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AN OPERATIONAL CALCULUS FOR THE Mould OPERAD

FRÉDÉRIC CHAPOTON, FLORENT HIVERT, JEAN-CHRISTOPHE NOVELLI, AND JEAN-YVES THIBON

ABSTRACT. The operad of moulds is realized in terms of an operational calculus of formal integrals (continuous formal power series). This leads to many simplifications and to the discovery of various suboperads. In particular, we prove a conjecture of the first author about the inverse image of non-crossing trees in the dendriform operad. Finally, we explain a connection with the formalism of noncommutative symmetric functions.

1. INTRODUCTION

A mould, as defined by Ecalle, is a "function of a variable number of variables", that is, a sequence $f_n(u_1, \ldots, u_n)$ of functions of n (continuous or discrete) variables. He developed around this notion a versatile formalism which is an essential technical tool in his theory of resurgence [10, 11] and in his later work on polyzetas [12, 13, 14] (see the lecture notes [7] for an elementary introduction).

In [6], the first author constructed an operad **Mould** from the set of (rational) moulds, and identified several (old and new) suboperads of it.

The aim of this article is to introduce an operational calculus on formal integrals, which allows to simplify considerably the arguments of [6], and also to obtain further results. In particular, we find that the operad Zinbiel introduced by Loday [19] is a sub-operad of **Mould**. As Zinbiel is based on permutations, this allows to consider the elements of the algebra **FQSym** of free quasi-symmetric functions as moulds. For instance, the classical Lie idempotents of Dynkin, Solomon and Klyachko give interesting examples of alternal moulds. We also find some other new suboperads, prove conjecture 5.7 of [6], and obtain some new examples of moulds.

This article is a continuation of [6]. In a few examples, we shall assume that the reader is familar with the notation of [18, 8].

2. Moulds as nonlinear operators

Let \mathcal{H} be a vector space of formal integrals

(1)
$$h(t) = \int h_u t^{u-1} d\mu(u) ,$$

where h_u are homogeneous elements of degree u in some graded associative algebra \mathcal{A} . We will only need the cases where μ is the Lebesgue measure on \mathbb{R} or \mathbb{R}_+ , or the discrete measure on \mathbb{N} , which gives back power series in t with noncommutative

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coefficients. In these cases, the object (1) can be interpreted as a linear map $\mathcal{V} \to \mathcal{A}$ on the vector space with basis (t^u) for u in the support of μ , and the theory is completely similar to that of formal power series.

A mould $f = (f_n(u_1, \ldots, u_n))$ can be interpreted as a nonlinear operator F on \mathcal{H} , by setting

(2)
$$F[h] = \sum_{n \ge 0} \int \cdots \int f_n(u_1, \dots, u_n) h_{u_1} \cdots h_{u_n} t^{u_1 + \dots + u_n} d\mu(u_1) \cdots d\mu(u_n)$$

It will be convenient to set

(3)
$$H(t) = \int_0^t h(\tau) d\tau = \int h_u \frac{t^u}{u} d\mu(u) d\tau$$

We also define the *polarization* of F as the collection of multilinear operators (the $h^{(i)}$ are arbitrary elements of \mathcal{H})

(4)
$$F_n[h^{(1)}, \dots, h^{(n)}] = \int \cdots \int f_n(u_1, \dots, u_n) h^{(1)}_{u_1} \cdots h^{(n)}_{u_n} t^{u_1 + \dots + u_n} d\mu(u_1) \cdots d\mu(u_n).$$

3. EXAMPLES OF MOULDS

In this section, we translate all the examples of [6] into the new formalism, and provide some new ones.

Example 3.1. The mould

(5)
$$f_n(u_1,\ldots,u_n) = \frac{1}{u_1\cdots u_n}$$

corresponds to the operators

(6)
$$F_n[h^{(1)}, \dots, h^{(n)}] = H^{(1)}(t) \cdots H^{(n)}(t) .$$

Example 3.2. The time-ordered exponential

(7)
$$U(t) = T \exp\left\{\int_0^t h(\tau) d\tau\right\},$$

i.e., the unique solution of U'(t) = U(t)h(t) with U(0) = 1, is given by the mould

(8)
$$f_n(u_1, \dots, u_n) = \frac{1}{u_1(u_1 + u_2) \cdots (u_1 + u_2 + \dots + u_n)}$$

Example 3.3. More generally, for a permutation $\sigma \in \mathfrak{S}_n$, the mould

(9)
$$f_{\sigma}(u_1, \dots, u_n) = \frac{1}{u_{\sigma(1)}(u_{\sigma(1)} + u_{\sigma(2)}) \cdots (u_{\sigma(1)} + u_{\sigma(2)} + \dots + u_{\sigma(n)})}$$

integrates over the simplex
$$\Delta_{\sigma}(t) = \{0 < t_{\sigma(1)} < t_{\sigma(2)} < \dots < t_{\sigma(n)} < t\}$$
:

(10)
$$F_{\sigma}[h^{(1)}, \dots, h^{(n)}] = \int_{\Delta_{\sigma}(t)} h^{(1)}(t_1) \cdots h^{(n)}(t_n) dt_1 \cdots dt_n$$

It follows from the well-known decomposition of a product of simplices as a union of simplices that these moulds form a subalgebra, isomorphic to the algebra of free quasi-symmetric functions **FQSym**, under the correspondence $f_{\sigma} \mapsto \mathbf{F}_{\sigma}$ (cf. [8]).

Example 3.4. To each planar binary tree T, we can associate an operator F_T defined by $F_{\bullet}[h] = H$ and, if $T = T_1 \wedge T_2$ has T_1 and T_2 as left and right subtrees

(11)
$$F_T[h] = \int_0^t F_{T_1}[h](\tau)h(\tau)F_{T_2}[h](\tau)d\tau$$

The kernels of these operators are the moulds associated to trees in [6], which can be computed graphically as follows. All the leaves of T are labelled by 1, and the internal nodes are labelled by t^{u_i-1} , in such a way that flattening the tree yields the t^{u_i-1} in their natural order

(12)
$$\begin{array}{c} t^{u_{1}-1} \\ t^{u_{1}-1} \\ t^{u_{3}-1} \\ t^{u_{3}-1} \\ 1 \end{array} \\ t^{u_{3}-1} \\ 1 \end{array}$$

The mould $f_T(u_1, \ldots, u_n)$ is obtained by evaluating the tree according to the following rule: the outgoing flow of each node is the integral $\int_0^t L(\tau)v(\tau)R(\tau)d\tau$, where L(t)and R(t) are the outputs of its left and right subtrees, and v(t) its label. For example, the above tree evaluates to $u_1+u_2+u_3+u_4$

(13)
$$\frac{t^{u_1+u_2+u_3+u_4}}{u_1u_3(u_3+u_4)(u_1+u_2+u_3+u_4)}$$

as can be seen on the following picture



and the corresponding mould is obtained by setting t = 1. Each F_T is a sum of operators F_{σ} (sum over all σ such that the decreasing tree of σ^{-1} has shape T). This can be used as in [16] to derive the hook-length formula for binary trees.

Example 3.5. The moulds associated to planar binary trees are related to the solution of the quadratic differential equation

(15)
$$\frac{dx}{dt} = b(x,x), \ x(0) = 1$$

where the bilinear map b(x, y) is assumed to have an integral representation of the type

(16)
$$b(x,y) = \int x_u b_u y_u t^{u-1} d\mu(u) = (x * b * y)(t)$$

the convolution * being defined by

(17)
$$(x*y)(t) = \int x_u y_u t^{u-1} d\mu(u)$$

and b(t) = b(1, 1)(t). This can be recast in the form

$$(18) x = 1 + B(x, x)$$

where

(19)
$$B(x,y) = \int_0^t b(x,y)(\tau)d\tau$$

so that

(20)
$$x = 1 + B(1,1) + B(B(1,1),1) + B(1,B(1,1)) + \dots = \sum_{T \in \mathbf{CBT}} B_T(1)$$

where **CBT** is the set of (complete) binary trees, and for a tree T, $B_T(a)$ is the result of evaluating the expression formed by labeling by a the leaves of T and by B its internal nodes. Then, the term $B_T(1)$ in the binary tree solution is $F_T[b]$.

Example 3.6. The mould [6, (103)]

(21)
$$y_{p,q}(u_1, \dots, u_n) = \frac{u_p}{u_1 \cdots u_n (u_1 + \dots + u_n)}$$

(sum over all binary trees of type (p,q)) corresponds to the operator

(22)
$$Y_{p,q}[h^{(1)},\ldots,h^{(n)}] = \int_0^t H^{(1)}(\tau)\cdots H^{(p-1)}(\tau)h^{(p)}(\tau)H^{(p+1)}(\tau)\cdots H^{(n)}(\tau)d\tau$$

Example 3.7. The mould TY defined by [6, (104)]

(23)
$$TY_n = \sum_{i=1}^n \alpha^{i-1} y_{i,n-i}$$

corresponds to the operator

(24)
$$F[h] = \int_0^t (1 - \alpha H(\tau))^{-1} h(\tau) (1 - H(\tau))^{-1} d\tau.$$

When h is scalar (the h_u commute), this reduces to

(25)
$$F[h] = \int_0^t (1 - \alpha H(\tau))^{-1} (1 - H(\tau))^{-1} dH(\tau) = \frac{1}{1 - \alpha} \log\left(\frac{1 - \alpha H(t)}{1 - H(t)}\right).$$

Example 3.8. The mould [6, (106)]

(26)
$$\sum_{i=1}^{n} i y_{i,n-i}$$

corresponds to the operator

(27)
$$F[h] = \int_0^t (1 - H(\tau))^{-2} h(\tau) (1 - H(\tau))^{-1} d\tau$$

When h is scalar, this reduces to

(28)
$$F[h] = \int_0^t (1 - H(\tau))^{-2} (1 - H(\tau))^{-1} dH(\tau) = \frac{H(t)(2 - H(t))}{2(1 - H(t))^2}.$$

Example 3.9. The following modified mould

(29)
$$\sum_{i=1}^{n} [i]_{q} y_{i,n-i},$$

where $[i]_q$ is the quantum number $1 + q + \cdots + q^{i-1}$, corresponds to the operator

(30)
$$F[h] = \int_0^t (1 - qH(\tau))^{-1} (1 - H(\tau))^{-1} h(\tau) (1 - H(\tau))^{-1} d\tau$$

When h is scalar, this reduces to (31)

$$F[h] = \int_0^t (1 - qH(\tau))^{-1} (1 - H(\tau))^{-2} dH(\tau) = \frac{1}{1 - q} \left(\frac{H(t)}{1 - H(t)} - \frac{q}{1 - q} \log \left(\frac{1 - H(t)}{1 - qH(t)} \right) \right)$$

Example 3.10. The Connes-Moscovici series ([6, (109)]) is given by the mould

(32)
$$\frac{1}{n!} \sum_{k=1}^{n} (-1)^{n-k} \binom{n}{k} k y_{k,n-k}$$

and the corresponding operator is

(33)
$$F[h] = \int_0^t e^{H(\tau)} h(\tau) e^{-H(\tau)} d\tau$$

which reduces to H(t) in the scalar case.

Example 3.11. From the Solomon Lie idempotent, one can define the following mould

(34)
$$\frac{1}{n} \sum_{\sigma \in \mathfrak{S}_n} (-1)^{d(\sigma)} {\binom{n-1}{d(\sigma)}}^{-1} f_{\sigma}$$

Its output is the logarithm of U(t) as defined by (7). It is also called the first Eulerian idempotent.

The q-deformation obtained in [18] yields a one-parameter family of moulds

(35)
$$\frac{1}{n} \sum_{\sigma \in \mathfrak{S}_n} (-1)^{d(\sigma)} \begin{bmatrix} n-1\\ d(\sigma) \end{bmatrix}^{-1} q^{\operatorname{maj}(\sigma) - \binom{d(\sigma)+1}{2}} f_{\sigma}$$

where $\begin{bmatrix} n-1\\ d(\sigma) \end{bmatrix}$ is a quantum binomial coefficient.

Example 3.12. The mould

(36)
$$D_n = \sum_{i=0}^{n-1} (-1)^i \frac{1}{(u_1 u_{12} u_{123} \cdots u_{123..i}) u_{1..n} (u_{i+1..n} \cdots u_{n-1n} u_n)}$$

(sum over trees of the form (left comb) \wedge (right comb) corresponds to Dynkin's idempotent, more precisely

(37)
$$D_n[h] = \int_{\Delta_n} [...[h(t_1), h(t_2)], h(t_3)]..., h(t_n)] d\mu(t_1) \cdots d\mu(t_n).$$

Example 3.13. The mould PO, defined in [6, (113)] by

(38)
$$PO_n = \frac{1}{u_1} \prod_{i=2}^n \frac{u_1 + \dots + u_{i-1} + qu_i}{u_i(u_1 + \dots + u_i)}$$

can be decomposed on the permutations f_{σ} as

(39)
$$PO_n = \sum_{\sigma \in \mathfrak{S}_n} q^{s(\sigma^{-1})-1} f_{\sigma},$$

where $s(\sigma)$ is the number of saillances of σ , *i.e.*, the number of *i* such that $\sigma_i > \sigma_j$ for all j < i. This statistics has the same distribution as the number of cycles.

Example 3.14. A mould is *alternal* if and only if it satisfies

(40)
$$F[h_1 + h_2] = F[h_1] + F[h_2]$$

whenever h_1 and h_2 commute. Typically, \mathcal{H} is a Lie algebra and F takes its values in a completion of $U(\mathcal{H})$. Then, F is alternal if and only if it preserves primitive elements. For example, (34), (35) and (36) are alternal. Similarly, F is symmetral if it maps primitive elements to group-like elements. Otherwise said,

(41)
$$F[h_1 + h_2] = F[h_1] \cdot F[h_2]$$

as soon as h_1 and h_2 commute.

Example 3.15. The dendriform products \prec and \succ are given by (42)

$$(F \succ G)[h] = \int_0^t F[h](\tau) \cdot \frac{d}{d\tau} G[h](\tau) d\tau , \quad (F \prec G)[h] = \int_0^t \frac{d}{d\tau} F[h](\tau) \cdot G[h](\tau) d\tau .$$

On permutational moulds f_{σ} , these coincide with the half-shifted shuffles, e.g., $312 \prec 12 = (31 \pm 45) \cdot 2$.

Example 3.16. The preLie product $F \curvearrowleft G = F \succ G - G \prec F$ is given by

(43)
$$F \curvearrowleft G[h] = \int_0^t [F[h], G'[h]](\tau) d\tau \,,$$

where G'[h] denotes the derivative with respect to τ . On this expression it is clear that if h is primitive, so is $F \curvearrowleft G[h]$ if F and G are alternal.

4. Operadic operations on operators

The *i*th operadic composition of two homogeneous moulds f_m and g_n , as defined in [6], corresponds to the operator whose polarization is

(44)
$$F_m \circ_i G_n[h^{(1)}, \dots, h^{(i-1)}; h^{(i)}, \dots, h^{(i+n-1)}; h^{(i+n)}, \dots, h^{(m+n-1)}]$$

= $F_m[h^{(1)}, \dots, h^{(i-1)}; \frac{d}{dt}G_n[h^{(i)}, \dots, h^{(i+n-1)}]; h^{(i+n)}, \dots, h^{(m+n-1)}].$

It follows from this description that the linear span of the F_{σ} is stable under these operations, hence form a suboperad.

Example 4.1. According to the definition of [6],

(45)
$$f_{312} \circ_2 f_{12} = \frac{1}{u_4 \left(u_4 + u_1\right) \left(u_2 + u_4 + u_3 + u_1\right) u_2} = f_{2413} + f_{4213} + f_{4123} \,.$$

and

(46)
$$F_{312} \circ_2 F_{12}[h^{(1)}, h^{(2)}, h^{(3)}, h^{(4)}] = F_{312}[h^{(1)}, \frac{d}{dt}F_{12}[h^{(2)}, h^{(3)}], h^{(4)}],$$

where

(47)
$$F_{12}[h^{(2)}, h^{(3)}] = \int_0^t dt_3 \int_0^{t_3} dt_2 h^{(2)}(t_2) h^{(3)}(t_3)$$

has as derivative, evaluated at t_3

(48)
$$F_{12}[h^{(2)}, h^{(3)}]'(t_3) = \int_0^{t_3} dt_2 h^{(2)}(t_2) h^{(3)}(t_3)$$

When plugged into F_{312} , with the shifts $312 \rightarrow 413$, this yields

(49)
$$\int_{\Delta_{413;2}(t,t_3)} h^{(1)}(t_1) h^{(2)}(t_2) h^{(3)}(t_3) h^{(4)}(t_4) dt_1 dt_2 dt_3 dt_4$$

where the integration domain decomposes as (50)

 $\Delta_{413;2}(t,t_3) := \{ 0 < t_4 < t_1 < t_3 < t; 0 < t_2 < t_3 \} = \Delta_{2413}(t) \cup \Delta_{4213}(t) \cup \Delta_{4123}(t) ,$ as expected.

To give the general rule, it is sufficient to compute

(51)
$$F_{\mathrm{Id}_m} \circ_i F_{\mathrm{Id}_n} = \sum F_o$$

where the sum is over permutations σ in the shuffle

(52)
$$((1,\ldots,i-1)\amalg(i,\ldots,i+n-2))\cdot(i+n-1,\ldots,m+n-1)).$$

Example 4.2.

(53)
$$F_{123} \circ_1 F_{123} = F_{12345}$$

(54)
$$F_{123} \circ_2 F_{123} = F_{12345} + F_{21345} + F_{23145}$$

(55)
$$F_{123} \circ_3 F_{123} = F_{12345} + F_{13245} + F_{13425} + F_{31245} + F_{31425} + F_{34125}$$

This operad is anticyclic. It is in fact isomorphic to Zinbiel (cf. [20]), up to mirror image of permutations. The action of the (n + 1)-cycle γ on a homogenous mould $f(u_1, \ldots, u_n)$ of degree n is defined by

(56)
$$\gamma f(u_1, \dots, u_n) = f(u_2, u_3, \dots, u_n, -u_1 - u_2 - \dots - u_n).$$

The subspace spanned by permutational moulds f_{σ} is stable under the action of γ . Explicitly,

(57)
$$\gamma f_{\sigma} = (-1)^{|v|} \sum_{\tau \in u \amalg v} f_{\tau}$$

where the words u and v are defined as follows. Let $\sigma'(i) = \sigma(i) + 1 \mod n$, write $\sigma' = u 1 w$ and $v = 1 \overline{w}$ (where \overline{w} is the mirror image of w).

This follows easily from the product formula for permutational moulds. For example,

(58)
$$\gamma f_{1432} = -f_{2134} - f_{1234} - f_{1324} - f_{1342} = -f_2 f_{134}$$

(59)
$$\gamma f_{2143} = f_{3214} + f_{3124} + f_{3142} + f_{1342} + f_{1324} + f_{1432} = f_{32}f_{14}$$

Example 4.3. The operadic preLie product $F \circ G$ is

(60)
$$(F \circ G)[h] = \sum_{i=1}^{m} (F \circ_{i} G)[h] = DF[h](G'[h]),$$

that is, the differential DF[h] of F at the point h, evaluated on the vector G'[h], where, as above, G'[h] denotes the *t*-derivative. On this description, it is clear that \circ preserves alternality.

Example 4.4. The derivation ∂ of [6, (85)] is

(61)
$$(\partial F)[h] = DF[h](1) := \lim_{\varepsilon \to 0} \frac{F[h+\varepsilon] - F[h]}{\varepsilon}$$

the derivative of F at h in the direction on the constant function 1. On this description, it is easy to check that ∂ is a derivation for the various products. For example,

$$\partial(F \succ G)[h] = \int_0^t \{DF[h](1)G'[h] + F[h]DG'[h](1)\}d\tau = (\partial F \succ G + F \succ \partial G)[h].$$

For those moulds such that F[h] reduces to an analytic function F(H) of H in the scalar case, $\partial F[h]$ reduces to the derivative of F(H) with respect to H.

Example 4.5. The over and under operations are given by

(63)
$$(F/G)[h^{(1)},\ldots,h^{(m+n)}] = G[F[h^{(1)},\ldots,h^{(n)}]h^{(n+1)},h^{(n+2)},\ldots,h^{(m+n)}]$$

(64)
$$(F \setminus G)[h^{(1)}, \dots, h^{(m+n)}] = F[h^{(1)}, \dots, h^{(n-1)}, h^{(n)}G[h^{(n+1)}, \dots, h^{(m+n)}]].$$

Example 4.6. The ARIT map is

(65)
$$\operatorname{ARIT}(F,G)[h] = DF[h](G[h]h - hG[h]).$$

The ARI map is

$$ARI(F,G)[h] = DF[h](G[h]h - hG[h]) - DG[h](F[h]h - hF[h]) + F[h]G[h] - G[h]F[h].$$

5. Non-crossing trees and non-interleaving forests

In [6], the first author has constructed an operad on the set of non-crossing trees, and formulated a conjecture about the inverse image of non-crossing trees in the dendriform operad. In this section, we prove this conjecture by means of a new presentation of this operad. The reader is referred to [6] for the background on non-crossing trees.



FIGURE 1. A non-crossing tree, and the corresponding labeling

5.1. A bijection.

Definition 5.1. A non-interleaving forest is a labeled rooted forest such that the set of labels of any subtree is an interval.

In particular, the labels of each connected component is an interval. A noninterleaving tree is a non-interleaving forest with a single component. Our new presentation of NCT will be based on non-interleaving trees.

Let T be a non-crossing tree. We define a poset P from T as follows. Fist, label each diagonal edge of T by the number of the unique open side which it separates from the base, and each side edge by its own number. Then, set $i <_P j$ iff the edge iis separated from the base by the edge j.

Lemma 5.2. If P is constructed from a non-crossing tree T by the above process, its Hasse diagram F is a non-interleaving forest. Moreover, the correspondence $T \mapsto F$ is a bijection between non-crossing trees and non-interleaving forests.

Proof. The roots of the trees are the labels of the edges having the base on their external sides. The edges α which are on the other sides of the root edges are labeled by disjoint intervals of [1, n], and these intervals are the labels of the edges which are separated from the bases by those α . Conversely, to each vertex v of a non-interleaving forest, on can associate an edge from the left side of $\min\{k|k <_P v\}$ to the right side of $\max\{k|k <_P v\}$. This yields a non-crossing tree mapped to P by the previous algorithm. Hence, the correspondence is onto. Finally, non-crossing trees and non-interleaving forests have the same grammar, hence in particular the same generating series.

For example, the non-interleaving forest associated to the non-crossing tree on Figure 1 is



5.2. Associated rational functions. In [6], one associates a rational function f_T to a non-crossing tree by the following rule:

(68)
$$f_T = \prod_{e \in E(T)} \frac{1}{\operatorname{ev}(e)}$$

where E(T) is the set of edges of T, and the evaluation of an edge is given by

(69)
$$\operatorname{ev}(e) = \sum_{i} u_{i},$$

where i runs over the labels of the edges separated from 0 by e.

It follows from the above arguments that

(70)
$$f_T = \prod_{i=1}^n \frac{1}{\sum_{j \le P^i} u_j}.$$

Lemma 5.3. The fraction associated to T is the sum of the linear extensions of P:

(71)
$$f_T = \sum_{\sigma \in L(P)} f_{\sigma} \,.$$

Proof. f_T is in **FQSym**, since NCT is a suboperad of Dend,

(72)
$$f_T = \sum c_\sigma(T) f_\sigma,$$

and $c_{\sigma}(T)$ is the iterated residue of $f_T T$ at $x_{\sigma_1} = 0, x_{\sigma_2} = 0, \ldots$ so that $c_{\sigma}(T) = 0$ if $\sigma \notin L(P)$, and $c_{\sigma}(T) = 1$ otherwise.

5.3. **Proof of the conjecture.** Hence, the morphism form the free NCT-algebra on one generator to the free dendriform algebra on one generator **PBT**, regarded as a subalgebra of **FQSym**, consists in mapping a non-interleaving forest on the sum of its linear extensions:

(73)
$$T \mapsto P \mapsto F \mapsto \sum_{\sigma \in L(P)} \mathbf{F}_{\sigma} = \sum_{t \in I} \mathbf{P}_{t},$$

where \mathbf{P}_t is the natural basis of **PBT**, and *I* a set of binary trees. Conjecture 6.5 of [6] is the following:

Theorem 5.4. I is an interval of the Tamari order.

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Proof. Under this morphism, a forest becomes the product of its connected components. It is therefore sufficient to prove that the linear extensions of a non-interleaving tree have the required properties. The linear extensions of a tree are computed recursively by shuffling the linear extensions of the subtrees of the root and concatenating the root at the end. By definition of a non-interleaving tree, these form an interval of the permutohedron, whose minimum avoids the pattern 312 and maximum avoids 132. This is a known characterization of Tamari intervals. \Box

5.4. Another approach. One can also start with an operad NIT defined directly on non-interleaving trees.

There are two natural binary operations on non-interleaving trees. Let T_1 and T_2 be two such trees. Let k be the number of vertices of T_1 , and denote by T'_2 the result of shifting the labels of T_2 by k. Define

- $T_1 \prec T_2 =$ grafting of the root of T'_2 on the root of T_1
- $T_1 \succ T_2 = \text{grafting of the root of } T_1$ on the root of T'_2

These are two magmatic operations, satisfying the single relation

(74)
$$(x \succ y) \prec z = x \succ (y \prec z).$$

Consider now the free algebra on one generator. Its monomials can be represented by bicolored complete binary trees, whose internal vertices are colored by \prec or \succ . Relation (74) implies that a basis is formed by the trees having no right edge from a vertex \succ to a vertex \prec . Loday [21] has presented a general method (relying on Koszul duality for quadratic operads) for counting such k colored binary trees avoiding a set Y of edges. Their generating series (with alternating signs) g(t) is obtained by inverting (for the composition of power series) the series $f(t) = -t + kt^2 - |X_2|t^3 + |X_3|t^4 - \cdots$, where X_n is the set of trees with n internal nodes whose all edges are in Y. Here k = 2, and there is only one tree, with two internal vertices, having all edges in Y. Hence, $f(t) = -t + 2t^2 - t^3$, and we get the sequence A006013 of [25] $g(t) = -t + 2t^2 - 7t^3 + 30t^4 - 143t^5 + \dots$ (based non-crossing trees).

6. Appendix: Moulds over the positive integers

When the variables u_k take only positive integer values, we denote them by i_k and write $f_I = f_{i_1,\ldots,i_r}$ instead of $f(i_1,\ldots,i_r)$. This corresponds to the choice

(75)
$$d\mu(t) = \sum_{n \ge 1} \delta(t-n)$$

In this case, there is a close connection with the formalism of noncommutative symmetric functions, which can also represent nonlinear operators on powers series with noncommuting coefficients.

In this appendix, we will give the interpretation of some of the previous examples in this context, as well as of some new ones. We assume here that the reader is familiar with the notation of [18]. 6.1. Generating sequences of noncommutative symmetric functions. By definition, Sym is a graded free associative algebra, with exactly one generator for each degree. Several sequences of generators are of common use, some of which being composed of primitive elements, whilst other are sequences of divided powers, so that their generating series is group-like. Each pair of such sequences (U_n) , (V_n) defines two moulds, whose coefficients express the expansions of the V_n on the U^I , and vice-versa. Ecalle's four fundamental symmetries reflect the four possible combinations of the primitive or group-like characteristics.

If we denote by \mathcal{L} the (completed) primitive Lie algebra of **Sym** and by $\mathcal{G} = \exp \mathcal{L}$ the associated multiplicative group, we have the following table

$\mathcal{L} ightarrow \mathcal{L}$	Alternal
$\mathcal{L} ightarrow \mathcal{G}$	Symmetral
$\mathcal{G} ightarrow \mathcal{L}$	Alternel
$\mathcal{G} \to \mathcal{G}$	Symmetrel

The characterization of alternal moulds in terms of shuffles is equivalent to Ree's theorem (cf. [24]): the orthogonal of the free Lie algebra in the dual of the free associative algebra is spanned by proper shuffles.

The composition of moulds is the usual composition of the corresponding operators. Since the relationship between two sequences of generators of the same type (divided powers or grouplike) can always be written in the form

(76)
$$V_n(A) = U_n(XA)$$
 (or $V(t) = U(t) * \sigma_1(XA)$),

where X is a virtual alphabet (commutative and ordered, *i.e.*, a specialization of QSym), the composition of alternal or symmetrel moulds can also be expressed by means of the internal product.

6.2. S_n and Λ_n : symmetrel. The simplest example just gives the coefficients of the inverse of a generic series regarded as $\lambda_{-t}(A)$. It is a symmetrel mould:

(77)
$$S_n = \sum_{I \models n} f_I \Lambda^I, \quad f_I = (-1)^{n-l(I)}$$

6.3. S and Ψ : symmetral/alternel. The mould

(78)
$$f_I = \frac{1}{i_1(i_1 + i_2)\dots(i_1 + \dots + i_r)}$$

gives the expression of S_n over Ψ^I :

(79)
$$S_n = \sum_{I \vDash n} f_I \Psi^I \,.$$

Since $\sigma'(t) = \sigma(t) \psi(t)$, this expresses the solution of the differential equation in terms of iterated integrals

(80)
$$\sigma(t) = 1 + \int_0^t dt_1 \,\psi(t_1) + \int_0^t dt_1 \int_0^{t_1} dt_2 \,\psi(t_2) \psi(t_1) + \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \,\psi(t_3) \psi(t_2) \psi(t_1) + \cdots = T \exp\left\{\int_0^t \psi(s) ds\right\},$$

or as Dyson's T-exponential.

6.4. An alternal mould: the Magnus expansion. The expansion of Ψ_n in the basis (Φ^K) is given by

(81)
$$\Psi_n = \sum_{|K|=n} \left[\sum_{i=1}^{\ell(K)} (-1)^{i-1} \binom{\ell(K)-1}{i-1} k_i \right] \frac{\Phi^K}{\ell(K)!\pi(K)} ,$$

where $\pi(K) = k_1 \cdots k_r$. Using the symbolic notation (82) $\{\Phi_{i_1} \cdots \Phi_{i_r}, F\} = \operatorname{ad} \Phi_{i_1} \operatorname{ad} \Phi_{i_2} \cdots \operatorname{ad} \Phi_{i_r}(F) = [\Phi_{i_1}, [\Phi_{i_2}, [\dots [\Phi_{i_r}, F] \dots]]]$ and the classical identity

(83)
$$e^{a}be^{-a} = \sum_{n\geq 0} \frac{(\operatorname{ad} a)^{n}}{n!} b = \{e^{a}, b\}$$

we obtain

(84)
$$\psi(t) = \sum_{n \ge 0} \frac{(-1)^n}{(n+1)!} \{ \Phi(t)^n \,, \, \Phi'(t) \} = \left\{ \frac{1 - e^{-\Phi(t)}}{\Phi(t)} \,, \, \Phi'(t) \right\}$$

which by inversion gives the Magnus formula:

(85)
$$\Phi'(t) = \left\{ \frac{\Phi(t)}{1 - e^{-\Phi(t)}}, \, \psi(t) \right\} = \sum_{n \ge 0} \frac{B_n}{n!} (\operatorname{ad} \Phi(t))^n \, \psi(t)$$

the B_n being the Bernoulli numbers.

6.5. Another alternal mould: the continuous BCH expansion. The expansion of $\Phi(t)$ in the basis (Ψ^I) is given by the series

(86)
$$\Phi(t) = \sum_{r \ge 1} \int_0^t dt_1 \cdots \int_0^{t_{r-1}} dt_r \sum_{\sigma \in \mathbf{S}_r} \frac{(-1)^{d(\sigma)}}{r} {\binom{r-1}{d(\sigma)}}^{-1} \psi(t_{\sigma(r)}) \cdots \psi(t_{\sigma(1)}) .$$

Thus, the coefficient of $\Psi^{I} = \Psi_{i_{1}} \cdots \Psi_{i_{r}}$ in the expansion of Φ_{n} is equal to

(87)
$$n \int_0^1 dt_1 \cdots \int_0^{t_{r-1}} dt_r \sum_{\sigma \in \mathbf{S}_r} \frac{(-1)^{d(\sigma)}}{r} {\binom{r-1}{d(\sigma)}}^{-1} t_{\sigma(r)}^{i_1-1} \cdots t_{\sigma(1)}^{i_r-1} .$$

It is worth observing that this expansion, together with a simple expression of Ψ_n in terms of the dendriform operations of **FQSym**, recently led Ebrahimi-Fard,

Manchon, and Patras [9], to an explicit solution of the Bogoliubov recursion for renormalization in Quantum Field Theory.

6.6. Moulds related to the Fer-Zassenhaus series. The noncommutative power sums of the third kind Z_n are defined by

(88)
$$\sigma(A;t) = \exp(Z_1 t) \, \exp(\frac{Z_2}{2} t^2) \, \dots \, \exp(\frac{Z_n}{n} t^n) \, \dots$$

The first values of Z_n are

$$\begin{aligned} Z_1 &= \Psi_1 \ , \ Z_2 &= \Psi_2 \ , \ Z_3 &= \Psi_3 + \frac{1}{2} \left[\Psi_2, \Psi_1 \right] \ , \\ Z_4 &= \Psi_4 + \frac{1}{3} \left[\Psi_3, \Psi_1 \right] + \frac{1}{6} \left[\left[\Psi_2, \Psi_1 \right], \Psi_1 \right] \ , \\ Z_5 &= \Psi_5 + \frac{1}{4} \left[\Psi_4, \Psi_1 \right] + \frac{1}{3} \left[\Psi_3, \Psi_2 \right] + \frac{1}{12} \left[\left[\Psi_3, \Psi_1 \right], \Psi_1 \right] \ , \\ &- \frac{7}{24} \left[\Psi_2, \left[\Psi_2, \Psi_1 \right] \right] + \frac{1}{24} \left[\left[\left[\Psi_2, \Psi_1 \right], \Psi_1 \right], \Psi_1 \right] \ . \end{aligned}$$

This defines interesting alternal moulds. There is no known expression for Z_n on the Ψ^I , but Goldberg's explicit formula (see [24]) for the Hausdorff series gives the decomposition of Φ_n on the basis Z^I .

The fact that Z_n is a Lie series is known as the Fer-Zassenhaus "formula".

6.7. A one-parameter family. It follows from the characterization of Lie idempotents in the descent algebra that $P_n(A;q) = (1-q^n)\Psi_n\left(\frac{A}{1-q}\right)$ is a noncommutative power sum. The corresponding Lie idempotent is

(89)
$$\varphi_n(q) = \frac{1}{n} \sum_{|I|=n} \frac{(-1)^{d(\sigma)}}{\begin{bmatrix} n-1\\ d(\sigma) \end{bmatrix}} q^{\max(\sigma) - \binom{d(\sigma)+1}{2}} \sigma$$

It specializes to

(90)
$$\varphi_n(0) = \theta_n, \qquad \varphi_n(1) = \phi_n \qquad \varphi_n(\omega) = \kappa_n$$

where ω is a primitive *n*th root of unity (and $\varphi_n(\infty) = \theta_n^*$). The nonlinear operator $E_q[h(t)]$, where $h(t) = \sum_{n \ge 1} H_n t^{n-1}$, is

(91)
$$E_q[h(t)] = \sum_I c_I(q) H^I t^{|I|}$$

Then,

(92)
$$E_1[h(t)] = \exp \int_0^t h(s)ds = H(t)$$

while E_0 is Dyson's chronological exponential

(93)
$$E_0[h(t)] = T \exp \int_0^t h(s) ds = 1 + \int_0^t dt_1 h(t_1) + \int_0^t dt_1 \int_0^{t_1} dt_2 h(t_2) h(t_1) + \cdots$$

6.8. Another one-parameter family. In [18], it is proved that there exists a unique sequence $\pi_n(q)$ of Lie idempotents which are left and right eigenvectors of $\sigma_1((1-q)A)$ for the internal product:

(94)
$$\sigma_1((1-q)A) * \pi_n(q) = \pi_n(q) * \sigma_1((1-q)A) = (1-q^n)\pi_n(q)$$

These elements have the following specializations:

(95)
$$\pi_n(1) = \frac{\Psi_n}{n}, \frac{1}{n} K_n(\zeta), \ \pi_n(0) = \frac{1}{n} Z_n.$$

In particular, the associated alternal moulds provide an interpolation between the T-exponential and the Fer-Zassenhaus expansion.

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