

# Moulds and Multiple Zeta Values

## 1 Moulds

**Definition 1.** *The standard definition is that a mould is a function on “a variable number of variables”. To flesh out this definition, in the general case, let  $\mathcal{A}, \mathcal{B}$  be sets and  $K$  be an algebra. A mould,  $M^\bullet = (M^\bullet, \mathcal{A}, K)$ , is a map from the free monoid  $\mathcal{A}^*$  into  $K$  and a bimould is defined as a function on the free monoid of the Cartesian product of two sets,  $(\mathcal{A} \times \mathcal{B})^*$ :*

$$\begin{array}{ll} \text{Mould} & M^\bullet : \mathcal{A}^* \rightarrow K \\ & \mathbf{w} = (w_1, \dots, w_r) \mapsto M^{\mathbf{w}} \\ \text{Bimould} & N^\bullet : (\mathcal{A} \times \mathcal{B})^* \rightarrow K \\ & \mathbf{w} = \begin{pmatrix} u_1, \dots, u_r \\ v_1, \dots, v_r \end{pmatrix} \mapsto N^{\mathbf{w}}. \end{array}$$

## 1.1 Examples

$Ze_*^\bullet$  is the bimould defined by

$$(Ze_*^\bullet, \mathbb{Q}/\mathbb{Z} \times \mathbb{N}^*, \mathbb{C}) := Ze_*^{\binom{\epsilon_1, \dots, \epsilon_r}{s_1, \dots, s_r}} = \sum_{n_1 > n_2 > \dots > n_r > 0} \prod n_k^{-s_k} e^{2\pi i \epsilon_k n_k}$$

with  $s_1 \geq 2$ . If we take  $\epsilon_i = 0 \forall i$  then we obtain the usual multiple zeta values. Sometimes people say that elements in the image of this mould are “colored multiple zeta values”.

$Wa_*^\bullet$  is the mould defined by

$$(Wa_*^\bullet, \{e^{2\pi i k}; k \in \mathbb{Q}\} \cup \{0\}, \mathbb{C}) := Wa_*^{e^{2\pi i \epsilon_1 0^{s_1-1}} \dots e^{2\pi i \epsilon_r 0^{s_r-1}}} = Ze_*^{\binom{\epsilon_r, \epsilon_{r-1}-\epsilon_r, \dots, \epsilon_1-\epsilon_2}{s_r, s_{r-1}, \dots, s_1}}.$$

Hence we require that the first term be a root of unity and the last term be 0.

## 1.2 Operations on Moulds

Given two moulds (resp. bimoulds)  $(M^\bullet, \mathcal{A}(\text{resp. } \times \mathcal{B}), K)$  and  $(N^\bullet, \mathcal{A}(\text{resp. } \times \mathcal{B}), K)$  addition and multiplication are given by

$$\begin{aligned} M^\bullet + N^\bullet &= C^\bullet : C^{\mathbf{w}} = M^{\mathbf{w}} + N^{\mathbf{w}} \\ M^\bullet \times N^\bullet &= mu(M^\bullet, N^\bullet) = C^\bullet : C^{\mathbf{w}} = \sum_{\mathbf{w}=\mathbf{w}^1 \cdot \mathbf{w}^2} M^{\mathbf{w}^1} \cdot N^{\mathbf{w}^2}. \end{aligned}$$

*Swap*

$$\begin{aligned} swap : (M^\bullet, \mathcal{A} \times \mathcal{B}, K) &\rightarrow (M^\bullet, \mathcal{B} \times \mathcal{A}, K) \\ swap(M^\bullet) \binom{u_1, \dots, u_r}{v_1, \dots, v_r} &= M \binom{v_r, \dots, v_1}{u_1 + \dots + u_r, u_1 + \dots + u_{r-1}, \dots, u_1} \end{aligned}$$

*Negation/Parity*

$$nepar(M^\bullet)^{(w_1, \dots, w_r)} = (-1)^r M^{(-w_1, \dots, -w_r)}$$

*Flexions*

$\mathcal{A}$ -semi-group,  $\mathcal{B}$ -abelian group

$$\begin{aligned} \mathbf{w} &= \dots \mathbf{w}^1 \cdot \mathbf{w}^2 \dots \\ \mathbf{w}^1 &= \begin{pmatrix} u_1 & \dots & u_r \\ v_1 & \dots & v_r \end{pmatrix}, \mathbf{w}^2 = \begin{pmatrix} u_{r+1} & \dots & u_s \\ v_{r+1} & \dots & v_s \end{pmatrix} \end{aligned}$$

$$\mathbf{w}^1 \rfloor := \begin{pmatrix} u_1 & \dots & u_{r-1} & \sum_{k=r}^s u_k \\ v_1 & \dots & v_{r-1} & v_r \end{pmatrix}$$

$$\mathbf{w}^1 \lceil := \begin{pmatrix} u_1 & \dots & u_r \\ v_1 - v_{r+1} & \dots & v_r - v_{r+1} \end{pmatrix}$$

$$\lceil \mathbf{w}^2 := \begin{pmatrix} \sum_{k=1}^{r+1} u_k & u_{r+2} & \dots & u_s \\ v_{r+1} & v_{r+2} & \dots & v_s \end{pmatrix}$$

$$\lfloor \mathbf{w}^2 := \begin{pmatrix} u_{r+1} & \dots & u_s \\ v_{r+1} - v_r & \dots & v_s - v_r \end{pmatrix}$$

### 1.3 Symmetries

**Definition 2.** A mould/bimould  $A^\bullet$  is *symmetral* (resp. *alternel*) if

$$\forall \mathbf{w}^1, \mathbf{w}^2, \quad \sum_{\mathbf{w} \in sha(\mathbf{w}^1, \mathbf{w}^2)} A^{\mathbf{w}} = A^{\mathbf{w}^1} A^{\mathbf{w}^2} \quad (\text{resp. } = 0),$$

where  $sha(\mathbf{w}^1, \mathbf{w}^2)$  denotes the *shuffle product of sequences*. We say such a mould is “*as*” (resp. “*al*”).  $Wa_\bullet^*$  is *as*.

A mould/bimould  $A^\bullet$  is *symmetrel* (resp. *alternel*) if

$$\forall \mathbf{w}^1, \mathbf{w}^2, \quad \sum_{\mathbf{w} \in she(\mathbf{w}^1, \mathbf{w}^2)} A^{\mathbf{w}} = A^{\mathbf{w}^1} A^{\mathbf{w}^2} \quad (\text{resp. } = 0),$$

where  $she(\mathbf{w}^1, \mathbf{w}^2)$  denotes the “*contracting shuffle*” or “*stuffle*” product of sequences, which is given by the recursion relation,

$$\mathbf{w}^1 = (a_1, \dots, a_r), \mathbf{w}^2 = (a_{r+1}, \dots, a_{r+s})$$

$$she(\mathbf{w}^i, \emptyset) = \mathbf{w}^i$$

$$she(\mathbf{w}^1, \mathbf{w}^2) = a_1 \cdot she((a_2, \dots, a_r), \mathbf{w}^2) \sqcup a_{r+1} \cdot she(\mathbf{w}^1, (a_{r+2}, \dots, a_{r+s})) \sqcup (a_1 + a_{r+1}) \cdot she((a_2, \dots, a_r), (a_{r+2}, \dots, a_{r+s})).$$

Such a mould is called *es* (resp. *el*).  $Ze_\bullet^*$  is *es*.

## 1.4 More Examples

The following examples of moulds define two generating series for multiple zeta values, and provide a method of regularization of multiple zeta values.

### Regularization

There exists a unique mould,  $Ze^\bullet$ , such that

- $Ze^\bullet = Ze_\bullet^\bullet$  wherever  $Ze_\bullet^\bullet$  is defined,
- $Ze^\bullet$  is defined on all of  $(\mathbb{Q}/\mathbb{Z} \times \mathbb{N}^*)^*$
- $Ze^{(1)} = 0$ ,
- $Ze^\bullet$  is symmetrel

Likewise, there exists a unique mould,  $Wa^\bullet$ , such that

- $Wa^\bullet = Wa_\bullet^\bullet$  wherever  $Wa_\bullet^\bullet$  is defined,
- $Wa^\bullet$  is defined on all  $\{e^{2\pi ik}; k \in \mathbb{Q}\} \cup \{0\}$ ,
- $Wa^{(1)} = Wa^{(0)} = 0$ ,
- $Wa^\bullet$  is symmetral.

### Generating Series

$$Zig^\bullet := Zig\left(\begin{smallmatrix} \epsilon_1 & \dots & \epsilon_r \\ v_1 & \dots & v_r \end{smallmatrix}\right) = \sum_{s_i \geq 1} Ze\left(\begin{smallmatrix} \epsilon_1 & \dots & \epsilon_r \\ s_1 & \dots & s_r \end{smallmatrix}\right) v_1^{s_1-1} \dots v_r^{s_r-1}.$$

$$Zag^\bullet := Zag\left(\begin{smallmatrix} u_1 & \dots & u_r \\ \epsilon_1 & \dots & \epsilon_r \end{smallmatrix}\right) = \sum_{s_i \geq 1} Wa\left(e^{2\pi i \epsilon_1 0^{s_1-1}}, \dots, e^{2\pi i \epsilon_r 0^{s_r-1}}\right) u_1^{s_1-1} (u_1 + u_2)^{s_2-1} \dots (u_1 + u_2 + \dots + u_r)^{s_r-1}.$$

$Zag^\bullet$  is symmetral, whereas  $Zig^\bullet$  satisfies another symmetry, *symmetril*, closely related to symmetrel.

## Conversion

$$\begin{aligned}
(\text{mono}^\bullet, \mathbb{Q}/\mathbb{Z} \times \mathbb{N}^*, \mathbb{C}) &:= 1 + \sum_{k=1} \text{mono} \binom{0^k}{1^k} t^k = \exp \left( \sum_{k=2} (-1)^{k-1} \zeta(k) \frac{t^k}{k} \right) \\
&:= 0 \text{ whenever } \begin{pmatrix} \epsilon_1 & \dots & \epsilon_r \\ s_1 & \dots & s_r \end{pmatrix} \neq \begin{pmatrix} 0 & \dots & 0 \\ 1 & \dots & 1 \end{pmatrix} \\
(\text{mini}^\bullet, \mathbb{Q}[u_i] \times \mathbb{Q}/\mathbb{Z}, \mathbb{C}) &:= \text{mini} \binom{\epsilon_1, \dots, \epsilon_r}{v_1, \dots, v_r} = \text{mono} \binom{\epsilon_1, \dots, \epsilon_r}{1, \dots, 1}.
\end{aligned}$$

**Proposition 3.**  $\text{mini}^\bullet \times \text{swap}(\text{Zag}^\bullet) = \text{Zig}^\bullet$

We say then that  $\text{Zag}^\bullet$  is *as/is*, since it's symmetral and its swap is symmetril (up to multiplication by a commutative bimould).

## 2 Key Results

### 2.1 ARI/GARI

In order to keep simplicity for this talk, we take the following definition, which is more restricted than the usual general definition.

**Definition 4.** Let  $ARI_{al/il}$  be the Lie algebra with the following definition.

- As a vector space over  $\mathbb{Q}$ ,

$$(ARI_{al/il}, \mathbb{Q}[u_i] \times \mathbb{Q}/\mathbb{Z}, \mathbb{C}[[u_i]]) := \langle M^\bullet : M^\emptyset = 0, M \text{ is al, swap}(M^\bullet) \text{ is alternil}^{**} \rangle,$$

- The Lie bracket is given by

$$\begin{aligned} \text{ari}(M^\bullet, N^\bullet)^{\mathbf{w}} = & \sum_{\mathbf{w}=\mathbf{w}^1\mathbf{w}^2} A^{\mathbf{w}^1} B^{\mathbf{w}^2} - B^{\mathbf{w}^1} A^{\mathbf{w}^2} + \sum_{\mathbf{w}=\mathbf{w}^2\mathbf{w}^3\mathbf{w}^4} M^{[\mathbf{w}^3} N^{\mathbf{w}^2]} \mathbf{w}^4 - N^{[\mathbf{w}^3} M^{\mathbf{w}^2]} \mathbf{w}^4 \\ & + \sum_{\mathbf{w}=\mathbf{w}^1\mathbf{w}^2\mathbf{w}^3} M^{\mathbf{w}^1} [\mathbf{w}^3} N^{\mathbf{w}^2}] - N^{\mathbf{w}^1} [\mathbf{w}^3} M^{\mathbf{w}^2}] \end{aligned}$$

(\*\* The alternil condition means “up to a multiplication by a commutative bimould”.)

*Remarks*

- The *ari* bracket is equal to the Lie-Poisson bracket  $\{, \}$ , up to a variable change, on the usual Lie algebra of multizeta values ( $\mathfrak{dm}$ ). However, the *ari* bracket can be defined on a more general set of vector spaces, which is a tool Ecalle uses in his proofs.
- The flexions ( $[\_, \_]$ ,  $[\_, \_]$ ,  $[\_]$ ) in the definition of the “*ari*” bracket correspond to the derivations,  $D_f(x) = 0$ ,  $D_f(y) = [y, f]$ , which give the definition of the above mentioned Poisson bracket.

**Definition 5.** By taking the ari-exponential of the Lie algebra,  $ARI_{al/il}$ , we obtain a Lie group,  $GARI_{as/is}$  which has the following presentation.

- As a set,

$$(GARI_{as/is}, \mathbb{Q}[u_i] \times \mathbb{Q}/\mathbb{Z}, \mathbb{C}[[u_i]]) := \{M^\bullet : M^\emptyset = 1, M \text{ is as, } \text{swap}(M^\bullet) \text{ is symmetril}^{**}\},$$

- The group law is given by

$$\text{gari}(A^\bullet, B^\bullet)^{\mathbf{w}} = \sum_{\mathbf{w}=\mathbf{a}^1\mathbf{b}^1\mathbf{c}^1\dots\mathbf{b}^s\mathbf{c}^s\mathbf{a}^{s+1}} A^{[\mathbf{b}^1]} \dots A^{[\mathbf{b}^s]} B^{\mathbf{a}^1} \dots B^{\mathbf{a}^{s+1}} (B^{-1})^{[\mathbf{c}^1]} \dots (B^{-1})^{[\mathbf{c}^s]},$$

where  $\mathbf{s} \geq 0$ ,  $\mathbf{b}^i \neq \emptyset$  ( $\forall 1 \leq i \leq \mathbf{s}$ ),  $\mathbf{c}^i \cdot \mathbf{a}^{i+1} \neq \emptyset$  ( $\forall 1 \leq i \leq \mathbf{s} - 1$ ) and  $(B^{-1})$  denotes the inverse for standard mould multiplication.

- $\text{invgari}(M^\bullet)$  is inverse of a mould  $M^\bullet$  for the gari product,

$$\text{gari}(\text{invgari}(A^\bullet), A^\bullet) = \text{gari}(A^\bullet, \text{invgari}(A^\bullet)) = \mathbf{1}^\bullet, \text{ where } \mathbf{1}^\emptyset = 1, \mathbf{1}^{\mathbf{w}} = 0.$$

## IMPORTANT FACT

The mould  $Zag^\bullet$  is an element of the Lie group, GARI.



## 2.2 Canonical Decomposition into Irreducibles

**Theorem 6.** *The mould  $Zag^\bullet$  may be decomposed into three factors,*

$$Zag^\bullet = gari(Zag_{I}^\bullet, Zag_{II}^\bullet, Zag_{III}^\bullet)$$

*such that:*

- *The even/odd length components of  $Zag_{I,II}^\bullet$  are even/odd functions of  $\mathbf{w}$ , while the even/odd length components of  $Zag_{III}^\bullet$  are odd/even functions of  $\mathbf{w}$ ;*
- *Each component is decomposed as a series in a basis of  $ARI_{al/il}$ , which when evaluated at  $\epsilon_i = 0$  are irreducible elements of the  $\mathbb{Q}$  algebra of multiple zeta values,  $\mathbb{Zeta}$ ;*
- *The irreducibles appearing as coefficients in the factors give us a factorization for the multiple zeta value algebra,*

$$\mathbb{Zeta} := \mathbb{Zeta}_I \otimes \mathbb{Zeta}_{II} \otimes \mathbb{Zeta}_{III}.$$

### 2.3 $Zag_{III}^\bullet$

- The factor  $Zag_{III}^\bullet$  is the most simple to express explicitly,

$$gari(Zag_{III}^\bullet, Zag_{III}^\bullet) = gari(nepar(inv\,gari(Zag^\bullet)), Zag^\bullet).$$

By linearizing, you can see that indeed this provides an odd/even function on components of even/odd length.

- The length 1 component is given by

$$Zag_{III}^{\binom{u_1}{0}} = \sum_{s \geq 3, \text{ odd}} \zeta(s) u_1^{s-1}.$$

- The associated factor in the multiple zeta value algebra,  $Zeta_{III}$ , is generated by irreducibles of odd depth, i.e. linear combinations of  $\zeta(s_1, \dots, s_r)$  where  $r$  is odd. The mould of such irreducibles is denoted by  $Irr_{III}^\bullet$ .
- We get an explicit expression for the set of irreducible multiple zeta values in factor  $Zag_{III}^\bullet$  in terms of a mould  $loma^\bullet$ , which is a generating mould which (vaguely speaking) forms a basis of rational polynomials for  $ARI_{al/il}$  (the explicit construction is out of the scope of this talk). We have

$$Zag_{III}^\bullet := \sum_{s_i \geq 1, r \text{ odd}} Irr_{III}^{s_1, \dots, s_r} loma_{s_1}^\bullet \cdots loma_{s_r}^\bullet,$$

where  $loma_{s_i}^\bullet$  is the restriction of  $loma^\bullet$  to the weight  $s_i$  terms.

## 2.4 $Zag_I^\bullet$

- $Zag_I^w \in \mathbb{Q}[[u_i, \pi^2]]$  (when  $\epsilon_1 = 0$ ), which in the language of zetas, means that the corresponding factor in the  $Zeta$  algebra,  $Zeta_I$ , is generated by  $6\zeta(2) = \pi^2$ .
- The explicit factorization of  $Zag_I^\bullet$  from  $Zag^\bullet$  is a very costly analytic construction, whose difficulty comes from getting rid of unwanted singularities. The formula is the following:

$$Zag_I^\bullet = gari(tal^\bullet, invgari(pal^\bullet), expari(roma^\bullet)),$$

and again the definition of  $pal$  and  $roma$  go out of the scope, since they are very long.

## 2.5 $Zag_{II}^\bullet$

- $Zag_{II}^\bullet$  is explicitly calculated by factoring  $Zag^\bullet$  by  $Zag_I^\bullet$  and  $Zag_{III}^\bullet$ .
- $Zag_{II}^\bullet$  may be factored as a generating series for the irreducible multiple zeta values of even depth in the same manner as  $Zag_{III}^\bullet$ , providing a set of “canonical” irreducibles for  $Zeta_{II}$ ,

$$Zag_{II}^\bullet := \sum_{s_i \geq 1, r \text{ even}} Irr_{II}^{s_1, \dots, s_r} loma_{s_1}^\bullet \cdots loma_{s_r}^\bullet.$$