{\ s\ } M \xrightarrow{\ p\ } N \xrightarrow{\ t\ } A$$

satisfying the following three conditions:

(1) t is injective

(2) s is injective; denote its complement R (the set of roots).

With $A = R + M$, define the walk-to-the-roots function $\sigma : A \to A$ by being the identity on R, and $e \mapsto t(p(e))$ for $e \in M$.

(3) $\forall x \in A : \exists k \in \mathbb{N} : \sigma^k(x) \in R$.

The interpretations of these axioms are similar to those following the definition of tree.

A *forest embedding* is by definition a diagram like (12), required now separately to be injective (whereas for trees this condition is automatic, for forests absence of the condition gies only etale maps).

An forest embedding is called a *root-preserving embedding* if it induces a bijection between the sets of roots. This is equivalent to being a sum of tree embeddings. By ideal embedding we understand an embedding such that the right-hand square of (12) is cartesian. This means that every edge and node above the subforest is also contained in the subforest. The most important example will be this: for a given tree S, the set of its leaves forms a forest, and the inclusion of this forest into S is an ideal embedding.

Just as for trees, root-preserving embeddings and ideal embeddings allow pushouts along each other (in the category of forests and forest embeddings). The important case is grafting a forest onto the leaves of a tree.

4.7. P-forests. The definition of P-forest if analogous to the definition of P-tree, and again the category of P-forest embeddings can be characterised as the finite-sum completion of $\mathbf{TEmb}_{/P}$ inside the slice category $\mathbf{Poly}_{/P}$.

We fix a polynomial endofunctor P (given by $I \leftarrow E \to B \to I$) and denote by $\mathbf{T}$ the groupoid of P-trees and by $\mathbf{F}$ the groupoid of P-forests.

4.8. Leaves and roots. To any P-tree we can associate it set of leaves; this is naturally an I-coloured set, defining a morphisms of groupoids called the *leaf map*,

$$L : \mathbf{T} \to \widetilde{I}.$$

An object in $\widetilde{I}$ can be interpreted as a *leaf profile*, and we can ask for those trees with a given leaf profile $N \in \widetilde{I}$. This is the homotopy fibre

$$
\begin{array}{ccc}
{}_N\mathbf{T} & \longrightarrow & \mathbf{T} \\
\downarrow & & \downarrow \\
1 & \xrightarrow{\ulcorner N \urcorner} & \widetilde{I}.
\end{array}
$$

Let $\mathbf{F}$ denote the groupoid of P-forests. There is a natural morphism, the *root map*

$$R : \mathbf{F} \to \widetilde{I},$$

which to a forest associates its I-coloured set of roots. For a fixed colour $N : X \to I$, the N-fibre,

$$
\begin{array}{ccc}
\mathbf{F}_N & \longrightarrow & \mathbf{F} \\
\downarrow & & \downarrow \\
1 & \xrightarrow{\ulcorner N \urcorner} & \widetilde{I}
\end{array}
$$

has the following characterisation:

Lemma. 4.9.

$$\mathbf{F}_N \simeq \boldsymbol{Grpd}_{/I}(N, \mathbf{T}).$$

Proof. Recall that the forest root map $\mathbf{F} \to \widetilde{I}$ is the family functor applied to the tree root map, that is, $\widetilde{R} : \widetilde{\mathbf{T}} \to \widetilde{I}$. Hence we can write, by adjunction:

$$\mathbf{F}_N \simeq \ulcorner N \urcorner^* \widetilde{R} \simeq \boldsymbol{Grpd}(1, \ulcorner N \urcorner^* \widetilde{R}) \simeq \boldsymbol{Grpd}_{/\widetilde{I}}(\ulcorner N \urcorner, \widetilde{R}).$$

It remains to establish the equivalence

$$\boldsymbol{Grpd}_{/\widetilde{I}}(\ulcorner N \urcorner, \widetilde{R}) \simeq \boldsymbol{Grpd}_{/I}(N, R).$$

Consider the commutative diagram

$$
\begin{array}{ccc}
\boldsymbol{Grpd}_{/I}(N, R) & \longrightarrow & \boldsymbol{Grpd}_{/\widetilde{I}}(\ulcorner N \urcorner, \widetilde{R}) \\
\downarrow & & \downarrow \\
\boldsymbol{Grpd}(X, \mathbf{T}) & \longrightarrow & \boldsymbol{Grpd}(1, \widetilde{\mathbf{T}}) \\
\downarrow & & \downarrow \\
\boldsymbol{Grpd}(X, I) & \longrightarrow & \boldsymbol{Grpd}(1, \widetilde{I})
\end{array}
$$

in which the vertical maps form the standard slice fibre sequences; the bottom vertical maps are postcomposition with R and $\widetilde{R}$, respectively. Each of the horizontal maps sends a family to its name. Since the bottom square is a pullback, we conclude that the top map is an equivalence. $\square$

Integrating over the fibres, we therefore find

$$\mathbf{F} \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \simeq \int^{N \in \widetilde{I}} \boldsymbol{Grpd}_{/I}(N, \mathbf{T}) \simeq \exp(\mathbf{T}),$$

corresponding again to the fact that forests are disjoint unions of trees.

5. FAÀ DI BRUNO EQUIVALENCE IN THE GROUPOID OF TREES

In this section we prove our main theorem, the equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$:

$$\int^{T \in \mathbf{T}} \mathrm{cut}(T) \simeq \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N \mathbf{T},$$

In Section 7 we will obtain the Faà di Bruno formula for the Green function in the bialgebra of trees by taking relative cardinality of both sides.

We fix a polynomial endofunctor P given by

$$I \leftarrow E \rightarrow B \rightarrow I.$$

Throughout this section the word 'tree' will mean a P-tree, a 'forest' will mean P-forest. Recall that we denote the categories of P-trees and P-forests by $\mathbf{T}$ and $\mathbf{F}$ respectively.

Recall (3.14) that $\widetilde{I}$ denotes the groupoid of finite sets over I and their isomorphisms. We have canonical morphisms

(13)

$$
\begin{array}{ccccc}
 & \mathbf{F} & & \mathbf{T} & \\
{}^{L}\swarrow & & {}^{R}\searrow \; {}^{L}\swarrow & & \searrow {}^{R} \\
\widetilde{I} & & \widetilde{I} & & I
\end{array}
$$

given by the leaf maps and the root maps. The map L associates to a tree or forest its I-coloured set of leaf edges, while R associates to a forest the I-coloured set of root edges and to a tree the colour of the unique root edge.

We use two-sided subscript notation to indicate the fibres of these maps. Hence, we denote by $\mathbf{T}_k$ the groupoid of trees with root colour $k \in I$ (or more precisely: with root colour isomorphic to k, and with a specified iso) and by $\mathbf{F}_N$ the groupoid of forests whose set of roots is $N \in \widetilde{I}$ (again, up to a specified iso). Similarly, for the fibres of L, we write ${}_N\mathbf{F}$ and ${}_N\mathbf{T}$ for the groupoids of forests and trees with leaf profile N. These are the groupoids of P-forests or P-trees with specified I-bijections between their leaves and N.

5.1. The groupoid of trees with a cut. In Section 2.3 we already defined a cut in a tree T to be a subtree S containing the root. For varying T, these form a groupoid which we denote $\mathbf{C}$: its objects are the root preserving inclusions $c : S \rightarrowtail T$, and its arrows are the isomorphisms of such arrows, i.e. commutative diagrams

$$(14) \qquad \begin{array}{ccc} T & \xrightarrow{\ \tau\ }_{\cong} & T' \\ c \big\uparrow & & \big\uparrow c' \\ S & \xrightarrow[\ \cong\ ]{\sigma} & S'. \end{array}$$

This groupoid comes equipped with canonical morphisms $m, r : \mathbf{C} \to \mathbf{T}$ and $w : \mathbf{C} \to \mathbf{F}$: when applied to a cut $c : S \rightarrowtail T$, the map m returns the total tree T, the map r returns the subtree (i.e. the tree S_c found below the cut), and the map w returns the forest P_c consisting of the ideal trees in T generated by the leaves of S. These maps and the morphisms L, R in (13) above form a commutative diagram

$$(15)$$

We denote by $_T\mathbf{C}$, $\mathbf{C}_S$ and $\mathbf{C}_N$ the fibres of the functors m, r and $L \circ r$.

For a fixed tree T, the arrows of the groupoid $_T\mathbf{C}$ are

$$\begin{array}{ccc} T & \xrightarrow{\ =\ } & T \\ \big\uparrow & & \big\uparrow \\ R & \xrightarrow[\ \cong\ ]{} & R' \end{array}$$

and since the vertical maps are monomorphisms, we see that this groupoid has no nontrivial automorphisms, and hence is equivalent to a discrete groupoid which we denote by $\mathrm{cut}(T)$; we refer to it objects as the cuts of T. In summary,

$$_T\mathbf{C} \ \simeq \ \pi_0(_T\mathbf{C}) \ = \ \mathrm{cut}(T).$$

Together with the double-counting lemma 3.11:

Lemma. 5.2. *We have equivalences of groupoids*

$$\int^{T \in \mathbf{T}} \mathrm{cut}(T) \ \simeq \ \int^{T \in \mathbf{T}} {}_T\mathbf{C} \ \simeq \ \mathbf{C} \ \simeq \ \int^{S \in \mathbf{T}} \mathbf{C}_S \ \simeq \ \int^{N \in \widetilde{I}} \mathbf{C}_N$$

The following Main Lemma states that the solid square face of (15) is a (homotopy) pullback square and enables us to identify the fibres $\mathbf{C}_S$ and $\mathbf{C}_N$.

Lemma. 5.3. *The canonical morphism to the product*

$$(w, r)\colon \mathbf{C} \longrightarrow \mathbf{F} \times \mathbf{T}$$

that sends $c : S \rightarrowtail T$ to (P_c, S_c), induces an equivalence

$$\mathbf{C} \simeq \mathbf{F} \times_{\widetilde{I}} \mathbf{T}.$$

Proof. Starting with an object $(P, S, L(S) \overset{\lambda}{\cong} R(P))$ of the pullback, we construct a tree with a cut by *grafting*. The isomorphism λ may be regarded as a root-preserving embedding of forests

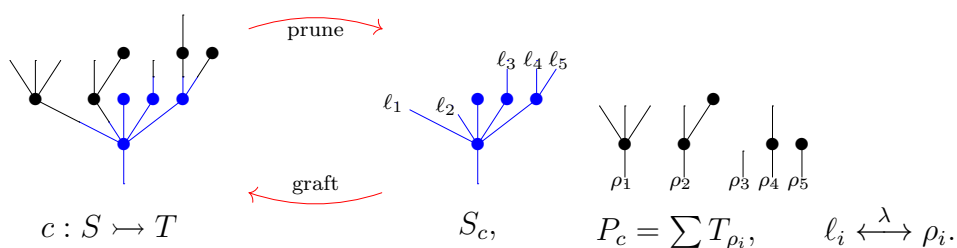$$LS \rightarrowtail P = \sum_{\ell \in LS} T_{\lambda(\ell)},$$

and we construct the pushout in the category of forests of this map and the ideal sub-forest embedding $LS \to S$,

$$
\begin{array}{ccc}
\sum T_{\lambda(\ell)} & \longrightarrow & T \\
\big\uparrow & & \big\uparrow \\
LS & \longrightarrow & S
\end{array}
$$

to obtain a root-preserving embedding $S \rightarrowtail T$ in the sense of 4.6. Note that since the forest S is a tree, T is again a tree. This assignment is functorial: an isomorphism (ρ, σ) from (P, S, λ) to (P', S', λ) induces an isomorphism of pushouts $\tau : T \cong T'$ extending σ as in (14).

In the reverse direction, we *prune* a root-preserving inclusion $S \rightarrowtail T$ to obtain $(\sum T_\ell, S, \mathrm{Id})$ where T_ℓ is the ideal subtree of T generated by the image of the leaf edge ℓ in T. An isomorphism of root-preserving inclusions (14) is sent to (τ, σ) where $\tau_\ell : T_\ell \to T'_{\tau\ell}$ is the restriction of τ to the ideal subtree T_ℓ. □

$$c : S \rightarrowtail T \qquad\qquad S_c, \qquad P_c = \sum T_{\rho_i}, \qquad \ell_i \overset{\lambda}{\longleftrightarrow} \rho_i.$$

Corollary. 5.4. *For $S \in \mathbf{T}$ and $N \in \widetilde{I}$ we have equivalences of groupoids*

$$\mathbf{C}_S \simeq (\mathbf{F} \times_{\widetilde{I}} \mathbf{T})_S \simeq \mathbf{F}_{LS},$$
$$\mathbf{C}_N \simeq \mathbf{F}_N \times {}_N\mathbf{T}.$$

Combining the previous results, we arrive at our main theorem:

Theorem. 5.5. *We have equivalences of groupoids*

$$\int^{T\in\mathbf{T}} \operatorname{cut}(T) \simeq \int^{S\in\mathbf{T}} \mathbf{F}_{LS}$$

$$\simeq \int^{N\in\widetilde{I}} \mathbf{F}_N \times {}_N\mathbf{T}.$$

We can regard this as an equivalence of groupoids over $\mathbf{F} \times \mathbf{T}$. For fixed T, the map from $\operatorname{cut}(T)$ to $\mathbf{F} \times \mathbf{T}$ is precisely

$$\sum_{c\in\operatorname{cut}(T)} 1 \xrightarrow{\ulcorner(P_c,S_c)\urcorner} \mathbf{F} \times \mathbf{T} .$$

To emphasise this, we can reformulate the result as

$$(16) \qquad \int^{T\in\mathbf{T}} \sum_{c\in\operatorname{cut}(T)} \{P_c\} \times \{S_c\} \simeq \int^{N\in\widetilde{I}} \mathbf{F}_N \times {}_N\mathbf{T}$$

Extracting the algebraic version of the Faà di Bruno formula 7.3 from 5.5 will be a matter of taking cardinality in a certain sense, which we explain in the next section.

If we take the fibres of the equivalence given in Theorem 5.5, over a fixed colour $v \in I$, we obtain:

Corollary. 5.6. *We have equivalences of groupoids*

$$\int^{T\in\mathbf{T}_v} \operatorname{cut}(T) \simeq \int^{N\in\widetilde{I}} \mathbf{F}_N \times {}_N\mathbf{T}_v.$$

6. GROUPOID CARDINALITY

6.1. Finiteness conditions. A groupoid X is called *finite* when $\pi_0(X)$ is a finite set and each $\pi_1(x)$ is a finite group. A morphism of groupoids is called finite when all its fibres are finite.

6.2. Cardinality. [2] The *cardinality* of a finite groupoid (sometimes called *groupoid cardinality* or *homotopy cardinality* if there is any danger of confusion) is the nonnegative rational number given by the formula

$$|X| := \sum_{x\in\pi_0 X} \frac{1}{|\operatorname{Aut}(x)|}$$

Here $|\operatorname{Aut}(x)|$ denotes the order of the vertex group at x. This is independent of the choice of the x in the same connected component since an arrow between two choices induces an isomorphism of vertex groups. The cardinality of a groupoid coincides with that of any skeleton, so the following fundamental result is clear from Lemma 3.7:

Lemma. 6.3. *Equivalent groupoids have the same cardinality.*

If X is a finite set considered as a groupoid, then the groupoid cardinality coincides with the set cardinality. If G is a group considered as a one-object groupoid, then the groupoid cardinality is the inverse of the order of the group. The groupoid cardinality is a standard construction in physics and combinatorics: you sum over the different (isomorphism classes of) objects and for each object divide out by the order of its symmetry group.

We have the following fundamental formulae for cardinality of sums and products of groupoids:

$$|X + Y| = |X| + |Y|$$
$$|X \times Y| = |X| \times |Y|$$

extending the analogous results for the cardinality of finite sets.

The following is one important feature of homotopy quotients and cardinality.

Lemma. 6.4. *For any action of a finite group G on a finite groupoid X, we have*

$$|X/G| = |X| \, / \, |G|$$

where $|G|$ denotes the order of the group G.

6.5. Cardinalities of families. For the sake of taking cardinalities we shall need the following 'numerical' description of the groupoid $\widetilde{I}$ of families of objects in I, cf. 3.14.

Let $v_1, \ldots, v_s$ be representatives of the isoclasses in I. Then every family

$$N : X \to I$$

is isomorphic to a sum (in the category of sets over I) of families of the kind $\ulcorner v_i \urcorner : 1 \to I$. Hence for uniquely determined natural numbers n_i we have

$$N \cong \sum_{i=1}^{s} n_i \ulcorner v_i \urcorner.$$

It follows that

$$\pi_0(\widetilde{I}) \simeq \mathbb{N}^s.$$

We compute the vertex group. The automorphism group of $\ulcorner v_i \urcorner : 1 \to I$ is $\mathrm{Aut}(v_i)$ and that of $n_i \ulcorner v_i \urcorner$ is $n_i! \, \mathrm{Aut}(v_i)^{n_i}$, since each point contributes with a factor $\mathrm{Aut}(v_i)$, and since the points can also be permuted. Altogether, we have

$$(17) \qquad\qquad \mathrm{Aut}(N) \cong \prod_{i=1}^{s} n_i! \, \mathrm{Aut}(v_i)^{n_i},$$

and the groupoid $\widetilde{I}$ can be described as

$$\widetilde{I} \simeq \sum_{(n_1,\ldots,n_s) \in \mathbb{N}^s} \frac{1}{\prod_i n_i! \operatorname{Aut}(v_i)^{n_i}}$$

6.6. Relative cardinality. Groupoid cardinality makes sense for more general groupoids than the finite ones: for example, the groupoid of finite sets and bijections has cardinality $\sum_{n \geq 0} \frac{1}{n!} = e$, see Baez–Dolan [2].

We shall instead make use of relative cardinality, which refers to the situation where one groupoid X is relatively finite over another groupoid, i.e. we have a morphism $p : X \to B$ with finite fibres. This notion is from [3]. In this situation we define the *relative cardinality* of X relative to B to be the following element in the completed vector space spanned by the symbols δ_b for $b \in \pi_0(B)$:

$$|p| := |X|_B := \sum_{b \in \pi_0 B} \frac{|X_b|}{|\operatorname{Aut}(b)|} \cdot \delta_b.$$

The notations $|X|_B$ is potentially ambiguous; it assumes the morphism $X \to B$ is clear from the context. Since the morphism has finite fibres X_b, the coefficients are well-defined nonnegative rational numbers.

The vector space spanned by the δ_b is nothing but the space of functions $\pi_0 B \to \mathbb{Q}$ with finite support, and we have an isomorphism between the completed vector space and $\mathbb{Q}^{\pi_0 B}$. For each $b \in \pi_0 B$ we identify the cardinality of the inclusion $\ulcorner b \urcorner : 1 \to B$ with a function

$$\delta_b = |1|_{\ulcorner b \urcorner} \; : \; \pi_0 B \; \longrightarrow \; \mathbb{Q}$$
$$x \; \longmapsto \; \begin{cases} 1 & \text{if } x \simeq b \\ 0 & \text{otherwise.} \end{cases}$$

Hence we identify the relative cardinality of $X \to B$ with the function

$$\pi_0 B \; \longrightarrow \; \mathbb{Q}$$
$$b \; \longmapsto \; |X_b| / |\operatorname{Aut}(b)| .$$

6.7. Relative cardinality as left Kan extension along π_0. We give a highbrow explanation of the above definition, which shows that the factor $1/|\operatorname{Aut}(b)|$ is not arbitrary, or just a convention, but in fact is forced upon us by general principles.

Any morphism of groupoids $p : X \to B$ naturally defines a groupoid-valued presheaf

$$B^{\mathrm{op}} \; \longrightarrow \; \boldsymbol{Grpd}$$
$$b \; \longmapsto \; X_b$$

which, composed with absolute cardinality $|-| : \boldsymbol{Grpd} \to \mathbb{Q}$ yields a function on B. However, we want our function spaces to be indexed

by *isomorphism classes* of objects in B, not by the groupoid B itself. Therefore we need to pass to $\pi_0 B$. The correct way to achieve this it to take left Kan extension along the projection map $B \to \pi_0 B$ of the groupoid valued presheaf. This is a standard construction in category theory and geometry; in the present case it has a very explicit description: it is obtained by first postcomposing the morphism p with the projection, and then taking the corresponding groupoid-valued presheaf

$$(\pi_0 B)^{\mathrm{op}} \; \longrightarrow \; \mathbf{Grpd}$$
$$b \; \longmapsto \; X_b / \operatorname{Aut}(b)$$

This automatically produces the quotient, as is readily seen by the pullback diagram

$$
\begin{array}{ccc}
E_b / \operatorname{Aut}(b) & \longrightarrow & E \\
\downarrow & & \downarrow{\scriptstyle p} \\
\{b\} / \operatorname{Aut}(b) & \longrightarrow & B \\
\downarrow & & \downarrow \\
\{b\} & \longrightarrow & \pi_0 B.
\end{array}
$$

The relative cardinality of $X \to B$ is now recovered by composing the presheaf $\pi_0 B \to \mathbf{Grpd}$ with the absolute cardinality, yielding the required function $\pi_0 B \to \mathbb{Q}$.

6.8. Properties of relative cardinality. When taking relative cardinality over a product of groupoids, $B \times B'$, the formal symbols are indexed by $(b, b') \in \pi_0 B \times \pi_0 B' \simeq \pi_0(B \times B')$. We shall then use notation $\delta_b \otimes \delta'_b$ instead of $\delta_{(b,b')}$. We shall need the following obvious compatibility with products: if

$$
\begin{array}{ccccc}
X \times X' & & X & & X' \\
\downarrow & = & \downarrow & \times & \downarrow \\
B \times B' & & B & & B'
\end{array}
$$

then

$$|X \times X'|_{B \times B'} = |X|_B \otimes |X'|_{B'} \, .$$

Consider the groupoid morphism $X \to X/G$ given by the action of a finite group on a groupoid. Then

$$|X/G|_{X/G} = \frac{|X|_{X/G}}{|G|}$$

and we have the following generalisation of Lemma 6.4:

Lemma. 6.9. *For any action of a finite group G on a groupoid X and a finite morphism $X/G \to A$, we have*

$$|X/G|_A = |X|_A / |G|$$

where $|G|$ denotes the order of the group G.

We need the following transitivity property of relative cardinality:

Lemma. 6.10. *Given groupoid morphisms $X \overset{p}{\to} B \overset{t}{\to} I$ with finite fibres, the relative cardinality of p is obtained from those of the restrictions $p_v : X_v \to B_v$,*

$$|p| = |X|_B = \sum_{v \in \pi_0 I} \frac{|p_v|}{|\mathrm{Aut}(v)|}.$$

Also the relative cardinality of X over I is obtained from the relative cardinality over B by substituting $\delta_{t(b)}$ for each δ_b. That is:

$$|X|_I = \sum_{b \in \pi_0 B} \frac{|X_b|}{|\mathrm{Aut}(b)|} \, \delta_{t(b)}.$$

In particular, any groupoid can be measured over itself via the identity morphism $\mathrm{Id} : X \to X$:

$$|X|_X = \sum_{x \in \pi_0 X} \frac{1}{|\mathrm{Aut}(x)|} \, \delta_x$$

Hence we get the following useful result.

Corollary. 6.11. *For $p : X \to B$ we have*

$$|X|_B = \sum_{x \in \pi_0 X} \frac{1}{|\mathrm{Aut}(x)|} \, \delta_{p(x)}.$$

7. The Faà di Bruno formula in the bialgebra of trees

7.1. Abstract Green functions as relative cardinality. There is a general notion of Green function which include the power series A in the Faà di Bruno algebra $\mathcal{F}$ and also our Green functions of P-trees. Let X be a groupoid with finite vertex groups, and consider first the relative cardinality of the identity functor $X \to X$,

$$\sum_{x \in \pi_0 X} \frac{1}{|\mathrm{Aut}(x)|} \cdot \delta_x.$$

Equally natural is to consider the inclusion $X \hookrightarrow \widetilde{X}$ into the groupoid of families of objects in X (cf. 3.14). We define the *Green function* as

the relative cardinality of this inclusion

$$
\begin{aligned}
G &= \sum_{x \in \pi_0 \widetilde{X}} \frac{|X_x|}{|\mathrm{Aut}(x)|} \cdot \delta_x \\
&= \sum_{x \in \pi_0 X} \frac{1}{|\mathrm{Aut}(x)|} \cdot \delta_x
\end{aligned}
$$

since the summand is zero when $x \notin \pi_0 X$. As an element of the ring $\mathbb{Q}^{\pi_0 \widetilde{X}}$, the Green function is

$$
\begin{aligned}
G : \pi_0 \widetilde{X} &\longrightarrow \mathbb{Q} \\
x &\longmapsto \begin{cases} 1/|\mathrm{Aut}(x)| & \text{if } x \in \pi_0 X \\ 0 & \text{otherwise} \end{cases}
\end{aligned}
$$

We observe the natural isomorphisms

$$
\mathbb{Q}^{\pi_0 \widetilde{X}} \cong \mathrm{Sym}(\mathbb{Q}^{\pi_0 X}) \cong \mathbb{Q}[[\delta_x]]_{x \in \pi_0 X}
$$

between the ring of functions and the power series in symbols δ_x for $x \in \pi_0 X$. This restricts to an isomorphism from those functions with finite support to the ring of polynomials.

7.2. Definition of the Green functions of trees. We define the total Green function as the relative cardinality of $\mathbf{T} \to \widetilde{\mathbf{T}} = \mathbf{F}$:

$$
G := \sum_{T \in \pi_0 \mathbf{T}} \frac{\delta_T}{|\mathrm{Aut}(T)|} \quad \in \quad \mathbb{Q}[[\delta_T; T \in \pi_0 \mathbf{T}]].
$$

We also define an individual Green function for each possible (isomorphism class of) root colour $v \in \pi_0 I$,

$$
G_v := \sum_{T \in \pi_0(\mathbf{T}_v)} \frac{\delta_T}{|\mathrm{Aut}_v(T)|}.
$$

Here the automorphism group $\mathrm{Aut}_v(T)$ consists of those automorphisms of T which fix the root colour v. This is the relative cardinality of the inclusion $\mathbf{T}_v \to \mathbf{T} \to \mathbf{F}$.

It follows from Lemma 6.10 that we have the relationship

$$
G = \sum_{v \in \pi_0 I} \frac{G_v}{|\mathrm{Aut}(v)|}.
$$

Let $s := |\pi_0 I|$ be the number of colours, and let $\mathbf{n} = (n_1, \ldots, n_s) \in \mathbb{N}^s$ be a multiindex, parametrising an isoclass of objects N in $\widetilde{I}$. Consider the relative cardinality of the inclusion of the homotopy fibre $_N \mathbf{T} \to \mathbf{T}$,

$$
G_{\mathbf{n}} := \sum_{T \in \pi_0(_N \mathbf{T})} \frac{\delta_T}{|\mathrm{Aut}_N(T)|}.
$$

We also consider the summands of the Green function corresponding to all trees with n_v leaves of each colour $v \in \pi_0 I$,

$$g_{\mathbf{n}} := \sum_{T \in \pi_0 \mathbf{T}, \, LT \cong N} \frac{\delta_T}{|\operatorname{Aut} T|}.$$

This is the relative cardinality of the *full subcategory* of $\mathbf{T}$ whose objects are those trees T with leaf profile N. This is equivalent to the weak quotient $_N\mathbf{T}/\operatorname{Aut} N$ of the homotopy fibre by the canonical action of $\operatorname{Aut} N$. Clearly,

$$g_{\mathbf{n}} \;=\; G_{\mathbf{n}}/|\operatorname{Aut} N|.$$

and hence

$$G = \sum_{\mathbf{n} \in \mathbb{N}^s} g_{\mathbf{n}}.$$

Theorem. 7.3. *The following Faà di Bruno formula holds for the Green function in the bialgebra of trees.*

(18)
$$\Delta(G) = \sum_{\mathbf{n} \in \mathbb{N}^s} G^{\mathbf{n}} \otimes g_{\mathbf{n}}.$$

Here $G^{\mathbf{n}}$ is to be interpreted as the product

$$G^{\mathbf{n}} = \prod_{v \in \pi_0 I} G_v^{n_v}.$$

To prove the theorem we first need a result about forests. Recall that the multiindices $\mathbf{n}$ classify the isomorphism classes of objects $N \in \widetilde{I}$.

Lemma. 7.4. *Let $N : X \to I$ be an object of $\widetilde{I}$ of class $\mathbf{n} = (n_1, \ldots, n_s)$. Then*

$$\mathbf{F}_N \simeq \prod_{i=1}^s \mathbf{T}_{v_i}{}^{n_i}$$

Proof. Combining Lemma 4.9 with 6.5, we find

$$\begin{aligned}
\mathbf{F}_N \;&\simeq\; \boldsymbol{Grpd}_{/I}(X, R) \\
&\simeq\; \boldsymbol{Grpd}_{/I}\left(\sum_{i=1}^s n_i \ulcorner v_i \urcorner, R\right) \\
&\simeq\; \prod_{i=1}^s \boldsymbol{Grpd}_{/I}(\ulcorner v_i \urcorner, R)^{n_i}.
\end{aligned}$$

Now $\ulcorner v_i \urcorner$ is the 'lowershriek' $\ulcorner v_i \urcorner_!(1)$ and so by adjunction (9) we have

$$\simeq\; \prod_{i=1}^s \boldsymbol{Grpd}(1, \ulcorner v_i \urcorner^* R)^{n_i} \;\simeq\; \prod_{i=1}^s \mathbf{T}_{v_i}{}^{n_i}$$

$\square$

Corollary. 7.5.

$$|\mathbf{F}_N| = G^{\mathbf{n}} = \prod_{i=1}^{s} G_{v_i}{}^{n_i}$$

7.6. Proof of the theorem. The left-hand side $\Delta(G)$ of (18) is the relative cardinality of the left-hand side of (16). It remains to show that the right-hand side of (18) is the relative cardinality of the right-hand side of (16). We have

$$\left| \int^{N \in \widetilde{I}} \mathbf{F}_N \times {}_N\mathbf{T} \right| = \sum_{N \in \pi_0 \widetilde{I}} |\mathbf{F}_N| \otimes |{}_N\mathbf{T}| / |\mathrm{Aut}\, N|$$

$$= \sum_{\mathbf{n} \in \mathbb{N}^s} G^{\mathbf{n}} \otimes g_{\mathbf{n}}.$$

$\square$

7.7. Summands of Green functions. If $v \in I$ and $\mathbf{n} \in \mathbb{N}^s$ is a multiindex parametrising an isoclass of an object $N \in \widetilde{I}$, define the Green function

$$g_{\mathbf{n},v} := |{}_N\mathbf{T}_v / \mathrm{Aut}\, N| \,.$$

We have

$$g_{\mathbf{n}} = \sum_{v \in \pi_0 I} \frac{g_{\mathbf{n},v}}{|\mathrm{Aut}(v)|}$$

and hence

$$G = \sum_{\mathbf{n}} \sum_{v \in \pi_0 I} \frac{g_{\mathbf{n},v}}{|\mathrm{Aut}(v)|}$$

Taking relative cardinality of Corollary 5.6 then gives

Theorem. 7.8. *For $v \in I$ and $\mathbf{n} \in \mathbb{N}^s$ we have*

$$\Delta(G_v) = \sum_{\mathbf{n} \in \mathbb{N}^s} G^{\mathbf{n}} \otimes g_{\mathbf{n},v}.$$

This is the version that most closely resembles the multi-variate Faà di Bruno formula and the formula of van Suijlekom.

8. Examples

In this section we specialise to some standard examples of the polynomial endofunctor P, and compare with the classical Faà di Bruno bialgebra. Fancier examples, more relevant to quantum field theory, are given in Section 9.

8.1. Naked trees. Consider the polynomial functor P represented by

$$1 \leftarrow \mathbf{Bij}' \rightarrow \mathbf{Bij} \rightarrow 1,$$

where $\mathbf{Bij}'$ denotes the groupoid of finite pointed sets and basepoint-preserving bijections, and 1 denotes a singleton set. This is the exponential functor

$$P(X) = \exp(X) = \sum_{n \in \mathbb{N}} X^n/n!.$$

There is a fibre of each finite cardinality $n \in \mathbb{N}$, and for every tree $A \leftarrow M \to N \to A$ there is a unique P-decoration

$$
\begin{array}{ccccccc}
A & \longleftarrow & M & \longrightarrow & N & \longrightarrow & A \\
\downarrow & & \downarrow{\scriptstyle\lrcorner} & & \downarrow & & \downarrow \\
1 & \longleftarrow & \mathbf{Bij}' & \longrightarrow & \mathbf{Bij} & \longrightarrow & 1
\end{array}
$$

(since a node of arity n must map to $n \in \mathbf{Bij}$, and since the choices of where to map the incoming edges to the fibre over n are all uniquely isomorphic). It follows that in this case P-trees are essentially the same thing as the naked trees defined in 4.1 (in the precise sense that the groupoid of P-trees is equivalent to the groupoid of naked trees).

8.2. Cyclic trees. If P is the polynomial endofunctor

$$1 \leftarrow \mathbb{C}' \to \mathbb{C} \to 1,$$

where $\mathbb{C}$ is the groupoid of finite cyclically ordered sets, and $\mathbb{C}'$ is the groupoid of finite cyclically ordered pointed sets (that's canonically equivalent to the $\mathbb{N}'$ of the following example), then the notion of P-tree is that of cyclic tree.

8.3. Planar trees. Consider the polynomial functor P represented by

$$1 \leftarrow \mathbb{N}' \to \mathbb{N} \to 1,$$

where $\mathbb{N}$ is the (discrete) groupoid of finite ordered sets, and $\mathbb{N}'$ is the (discrete) groupoid of finite ordered with a marked point, so that the fibre of the middle map is naturally a linearly ordered set). This functor is the geometric series

$$P(X) = \frac{1}{1 - X} = \sum_{n \in \mathbb{N}} X^n.$$

In this case the P-trees

$$
\begin{array}{ccccccc}
A & \longleftarrow & M & \longrightarrow & N & \longrightarrow & A \\
\downarrow & & \downarrow{\scriptstyle\lrcorner} & & \downarrow & & \downarrow \\
1 & \longleftarrow & \mathbb{N}' & \longrightarrow & \mathbb{N} & \longrightarrow & 1
\end{array}
$$

are naturally planar trees, since the cartesian square in the middle equips the incoming edges of each node in the tree with a linear order.

Note that the resulting bialgebra of planar trees is still commutative, unlike the planar-tree Hopf algebra studied by Foissy [17] and others. Since P-trees are rigid (this is true in general when P is represented

by discrete groupoids), there are no symmetries, so the Green function is the just the sum of all the formal symbols,

$$G = \sum_{T \in \pi_0 \mathbf{T}} \delta_T.$$

8.4. Planar binary trees. Consider now the diagram

$$1 \leftarrow 2 \rightarrow 1 \rightarrow 1$$

representing the polynomial functor $P(X) = 1 + X^2$. In this case P-trees are planar binary trees.

8.5. Injections. For the constant polynomial functor $P(X) = 1$, represented by

$$1 \leftarrow 0 \rightarrow 1 \rightarrow 1,$$

there are two possible P-trees:

$$x \mid \qquad y \, \pmb{\uparrow}$$

P-forests are disjoint unions of these. The groupoid $\mathbf{F}$ of P-forests is naturally equivalent to the groupoid whose objects are injections between finite sets, and whose arrows are the isomorphisms between such. The associated Faà di Bruno bialgebra is $\mathbb{Q}[\delta_x, \delta_y]$, with the comultiplication given by

$$\Delta(\delta_x) = \delta_x \otimes \delta_x$$
$$\Delta(\delta_y) = 1 \otimes \delta_y + \delta_y \otimes \delta_x.$$

Expanding we find

$$\Delta(\delta_y^n) = \sum_{k \leq n} \binom{n}{k} \delta_y^k \otimes \delta_y^{n-k} \delta_x^k.$$

After passing to the reduction (putting $x = 1$) we get the usual binomial Hopf algebra. The Green function is

$$G = \delta_x + \delta_y,$$

with $g_0 = \delta_y$ and $g_1 = \delta_x$, and the Faà di Bruno formula is immediate.

8.6. Linear trees. The identity functor $P(X) = X$ is represented by

$$1 \leftarrow 1 \rightarrow 1 \rightarrow 1.$$

Now P-trees are linear trees. We take a variable x_n for the isoclass of the linear tree with n nodes, and find the comultiplication formula

$$\Delta(x_n) = \sum_{i=0}^{n} x_i \otimes x_{n-i};$$

this is the ladder Hopf algebra, studied for example in [37].

8.7. Trivial trees. Consider the polynomial functor

$$P = (I \leftarrow 0 \rightarrow 0 \rightarrow I).$$

where I is a discrete groupoid. The only P-trees are the trivial trees, one for each $x \in \pi_0 I$. The groupoids of P-trees and P-forests are I and $\widetilde{I}$ respectively. In $\mathbb{Q}[\pi_0 I]$ all generators are grouplike, and we have

$$G = \sum_{x \in \pi_0 I} x$$

$$\Delta(G) = \sum_{x \in \pi_0 I} x \otimes x \;\; = \;\; \sum_{x \in \pi_0 I} |I_x \times {}_x I| \;\; = \;\; \sum_{x \in \pi_0 \widetilde{I}} |\widetilde{I}_x \times {}_x I|$$

(This is the monoid algebra on the free commutative monoid on $\pi_0 I$.)

8.8. Effective trees. Consider the polynomial functor represented by

$$1 \leftarrow \mathbf{B}' \rightarrow \mathbf{B} \rightarrow 1,$$

where $\mathbf{B}$ is the groupoid of non-empty finite sets and bijections (and $\mathbf{B}'$ the groupoid of non-empty finite pointed sets and basepoint-preserving bijections). The resulting endofunctor is $P(X) = \exp(X) - 1$. In this case P-trees are naked trees with no nullary operations, sometimes called 'effective' trees. These are the key to understanding the relationship with the classical Faà di Bruno bialgebra, cf. 1.2, as explained below.

Since effective trees have no nullary nodes, they always have a non-empty set of leaves, and therefore the leaf map can be seen to take values in $\mathbf{B}$. Furthermore, for each $n \in \mathbf{B}$, the homotopy fibre ${}_n\mathbf{T} \subset \mathbf{T}$ is discrete, since if an automorphism of a effective tree fixes the leaves then it fixes the whole tree.

The sub-bialgebra $\mathcal{B}_{\mathrm{eff}}$ of $\mathcal{B}$ is the polynomial algebra on the isomorphism classes of effective trees.

8.9. Stable trees. In a similar vein, we can consider P-trees for the polynomial functor $P(X) = \exp(X) - 1 - X$, represented by

$$1 \leftarrow \mathbf{Y}' \rightarrow \mathbf{Y} \rightarrow 1,$$

where $\mathbf{Y}$ is the groupoid of finite sets of cardinality at least 2. These are naked trees with no nullary and no unary nodes, called *reduced trees* by Ginzburg and Kapranov [20]. We adopt instead the term *stable trees*. Clearly stable trees are effective, so $L : \mathbf{T} \rightarrow \mathbf{B}$ is a discrete fibration. In this case it is furthermore finite: for a given number of leaves there is only a finite number of isoclasses of stable trees. This finiteness is convenient for computational purposes, and we include an instructive computation in the appendix for this case.

8.10. The classical Faà di Bruno: surjections versus effective trees. As far as we know, the classical Faà di Bruno bialgebra of surjections is not a bialgebra of P-trees for any P. There is nevertheless

a close relationship with the bialgebra of effective trees, which we now proceed to explain. The following construction work for any polynomial endofunctor without nullary operations.

Since effective trees have no nullary nodes, the leaf map can be seen as taking values in the groupoid $\mathbf{B}$ of non-empty finite sets. Pulling back along the leaf map $L : \mathbf{T} \to \mathbf{B}$

$$L^* : \mathbf{Grpd}_{/\mathbf{B}} \to \mathbf{Grpd}_{/\mathbf{T}},$$

sends $\ulcorner n \urcorner : 1 \to \mathbf{B}$ to the inclusion of the discrete fibre $_n\mathbf{T} \to \mathbf{T}$.

This yields a linear map

$$
\begin{array}{rcl}
\mathbb{Q}^{\pi_0 \mathbf{B}} & \longrightarrow & \mathbb{Q}^{\pi_0 \mathbf{T}} \\
A_n & \longmapsto & G_n \\
a_n & \longmapsto & g_n \\
A & \longmapsto & G.
\end{array}
$$

which extends to an algebra homomorphism

$$\Phi : \mathcal{F} = \mathbb{Q}[[A_n : n \in \pi_0 \mathbf{B}]] \longrightarrow \mathbb{Q}[[\delta_T : T \in \pi_0 \mathbf{T}]] = \mathcal{B}_{\mathrm{eff}}.$$

Lemma. 8.11. *The map Φ is a bialgebra homomorphism.*

Proof. We already noted that Φ preserves the Green functions. Now

$$
\begin{aligned}
(\Phi \otimes \Phi)(\Delta(A)) &= (\Phi \otimes \Phi)(\sum_n A^n \otimes a_n) \\
&= \sum_n (\Phi A)^n \otimes \Phi(a_n) \\
&= \sum_n G^n \otimes g_n \\
&= \Delta(\Phi(A)).
\end{aligned}
$$

It remains to recall that the comultiplication in $\mathcal{F}$ is determined by the comultiplication of the Green function. $\square$

To appreciate the amount of combinatorics hidden in these arguments, it is rewarding to work out the comultiplicativity of Φ by hand. We provide in the Appendix a direct combinatorial proof that $(\Phi \otimes \Phi)(\Delta A_4) = \Delta G_4$, but for simplicity we work with stable trees instead of effective trees.

9. Trees versus graphs

In this final section we explain how to derive Faà di Bruno formulae in bialgebras of graphs from our formulae for trees, and compare with van Suijlekom's Faà di Bruno formula, although this has not been sorted out completely. All the differences are due to our strictly operadic viewpoint. The results in this section are from the forthcoming paper

[28] and concern the relationship between Feynman graphs and P-trees. We reproduce the key points since this correspondence is the main motivation for the use of P-trees.

(All the pictures in this section are implicitly from massless ϕ^3 theory in six space-time dimensions.)

9.1. Trees in BPHZ renormalisation. The main use of trees in BPHZ renormalisation is to express nestings of Feynman graphs. The discovery of Kreimer [30] was that the combinatorics of the BPHZ procedure is elegantly encoded in a Hopf algebra of rooted trees. More information, related to the specifics of a particular theory, is encoded in the Hopf algebra of graphs [9], [10].

In order to understand the relationship between the two Hopf algebras well enough to transfer constructions and results such as the ones of the present paper, some modifications seem necessary both on the graphs and the tree side. On the tree side, we pass to operadic trees, as already explained. In the following figure,
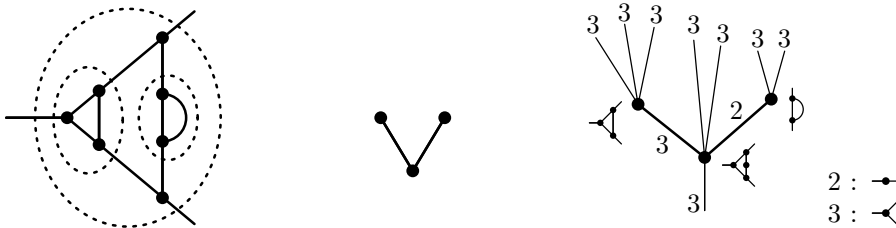
the small combinatorial tree in the middle expresses the nesting of 1PI subgraphs on the left; Kreimer showed that the information encoded by such trees is sufficient to account for the counter-term corrections of BPHZ. On the other hand, it is clear that such combinatorial trees do not capture anything related to symmetries of graphs.

For this, fancier trees are needed, as partially indicated on the right. First of all, each node in the tree should be decorated by the 1PI graph it corresponds to in the nesting [5], and second, to allow an operadic interpretation, the tree should have leaves (input slots) corresponding to the vertices of the graph. Just as vertices of graphs serve as insertion points, the leaves of a tree serve as input slots for grafting. The decorated tree should be regarded as a recipe for reconstructing the graph by inserting the decorating graphs into the vertices of the graphs of parent nodes. The numbers on the edges indicate the type constraint of each substitution: the outer interface of a graph must match the local interface of the vertex it is substituted into. But the type constraints on the tree decoration are not enough to reconstruct the graph, because for example the small graph ⫸ decorating the left-hand node could be substituted into various different vertices of the graph ⫸. The solution found in [28] is to consider P-trees, for P a certain polynomial endofunctor over groupoids, which depends on the theory. For this to work, a few modifications are needed on the graphs side:

9.2. Adjustmenst to the Hopf algebra of graphs. The first modification required is rather harmless. Traditionally, the Connes–Kreimer Hopf algebra of graphs is spanned by the 1PI graphs that are furthermore superficially divergent. This last condition excludes the one-vertex graphs given by the interaction labels themselves, and for this reason in the formula for comultiplication

$$\Delta(\Gamma) = 1 \otimes \Gamma + \Gamma \otimes 1 + \sum_{\gamma \subsetneq \Gamma} \gamma \otimes \Gamma/\gamma$$

the primitive part has to be specified separately since taking $\gamma = \Gamma$ would yield a term with the one-vertex graph $\Gamma/\gamma = \mathrm{res}(\Gamma)$. While of course excluding the one-vertex graphs is natural from the viewpoint of physics, from the strictly combinatorial viewpoint it appears as an ad hoc feature. This was perhaps first observed by Manchon [36] who introduced a bigger bialgebra, by including the interaction labels (one-vertex graphs) as generators. Since obviously these new generators have loop number zero, this bigger bialgebra is not connected, and therefore no longer Hopf. The difference is strictly analogous to the difference between reduced and non-reduced incidence algebras, as we saw in the classical Faà di Bruno case in Section 1; again, the standard Hopf algebra can be obtained by collapsing the degree-0 piece. It should also be noted here that in this setting the sum constituting the Green function for a vertex v does not start with 1, but rather with v considered as a graph with residue v.

The second modification is subtler. The Hopf algebra of graphs expresses contraction of subgraphs, but its dual Lie algebra is the one of insertions of graphs. One is allowed to substitute graphs with two external legs into internal lines of the receiving graph. This means that every internal line represents an ordered infinity of virtual insertion points. This does not look very good from the viewpoint of operadic trees, as it destroys the input slot correspondence between vertices in graphs and leaves in trees: the strict operadic viewpoint requires that grafting of trees only occurs at pre-existing leaves, and correspondingly in the setting of graphs, only insertions at vertices should be allowed.

This can be arranged by declaring each internal line to be an insertion point, for example by decorating it with a special 2-valent vertex, often indicated with a cross. It means that the bialgebra now has a generator for every term in the Lagrangian, even for the kinetic terms. Correspondingly one declares the residue of a graph with two external lines to be this new kind of vertex, instead of saying that the residue is just the line, and the Green function for the new interaction label $e = \text{—•—}$ looks like this:

$$G_e = \quad \text{—•—} + \tfrac{1}{2}\, \text{⬡} + \text{⬡} + \tfrac{1}{2}\, \text{⬡} + \cdots$$

and similarly, the Green functions for the proper interaction labels are refined by all possible appearances of the new vertex.

These issues seem to be closely related to the Z-factor comparing the bare and normalised Green functions, but we do not at this point understand the physics of this relationship.

9.3. Trees decorated with graphs. Having been specific about which graphs we consider, we can now explain how to encode the graph-decorated trees, in order to get the correct correspondence between graphs and trees, cf. [28]. The decorations are encoded P-trees, for P a certain polynomial endofunctor over groupoids, which depends on the theory. This formalism yields the correct symmetry factors.

To match the figure above, we consider a theory in which there are two interaction labels $\multimap$ and $\prec$; let I denote the groupoid of all such one-vertex graphs. Let B denote the groupoid of all connected 1PI graphs of the theory such that the residue belongs to I. Finally let E denote the groupoid of such graphs with a marked vertex. The polynomial endofunctor is now given by the diagram

$$(19) \qquad I \xleftarrow{\ s\ } E \xrightarrow{\ p\ } B \xrightarrow{\ t\ } I,$$

where the map s returns the one-vertex subgraph at the mark, p forgets the mark, and t returns the residue of the graph, i.e. the graph obtained by contracting everything to a point, but keeping the external lines. A P-tree is hence a diagram

$$(20) \qquad \begin{array}{ccccccc} A & \longleftarrow & M & \longrightarrow & N & \longrightarrow & A \\ \downarrow & \Leftarrow & \downarrow & \Rightarrow & \downarrow & \Rightarrow & \downarrow \\ I & \longleftarrow & E & \longrightarrow & B & \longrightarrow & I \, , \end{array}$$

with specified 2-cells, in which the first row is a tree in the sense of 4.1. These 2-cells carry much of the structure: for example the 2-cell on the right says that the 1PI graph decorating a given node must have the same residue as the decoration of the outgoing edge of the node — or more precisely, and more realistically: an isomorphism is specified (it's a bijection between external lines of one-vertex graphs). Similarly, the left-hand 2-cell specifies for each node-with-a-marked-incoming-edge $x' \in M$, an isomorphism between the one-vertex graph decorating that edge and the marked vertex of the graph decorating the marked node x'. Hence the structure of a P-tree is a complete recipe not only for which graphs should be substituted into which vertices, but also *how*: specific bijections prescribe which external lines should be identified with which lines in the receiving graph.

9.4. Graph nesting. A *graph nesting* is a Feynman graph (assumed to be 1PI and with residue belonging to I) with nested circles, such that every circle cuts a 1PI Feynman graph of the theory with residue

in I. The graph nestings form a groupoid $\mathbf{N}$, in which the maps are
graph isomorphisms compatible with the configuration of circles.

The following is the main theorem of [28], which draws from insights
from higher category theory [29].

Theorem. 9.5. ([28]) *There is an equivalence of groupoids between
the groupoid* $\mathbf{N}$ *of graph nestings and the groupoid* $\mathbf{T}$ *of P-trees. In
particular, the symmetries of a given graph nesting can be read off the
corresponding decorated tree and vice versa.*

It should be stressed that the use of groupoids as coefficients is crucial
for getting the decorations that make this correspondence to work. In
fact, a tree decorated in groupoids may have more symmetries than
the underlying tree. For example, the graph $\Gamma = \multimap\!\circ\!\!\multimap$ is 1PI and, as
a trivial nesting it corresponds to the tree $\curlyvee$ decorated with Γ at the
node, 3 at the leaves, and 2 at the root. More formally it is of course a
diagram like (20). It is straightforward to check that this P-tree has a
symmetry group of order 4, just as the graph Γ, whereas the underlying
tree clearly has a symmetry group of order 2.

9.6. Graphs with fixed residue. So far we are talking abstract
Feynman graphs, whereas in quantum field theory, the symmetries are
required to fix the external lines. Categorically, this means that we are
talking about the groupoid $\mathbf{G}_v$ defined as the (homotopy) fibre over
the residue $v = \multimap\!\!\multimap$. Inside this fibre, the symmetry group of the graph
$\Gamma = \multimap\!\circ\!\!\multimap$ is of order 2, the non-trivial symmetry being the one that fixes
the external lines and interchanges the two internal lines. Since v is an
object in the groupoid I, the tree corresponding to Γ belongs to the
fibre $\mathbf{T}_v$ of trees with root colour v. One can check directly that in this
groupoid, the tree has only one non-trivial automorphism, which in
fact is trivial on the underlying tree! Indeed, if we were to interchange
the two leaves of the tree, then by the compatibilities expressed by the
decoration, we would be interchanging the two vertices of Γ, and this
in turn would interchange the two external lines of $v = \multimap\!\!\multimap$, the residue
of Γ, but since we are inside the fibre $\mathbf{T}_v$ this automorphism is not
allowed.

9.7. Nestings versus graphs. By Theorem 9.5 we have an equiv-
alence of groupoids $\mathbf{N} \simeq \mathbf{T}$. There is an obvious projection functor
$\mathbf{N} \to \mathbf{G}$ which simply forgets the circles expressing the nesting on a
graph. This functor is a finite discrete fibration — this is just to say
that for a given graph there is a finite set of possible nestings to put
on it. Pullback along this projection defines a functor

$$\mathbf{Grpd}_{/\mathbf{G}} \longrightarrow \mathbf{Grpd}_{/\mathbf{N}} \stackrel{\sim}{\to} \mathbf{Grpd}_{/\mathbf{T}},$$

which associates to each graph the set of possible nestings on it, and
then the associated P-tree. Note that no coefficients appear in this

sum, but as illustrated in 9.11 below, there may be repetitions. This functor induces an injective linear map

$$\mathbb{Q}^{\pi_0 \mathbf{G}} \to \mathbb{Q}^{\pi_0 \mathbf{N}} \overset{\sim}{\rightrightarrows} \mathbb{Q}^{\pi_0 \mathbf{T}}$$

between the spaces of $\mathbb{Q}$-valued functions, which in turn extends to an algebra homomorphism

$$\Psi : \mathbb{Q}[[\Gamma \in \pi_0 \mathbf{G}]] \longrightarrow \mathbb{Q}[[T \in \pi_0 \mathbf{T}]].$$

Theorem. 9.8. ([28]) *The map* $\mathbb{Q}[[\Gamma \in \pi_0 \mathbf{G}]] \longrightarrow \mathbb{Q}[[T \in \pi_0 \mathbf{T}]]$ *is a bialgebra homomorphism. Here the bialgebra structure on* $\mathbb{Q}[[\Gamma \in \pi_0 \mathbf{G}]]$ *is the one of 9.2; the bialgebra structure on* $\mathbb{Q}[[T \in \pi_0 \mathbf{T}]]$ *is the one explained in Section 2.3.*

Proposition. 9.9. *The bialgebra homomorphism* $\mathbb{Q}[[\Gamma \in \pi_0 \mathbf{G}]] \longrightarrow \mathbb{Q}[[T \in \pi_0 \mathbf{T}]]$ *sends Green functions to Green functions.*

This is basically because the inverse image of the groupoid $\mathbf{G}_v$ is the whole groupoid $\mathbf{N}_v$. Since Ψ is injective we conclude:
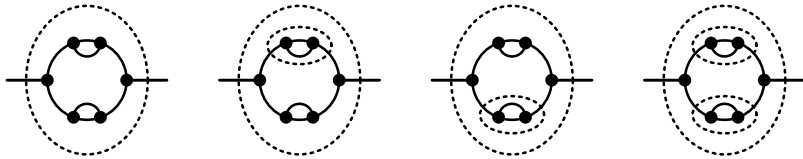
Corollary. 9.10. *The Faà di Bruno formula holds for the Green function in the bialgebra of graphs.*

We offer two examples to illustrate the significance of this result.

**9.11. Example: nestings breaking symmetry.** First we consider the graph Γ (with residue $v = \text{—•—}$):
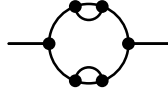
The fibre over Γ has four elements, named N_1, N_2, N_3, N_4:

The graph Γ has a automorphism group of order 8 (in $\mathbf{G}_v$), and thus appears in the Green function with a factor $\frac{1}{8}$. Hence $\Psi(\frac{1}{8}\Gamma) = \frac{1}{8}N_1 + \frac{1}{8}N_2 + \frac{1}{8}N_3 + \frac{1}{8}N_4$. Now N_2 and N_3 are isomorphic in $\mathbf{N}_v$, so we can also write the sum as $\frac{1}{8}N_1 + \frac{1}{4}N_2 + \frac{1}{8}N_4$, and these factors, $\frac{1}{8}, \frac{1}{4}, \frac{1}{8}$ are precisely the inverses of the orders of the symmetry groups of the three objects in $\mathbf{N}_v$. What the example shows is the fact that symmetries of a graph can be broken by imposing nestings, but the decrease in symmetry is precisely counter-balanced by the fact that a certain number of isomorphic nestings appear in the fibre.

9.12. Overlapping divergences. The second example concerns a graph with overlapping divergences. Consider the graph Ω (with residue $v = \text{—•—}$):
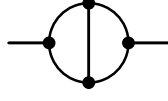
The fibre over Γ has three elements, denoted N_1, N_2, N_3:
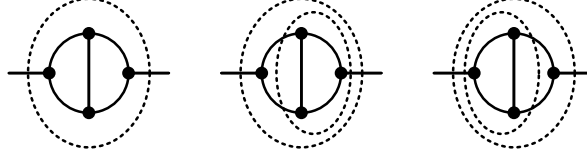
In this case Ω as well as the nestings N_1, N_2, N_3 all have an automorphism group of order 2 (over v). The interesting remark in this case is that the trees corresponding to the nestings N_2 and N_3 are *not* isomorphic inside the fibre $\mathbf{T}_v$ (although they *are* isomorphic as abstract P-trees). The reason for this is the observation already made earlier that the drawings of these trees, even with all the decorating graphs, is not the full picture. Interchanging the two branches is only possible over the non-trivial automorphism of $v = $ ➝. (In fact it is clear in the drawings of nestings that the two nestings are not isomorphic for fixed residue.)

APPENDIX

As an illustration of the content of Lemma 8.11, we check the identity

(21) $$(\Phi \otimes \Phi)(\Delta A_4) = \Delta \Phi A_4$$

by hand, where Φ is the map from the classical Faà di Bruno bialgebra $\mathcal{F}$ to the bialgebra of stable trees $\mathcal{B}$ that sends A_n to G_n.

Recall that the coproduct of A_4 in the classical Faà di Bruno bialgebra is given by

$$\Delta(A_4) = A_4 \otimes A_1 + \left(3\, A_2{}^2 + 4\, A_3 A_1\right) \otimes A_2 + 6\, A_2 A_1{}^2 \otimes A_3 + A_1{}^4 \otimes A_4.$$

In the bialgebra of trees we restrict for simplicity to the case of stable trees, with colours $I = \{*\}$. Recall that there are no non-trivial automorphisms in the homotopy fibre $_n\mathbf{T}$ of trees with n leaves, so the relative cardinality is

$$G_n \;=\; \sum_{T \in \pi_0(_n\mathbf{T})} \delta_T / \operatorname{Aut}_n(T) \;=\; \sum_{T \in \pi_0(_n\mathbf{T})} \delta_T.$$

The relative cardinality g_n of the *full* subcategory of trees with n leaves, which has fewer isomorphism classes, satisfies

$$g_n = G_n/n!\,.$$

We draw a tree for its corresponding symbol δ_T, and identify symbols for trees in $T \in \pi_0(_n\mathbf{T})$, if the trees coincide in $\pi_0\mathbf{T}$. The total Green function is

$$G = G_1 + G_2/2 + G_3/6 + G_4/24 + \dots$$

where

$$G_1 = |$$
$$G_2 = \curlyvee$$
$$G_3 = \curlyvee + 3\,\curlyveedownvee$$
$$G_4 = \curlyvee + 6\,\curlyveedownvee + 3\,\curlyveewye + 4\,\curlyveewye + 12\,\curlyveedownwye$$

The comultiplication applied to G_4 is then, by definition,

$$\Delta G_4 = |^4 \otimes \curlyvee + \curlyvee \otimes |$$
$$+6\left(|^4 \otimes \curlyveedownvee + \curlyveedownvee \otimes | \qquad\qquad + |^2\curlyvee \otimes \curlyvee\right)$$
$$+3\left(|^4 \otimes \curlyveewye + \curlyveewye \otimes | + \curlyvee^2 \otimes \curlyvee + 2|^2\curlyvee \otimes \curlyveedownvee\right)$$
$$+4\left(|^4 \otimes \curlyveewye + \curlyveewye \otimes | + |\,\curlyvee \otimes \curlyvee\right)$$
$$+12\left(|^4 \otimes \curlyveedownwye + \curlyveedownwye \otimes | + |\,\curlyveedownvee \otimes \curlyvee + |^2\curlyvee \otimes \curlyveedownvee\right)$$

The first two columns are simply $G_1^4 \otimes G_4$ and $G_4 \otimes G_1$ respectively. Less obvious is the simplification that occurs in the third column and the fourth column:

$$\left(3 \cdot \curlyvee^2 + 4 \cdot |\,\curlyvee + 12 \cdot |\,\curlyveedownvee\right) \otimes \curlyvee = (3G_2^2 + 4G_1G_3) \otimes G_2,$$
$$|^2\curlyvee \otimes \left(6 \cdot \curlyvee + 3 \cdot 2 \cdot \curlyveedownvee + 12 \cdot \curlyveedownvee\right) = G_1^2 G_2 \otimes 6G_3.$$

Thus we have shown that

$$\Delta G_4 = G_4 \otimes G_1 + \left(3\,G_2{}^2 + 4\,G_3 G_1\right) \otimes G_2 + 6\,G_2 G_1{}^2 \otimes G_3 + G_1{}^4 \otimes G_4.$$

and the relation (21) holds.

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