



# SINGLE-VALUED MOTIVIC PERIODS AND MULTIPLE ZETA VALUES

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## Abstract

The values at 1 of single-valued multiple polylogarithms span a certain subalgebra of multiple zeta values. The properties of this algebra are studied from the point of view of motivic periods.

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## 1. Introduction

The goal of this paper is to study a special class of multiple zeta values which occur as the values at 1 of single-valued multiple polylogarithms. The latter were defined in [11], and generalize the Bloch–Wigner dilogarithm

$$D(z) = \text{Im}(\text{Li}_2(z) + \log |z| \log(1 - z)), \quad (1.1)$$

which is a single-valued version of  $\text{Li}_2(z)$ , to the case of all multiple polylogarithms in one variable. These are defined for integers  $n_1, \dots, n_r \geq 1$  by

$$\text{Li}_{n_1, \dots, n_r}(z) = \sum_{0 < k_1 < \dots < k_r} \frac{z^{k_r}}{k_1^{n_1} \dots k_r^{n_r}},$$

and are iterated integrals on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  obtained by integrating along the straight-line path from 0 to 1 along the real axis. In the convergent case  $n_r \geq 2$ , their values at 1 are Euler’s multiple zeta values

$$\zeta(n_1, \dots, n_r) = \sum_{0 < k_1 < \dots < k_r} \frac{1}{k_1^{n_1} \dots k_r^{n_r}}. \quad (1.2)$$

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The values at 1 of the single-valued multiple polylogarithms define an interesting subclass of multiple zeta values, which we denote by

$$\zeta_{\text{sv}}(n_1, \dots, n_r) \in \mathbb{R}. \quad (1.3)$$

They satisfy  $\zeta_{\text{sv}}(2) = D(1) = 0$ , as one immediately sees from (1.1). These numbers are, in a precise sense, the values of iterated integrals on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ , which are obtained by integrating from 0 to 1 *independently of all choices of path*.

The numbers (1.3) have recently found several applications in physics: for example, in

- (1) O. Schnetz' theory of graphical functions for Feynman amplitudes [8, 27];
- (2) the coefficients of the closed super-string tree-level amplitude [29, 30]; and
- (3) wrapping functions in  $N = 4$  super Yang–Mills theory [24];

as well as in [7, 19, 20, 26], and also in mathematics as the coefficients of Deligne's associator. A general theme seems to be that a large class of (but not all) Feynman amplitudes in four-dimensional renormalizable quantum field theories lies in the subspace of single-valued multiple zeta values. This raises an interesting possibility of replacing general amplitudes with their single-valued versions (see Section 3), which should lead to considerable simplifications.

**1.1. Main result.** In [9], motivic multiple zeta values  $\zeta^{\text{m}}(n_1, \dots, n_r)$  were defined as elements of a certain graded algebra  $\mathcal{H}$ , equipped with a period homomorphism

$$\text{per} : \mathcal{H} \longrightarrow \mathbb{C}$$

which maps  $\zeta^{\text{m}}(n_1, \dots, n_r)$  to  $\zeta(n_1, \dots, n_r)$ . Furthermore, the algebra  $\mathcal{H}$  has an action of the de Rham motivic Galois group  $G_{\text{dR}}$  which is an affine group scheme over  $\mathbb{Q}$ . In this paper, 'single-valued motivic multiple zeta values'  $\zeta_{\text{sv}}^{\text{m}}(n_1, \dots, n_r)$  are defined. Their images under the map  $\text{per}$  are the numbers (1.3). They generate a subalgebra  $\mathcal{H}^{\text{sv}} \subset \mathcal{H}$  whose main properties can be summarized as follows.

**THEOREM 1.1.** *There is a natural homomorphism  $\mathcal{H} \rightarrow \mathcal{H}^{\text{sv}}$  which sends  $\zeta^{\text{m}}(n_1, \dots, n_r)$  to  $\zeta_{\text{sv}}^{\text{m}}(n_1, \dots, n_r)$ . In particular, the  $\zeta_{\text{sv}}^{\text{m}}(n_1, \dots, n_r)$  satisfy all motivic relations for multiple zeta values, together with the relation  $\zeta_{\text{sv}}^{\text{m}}(2) = 0$ .*

*The algebra  $\mathcal{H}^{\text{sv}}$  is isomorphic to the polynomial algebra generated by*

$$\zeta_{\text{sv}}^{\text{m}}(n_1, \dots, n_r),$$

*where  $n_i \in \{2, 3\}$  and  $(n_1, \dots, n_r)$  is a Lyndon word (for the ordering  $3 < 2$ ) of odd weight. Furthermore,  $\mathcal{H}^{\text{sv}}$  is preserved under the action of the group  $G_{\text{dR}}$ .*

In particular, the numbers  $\zeta_{\text{sv}}(n_1, \dots, n_r)$  satisfy the same double shuffle and associator relations as usual multiple zeta values, and many more relations besides: the space  $\mathcal{H}^{\text{sv}}$  is much smaller than  $\mathcal{H}$  (Section 7.4). By way of example,

$$\begin{aligned}\zeta_{\text{sv}}(2n+1) &= 2\zeta(2n+1) \quad \text{for all } n \geq 1 \\ \zeta_{\text{sv}}(5, 3) &= 14\zeta(3)\zeta(5) \\ \zeta_{\text{sv}}(3, 5, 3) &= 2\zeta(3, 5, 3) - 2\zeta(3)\zeta(3, 5) - 10\zeta(3)^2\zeta(5).\end{aligned}$$

The reader who is only interested in the single-valued multiple zeta values and not their motivic versions can turn directly to Section 5 for an elementary definition (which only uses the Ihara action, Section 4.2), and Section 7.4 for enumerative properties and examples.

**1.2. Motivic periods.** This paper seemed a good opportunity to clarify certain concepts relating to motivic multiple zeta values. There are two conflicting notions of motivic multiple zeta values in the literature, one due to Goncharov [22] (for which the motivic version of  $\zeta(2)$  vanishes), via the concept of framed objects in mixed Tate categories, and another for which the motivic version of  $\zeta(2)$  is nonzero [9], later simplified by Deligne [17]. It can be paraphrased as follows.

**DEFINITION 1.2.** Let  $\mathcal{M}$  be a Tannakian category of motives over  $\mathbb{Q}$ , with two fiber functors  $\omega_{dR}, \omega_B$ . A *motivic period* is an element of the affine ring of the torsor of tensor isomorphisms from  $\omega_{dR}$  to  $\omega_B$ :

$$\mathcal{P}_{\mathcal{M}}^{\text{m}} = \mathcal{O}(\text{Isom}_{\mathcal{M}}(\omega_{dR}, \omega_B)).$$

Given a motive  $M \in \mathcal{M}$ , and classes  $\eta \in \omega_{dR}(M)$ ,  $X \in \omega_B(M)^\vee$ , the *motivic period* [17] associated to this data is the function on  $\text{Isom}_{\mathcal{M}}(\omega_{dR}, \omega_B)$  defined by

$$[M, \eta, X]^{\text{m}} := (\phi \mapsto \langle \phi(\eta), X \rangle).$$

This definition is nothing other than the standard construction of the ring of functions on the Tannaka groupoid, and appears in a similar form in [1, 2, Section 23.5]. However, it is the interpretation and application of this concept which is of interest here; in particular, the idea that one can sometimes deduce results about periods from their motivic versions and vice versa (see, for example, [9, Section 4.1]). The ring of motivic periods is a bitorsor over the Tannaka groups  $(G_{\omega_{dR}}, G_{\omega_B})$  and thus gives rise to a Galois theory of motivic periods. In this paper, only the special case where  $\mathcal{M} = \mathcal{MT}(\mathbb{Z})$  is the category of mixed Tate motives over  $\mathbb{Z}$  is considered: the generalization to other categories of mixed Tate motives [18] is relatively straightforward if one replaces  $\omega_{dR}$  with the canonical fiber functor, and bears in mind that there can be several different Betti realizations.

In a similar vein, one can replace  $\omega_{dR}, \omega_B$  with any pair of fiber functors, to obtain various different notions of motivic period. One can consider the ring of *de Rham periods*  $\mathcal{P}_{\mathcal{M}}^{\partial\tau}$ , where we replace  $m = (\omega_{dR}, \omega_B)$  with  $\partial\tau = (\omega_{dR}, \omega_{dR})$ , and a weaker notion of *unipotent de Rham periods*  $\mathcal{P}_{\mathcal{M}}^u$  which are their restriction to the unipotent radical  $U_{\omega_{dR}}$  of the Tannaka group  $G_{\omega_{dR}}$ . The latter are precisely the ‘framed objects’ studied in [5, 6, 22], and the unipotent de Rham versions of multiple zeta values are the objects that Goncharov calls motivic multiple zeta values. Although there is no complex period (integration) map for de Rham motivic periods, we construct a related notion in Section 3 in the case  $\mathcal{M} = \mathcal{MT}(\mathbb{Z})$ , which we call the single-valued motivic period. It gives a well-defined homomorphism from unipotent de Rham periods to motivic periods:

$$sv^m : \mathcal{P}_{\mathcal{M}}^u \longrightarrow \mathcal{P}_{\mathcal{M}}^m.$$

Composing with the period map attaches a complex number to de Rham periods. This gives a transcendental pairing between a de Rham cohomology class and a de Rham homology class. In the case of  $\mathcal{MT}(\mathbb{Z})$ , the numbers one obtains are precisely the single-valued multiple zeta values (1.3). Since the definition of  $sv^m$  requires nothing more than complex conjugation and the weight grading, it comes perhaps as a surprise that this map is already so intricate in this special case (see, for example, (7.4)). A similar construction works for more general categories of mixed Tate motives over a number field with a real embedding.

**1.3. Contents.** Section 2 consists of generalities on motivic and de Rham periods, some of which are new, and may be of independent interest. In particular, it should hopefully clarify the role of  $\zeta(2)$  and statements of the sort ‘ $2\pi i = 0$ ’ versus ‘ $2\pi i = 1$ ’ that one sometimes encounters. Section 3 defines the motivic single-valued map  $sv^m$ . The remainder of the paper applies this construction to the case of the motivic fundamental groupoid of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . Section 4 consists of reminders, and Section 5 gives a completely elementary definition of  $\zeta_{sv}$ . Section 6 defines the motivic versions  $\zeta_{sv}^m$ , and Section 6.3 constructs the single-valued multiple polylogarithms from first principles from the point of view of the unipotent fundamental groupoid.

The multiple polylogarithms  $Li_{n_1, \dots, n_r}(z)$  are coefficients of the function  $L(z)$ , which is the unique solution to the Knizhnik–Zamolodchikov equation

$$\begin{aligned} \frac{\partial}{\partial z} L(z) &= L(z) \left( \frac{e_0}{z} + \frac{e_1}{1-z} \right) \\ \frac{\partial}{\partial \bar{z}} L(z) &= 0, \end{aligned}$$

normalized with respect to the tangent vector 1 at 0. The single-valued versions are the coefficients of the function  $\mathcal{L}(z)$ , which is the unique solution to the equations

$$\begin{aligned} \frac{\partial}{\partial z} \mathcal{L}(z) &= \mathcal{L}(z) \left( \frac{e_0}{z} + \frac{e_1}{1-z} \right) \\ (\mathcal{M}_i - \text{id})L(z) &= 0 \quad \text{for } i = 0, 1, \infty, \end{aligned}$$

where  $\mathcal{M}_i$  denotes analytic continuation around a small loop encircling the point  $i$ , again normalized with respect to the tangent vector 1 at 0. The general single-valued principle derives the formula for  $\mathcal{L}(z)$  in terms of  $L(z)$  which was given in [11]. Up to this point, all constructions in this paper are rather general and do not use any deep results about the structure of multiple zeta values or mixed Tate motives. Finally, Section 7 applies the main theorem of [9] to deduce structural results about  $\mathcal{H}^{\text{sv}}$ .

1.3.1. *Conventions.* All tensor products are over  $\mathbb{Q}$  unless stated otherwise.

## 2. Generalities on periods and mixed Tate motives

See [18, Section 2] for the background material on mixed Tate motives required in this section. Much of what follows applies to any category of mixed Tate motives over a number field, provided that one replaces the de Rham fiber functor with the canonical fiber functor  $\omega = \bigoplus_n \omega_n$ , where

$$\omega_n(M) = \text{Hom}_{\mathcal{MT}}(\mathbb{Q}(-n), \text{gr}_{2n}^W M),$$

which is defined over  $\mathbb{Q}$  (see [18, Section 1.1]). A Betti realization functor will be relative to an embedding of the number field into  $\mathbb{C}$ .

**2.1. Mixed Tate motives over  $\mathbb{Z}$ .** Let  $\mathcal{M} = \mathcal{MT}(\mathbb{Z})$  denote the  $\mathbb{Q}$ -linear Tannakian category of mixed Tate motives over  $\mathbb{Z}$  [18, 25]. Its canonical fiber functor is equal to the fiber functor  $\omega_{dR}$  given by the de Rham realization, and it is equipped with a fiber functor  $\omega_B$  given by the Betti realization with respect to the unique embedding  $\mathbb{Q} \hookrightarrow \mathbb{C}$ . Let  $G_{dR}$  and  $G_B$  denote the corresponding Tannaka groups. They are affine group schemes over  $\mathbb{Q}$ . We shall mainly focus on  $G_{dR}$ .

The action of  $G_{dR}$  on  $\mathbb{Q}(-1) \in \mathcal{M}$  defines a map  $G_{dR} \rightarrow \mathbb{G}_m$  whose kernel is denoted by  $\mathcal{U}_{dR}$ . Note that our convention for the degree differs from that in [18]. The group  $\mathcal{U}_{dR}$  is a pro-unipotent affine group scheme over  $\mathbb{Q}$ . Furthermore, since  $\omega_{dR}$  is graded,  $G_{dR}$  admits a decomposition as a semidirect product ([18, Section 2.1]):

$$G_{dR} \cong \mathcal{U}_{dR} \rtimes \mathbb{G}_m. \tag{2.1}$$

A mixed Tate motive  $M \in \mathcal{M}$  can be represented by a finite-dimensional graded  $\mathbb{Q}$ -vector space  $M_{dR} = \omega_{dR}(M)$  equipped with an action of  $\mathcal{U}_{dR}$  which is compatible with the grading. We shall write  $(M_{dR})_n$  for the component in degree  $n$ ; that is,  $(M_{dR})_n = (W_{2n} \cap F^n)M_{dR}$ . The Betti realization of  $M$ , denoted  $M_B = \omega_B(M)$ , is a finite-dimensional  $\mathbb{Q}$ -vector space equipped with an increasing filtration  $W_\bullet M_B$ .

The two are related by a canonical comparison isomorphism,

$$\text{comp}_{B,dR} : M_{dR} \otimes_{\mathbb{Q}} \mathbb{C} \xrightarrow{\sim} M_B \otimes_{\mathbb{Q}} \mathbb{C}, \tag{2.2}$$

which can be computed by integrating differential forms. We shall often use the fact that  $\mathbb{Q}(0) \in \mathcal{M}$  has rational periods, that is,

$$\text{comp}_{B,dR} : \mathbb{Q}(0)_{dR} \xrightarrow{\sim} \mathbb{Q}(0)_B. \tag{2.3}$$

In general, given any pair of fiber functors  $\omega_1, \omega_2$  on  $\mathcal{M}$ , let

$$\mathfrak{F}_{\omega_1, \omega_2} = \text{Isom}(\omega_1, \omega_2)$$

denote the set of isomorphisms of fiber functors from  $\omega_1$  to  $\omega_2$ . It is a scheme over  $\mathbb{Q}$ , and is a bitorsor over  $(G_{\omega_1}, G_{\omega_2})$ , where  $G_{\omega_i} = \mathfrak{F}_{\omega_i, \omega_i}$  is the Tannaka group scheme relative to  $\omega_i$ , for  $i = 1, 2$ . The comparison map defines a complex point:

$$\text{comp}_{B,dR} \in \mathfrak{F}_{\omega_{dR}, \omega_B}(\mathbb{C}).$$

**2.2. Motivic periods.** There are two conflicting notions of motivic multiple zeta values in the literature, one due to [22] and the other due to [9]. One can reconcile the two definitions with minimal damage to existing terminology as follows.

DEFINITION 2.1. Let  $\omega_1, \omega_2$  be two fiber functors on  $\mathcal{M}$ . Let  $M \in \text{Ind}(\mathcal{M})$ , and let  $\eta \in \omega_1(M)$ , and  $X \in \omega_2(M)^\vee$ . A *motivic period* of  $M$  of type  $(\omega_1, \omega_2)$ ,

$$[M, \eta, X]^{\omega_1, \omega_2} \in \mathcal{O}(\mathfrak{F}_{\omega_1, \omega_2}), \tag{2.4}$$

is the function  $\mathfrak{F}_{\omega_1, \omega_2} \rightarrow \mathbb{A}^1$  defined by  $\phi \mapsto \langle \phi(\eta), X \rangle = \langle \eta, {}^t\phi(X) \rangle$ .

One can clearly extend Definition 2.1 to other Tannakian categories (of motives), but only  $\mathcal{M} = \mathcal{MT}(\mathbb{Z})$  will be considered in this paper.

Definition 2.1 in the case  $(\omega_1, \omega_2) = (\omega_{dR}, \omega_B)$  is due to Deligne [17], and simplifies the definition in [9]. Since this is the case of primary interest for us, we shall call (2.4) a *motivic period*, and denote the pair  $(\omega_{dR}, \omega_B)$  simply

by  $m$ . We shall also consider the case  $(\omega_1, \omega_2) = (\omega_{dR}, \omega_{dR})$ . We shall call the corresponding period (2.4) a *de Rham period*, and denote the pair  $(\omega_{dR}, \omega_{dR})$  by  $\partial\tau$ .

DEFINITION 2.2. Let  $M \in \mathcal{M}$ , and let  $\omega_1, \omega_2$  be a pair of fiber functors as above. We shall denote the space of all motivic periods of type  $(\omega_1, \omega_2)$  by

$$\mathcal{P}^{\omega_1, \omega_2} = \mathcal{O}(\mathfrak{P}_{\omega_1, \omega_2}), \quad (2.5)$$

and we shall write  $\mathcal{P}^{\omega_1, \omega_2}(M)$  for the  $\mathbb{Q}$ -(vector)subspace of  $\mathcal{P}^{\omega_1, \omega_2}$  spanned by the motivic periods of  $M$  of type  $(\omega_1, \omega_2)$ .

It follows from (2.5) that the set of all motivic periods forms an algebra over  $\mathbb{Q}$ . The schemes  $\mathfrak{P}$  form a groupoid on  $\mathcal{M}$  with respect to composition,

$$\mathfrak{P}_{\omega_1, \omega_2} \times \mathfrak{P}_{\omega_2, \omega_3} \rightarrow \mathfrak{P}_{\omega_1, \omega_3},$$

for any three fiber functors  $\omega_1, \omega_2, \omega_3$ . Dualizing, we obtain a coalgebroid structure on spaces of motivic periods:

$$\mathcal{P}^{\omega_1, \omega_3} \longrightarrow \mathcal{P}^{\omega_1, \omega_2} \otimes \mathcal{P}^{\omega_2, \omega_3}, \quad (2.6)$$

which, in the case  $\omega_1 = \omega_2 = \omega_{dR}$ , and  $\omega_3 = \omega_B$  becomes a coaction:

$$\Delta^{\partial\tau, m} : \mathcal{P}^m \longrightarrow \mathcal{P}^{\partial\tau} \otimes \mathcal{P}^m, \quad (2.7)$$

where  $\mathcal{P}^{\partial\tau}$  is a Hopf algebra over  $\mathbb{Q}$ . By the definition of the Tannaka group,

$$G_{dR} = \text{Spec}(\mathcal{P}^{\partial\tau}), \quad (2.8)$$

and so (2.7) makes the space of motivic periods  $\mathcal{P}^m$  into a  $G_{dR}$ -representation. Since  $\omega_{dR}$  is graded, the (left) action of  $\mathbb{G}_m \subset G_{dR}$  corresponds to a grading on  $\mathcal{P}^{\omega_{dR}, \omega}$  for any fiber functor  $\omega$ . The standard terminology for multiple zeta values sometimes requires one to call the degree the weight. It is one half of the Hodge-theoretic weight; that is,  $\mathbb{Q}(-n)$  has degree  $n$ .

The notions of motivic and de Rham periods are fundamentally different. In the case of motivic periods, pairing with the element (2.2) defines the period homomorphism:

$$\text{per} : \mathcal{P}^m \longrightarrow \mathbb{C}. \quad (2.9)$$

The point  $1 \in G_{dR}$  defines a map  $\mathcal{P}^{\partial\tau} \rightarrow \mathbb{Q}$ . The period map *per se* is not available for de Rham periods, although we shall define a substitute in Section 3.

**2.3. Formulae.** By the main construction of Tannaka theory [14, Section 4.7], motivic periods are spanned by symbols  $[M, \eta, X]^{\omega_1, \omega_2}$ , where  $M \in \mathcal{M}$ ,

$\eta \in \omega_1(M)$ , and  $X \in \omega_2(M)^\vee$ , modulo the equivalence relation generated by

$$\begin{aligned} [M, \lambda_1 \eta_1 + \lambda_2 \eta_2, X]^{\omega_1, \omega_2} &\sim \lambda_1 [M, \eta_1, X]^{\omega_1, \omega_2} + \lambda_2 [M, \eta_2, X]^{\omega_1, \omega_2} \\ [M, \eta, \lambda_1 X_1 + \lambda_2 X_2]^{\omega_1, \omega_2} &\sim \lambda_1 [M, \eta, X_1]^{\omega_1, \omega_2} + \lambda_2 [M, \eta, X_2]^{\omega_1, \omega_2}, \end{aligned}$$

where  $\lambda_1, \lambda_2 \in \mathbb{Q}$  (linearity in  $\eta$  and  $X$ ) and by the relation

$$[M_1, \eta_1, X_1]^{\omega_1, \omega_2} \sim [M_2, \eta_2, X_2]^{\omega_1, \omega_2} \quad (2.10)$$

for every morphism  $\rho : M_1 \rightarrow M_2$  such that  $\eta_2 = \omega_1(\rho)\eta_1$ , and  $X_1 = \omega_2(\rho)^\vee X_2$ .

The multiplication on motivic periods is given concretely by the formula

$$\mathcal{P}^{\omega_1, \omega_2}(M_1) \times \mathcal{P}^{\omega_1, \omega_2}(M_2) \longrightarrow \mathcal{P}^{\omega_1, \omega_2}(M_1 \otimes M_2) \quad (2.11)$$

$$[M_1, \eta_1, X_1]^{\omega_1, \omega_2} \times [M_2, \eta_2, X_2]^{\omega_1, \omega_2} = [M_1 \otimes M_2, \eta_1 \otimes \eta_2, X_1 \otimes X_2]^{\omega_1, \omega_2}.$$

In particular, if  $M$  is an algebra object in  $\text{Ind}(\mathcal{M})$ , then  $\mathcal{P}^{\omega_1, \omega_2}(M)$  is a commutative ring, and its spectrum is an affine scheme over  $\mathbb{Q}$ .

Given three fiber functors  $\omega_1, \omega_2, \omega_3$ , the Hopf algebroid structure (2.6) can be computed explicitly by the usual coproduct formula for endomorphisms:

$$\Delta^{\omega_1, \omega_2, \omega_3} : \mathcal{P}^{\omega_1, \omega_3}(M) \longrightarrow \mathcal{P}^{\omega_1, \omega_2}(M) \otimes \mathcal{P}^{\omega_2, \omega_3}(M) \quad (2.12)$$

$$[M, \eta, X]^{\omega_1, \omega_3} \mapsto \sum_v [M, \eta, v^\vee]^{\omega_1, \omega_2} \otimes [M, v, X]^{\omega_2, \omega_3},$$

where  $\{v\}$  is a basis of  $\omega_2(M)$  and  $\{v^\vee\}$  is the dual basis. The previous formula does not depend on the choice of basis (if one prefers, one can write (2.12) in terms of the coevaluation map  $1 \rightarrow M^\vee \otimes M$ ). In the case  $\omega_1 = \omega_2 = \omega_{dR}$ , Equation (2.12) gives the following formula for the degree of a motivic period:

$$\text{deg}[M, \eta, X]^{\omega_{dR}, \omega} = m, \quad (2.13)$$

whenever  $\eta \in (M_{dR})_m$  has degree  $m$ , and  $\omega$  is any fiber functor.

Finally, given a motivic period  $[M, \eta, X]^m \in \mathcal{P}^m$ , its period is given by

$$\text{per}([M, \eta, X]^m) = \langle \text{comp}_{B, dR}(\eta), X \rangle \in \mathbb{C}. \quad (2.14)$$

In principle, it can always be computed by integrating differential forms representing  $\eta$  along topological cycles representing  $X$ .

**2.4. Unipotent de Rham periods.** There is yet another notion of de Rham period which is obtained by restricting to the unipotent radical  $U_{dR} \subset G_{dR}$ .

**DEFINITION 2.3.** Let  $v \in M_{dR}$ , and let  $f \in M_{dR}^\vee$ . A *unipotent de Rham period* is the image of  $[M, v, f]^{\text{or}}$  under the map  $\mathcal{O}(G_{dR}) \rightarrow \mathcal{O}(U_{dR})$ . Denote it by

$$[M, v, f]^u \in \mathcal{O}(U_{dR}),$$

and denote the ring of unipotent de Rham periods by

$$\mathcal{P}^u \cong \mathcal{O}(U_{dR}). \quad (2.15)$$

Unipotent de Rham periods are equivalent to the notion of framed objects in mixed Tate categories considered, for example, in [22, Section 2]. There is a natural map

$$\pi^{u, \text{dr}} : \mathcal{P}^{\text{dr}} \longrightarrow \mathcal{P}^u,$$

and hence, by taking  $\omega_1 = \omega_2 = \omega_{dR}$  and  $\omega_3 = \omega_B$  and restricting the left-hand factor of the right-hand side of (2.12) to  $\mathcal{P}^u$ , we obtain a coaction:

$$\Delta^{u, m} : \mathcal{P}^m \longrightarrow \mathcal{P}^u \otimes \mathcal{P}^m. \quad (2.16)$$

The action of  $\mathbb{G}_m$  by conjugation gives  $\mathcal{O}(U_{dR})$  a grading. A (nonzero) unipotent de Rham period  $[M, v_m, f_n]^u$  is homogeneous of degree

$$\deg[M, v_m, f_n]^u = m - n \quad (2.17)$$

whenever  $v_m \in (M_{dR})_m$ , and  $f_n \in ((M_{dR})_n)^\vee$ . Note that the formula only agrees with (2.13) when  $n = 0$ . Since  $\mathcal{O}(U_{dR})$  has degrees  $\geq 0$ ,  $[M, v_m, f_n]^u$  vanishes if  $m < n$ . With these definitions, the coaction (2.16) is homogeneous in the degree.

REMARK 2.4. In [22], it is assumed that one framing, namely  $f_n$ , is in degree 0. This defines a smaller space of de Rham periods for a given motive  $M$  than those which are considered here, and the corresponding coproduct formula requires an extra Tate twist in the left-hand factor. See Remark 2.9.

It is expected (see, for example, [18, Section 5.28]) that unipotent de Rham periods for  $\mathcal{MT}(\mathbb{Z})$  should have natural  $p$ -adic period homomorphisms

$$\text{per}_p : \mathcal{P}^u \longrightarrow \mathbb{Q}_p$$

for all primes  $p$ . One expects that there exists a functorial Frobenius automorphism  $F_p : M_{dR} \otimes \mathbb{Q}_p \rightarrow M_{dR} \otimes \mathbb{Q}_p$ , which, by the Tannakian formalism, corresponds to an element  $c_p \in U^{dR}(\mathbb{Q}_p)$  (after rescaling so that  $F_p$  acts as the identity on  $\mathbb{Q}_p(-1)$ ). The  $p$ -adic period should be obtained by pairing with  $c_p$ . See also [4, 21]. Our single-valued period, to be defined below, is a version of  $\text{per}_p$  at the infinite prime.

**2.5. Motives generated by motivic periods.** It is very useful to think of a space of motivic periods  $\mathcal{P}^m(M)$  as a motive in its own right.

DEFINITION 2.5. Let  $\xi \in \mathcal{P}^m$  be a motivic period. Let  $M(\xi)_{dR}$  denote the graded  $\mathcal{O}(U_{dR})$ -comodule it generates via the coaction (2.16).

By the Tannakian formalism, this is the de Rham realization of a motive we denote by  $M(\xi) \in \mathcal{M}$ . Define *the motive generated by the motivic period*  $\xi$  to be  $M(\xi)$ .

LEMMA 2.6. *For any  $\xi \in \mathcal{P}^m$ ,  $\xi$  is a motivic period of  $M(\xi)$ .*

*Proof.* If we represent  $\xi$  by a triple  $[M, \eta, X]^m$ , then the de Rham orbit  $G_{dR}\eta$  defines a submotive  $M^1 \subset M$  such that  $M^1_{dR} = G_{dR}\eta$ . Inclusion gives an equivalence:

$$[M^1, \eta, X^1]^m \sim [M, \eta, X]^m = \xi,$$

where  $X^1$  is the image of  $X$  in  $(M^1_B)^\vee$ . Now define  $M^2$  to be the quotient motive of  $M^1$  whose de Rham realization is  $M^1_{dR}/(\mathfrak{P}_{dR,B}X^1)^\perp$ . The dual of its Betti realization is  $(M^2_B)^\vee = G_B X^1 \subset (M^1_B)^\vee$ . Then

$$[M^1, \eta, X^1]^m \sim [M^2, \eta_2, X^1]^m$$

are equivalent, where  $\eta_2$  is the image of  $\eta$  in  $M^2_{dR}$ . In particular,  $\xi$  is a motivic period of  $M^2$ . The de Rham realization of  $M_2$  is exactly

$$\frac{G_{dR}\eta}{G_{dR}\eta \cap (\mathfrak{P}_{dR,B}X)^\perp},$$

which is isomorphic to the  $G_{dR}$ -module generated by  $[M, \eta, X]^m \in \mathcal{P}^m$ . Therefore  $M^2_{dR} = M(\xi)_{dR}$ , and hence  $M^2 = M(\xi)$ .  $\square$

Thus  $M(\xi)$  is the smallest subquotient motive  $M'$  of  $M$  such that  $\xi \in \mathcal{P}^m(M')$ .

**2.6. Geometric periods.** The notions of de Rham and motivic periods can be related to each other via the following algebra of geometric periods.

DEFINITION 2.7. Let  $\mathcal{P}^{m,+} \subset \mathcal{P}^m$  be the largest graded subalgebra of  $\mathcal{P}^m$  such that

- (i)  $\mathcal{P}^{m,+}$  has weights  $\geq 0$ ;
- (ii)  $\mathcal{P}^{m,+}$  is a comodule for the coaction by  $\mathcal{P}^u$ ; that is,

$$\Delta^{u,m} : \mathcal{P}^{m,+} \longrightarrow \mathcal{P}^u \otimes \mathcal{P}^{m,+}. \quad (2.18)$$

Suppose that  $M \in \mathcal{M}$  has nonnegative weights; that is,  $W_{-1}M = 0$ . Then

$$\mathcal{P}(M) \subset \mathcal{P}^{m,+}.$$

LEMMA 2.8. *The algebra  $\mathcal{P}^{m,+}$  is generated by the motivic periods of  $M$ , where  $M$  has nonnegative weights ( $W_{-1}M = 0$ ).*

*Proof.* The graded vector space  $\mathcal{P}^{m,+}$  is an  $\mathcal{O}(U_{dR})$ -comodule by (2.18). It is therefore the de Rham realization of an object  $\mathbb{P} \in \text{Ind}(\mathcal{M})$  which has weights  $\geq 0$  by 2.7(i). By Lemma 2.6, every  $\xi \in \mathcal{P}^{m,+}$  is a motivic period of  $\mathbb{P}$ .  $\square$

It follows from Lemma 2.8 that

$$\mathcal{P}_0^{m,+} \cong \mathbb{Q}. \quad (2.19)$$

This is because a motivic period of weight 0 of a motive  $M$  satisfying  $W_{-1}M = 0$  is equivalent to a period of  $\mathbb{Q}(0)$ , which is rational. Note that the isomorphism (2.19) uses  $\text{comp}_{B,dR}$  via (2.3). As a consequence, there is an augmentation map

$$\varepsilon : \mathcal{P}^{m,+} \longrightarrow \mathbb{Q}$$

given by projection onto  $\mathcal{P}_0^{m,+}$ . This defines a map

$$\pi^{u,m,+} : \mathcal{P}^{m,+} \longrightarrow \mathcal{P}^u \quad (2.20)$$

by composing the coaction  $\Delta^{u,m} : \mathcal{P}^{m,+} \longrightarrow \mathcal{P}^u \otimes \mathcal{P}^{m,+}$  with  $\text{id} \otimes \varepsilon$ . The map  $\pi^{u,m,+}$  respects the weight gradings, and is an isomorphism in weight 0, i.e.,  $\pi^{u,m,+} : \mathcal{P}_0^{m,+} \cong \mathcal{P}_0^u$ .

The map  $\pi^{u,m,+}$  can be computed another way. Let  $M$  satisfy  $W_{-1}M = 0$ . Then  $W_0M$  is a direct sum of copies of  $\mathbb{Q}(0)$ , which has rational periods (2.3). We have

$$\text{gr}_0^W M_{dR} = W_0 M_{dR} \xrightarrow{\text{comp}_{B,dR}} W_0 M_B \hookrightarrow M_B.$$

Since  $M_{dR}$  is graded, we can first apply the projection  $M_{dR} \rightarrow \text{gr}_0^W M_{dR}$  and then apply the previous map. This defines a rational comparison morphism,

$$c_0 : M_{dR} \longrightarrow M_B, \quad (2.21)$$

whose dual is  ${}^t c_0 : M_B^\vee \rightarrow M_{dR}^\vee$ . Then (2.20) is given by the formula

$$\begin{aligned} \pi^{u,m,+} : \mathcal{P}^m(M) &\longrightarrow \mathcal{P}^u(M) \\ [M, \eta, X]^m &\mapsto [M, \eta, {}^t c_0(X)]^u \end{aligned} \quad (2.22)$$

for all  $\eta \in M_{dR}$ ,  $X \in M_B^\vee$ . It only depends on the restriction of  $X$  to  $W_0 M_B$ .

**2.7. Example: the Lefschetz motive.** Let  $M = H^1(\mathbb{G}_m) \cong \mathbb{Q}(-1)$ . Then  $M_{dR} = H_{dR}^1(\mathbb{G}_m; \mathbb{Q}) \cong \mathbb{Q}\omega_0$ , and  $M_B^\vee = H_1(\mathbb{C}^\times; \mathbb{Q}) = \mathbb{Q}\gamma_0$ , where  $\omega_0 = [dz/z]$ , and  $\gamma_0$  is the homology class of a loop winding around 0 in the positive direction. Denote the Lefschetz motivic period by

$$\mathbb{L}^m = [M, \omega_0, \gamma_0]^m, \quad (2.23)$$

whose degree is 1 and whose period is

$$\text{per}(\mathbb{L}^m) = \int_{\gamma_0} \omega_0 = 2\pi i.$$

The element  $\mathbb{L}^m$  is invertible in  $\mathcal{P}^m$ . We only use the notation  $\mathbb{L}^m$  in order to avoid the rather ugly alternative  $(2\pi i)^m$ . Define the Lefschetz de Rham period by

$$\mathbb{L}^{\text{dr}} = [M, \omega_0, \omega_0^\vee]^{\text{dr}}. \quad (2.24)$$

It is group-like for the coproduct on  $\mathcal{O}(G_{dR})$ :  $\Delta^{\text{dr}, \text{dr}} \mathbb{L}^{\text{dr}} = \mathbb{L}^{\text{dr}} \otimes \mathbb{L}^{\text{dr}}$ . Since  $U_{dR}$  acts trivially on  $\mathbb{Q}(-1)$ , the unipotent de Rham Lefschetz period is the trivial function:

$$\mathbb{L}^u = \pi^{u, \text{dr}}(\mathbb{L}^{\text{dr}}) = 1. \quad (2.25)$$

By definition,  $\mathbb{L}^{\text{dr}}$  can be viewed as a coordinate on  $\mathbb{G}_m$ , and

$$\mathbb{G}_m \cong \text{Spec } \mathbb{Q}[(\mathbb{L}^{\text{dr}})^{-1}, \mathbb{L}^{\text{dr}}]. \quad (2.26)$$

On the other hand,  $\text{gr}_0^W M = 0$ , so  $c_0([\gamma_0]) = 0$ , and therefore

$$\pi^{u, m+}(\mathbb{L}^m) = [M, \omega_0, c_0(\gamma_0)]^u = 0. \quad (2.27)$$

By (2.12), the coaction  $\Delta^{\text{dr}, m} : \mathcal{P}^m \rightarrow \mathcal{P}^{\text{dr}} \otimes \mathcal{P}^m$  acts on the motivic Lefschetz period by  $\Delta^{\text{dr}, m} \mathbb{L}^m = \mathbb{L}^{\text{dr}} \otimes \mathbb{L}^m$ . By (2.25), the coaction  $\Delta^{u, m} : \mathcal{P}^m \rightarrow \mathcal{P}^u \otimes \mathcal{P}^m$  satisfies

$$\Delta^{u, m}(\mathbb{L}^m) = 1 \otimes \mathbb{L}^m. \quad (2.28)$$

**2.8. Structure of de Rham periods.** The fact that  $G_{dR}$  is canonically a semidirect product (2.1) implies that  $G_{dR} \cong U_{dR} \times \mathbb{G}_m$  as schemes, and hence

$$\mathcal{P}^{\text{dr}} \cong \mathcal{P}^u \otimes \mathbb{Q}[(\mathbb{L}^{\text{dr}})^{-1}, \mathbb{L}^{\text{dr}}]. \quad (2.29)$$

The coaction of  $\mathcal{P}^u$  on the right-hand side is given by the formula  $\Delta^{u, \text{dr}}(\mathbb{L}^{\text{dr}}) = 1 \otimes \mathbb{L}^{\text{dr}}$ , by (2.25). Equivalently, the map  $\mathbb{G}_m \rightarrow G_{dR}$  induces a projection

$$\pi_{\mathbb{L}, \text{dr}} : \mathcal{P}^{\text{dr}} \longrightarrow \mathbb{Q}[(\mathbb{L}^{\text{dr}})^{-1}, \mathbb{L}^{\text{dr}}], \quad (2.30)$$

or explicitly  $\pi_{\mathbb{L}, \text{dr}}([M, v, f]^{\text{dr}}) = f(v) (\mathbb{L}^{\text{dr}})^n$  if  $v \in (M_{dR})_n$ . The isomorphism (2.29) is then induced by composing the coaction  $\Delta^{u, \text{dr}} : \mathcal{P}^{\text{dr}} \rightarrow \mathcal{P}^u \otimes \mathcal{P}^{\text{dr}}$  with  $\text{id} \otimes \pi_{\mathbb{L}, \text{dr}}$ .

REMARK 2.9. If  $v \in (M_{dR})_m$  and  $f \in ((M_{dR})_n)^\vee$  are of degrees  $m$  and  $n$ , respectively, with  $m > n$ , then the image of  $[M, v, f]^u$  under the implied section  $\mathcal{P}^u \rightarrow \mathcal{P}^{\text{dr}}$  is  $[M(n), v, f]$ , where  $v$  now sits in degree  $m - n$ , and  $f$  in degree 0. The literature on framed mixed Tate objects essentially identifies  $\mathcal{P}^u$  with its image in  $\mathcal{P}^{\text{dr}}$ .

**2.9. Structure of motivic periods.** Rather than using the canonical isomorphism of fiber functors  $\text{comp}_{dR,B}$ , which is defined over  $\mathbb{C}$ , we prefer to choose rational isomorphisms, which are noncanonical.

PROPOSITION 2.10. *There exists an isomorphism of fiber functors from  $\omega_B$  to  $\omega_{dR}$ .*

*Proof.* See the proof of Proposition 8.10 in [15]. □

By choosing such an element  $s \in \text{Isom}(\omega_B, \omega_{dR})$ , we obtain an isomorphism:

$$\text{Isom}(\omega_{dR}, \omega_B) \xrightarrow{\sim} \text{Isom}(\omega_{dR}, \omega_{dR}). \tag{2.31}$$

Dually, this gives  $s^t : \mathcal{P}^{dr} \xrightarrow{\sim} \mathcal{P}^m$ , and so (2.29) gives a noncanonical isomorphism:

$$s^t : \mathcal{P}^u \otimes \mathbb{Q}[(\mathbb{L}^{dr})^{-1}, \mathbb{L}^{dr}] \xrightarrow{\sim} \mathcal{P}^m.$$

By Section 2.7, we can assume that  $s^t(\mathbb{L}^{dr}) = \mathbb{L}^m$ , and write the previous isomorphism as

$$\mathcal{P}^m \cong \mathcal{P}^u \otimes \mathbb{Q}[(\mathbb{L}^m)^{-1}, \mathbb{L}^m] \quad (\text{depending on } s). \tag{2.32}$$

It is compatible with the coaction  $\Delta^{u,m} : \mathcal{P}^m \rightarrow \mathcal{P}^u \otimes \mathcal{P}^m$ , and the weight gradings.

COROLLARY 2.11. *There is a noncanonical decomposition*

$$\mathcal{P}^{m,+} \cong \mathcal{P}^u \otimes \mathbb{Q}[\mathbb{L}^m]. \tag{2.33}$$

*Proof.* The decomposition (2.32) is induced by  $(\text{id} \otimes \pi_{\mathbb{L}^m}) \circ \Delta^{u,m}$ , where  $\pi_{\mathbb{L}^m}$  is given by  $(s^t)^{-1}$  followed by (2.30), and  $\mathbb{L}^{dr} \mapsto \mathbb{L}^m$ . Since  $\mathcal{P}^{m,+}$  has weights  $\geq 0$ , and is closed under the coaction by  $\mathcal{P}^u$ , it follows that the restriction of (2.32) to  $\mathcal{P}^{m,+}$  has nonnegative degrees in  $\mathbb{L}^m$ , and therefore gives an injective map:

$$\mathcal{P}^{m,+} \longrightarrow \mathcal{P}^u \otimes \mathbb{Q}[\mathbb{L}^m].$$

Identify  $\mathcal{P}^u \otimes \mathbb{Q}[\mathbb{L}^m]$  with its image in  $\mathcal{P}^m$ , by the map (2.32). It is a subalgebra which has weights  $\geq 0$ , and is  $G_{dR}$ -stable. Since  $\mathcal{P}^{m,+}$  is the largest subalgebra of  $\mathcal{P}^m$  with this property, the previous map is an isomorphism. □

Sending  $\mathbb{L}^m$  to 0 in (2.33) gives back the map  $\pi^{u,m,+} : \mathcal{P}^{m,+} \rightarrow \mathcal{P}^u$ .

**2.10. Real Frobenius.** Since there is a unique embedding from  $\mathbb{Q}$  to  $\mathbb{C}$ , complex conjugation defines the real Frobenius  $c : M_B \rightarrow M_B$ . It induces an involution,

$$c : \mathcal{P}^m \longrightarrow \mathcal{P}^m \tag{2.34}$$

$$[M, \eta, X]^m \mapsto [M, \eta, c(X)]^m,$$

which is compatible, via the period homomorphism, with complex conjugation on  $\mathbb{C}$ . If  $\Delta^{u,m} : \mathcal{P}^m \rightarrow \mathcal{P}^u \otimes \mathcal{P}^m$  denotes the coaction, then clearly  $\Delta^{u,m}c = (\text{id} \otimes c)\Delta^{u,m}$ . Since, by Example 2.7,

$$c(\mathbb{L}^m) = -\mathbb{L}^m,$$

it follows that  $c$  acts on a decomposition (2.33) by multiplying  $(\mathbb{L}^m)^n$  by  $(-1)^n$ .

**COROLLARY 2.12.** *If  $\mathcal{P}_{\mathbb{R}}^{m,+}$  (respectively  $\mathcal{P}_{i\mathbb{R}}^{m,+}$ ) denotes the subspace of  $\mathcal{P}^{m,+}$  of invariants (anti-invariants) of the map  $c$ , then we have*

$$\mathcal{P}_{i\mathbb{R}}^{m,+} \cong \mathcal{P}_{\mathbb{R}}^{m,+} \mathbb{L}^m$$

and  $\mathcal{P}_{\mathbb{R}}^{m,+} \cong \mathcal{P}^u \otimes \mathbb{Q}[(\mathbb{L}^m)^2]$

with respect to some choice of decomposition (2.33).

**2.11. Universal comparison map.** The identity map  $\text{id} : \mathcal{P}^m \rightarrow \mathcal{P}^m$  defines a canonical element in  $(\text{Spec } \mathcal{P}^m)(\mathcal{P}^m)$  which we denote by

$$\text{comp}_{B,dR}^m \in \text{Isom}_{\omega_{dR},\omega_B}(\mathcal{P}^m).$$

It reduces to the usual comparison map  $\text{comp}_{B,dR}$  after applying the period homomorphism to the coefficient ring  $\mathcal{P}^m$ . It is given for  $M \in \mathcal{M}$  by

$$\text{comp}_{B,dR}^m : M_{dR} \longrightarrow M_B \otimes \mathcal{P}^m(M) \tag{2.35}$$

$$\eta \mapsto \sum_x x \otimes [M, \eta, x^\vee]^m,$$

where the sum ranges over a basis  $\{x\}$  of  $M_B$ , and  $\{x^\vee\}$  is the dual basis. We can also write (2.35) as an isomorphism after tensoring with all motivic periods:

$$\text{comp}_{B,dR}^m : M_{dR} \otimes \mathcal{P}^m \xrightarrow{\sim} M_B \otimes \mathcal{P}^m. \tag{2.36}$$

In the other direction, we have a universal map,

$$\text{comp}_{dR,B}^m : M_B \longrightarrow M_{dR} \otimes \mathcal{P}^{\omega_B,\omega_{dR}}(M),$$

which is defined in a similar way. It will not be used here.

The universal comparison maps can be used to compare the action of the de Rham motivic Galois group  $G_{dR}$  with the action of the Betti group  $G_B$  on  $\mathcal{P}^m$ .

### 3. Single-valued motivic periods

The single-valued period is an analogue of the period homomorphism for de Rham periods. First, we construct a well-defined map which we call the single-valued motivic period,

$$sv^m : \mathcal{P}^u \longrightarrow \mathcal{P}^{m,+},$$

and define the single-valued period to be the homomorphism

$$sv : \mathcal{P}^u \longrightarrow \mathbb{C}$$

obtained by composing with the usual period  $per : \mathcal{P}^m \rightarrow \mathbb{C}$ . The map  $sv$  is similar to what is sometimes referred to as the ‘real period’ in the literature [3, 23, Section 4]. Since multiple zeta values are already real numbers, this terminology could lead to confusion, so we prefer not to use it. Note that the single-valued periods of a motive  $M$  are not in fact periods of  $M$ , but are periods of the Tannakian subcategory of  $\mathcal{M}$  generated by  $M$ .

In the second half of the paper, we shall compute the single-valued versions of motivic multiple zeta values using the motivic fundamental groupoid of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . More precisely, we compute the map

$$\mathcal{P}^{m,+} \xrightarrow{\pi^{u,m,+}} \mathcal{P}^u \xrightarrow{sv^m} \mathcal{P}^{m,+}$$

on the subspace  $\mathcal{H} \subset \mathcal{P}^{m,+}$  of motivic multiple zeta values. Since we know by [9] that  $\mathcal{H}$  is equal to  $\mathcal{P}_{\mathbb{R}}^{m,+}$ , this computation in fact yields all single-valued motivic periods of the category  $\mathcal{MT}(\mathbb{Z})$ .

**3.1. Single-valued motivic periods.** The weight grading on  $\mathcal{P}^m$  is given by an action of  $\mathbb{G}_m$ , which we shall denote by  $\tau$ . Thus  $\tau(\lambda)$  is the map which in weight  $n$  acts via multiplication by  $\lambda^n$ , for any  $\lambda \in \mathbb{Q}^\times = \mathbb{G}_m(\mathbb{Q})$ .

DEFINITION 3.1. Let  $\sigma : \mathcal{P}^m \longrightarrow \mathcal{P}^m$  be the involution

$$\sigma = \tau(-1)c, \tag{3.1}$$

where  $c$  is the real Frobenius of Section 2.10. For example,  $\sigma(\mathbb{L}^m) = \mathbb{L}^m$ .

To spell this out, the map  $\text{Spec}(\sigma)$  is a morphism of schemes from  $\text{Isom}(\omega_{dR}, \omega_B)$  to itself which acts on  $\phi \in \text{Isom}(\omega_{dR}, \omega_B)$  by

$$(M_{dR} \xrightarrow{\phi} M_B) \mapsto (M_{dR} \xrightarrow{\tau(-1)} M_{dR} \xrightarrow{\phi} M_B \xrightarrow{c} M_B).$$

On the level of motivic periods,  $\sigma[M, v, X]^m = [M, \tau(-1)v, c(X)]^m$ .

REMARK 3.2. If  $\Delta^{u,m} : \mathcal{P}^m \rightarrow \mathcal{P}^u \otimes \mathcal{P}^m$  denotes the coaction, then

$$\Delta^{u,m}\sigma = (\bar{\sigma} \otimes \sigma) \circ \Delta^{u,m},$$

where  $\bar{\sigma} : \mathcal{P}^u \rightarrow \mathcal{P}^u$  is given by the action of  $\tau(-1)$  on  $\mathcal{P}^u$  by conjugation. In other words,  $\bar{\sigma}$  acts by multiplication by  $(-1)^n$  in degree  $n$ , where the degree is (2.17).

Consider the following affine scheme over  $\mathbb{Q}$ :

$$\mathbb{P} = \text{Spec}(\mathcal{P}^m) \quad (= \text{Isom}(\omega_{dR}, \omega_B)).$$

The coaction  $\mathcal{P}^m \rightarrow \mathcal{P}^{dr} \otimes \mathcal{P}^m$  defines an action we denote by  $\circ$ :

$$\circ : G_{dR} \times \mathbb{P} \longrightarrow \mathbb{P},$$

and makes  $\mathbb{P}$  a torsor over  $G_{dR}$  (by Proposition 2.10). We use the notation  $\circ$  to be consistent with the Ihara action which will be denoted by the same symbol later on. The maps  $\text{id}, \sigma : \mathcal{P}^m \rightarrow \mathcal{P}^m$  can be viewed as elements  $\text{id}, \sigma \in \mathbb{P}(\mathcal{P}^m)$ .

DEFINITION 3.3. Define  $\text{sv}^m$  to be the unique element of  $G_{dR}(\mathcal{P}^m)$  such that

$$\text{sv}^m \circ \sigma = \text{id}. \tag{3.2}$$

We can view  $\text{sv}^m : \mathcal{P}^{dr} \rightarrow \mathcal{P}^m$  as an algebra homomorphism. In order to compute  $\text{sv}^m(\mathbb{L}^{dr})$ , use the fact that  $\Delta^{dr,m}\mathbb{L}^m = \mathbb{L}^{dr} \otimes \mathbb{L}^m$ , which gives

$$\mathbb{L}^m = (\text{sv}^m \circ \sigma)(\mathbb{L}^m) = \mu(\text{sv}^m \otimes \sigma)(\mathbb{L}^{dr} \otimes \mathbb{L}^m) = \text{sv}^m(\mathbb{L}^{dr})\sigma(\mathbb{L}^m),$$

where  $\mu$  denotes multiplication. Since  $\sigma(\mathbb{L}^m) = \mathbb{L}^m$ , we deduce that  $\text{sv}^m(\mathbb{L}^{dr}) = 1$ . Therefore  $\text{sv}^m$  actually lies in the image of  $U_{dR}(\mathcal{P}^m)$  in  $G_{dR}(\mathcal{P}^m)$ , and we can view it as an algebra homomorphism  $\text{sv}^m : \mathcal{P}^u \longrightarrow \mathcal{P}^m$ . Even more precisely, we have the following.

PROPOSITION 3.4. For all  $g \in G_{dR}$ , and  $\xi \in \mathcal{P}^u$ ,

$$\text{sv}^m(c_g \xi) = g \text{sv}^m(\xi), \tag{3.3}$$

where  $c_g$  denotes the action of  $g \in G_{dR}$  on  $\mathcal{P}^u$  by twisted conjugation:

$$c_g(\xi) = g \xi \bar{g}^{-1},$$

where  $\bar{g} = \tau(-1) g \tau(-1)$ . In particular,  $\text{sv}^m$  defines an algebra homomorphism,

$$\text{sv}^m : \mathcal{P}^u \longrightarrow \mathcal{P}^{m,+}, \tag{3.4}$$

which is homogeneous for the weight gradings on both sides.

*Proof.* For any  $g \in G_{dR}$ , define  $sv_g^m : \mathcal{P}^u \rightarrow \mathcal{P}^m$  to be  $sv_g^m(x) = g sv^m(x)$ , and similarly define  $\sigma_g, id_g \in \mathbb{P}(\mathcal{P}^m)$ , where  $\sigma_g(x) = g \sigma(x)$ ,  $id_g(x) = g id(x)$ , and the action of  $g$  is on the ring of coefficients  $\mathcal{P}^m$ . By the definition (3.2) of  $sv^m$ , we have

$$sv_g^m \circ \sigma_g = id_g.$$

Clearly,  $id_g = g$ . By an identical argument to Remark 3.2, we have the equation  $\Delta^{\text{tr},m} \sigma = (\bar{\sigma} \otimes \sigma) \circ \Delta^{\text{tr},m}$ , where  $\Delta^{\text{tr},m} : \mathcal{P}^m \rightarrow \mathcal{P}^{\text{tr}} \otimes \mathcal{P}^m$  is the coaction by  $\mathcal{P}^{\text{tr}}$  and  $\bar{\sigma}$  is conjugation by  $\tau(-1)$ . This implies that

$$\mu(g \otimes id) \Delta^{\text{tr},m} \sigma = \mu(\bar{g} \otimes \sigma) \Delta^{\text{tr},m},$$

where  $g, \bar{g}$  are viewed as maps  $\mathcal{P}^{\text{tr}} \rightarrow \mathbb{Q}$  and  $\mu : \mathbb{Q} \otimes \mathcal{P}^m \rightarrow \mathcal{P}^m$  is multiplication. The previous equation states that  $\sigma_g = \bar{g} \circ \sigma$ . Therefore

$$sv_g^m \circ \bar{g} \circ \sigma = g.$$

Since  $\mathbb{P}$  is a torsor over  $G_{dR}$ , this has the unique solution  $sv_g^m = g \circ sv^m \circ \bar{g}^{-1}$ , which is precisely (3.3). Since the weight grading on  $\mathcal{P}^u$  is given by conjugation by  $g$  for  $g \in \mathbb{G}_m$  and  $\bar{g} = g$  for such  $g$  (because  $\mathbb{G}_m$  is commutative), we deduce from (3.3) that  $sv^m$  is homogeneous in the weight. In particular, since  $\mathcal{P}^u$  has weight  $\geq 0$ , the image of  $sv^m$  has weight  $\geq 0$ , is stable under  $G_{dR}$ , and hence is contained in  $\mathcal{P}^{m,+}$ .  $\square$

As pointed out by the referee, another way to see that  $\sigma_g = \bar{g} \circ \sigma$  is to note that  $\text{Spec}(\sigma_g)$  corresponds to the isomorphism of  $\text{Isom}(\omega_{dR}, \omega_B)$  in which we first act by  $g \in \text{Isom}(\omega_{dR}, \omega_{dR})$  then apply  $\text{Spec}(\sigma)$ :

$$\begin{aligned} (M_{dR} \xrightarrow{\phi} M_B) &\mapsto (M_{dR} \xrightarrow{g} M_{dR} \xrightarrow{\phi} M_B) \\ &\mapsto (M_{dR} \xrightarrow{\tau(-1)} M_{dR} \xrightarrow{g} M_{dR} \xrightarrow{\phi} M_B \xrightarrow{c} M_B) \end{aligned}$$

and  $\bar{g} \circ \sigma$  corresponds to the same map:

$$(M_{dR} \xrightarrow{\phi} M_B) \mapsto (M_{dR} \xrightarrow{\bar{g}} M_{dR} \xrightarrow{\tau(-1)} M_{dR} M \xrightarrow{\phi} M_B \xrightarrow{c} M_B).$$

**DEFINITION 3.5.** Let  $\mathcal{P}^{sv} \subset \mathcal{P}^{m,+}$  denote the image of the map  $sv^m$ . We shall call it the ring of single-valued motivic periods.

**REMARK 3.6.** Formula (3.3) can be translated into coactions as follows. Let

$$\mathcal{L}^u = \frac{\mathcal{P}_{>0}^u}{\mathcal{P}_{>0}^u \mathcal{P}_{>0}^u}$$

denote the Lie coalgebra of indecomposable elements of  $\mathcal{P}^u$ . Projecting from  $\mathcal{P}_{>0}^u$  to  $\mathcal{L}^u$  defines infinitesimal versions of the usual coactions (2.12):

$$\begin{aligned}\delta &: \mathcal{P}^m \longrightarrow \mathcal{L}^u \otimes \mathcal{P}^m \\ \delta_L &: \mathcal{P}^u \longrightarrow \mathcal{L}^u \otimes \mathcal{P}^u \\ \delta_R &: \mathcal{P}^u \longrightarrow \mathcal{P}^u \otimes \mathcal{L}^u \cong \mathcal{L}^u \otimes \mathcal{P}^u,\end{aligned}$$

where  $\delta_L, \delta_R$  are obtained from the left and right coactions of  $\mathcal{P}^u$  on itself. Then

$$\delta \operatorname{sv}^m(\xi) = (\operatorname{id} \otimes \operatorname{sv}^m)(\delta_L \xi) + (\bar{S} \otimes \operatorname{sv}^m)(\delta_R \xi), \quad (3.5)$$

where  $\bar{S} : \mathcal{L}^u \rightarrow \mathcal{L}^u$  is multiplication by  $(-1)^n$  in degree  $n$  followed by the infinitesimal antipode  $S = -\operatorname{id} : \mathcal{L}^u \rightarrow \mathcal{L}^u$ . Thus  $\bar{S}$  is multiplication by  $(-1)^{n+1}$  in degree  $n$ .

**3.2. Properties of the single-valued motivic period.** For computations, it is convenient to trivialize the torsor  $\mathbb{P}$  as follows. By Proposition 2.10, we can choose an isomorphism of fiber functors  $s' \in \operatorname{Isom}(\omega_B, \omega_{dR})$ . It defines an isomorphism (2.31),

$$s : \mathcal{O}(G_{dR}) = \mathcal{P}^{\text{or}} \xrightarrow{\sim} \mathcal{P}^m, \quad (3.6)$$

where  $s = (s')^t$ , which we view as a  $\mathcal{P}^m$ -valued point of  $G_{dR}$ , denoted  $s \in G_{dR}(\mathcal{P}^m)$ . The action of the involution (3.1) on its coefficients will be denoted by  $\sigma$ . Via the isomorphism (3.6), the element  $\operatorname{id} \in \mathbb{P}(\mathcal{P}^m)$  (respectively  $\sigma \in \mathbb{P}(\mathcal{P}^m)$ ) corresponds to  $s \in G_{dR}(\mathcal{P}^m)$  (respectively  ${}^\sigma s \in G_{dR}(\mathcal{P}^m)$ ). Therefore  $\operatorname{sv}^m \in G_{dR}(\mathcal{P}^m)$  is

$$\operatorname{sv}^m = s \circ ({}^\sigma s)^{\circ-1}, \quad (3.7)$$

where the inversion and multiplication  $\circ$  take place in the group  $G_{dR}$ .

**REMARK 3.7.** To check that (3.7) is well defined, let  $s'_1, s'_2 \in \operatorname{Isom}(\omega_B, \omega_{dR})(\mathbb{Q})$ . Since the latter is a  $(G_B, G_{dR})(\mathbb{Q})$ -bitorsor, there exists an element  $\rho' \in G_{dR}(\mathbb{Q})$  such that  $s'_2 = \rho' s'_1$ . Transposing gives  $s_2 = s_1 \circ \rho$ , where  $\rho$  is the image of  $\rho'$  in  $G_{dR}(\mathcal{P}^m)$  via  $\mathbb{Q} \subset \mathcal{P}^m$ . In particular,  ${}^\sigma \rho = \rho$ , since its coefficients are rational of weight 0. Thus

$$s_2 \circ ({}^\sigma s_2)^{\circ-1} = s_1 \circ \rho \circ ({}^\sigma \rho)^{\circ-1} \circ ({}^\sigma s_1)^{\circ-1} = s_1 \circ ({}^\sigma s_1)^{\circ-1},$$

and (3.7) is well defined, as expected.

**DEFINITION 3.8.** Let  $\mathcal{P}^{m,0} \subset \mathcal{P}^{m,+}$  denote the subring of motivic periods

$$\mathcal{P}^{m,0} = \bigcap_s s(\mathcal{P}^u),$$

where  $s$  ranges over maps  $s : \mathcal{P}^u \rightarrow \mathcal{P}^{m,+}$  induced by decompositions (2.33). Since  $\pi^{u,m+}_s$  is the identity on  $\mathcal{P}^u$ , it follows that  $\pi^{u,m+}$  is injective on  $\mathcal{P}^{m,0}$ .

LEMMA 3.9. *We have  $\mathcal{P}^{sv} \subset \mathcal{P}^{m,0}$ . In particular,  $\pi^{u,m+} : \mathcal{P}^{sv} \rightarrow \mathcal{P}^u$  is injective. The compositum  $\pi^{u,m+}_{sv^m} : \mathcal{P}^u \rightarrow \mathcal{P}^u$  is given by the element*

$$\text{id} \circ \sigma^{\circ-1} \in U_{dR}(\mathcal{P}^u). \quad (3.8)$$

*Proof.* A choice of isomorphism (2.32) defines a map  $s : \mathcal{P}^u \rightarrow \mathcal{P}^{m,+}$  (and hence an element  $s \in U_{dR}(\mathcal{P}^m)$ ) which we can use to compute  $sv^m$ . By a similar argument to the discussion preceding (3.7), except that we work in  $U_{dR}$  instead of  $G_{dR}$ , we have  $sv^m = s \circ (\sigma_s)^{\circ-1}$ . The coefficients of  $s$ , and a fortiori  $sv^m$ , lie in the subspace  $s(\mathcal{P}^u) \subset \mathcal{P}^{m,+}$ . This proves the first statement.

For the second statement, observe that  $\pi^{u,m+}_s$  is the identity map on  $\mathcal{P}^u$ , and therefore  $\pi^{u,m+}_{sv^m} = \text{id} \circ (\sigma \text{id})^{\circ-1}$ , which gives exactly (3.8).  $\square$

In particular, the map  $\pi^{u,m+}_{sv^m} : \mathcal{P}^u \rightarrow \mathcal{P}^u$  is not the identity, and it has a large kernel. The previous lemma will be used in Section 6.2 to determine the structure of  $\mathcal{P}^{sv}$ .

**3.3. Formulae.** Expression (3.7) can be translated into a formula for the single-valued periods of an object  $M \in \mathcal{M}$  in terms of products of motivic periods of Tate twists of  $M$ . The formula is ugly (see [arXiv:1309.5309](https://arxiv.org/abs/1309.5309), Section 3.3) and probably of limited use, so it is not included here.

#### 4. The motivic fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

The main references for this section are [9, 15, 16, 18].

Let  $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ , and let  $\vec{1}_0, -\vec{1}_1$  denote the tangential base points on  $X$  given by the vector 1 at 0, and the vector  $-1$  at 1. Denote the motivic fundamental torsor of paths on  $X$  by

$${}_0\Pi_1^m = \pi_1^m(X, \vec{1}_0, -\vec{1}_1).$$

It is an affine scheme in the category  $\mathcal{MT}(\mathbb{Z})$ . This means that there is a commutative algebra object  $\mathcal{O}({}_0\Pi_1^m) \in \text{Ind } \mathcal{MT}(\mathbb{Z})$ , and  $\omega({}_0\Pi_1^m)$  is defined to be  $\text{Spec}$  of the commutative algebra  $\omega(\mathcal{O}({}_0\Pi_1^m))$ , for any fiber functor  $\omega$ .

We shall denote the de Rham realization  $\omega_{dR}({}_0\Pi_1^m)$  of  ${}_0\Pi_1^m$  simply by

$${}_0\Pi_1 = \text{Spec } \mathcal{O}({}_0\Pi_1),$$

where  $\mathcal{O}({}_0\Pi_1)$  is isomorphic to  $H^0(B(\Omega_{\log}^\bullet(\mathbb{P}^1 \setminus \{0, 1, \infty\}; \mathbb{Q})))$ , where  $B$  is the bar complex. Writing  $e^0$  for  $dz/z$  and  $e^1$  for  $dz/1 - z$ , we can identify the latter with the graded  $\mathbb{Q}$ -algebra

$$\mathcal{O}({}_0\Pi_1) \cong \mathbb{Q}\langle e^0, e^1 \rangle.$$

Its underlying vector space is spanned by the set of words  $w$  in the letters  $e^0, e^1$ , together with the empty word, and the multiplication is given by the shuffle product  $\text{III} : \mathbb{Q}\langle e^0, e^1 \rangle \otimes \mathbb{Q}\langle e^0, e^1 \rangle \rightarrow \mathbb{Q}\langle e^0, e^1 \rangle$  which is defined recursively by

$$(e^i w) \text{III} (e^j w') = e^i (w \text{III} e^j w') + e^j (e^i w \text{III} w')$$

for all words  $w, w'$  in  $\{e^0, e^1\}$  and  $i, j \in \{0, 1\}$ . The empty word will be denoted by 1. It is the unit for the shuffle product:  $1 \text{III} w = w \text{III} 1$  for all  $w$ .

The de Rham realization  ${}_0\Pi_1$  is therefore isomorphic to  $\text{Spec } \mathbb{Q}\langle e^0, e^1 \rangle$ . It is the affine scheme over  $\mathbb{Q}$  which to any commutative unitary  $\mathbb{Q}$ -algebra  $R$  associates the set of group-like formal power series in two noncommuting variables  $e_0$  and  $e_1$ :

$${}_0\Pi_1(R) = \{S \in R\langle\langle e_0, e_1 \rangle\rangle^\times : \Delta S = S \widehat{\otimes} S\}.$$

Here,  $\Delta$  is the completed coproduct  $R\langle\langle e_0, e_1 \rangle\rangle \rightarrow R\langle\langle e_0, e_1 \rangle\rangle \widehat{\otimes}_R R\langle\langle e_0, e_1 \rangle\rangle$  for which the elements  $e_0$  and  $e_1$  are primitive:  $\Delta e_i = 1 \otimes e_i + e_i \otimes 1$  for  $i = 0, 1$ .

Since the bar complex is augmented, we have an augmentation map  ${}_0\Pi_1 \rightarrow \mathbb{Q}$  which is the projection onto the empty word. Dually, this corresponds to an element denoted

$${}_0 1_1 \in {}_0\Pi_1(\mathbb{Q})$$

which is called the canonical de Rham path from  $\vec{1}_0$  to  $-\vec{1}_1$ .

On the other hand, the Betti realization of  ${}_0\Pi_1^m$  is the affine scheme over  $\mathbb{Q}$  given by the Mal'cev completion of the topological fundamental torsor of paths

$$\omega_B({}_0\Pi_1^m) \cong \pi_1^{un}(X(\mathbb{C}), \vec{1}_0, -\vec{1}_1).$$

There is a natural map  $\pi_1(X(\mathbb{C}), \vec{1}_0, -\vec{1}_1) \rightarrow \pi_1^{un}(X(\mathbb{C}), \vec{1}_0, -\vec{1}_1)(\mathbb{Q})$ .

**4.1. Drinfeld's associator.** There is a canonical straight-line path ('droit chemin')

$$\text{dch} \in \pi_1(X(\mathbb{C}), \vec{1}_0, -\vec{1}_1) \tag{4.1}$$

which therefore corresponds to an element in  $\omega_B({}_0\Pi_1^m)$ . Via the isomorphism (2.2), it defines an element in  ${}_0\Pi_1(\mathbb{C})$ , which we denote by

$$Z(e_0, e_1) \in {}_0\Pi_1(\mathbb{C}).$$

It is precisely Drinfeld's associator, and is given in low degrees by the formula

$$Z(e_0, e_1) = 1 + \zeta(2)[e_1, e_0] + \zeta(3)([e_1, [e_1, e_0]] + [e_0, [e_0, e_1]]) + \dots \quad (4.2)$$

In general, the coefficients are multiple zeta values. In fact, (4.2) is the noncommutative generating series of (shuffle-regularized) multiple zeta values

$$Z(e_0, e_1) = \sum_{w \in \{e_0, e_1\}^\times} \zeta(w) w.$$

The coefficient  $\zeta(w)$  is given by the regularized iterated integral

$$\zeta(e_{a_1} \dots e_{a_n}) = \int_{\text{dch}} \omega_{a_1} \dots \omega_{a_n} \quad \text{for } a_i \in \{0, 1\},$$

where  $\omega_0 = dt/t$  and  $\omega_1 = dt/1-t$ , and the integration begins on the left. One shows that the  $\zeta(w)$  are linear combinations of multiple zeta values (1.2) and that, for  $n_r \geq 2$ ,

$$\zeta(e_1 e_0^{n_1-1} e_1 e_0^{n_2-1} \dots e_1 e_0^{n_r-1}) = \zeta(n_1, \dots, n_r).$$

**4.2. The Ihara action.** Since  $\mathcal{O}({}_0\Pi_1)$  is the de Rham realization of an Ind object in the category  $\mathcal{MT}(\mathbb{Z})$ , it inherits an action of the motivic Galois group

$$\mathcal{U}_{dR} \times {}_0\Pi_1 \longrightarrow {}_0\Pi_1.$$

The action of  $\mathcal{U}_{dR}$  on the element  ${}_0 1_1 \in {}_0\Pi_1$  defines a map

$$g \mapsto g({}_0 1_1) : \mathcal{U}_{dR} \longrightarrow {}_0\Pi_1, \quad (4.3)$$

and one shows [18, Section 5.8] that the action of  $\mathcal{U}_{dR}$  on  ${}_0\Pi_1$  factors through a map

$$\circ : {}_0\Pi_1 \times {}_0\Pi_1 \longrightarrow {}_0\Pi_1 \quad (4.4)$$

which, on the level of formal power series, is given by the following formula:

$$\begin{aligned} R\langle\langle e_0, e_1 \rangle\rangle^\times \times R\langle\langle e_0, e_1 \rangle\rangle &\longrightarrow R\langle\langle e_0, e_1 \rangle\rangle \quad (4.5) \\ F(e_0, e_1) \circ G(e_0, e_1) &= G(e_0, F(e_0, e_1)e_1 F(e_0, e_1)^{-1})F(e_0, e_1), \end{aligned}$$

which was first considered by Y. Ihara. The action (4.4) makes  ${}_0\Pi_1$  into a torsor over  ${}_0\Pi_1$  for  $\circ$ . More prosaically, given two invertible formal power series  $G, H$ , one can solve  $F \circ G = H$  for  $F$  recursively by writing Equation (4.5) as

$$F = G(e_0, F e_1 F^{-1})^{-1} H. \quad (4.6)$$

If all the coefficients in  $F$  of words of length  $\leq N$  have been determined, then the coefficients of  $F e_1 F^{-1}$ , and hence  $G(e_0, F e_1 F^{-1})$ , are determined up to length  $N + 1$ . Equation (4.6) determines the coefficients of  $F$  in length  $N + 1$ . A similar recurrence based on the number of occurrences of  $e_1$  in a word (the depth) sometimes allows one to write down closed formulae in low depth and in all weights (Section 7.4).

**4.3. Motivic multiple zeta values.** Let  $\text{dch}_B \in \omega_B({}_0\Pi_1^m)(\mathbb{Q})$  denote the Betti image of the straight-line path (4.1). It defines an element  $\text{dch}_B \in \omega_B({}_0\Pi_1^m)^\vee$ . Let  $w$  be any word in  $\{e^0, e^1\}$ . It defines an element  $w \in \mathcal{O}({}_0\Pi_1) \cong \mathbb{Q}\langle e^0, e^1 \rangle$ , the de Rham realization of  $\mathcal{O}({}_0\Pi_1^m)$ .

DEFINITION 4.1. The *motivic multiple zeta value*  $\zeta^m(w)$  is the motivic period:

$$\zeta^m(w) = [\mathcal{O}({}_0\Pi_1^m), w, \text{dch}_B]^m.$$

The *algebra of motivic multiple zeta values*  $\mathcal{H} \subset \mathcal{P}^m$  is the graded  $\mathbb{Q}$ -algebra spanned by the  $\zeta^m(w)$ , that is, the image of the map  $w \mapsto \zeta^m(w) : \mathbb{Q}\langle e^0, e^1 \rangle \rightarrow \mathcal{P}^m$ .

Since  $\mathcal{O}({}_0\Pi_1^m)$  has weights  $\geq 0$ , and is stable under  $U_{dR}$ , it follows that  $\mathcal{H} \subset \mathcal{P}^{m,+}$ , by Definition 2.7. Thus  $\mathcal{H} = \bigoplus_{n \geq 0} \mathcal{H}_n$  is positively graded, and there is a natural map

$$\begin{aligned} \mathbb{Q}\langle e^0, e^1 \rangle &\longrightarrow \mathcal{H} \\ w &\mapsto \zeta^m(w) \end{aligned} \tag{4.7}$$

which is a homomorphism for the shuffle product. The period map (2.9) yields

$$\begin{aligned} \text{per} : \mathcal{H} &\longrightarrow \mathbb{R} \\ \zeta^m(w) &\mapsto \zeta(w), \end{aligned} \tag{4.8}$$

and the periods of motivic multiple zeta values are the usual multiple zeta values.

There is a corresponding notion of unipotent de Rham multiple zeta value. Instead of  $\text{dch}_B$ , we now take a de Rham framing  ${}_0 1_1 \in {}_0\Pi_1(\mathbb{Q}) \subset \mathcal{O}({}_0\Pi_1)^\vee$ .

DEFINITION 4.2. The *unipotent de Rham multiple zeta value*  $\zeta^u(w)$  is

$$\zeta^u(w) = [\mathcal{O}({}_0\Pi_1^m), w, {}_0 1_1]^u.$$

The *algebra of unipotent de Rham multiple zeta values*  $\mathcal{A} \subset \mathcal{P}^u$  is the graded  $\mathbb{Q}$ -algebra spanned by the  $\zeta^u(w)$ , that is, the image of the map  $w \mapsto \zeta^u(w) : \mathbb{Q}\langle e^0, e^1 \rangle \rightarrow \mathcal{P}^u$ . The objects  $\zeta^u(w)$  were denoted by  $\zeta^\alpha(w)$  in [10].

Since  $\mathcal{O}({}_0\Pi_1^m)$  has nonnegative weights, and because the de Rham image  $Z(e_0, e_1)$  of  $\text{dch}$  has leading term 1 (see (4.2)), we verify that

$${}^t c_0(\text{dch}_B) = {}_0 1_1.$$

By Equation (2.20), we deduce a surjective homomorphism

$$\begin{aligned} \pi^{u,m+} : \mathcal{H} &\longrightarrow \mathcal{A} \\ \zeta^m(w) &\mapsto \zeta^u(w). \end{aligned} \tag{4.9}$$

The motivic multiple zeta values  $\zeta^m(w)$  were defined in [9], and simplified by Deligne [17]. The unipotent de Rham multiple zeta values  $\zeta^u(w)$  are equivalent to the ‘motivic multiple zeta values’ considered in [22].

REMARK 4.3. It is important to note that  $\zeta^m(2) \neq 0$ , whereas  $\zeta^u(2) = 0$  [9].

The algebra  $\mathcal{A} = \bigoplus_{n \geq 0} \mathcal{A}_n$  is again positively graded, and is a commutative Hopf algebra by (2.6). We have a commutative diagram:

$$\begin{array}{ccc} \mathcal{H} & \longrightarrow & \mathcal{A} \otimes \mathcal{H} \\ \downarrow & & \downarrow \\ \mathcal{A} & \longrightarrow & \mathcal{A} \otimes \mathcal{A}. \end{array}$$

Let us write  $\mathbb{A} = \text{Spec}(\mathcal{A})$ , and  $\mathbb{H} = \text{Spec}(\mathcal{H})$ . Then  $\mathbb{A}$  is isomorphic to the image of  $\mathcal{O}({}_0\Pi_1)$  in  $\mathcal{O}(\mathcal{U}_{dR})$  via the map (4.3). Furthermore,  $\mathbb{A}$  is a pro-unipotent affine group scheme over  $\mathbb{Q}$ , which embeds in  $\mathbb{H}$  via (4.9), and acts upon it on the left:

$$\mathbb{A} \times \mathbb{H} \longrightarrow \mathbb{H}. \tag{4.10}$$

See [9, Section 2] for further details.

**4.4. Compatibility with the Ihara action.** The fact that the action of the motivic Galois group factors through the Ihara action (Section 4.2) can be expressed by the following commutative diagram, where the maps  $\mathbb{A} \hookrightarrow \mathbb{H} \hookrightarrow {}_0\Pi_1$  are induced by (4.9), (4.7):

$$\begin{array}{ccc} \mathbb{A} \times \mathbb{H} & \longrightarrow & \mathbb{H} \\ \downarrow & \downarrow & \downarrow \\ {}_0\Pi_1 \times {}_0\Pi_1 & \longrightarrow & {}_0\Pi_1, \end{array}$$

and the map along the bottom is the Ihara action  $\circ : {}_0\Pi_1 \times {}_0\Pi_1 \rightarrow {}_0\Pi_1$ . Dually, we have the following commutative diagram [9, Section 2.2]:

$$\begin{array}{ccc} \mathcal{O}({}_0\Pi_1) & \longrightarrow & \mathcal{O}({}_0\Pi_1) \otimes \mathcal{O}({}_0\Pi_1) \\ \downarrow & & \downarrow \\ \mathcal{H} & \longrightarrow & \mathcal{A} \otimes \mathcal{H}, \end{array}$$

where the map along the top is the Ihara coaction, which can be effectively replaced with an explicit formula which is due to Goncharov (who proved it for unipotent de Rham periods  $\zeta^u$ , that is modulo  $\zeta^m(2)$ , but in fact gives the correct coaction for  $\zeta^m$  also. See [13] for a direct and short proof using the Ihara coaction).

**4.5. The motivic Drinfeld associator.** In this section, all the Hom's are in the category of commutative unitary  $\mathbb{Q}$ -algebras.

DEFINITION 4.4. Define the *motivic version of the Drinfeld associator* by

$$Z^m(e_0, e_1) = \sum_{w \in \{e_0, e_1\}^\times} \zeta^m(w) w \in {}_0\Pi_1(\mathcal{H}) \subset \mathcal{H}\langle\langle e_0, e_1 \rangle\rangle.$$

Define the *unipotent de Rham version of the Drinfeld associator* by

$$Z^u(e_0, e_1) = \sum_{w \in \{e_0, e_1\}^\times} \zeta^u(w) w \in {}_0\Pi_1(\mathcal{A}) \subset \mathcal{A}\langle\langle e_0, e_1 \rangle\rangle.$$

It is useful to view  $Z^m$  as a morphism via the following general nonsense. For any commutative unitary ring  $R$ , we have an isomorphism

$$\mathrm{Hom}(\mathbb{Q}\langle e^0, e^1 \rangle, R) \xrightarrow{\sim} R\langle\langle e_0, e_1 \rangle\rangle.$$

The subspace of algebra homomorphisms on the left maps to the set of group-like formal power series on the right. Via this isomorphism, we see that  $Z^m$  is simply the image of the canonical map (4.7). Composing with (4.7) gives a map:

$$\mathrm{Hom}(\mathcal{H}, R) \longrightarrow \mathrm{Hom}(\mathbb{Q}\langle e^0, e^1 \rangle, R) \longrightarrow R\langle\langle e_0, e_1 \rangle\rangle.$$

Restricting to algebra homomorphisms retrieves the morphism  $\mathbb{H}(R) \hookrightarrow {}_0\Pi_1(R)$ . Setting  $R = \mathcal{H}$ , we can view the motivic Drinfeld associator as the image of the identity map

$$\mathrm{id}_{\mathcal{H}} \in \mathrm{Hom}(\mathcal{H}, \mathcal{H}) \longrightarrow Z^m \in \mathcal{H}\langle\langle e_0, e_1 \rangle\rangle. \quad (4.11)$$

The usual Drinfeld associator is the image of the element

$$\mathrm{per} \in \mathrm{Hom}(\mathcal{H}, \mathbb{C}) \longrightarrow Z \in \mathbb{C}\langle\langle e_0, e_1 \rangle\rangle.$$

The unipotent de Rham Drinfeld associator is the image of the map (4.9):

$$\pi^{u, m^+} \in \mathrm{Hom}(\mathcal{H}, \mathcal{A}) \longrightarrow Z^u \in \mathcal{A}\langle\langle e_0, e_1 \rangle\rangle.$$

**4.6. Decomposition with respect to  $\zeta^m(2)$ 's.**

LEMMA 4.5 (See also [9, Lemma 3.2]). *We have*

$$\zeta^m(2) = -\frac{(\mathbb{L}^m)^2}{24}. \quad (4.12)$$

*Proof.* The action of  $U_{dR}$  on  $\zeta^m(2)$  is trivial, by [9, Section 3.2]. Since  $\zeta^m(2)$  has degree 2, it must be equal to a rational multiple of  $(\mathbb{L}^m)^2$ . The rational multiple is determined by applying the period map and using Euler's formula  $\zeta(2) = \pi^2/6$ .  $\square$

REMARK 4.6. The analogue of Euler's theorem (4.12) is false for de Rham periods, since  $\zeta^{dr}(2) = 0$ , but  $\mathbb{L}^{dr}$  is nonzero.

LEMMA 4.7 [9, Section 2.3]. *There is a noncanonical isomorphism*

$$\mathcal{H} \cong \mathcal{A} \otimes \mathbb{Q}[\zeta^m(2)]. \quad (4.13)$$

*Proof.* Since the motive  $\mathcal{O}({}_0\Pi_1^m)$  has weights  $\geq 0$ , and is stable under  $U_{dR}$ ,  $\mathcal{H}$  is contained in  $\mathcal{P}^{m,+}$ . Furthermore, since the path dch is invariant under complex conjugation, we deduce that  $\mathcal{H} \subset \mathcal{P}_{\mathbb{R}}^{m,+}$ . By Corollary 2.12, there is an injective map

$$\mathcal{H} \longrightarrow \mathcal{P}^u \otimes \mathbb{Q}[(\mathbb{L}^m)^2] \cong \mathcal{P}^u \otimes \mathbb{Q}[\zeta^m(2)], \quad (4.14)$$

which is compatible with the  $\mathcal{P}^u$ -coaction. Since, by definition,  $\pi^{u,m+}(\mathcal{H}) = \mathcal{A}$ , and because  $\zeta^m(2) \in \mathcal{H}$ , the image of (4.14) is equal to  $\mathcal{A} \otimes \mathbb{Q}[\zeta^m(2)]$ .  $\square$

A choice of decomposition (4.13) defines a homomorphism  $Z_o^m : \mathcal{A} \rightarrow \mathcal{H}$ . Applying  $\varepsilon \otimes \text{id}$ , where  $\varepsilon$  is the augmentation on  $\mathcal{P}^u$ , defines a homomorphism  $\gamma^m : \mathcal{H} \rightarrow \mathbb{Q}[\zeta^m(2)]$ .

COROLLARY 4.8. *There exist elements  $\gamma^m \in \mathbb{H}(\mathbb{Q}[\zeta^m(2)])$ , and  $Z_o^m \in \mathbb{A}(\mathcal{H})$  such that*

$$Z^m = Z_o^m \circ \gamma^m. \quad (4.15)$$

*Proof.* The map  $\mathcal{H} \rightarrow \mathcal{A} \otimes \mathbb{Q}[\zeta^m(2)] \rightarrow \mathcal{H}$  is the identity, where the second map is  $\mu(Z_o^m \otimes \text{id})$  and  $\mu$  denotes multiplication. This implies that  $\text{id}_{\mathcal{H}} = \mu(Z_o^m \otimes \gamma^m)\Delta$ ; that is,  $\text{id}_{\mathcal{H}}$  is the convolution product of  $Z_o^m$  and  $\gamma^m$ . This is exactly (4.15), by (4.11).  $\square$

## 5. A class of multiple zeta values (elementary version)

The class of single-valued multiple zeta values is constructed in this section in a completely ‘elementary’ way, that is, with no reference to motivic periods.

**5.1. Deligne’s canonical associator.** Consider the continuous antilinear map

$$\begin{aligned} \sigma : \mathbb{C}\langle\langle e_0, e_1 \rangle\rangle &\longrightarrow \mathbb{C}\langle\langle e_0, e_1 \rangle\rangle \\ \sigma(e_i) &\mapsto -e_i \end{aligned} \tag{5.1}$$

which acts by complex conjugation on the coefficients of words. Let  $Z \in \mathbb{R}\langle\langle e_0, e_1 \rangle\rangle$  denote the Drinfeld associator (4.2).

LEMMA 5.1. *There exists a unique element  $W \in \mathbb{R}\langle\langle e_0, e_1 \rangle\rangle$  such that*

$$W \circ^\sigma Z = Z. \tag{5.2}$$

*Proof.* By Section 4.2, the Ihara action is transitive and faithful. Equation (5.2) can be solved recursively using (4.6) and the comments which follow.  $\square$

The series  $W$  is Deligne’s associator. We show in Section 6.1 that it is indeed an associator.

**5.2. Single-valued multiple polylogarithms.** We briefly recall the construction given in [11]. See Section 6.3 for a more conceptual derivation. The conventions for iterated integrals will be switched relative to [11] in order to remain compatible with the above. The generating series of multiple polylogarithms is

$$L_{e_0, e_1}(z) = \sum_{w \in \{e_0, e_1\}^\times} L_w(z)w,$$

and is defined to be the unique solution to the Knizhnik–Zamolodchikov equation

$$\frac{d}{dz} L_{e_0, e_1}(z) = L(z) \left( \frac{e_0}{z} + \frac{e_1}{1-z} \right)$$

which is equal to  $h(z) \exp(e_0 \log(z))$  near the origin, where  $h(z)$  is a holomorphic function at 0, where it takes the value 1.

DEFINITION 5.2. There is a unique element  $e'_1 \in {}_0\Pi_1(\mathbb{R}) = \mathbb{R}\langle\langle e_0, e_1 \rangle\rangle$  which satisfies the fixed-point equation:

$$Z(-e_0, -e'_1)e'_1 Z(-e_0, -e'_1)^{-1} = Z(e_0, e_1)e_1 Z(e_0, e_1)^{-1}. \tag{5.3}$$

One can easily show that (5.3) can be solved recursively in the weight, and so  $e'_1$  does indeed exist and is unique [11].

The generating series of single-valued multiple polylogarithms was defined by

$$\mathcal{L}(z) = \tilde{L}_{e_0, e'_1}(\bar{z}) L_{e_0, e_1}(z), \quad (5.4)$$

where  $\tilde{\phantom{x}}$  denotes reversal of words. Since the antipode in the Hopf algebra  $\mathbb{C}\langle\langle e_0, e_1 \rangle\rangle$  is given by  $e_{i_1} \dots e_{i_n} \mapsto (-1)^n e_{i_n} \dots e_{i_1}$ , and since  $L(z)$  is group like, we have

$$L_{e_0, e_1}(z)^{-1} = \tilde{L}_{-e_0, -e_1}(z), \quad (5.5)$$

and therefore we can rewrite (5.4) as

$$\mathcal{L}(z) = (L_{-e_0, -e'_1}(\bar{z}))^{-1} L_{e_0, e_1}(z). \quad (5.6)$$

In [11], it was shown that the coefficients  $\mathcal{L}_w(z)$  of  $w$  in the generating series  $\mathcal{L}(z)$  are single-valued functions of  $z$ , are linearly independent over  $\mathbb{C}$ , and satisfy the same shuffle and differential equations (with respect to  $\partial/\partial z$ ) as  $L_w(z)$ . The last two properties are obvious from (5.4). Their values at 1 are given by

$$\mathcal{L}(1) = (Z(-e_0, -e'_1))^{-1} Z(e_0, e_1). \quad (5.7)$$

**5.3. Values of single-valued multiple polylogarithms at 1.** The values of single-valued multiple polylogarithms at 1 are exactly the coefficients of Deligne's associator.

LEMMA 5.3. Equation (5.3) has the unique solution  $e'_1 = W e_1 W^{-1}$ .

*Proof.* By the formula for the Ihara action (4.5), we have

$$W \circ {}^\sigma Z(e_0, e_1) = {}^\sigma Z(e_0, W e_1 W^{-1}) W. \quad (5.8)$$

Let  $e'_1 = W e_1 W^{-1}$ , and write  $Z' = Z(e_0, e'_1)$ , and  ${}^\sigma Z' = Z(-e_0, -e'_1)$ . We have

$${}^\sigma Z' \stackrel{(5.8)}{=} (W \circ {}^\sigma Z) W^{-1} \stackrel{(5.2)}{=} Z W^{-1}, \quad (5.9)$$

which implies that  ${}^\sigma Z' e'_1 ({}^\sigma Z')^{-1} = Z W^{-1} (W e_1 W^{-1}) W Z^{-1} = Z e_1 Z^{-1}$ .

For the uniqueness, any solution to (5.3) is of the form  $e'_1 = A e_1 A^{-1}$  for some group-like series  $A$  whose coefficient of  $e_1$  vanishes (this is the case for  $Z$ ). Then Equation (5.3) is just  $(A \circ {}^\sigma Z) e_1 (A \circ {}^\sigma Z)^{-1} = Z e_1 Z^{-1}$ . This readily implies that  $A \circ {}^\sigma Z = Z$ , since the unique group-like series  $B$  satisfying  $B e_1 B^{-1} = e_1$  with vanishing coefficient of  $e_1$  is  $B = 1$ . We conclude that  $A = W$  by (5.2).  $\square$

By Equation (5.7),  $\mathcal{L}(1)$  is  $({}^\sigma Z')^{-1} Z$ , which is exactly  $W$  by (5.9).

COROLLARY 5.4.  $\mathcal{L}(1) = W$ .

In other words, the coefficients of Deligne's associator  $W$  are the values at 1 of single-valued multiple polylogarithms.

## 6. The single-valued associator (motivic version)

**6.1. Single-valued motivic multiple zeta values.** Recall that  $Z^m \in \mathbb{H}(\mathcal{H})$  is the motivic Drinfeld associator (4.11), and that the action of  $\sigma$  (definition 3.1) on the ring  $\mathcal{H}$  of coefficients of  $\mathbb{H}(\mathcal{H})$  is denoted by  $^\sigma$ . Since the straight-line path  $dch$  is invariant under complex conjugation, it follows that  $\sigma$  acts by  $(-1)^n$  on motivic multiple zeta values of weight  $n$ . Recall from Section 3 that  $\bar{\sigma}$  is the induced action on  $\mathcal{A}$ , and that it also acts by  $(-1)^n$  in weight  $n$ .

LEMMA 6.1. *There exists a unique  $W^m \in \mathbb{A}(\mathcal{H})$  such that*

$$W^m \circ {}^\sigma Z^m = Z^m. \tag{6.1}$$

*Proof.* One can follow a similar argument to Lemma 5.1. Alternatively, use a decomposition  $Z^m = Z_o^m \circ \gamma^m$  (4.15), and set  $W^m = Z_o^m \circ ({}^\sigma Z_o^m)^{\circ-1}$ , where the inversion and multiplication take place in the group  $\mathbb{A}(\mathcal{H})$ . Since  $\sigma$  acts trivially on the coefficients of  $\gamma^m$ , it is independent of the chosen decomposition: replacing  $(Z_o^m, \gamma^m)$  with  $(Z_o^m \circ h, h^{\circ-1} \circ \gamma^m)$ , where  ${}^\sigma h = h$ , gives rise to the same element.

Then  $W^m \circ {}^\sigma Z_o^m = Z_o^m$ , which implies (6.1).  $\square$

The element  $W^m$  is the motivic version of Deligne's associator  $W$ .

Via  $\mathbb{A}(\mathcal{H}) = \text{Hom}(\mathcal{A}, \mathcal{H})$ , we view  $W^m$  as an algebra morphism

$$W^m : \mathcal{A} \longrightarrow \mathcal{H}.$$

Composing with  $\mathbb{Q}\langle e^0, e^1 \rangle \rightarrow \mathcal{H} \rightarrow \mathcal{A}$  gives a map we also denote by

$$W^m : \mathbb{Q}\langle e^0, e^1 \rangle \rightarrow \mathcal{H}.$$

DEFINITION 6.2. For every word  $w \in \{e^0, e^1\}$ , define the single-valued motivic multiple zeta value to be the image of  $w$  under the map  $W^m$ . Denote it by

$$\zeta_{\text{sv}}^m(w) \in \mathcal{H}.$$

Let  $\mathcal{H}^{\text{sv}} \subset \mathcal{H}$  be the algebra spanned by the  $\zeta_{\text{sv}}^m(w)$ .

The fact that the map  $\mathbb{Q}\langle e^0, e^1 \rangle \rightarrow \mathcal{H}^{\text{sv}}$  factors through  $\mathcal{A}$  means the following.

COROLLARY 6.3. *The elements  $\zeta_{\text{sv}}^m(w)$  satisfy all the motivic relations between motivic multiple zeta values, together with the relation*

$$\zeta_{\text{sv}}^m(2) = 0.$$

In particular, the  $\zeta_{sv}^m(w)$  satisfy the usual double shuffle equations and associator relations. Note, however, that the map  $\mathcal{A} \rightarrow \mathcal{H}^{sv}$  is not injective, so the elements  $\zeta_{sv}^m$  satisfy many more relations than their usual counterparts.

We can write the element  $W^m$  as a generating series:

$$W^m = \sum_w \zeta_{sv}^m(w) w.$$

Its period  $\text{per}(W^m)$  is precisely  $W$  defined in (5.2), which shows that  $W$  is an associator. Therefore, by Corollary 5.4, the period of  $\zeta_{sv}^m(w)$  is given by the value at 1 of the corresponding single-valued multiple polylogarithm:

$$\text{per}(\zeta_{sv}^m(w)) = \mathcal{L}_w(1). \quad (6.2)$$

**6.2. Structure of  $\mathcal{H}^{sv}$ .** Let  $\mathcal{A}^{sv} \subset \mathcal{A}$  denote the image of  $\mathcal{H}^{sv}$  under  $\pi^{u,m+}$ .

LEMMA 6.4. *The map  $\pi^{u,m+} : \mathcal{H}^{sv} \rightarrow \mathcal{A}^{sv}$  is an isomorphism, and  $\mathcal{H}^{sv} \cong \mathcal{A}^{sv}$  is the image of  $\mathcal{A}$  under the homomorphism*

$$\text{sv}_{\mathcal{A}} := \text{id} \circ \bar{\sigma}^{-1} : \mathcal{A} \longrightarrow \mathcal{A}, \quad (6.3)$$

where the multiplication  $\circ$  and inverse take place in the group  $\mathbb{A}(\mathcal{A})$ .

*Proof.* This follows from Lemma 3.9 since  $\mathcal{H}^{sv} \subset \mathcal{P}^{sv}$ . □

Denote the Lie coalgebra of indecomposable elements of  $\mathcal{A}$  by

$$\mathcal{L} = \frac{\mathcal{A}_{>0}}{\mathcal{A}_{>0}\mathcal{A}_{>0}}.$$

Since  $\mathcal{A}$  is a commutative graded Hopf algebra, it follows from standard facts that  $\mathcal{A}$  is isomorphic to the polynomial algebra generated by the elements of  $\mathcal{L}$ .

PROPOSITION 6.5. *The algebra  $\mathcal{H}^{sv}$  of single-valued motivic multiple zetas is isomorphic to the polynomial algebra generated by elements  $\mathcal{L}^{\text{odd}}$  of  $\mathcal{L}$  of odd weight.*

*Proof.* By Lemma 6.4,  $\mathcal{H}^{sv} \cong \text{sv}_{\mathcal{A}}(\mathcal{A})$ , where  $\text{sv}_{\mathcal{A}} = \text{id} \circ \bar{\sigma}^{-1}$ . Since  $\text{sv}_{\mathcal{A}}$  is a homomorphism, it defines a map  $\text{sv}_{\mathcal{L}} : \mathcal{L} \rightarrow \mathcal{L}$ . Writing  $\text{sv}_{\mathcal{A}} = \mu(\text{id} \otimes \bar{\sigma}^{-1})\Delta$ , where  $\Delta : \mathcal{A} \rightarrow \mathcal{A} \otimes \mathcal{A}$  is the coproduct, and  $\mu$  is the multiplication on  $\mathcal{A}$ , we see that

$$\text{sv}_{\mathcal{A}} \equiv \text{id} - \bar{\sigma} \quad (\text{modulo products}),$$

and therefore  $sv_{\mathcal{L}} = 2\pi^{\text{odd}}$ , where  $\pi^{\text{odd}} : \mathcal{L} \rightarrow \mathcal{L}^{\text{odd}}$  is the projection onto the part of odd weight. It follows that the images of odd generators in  $\mathcal{A}$  under the map  $sv_{\mathcal{A}}$  are algebraically independent.

On the other hand, applying  $\sigma$  to the defining equation  $W^m \circ^\sigma Z^m = Z^m$  implies that  ${}^\sigma W^m \circ Z^m = {}^\sigma Z^m$ , and hence  ${}^\sigma W^m \circ W^m \circ Z^m = Z^m$ . By uniqueness,

$${}^\sigma W^m \circ W^m = 1,$$

which implies the equation  $\mu(\bar{\sigma}sv_{\mathcal{A}} \otimes sv_{\mathcal{A}})\Delta = \varepsilon$  on  $\mathcal{A}$ , where  $\varepsilon$  is the augmentation. Using Sweedler's notation  $\Delta(\xi) = \xi \otimes 1 + 1 \otimes \xi + \sum \xi' \otimes \xi''$ , this gives

$$sv_{\mathcal{A}}(\bar{\sigma}\xi) + sv_{\mathcal{A}}(\xi) + \sum sv_{\mathcal{A}}(\bar{\sigma}\xi')sv_{\mathcal{A}}(\xi'') = 0, \tag{6.4}$$

since  $sv_{\mathcal{A}}$  is homogeneous in the weight, and hence commutes with  $\bar{\sigma}$ . This implies that, if  $\xi$  is  $\bar{\sigma}$ -invariant of weight  $\geq 1$  (that is, of even weight  $\geq 2$ ), then  $sv_{\mathcal{A}}(\xi)$  is a product of elements in  $\mathcal{A}^{\text{sv}}$  of strictly smaller weight. It follows that, for any  $\xi \in \mathcal{A}$ ,  $sv_{\mathcal{A}}(\xi)$  is a polynomial in  $sv_{\mathcal{A}}(\xi_i)$ , where  $\xi_i$  are generators of odd weights only. □

**6.3. Single-valued multiple polylogarithms revisited.** We can rederive the construction of the single-valued multiple polylogarithms of [11] and Section 5.2 as follows. Single-valued versions of classical polylogarithms were considered in [31, 32].

Consider  $X = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ , with the base points  $\{\vec{1}_0, -\vec{1}_1, z\}$  for some  $z \in X(\mathbb{C})$ . Its de Rham fundamental groupoid consists of a copy of  $\mathbb{Q}\langle e^0, e^1 \rangle$  for each pair of these base points. We shall only consider the copies  ${}_0\Pi_0, {}_0\Pi_1, {}_0\Pi_z$ , corresponding to the canonical de Rham paths between the base points indicated by their subscripts.

Let  $Aut$  denote the group of automorphisms of  $\pi_1(X, \{\vec{1}_0, -\vec{1}_1, z\})$  which fixes the copy of  $\exp(e_0)$  in  ${}_0\Pi_0$  and  $\exp(e_1)$  in  ${}_0\Pi_1$ . Modifying [18, Proposition 5.9], accordingly, the action of  $Aut$  on the elements  ${}_01_1, {}_01_z$  defines an injective map

$$\begin{aligned} Aut &\hookrightarrow {}_0\Pi_1 \times {}_0\Pi_z \\ a &\mapsto (a_1, a_z), \end{aligned} \tag{6.5}$$

where, for any  $a \in Aut$ , we write  $a_z = a({}_01_z)$  and  $a_1 = a({}_01_1)$ . We leave to the reader the verification that this is an isomorphism of schemes. Since  ${}_0\Pi_z$  is a left  ${}_0\Pi_0$ -torsor, we immediately deduce a formula for the generalized Ihara action,

$$\begin{aligned} Aut \times {}_0\Pi_z &\longrightarrow {}_0\Pi_z \\ a \circ b &= \langle a_1 \rangle_0(b) \cdot a_z, \end{aligned} \tag{6.6}$$

where  $\langle a \rangle_0$  denotes the action of  $a \in {}_0\Pi_1$  on  ${}_0\Pi_0$  ([18, (5.9.4)]). Concretely,

$$\begin{aligned} ({}_0\Pi_1 \times {}_0\Pi_z) \times ({}_0\Pi_1 \times {}_0\Pi_z) &\longrightarrow ({}_0\Pi_1 \times {}_0\Pi_z) & (6.7) \\ (F_1, F_z) \circ (G_1, G_z) &= (G_1(e_0, F_1 e_1 F_1^{-1})F_1, G_z(e_0, F_1 e_1 F_1^{-1})F_z). \end{aligned}$$

The action of  ${}_0\Pi_1 \times {}_0\Pi_z$  on  ${}_0\Pi_1$  factors through the usual Ihara action of  ${}_0\Pi_1$  on  ${}_0\Pi_1$ .

Let us fix a path  $\text{ch}_z$  from  $\vec{1}_0$  to  $z$  in  $X(\mathbb{C})$ . Its de Rham image in  ${}_0\Pi_z(\mathbb{C})$  is exactly (some branch of) the generating series of multiple polylogarithms (Section 5.2)

$$\text{ch}_z^{dR} = L(z) \in {}_0\Pi_z(\mathbb{C}).$$

By the general single-valued principle, we seek an element  $W = (W_1, W_z)$  in the group  $\text{Aut}(\mathbb{C}) \cong {}_0\Pi_1(\mathbb{C}) \times {}_0\Pi_z(\mathbb{C})$  such that

$$W \circ ({}^\sigma Z, {}^\sigma L(z)) = (Z, L(z)).$$

It has a solution since  ${}_0\Pi_1 \times {}_0\Pi_z$  is a torsor over  $\text{Aut} \cong {}_0\Pi_1 \times {}_0\Pi_z$ . By the formula for the action (6.7), this is equivalent to the pair of equations

$$\begin{aligned} {}^\sigma L_{e_0, W_1 e_1 W_1^{-1}}(z) W_z &= L(z) & (6.8) \\ {}^\sigma Z(e_0, W_1 e_1 W_1^{-1}) W_1 &= Z, \end{aligned}$$

and so  $W_1 \circ {}^\sigma Z = Z$ , and  $W_1$  is equal to the element  $W$  defined in (5.2). As in Section 5.2, write  $e'_1 = W e_1 W^{-1}$ . Therefore, by (6.8), we deduce the following formula for  $W_z$ :

$$W_z = L_{-e_0, -e'_1}^{-1}(\bar{z}) L(z).$$

It is independent of the choice of path  $\text{ch}_z$ , and is therefore single valued (compare (5.6)). This gives another derivation of the construction in [11].

## 7. Generators for $\mathcal{H}^{\text{sv}}$ and examples

Up to this point we have used no deep results about the category of mixed Tate motives, nor about the structure of motivic multiple zeta values.

**7.1. Periods of mixed Tate motives.** In [9], it was shown that

$$\mathcal{A} \cong \mathcal{O}(U_{dR}) = \mathcal{P}^u. \quad (7.1)$$

The following proposition, due to Deligne [17], is a more precise statement about periods of mixed Tate motives than the one stated in [9].

PROPOSITION 7.1 [17]. Let  $M \in \mathcal{MT}(\mathbb{Z})$  be a mixed Tate motive over  $\mathbb{Z}$  with nonnegative weights; that is,  $W_{-1}M = 0$ . Let  $\eta \in (M_{dR})_n$  and  $X \in M_B^\vee$ .

- (i) If  $c(X) = X$ , then the motivic period  $[M, \eta, X]^m$  is a rational linear combination of motivic multiple zeta values of weight  $n$ .
- (ii) If  $c(X) = -X$ , then the motivic period  $[M, \eta, X]^m$  is a rational linear combination of motivic multiple zeta values of weight  $n-1$ , multiplied by  $\mathbb{L}^m$ .

*Proof.* By (7.1), and Section 4.6,  $\mathcal{H} \cong \mathcal{P}^u \otimes \mathbb{Q}[(\mathbb{L}^m)^2] \cong \mathcal{P}_{\mathbb{R}}^{m,+}$ . The result then follows immediately from the definitions of  $\mathcal{P}_{\mathbb{R}}^{m,+}$  and  $\mathcal{P}_{i\mathbb{R}}^{m,+}$ , and Corollary 2.12.  $\square$

The methods of [17] give an equivalent but slightly different proof of Corollary 2.12.

**7.2. A model for  $\mathcal{H}^{sv}$ .** Applying a choice of trivialization (2.32) and a choice of generators for  $\mathcal{O}(U_{dR})$  to (7.1) gives a noncanonical isomorphism [9, Section 2.5]:

$$\mathcal{H} \cong \mathcal{U} \otimes \mathbb{Q}[f_2] \tag{7.2}$$

such that the natural map  $\pi^{u,m+} : \mathcal{H} \rightarrow \mathcal{A}$  induces an isomorphism  $U \cong \mathcal{A}$ , where

$$U = \mathbb{Q}\langle f_3, f_5, f_7, \dots \rangle$$

is the graded Hopf algebra cogenerated by one element  $f_{2n+1}$  in every odd degree  $2n+1 \geq 3$ , equipped with the shuffle product and the deconcatenation coproduct

$$\Delta^{dec}(f_{i_1} \dots f_{i_n}) = \sum_{k=0}^n f_{i_1} \dots f_{i_k} \otimes f_{i_{k+1}} \dots f_{i_n}.$$

The element  $f_2$  corresponds to  $(\mathbb{L}^m)^2$ , and satisfies  $\Delta(f_2) = 1 \otimes f_2$ .

The map  $sv : \mathcal{A} \rightarrow \mathcal{A}$  defines a homomorphism

$$\begin{aligned} sv : \mathcal{U} &\longrightarrow \mathcal{U} \\ w &\longmapsto \sum_{uv=w} u \text{ III } \tilde{v}, \end{aligned} \tag{7.3}$$

where  $\tilde{\phantom{x}}$  denotes reversal of words. To see this, note that  $\sigma : \mathcal{U} \rightarrow \mathcal{U}$  is the map  $f_{2n+1} \mapsto -f_{2n+1}$ , and the antipode  $S$  on  $\mathcal{U}$  is given by  $w \mapsto \sigma(\tilde{w})$ . By formula (6.3), we have  $sv = \mu(\text{id} \otimes \sigma S) \Delta^{dec}$ , where  $\mu$  is multiplication, which gives (7.3).

Since  $\pi^{u,m+} : \mathcal{H}^{sv} \cong \mathcal{A}^{sv}$  by Lemma 6.4, we conclude that

$$\mathcal{H}^{sv} \cong \mathcal{A}^{sv} \cong \mathcal{U}^{sv},$$

where  $\mathcal{U}^{\text{sv}}$  is the image of the map (7.3). By way of example,

$$\begin{aligned} \text{sv}(f_a) &= 2f_a, & \text{sv}(f_a f_b) &= 2(f_a f_b + f_b f_a) \\ \text{sv}(f_a f_b f_c) &= 2(f_a f_b f_c + f_a f_c f_b + f_c f_a f_b + f_c f_b f_a), \end{aligned}$$

where  $a, b, c$  are odd integers  $\geq 3$ . In general, we have formula (3.5), which implies, in particular, that

$$\text{sv}(f_a w f_b) = f_a \text{sv}(w f_b) + f_b \text{sv}(f_a w)$$

for any word  $w \in \{f_{2n+1}\}$ , and  $a, b$  odd integers  $\geq 3$ . This also follows immediately from (7.3), since, via the recursive definition of  $\text{sv}$ , we have

$$f_a u \text{sv} f_b \tilde{v} = f_a (u \text{sv} f_b \tilde{v}) + f_b (f_a u \text{sv} \tilde{v}).$$

Formula (7.3) makes it obvious that

$$\text{sv}(f_{i_1} \dots f_{i_{2n+1}}) \equiv 2f_{i_1} \dots f_{i_{2n+1}} \pmod{\text{products}}$$

for all words of odd weight. An immediate corollary of (7.3) is

$$\text{sv}(w) = \text{sv}(\tilde{w}).$$

Recall that the map  $u \mapsto (-1)^{|u|} \tilde{u}$  is the antipode on  $\mathcal{U}$ , giving

$$\sum_{uv=w} (-1)^{|u|} \tilde{u} \text{sv} v = \varepsilon(w).$$

Applying  $\text{sv}$  implies the following explicit version of Equation (6.4)

$$2 \text{sv}(f_{i_1} \dots f_{i_{2n}}) + \sum_{k=1}^{2n-1} (-1)^k \text{sv}(f_{i_1} \dots f_{i_k}) \text{sv}(f_{i_{k+1}} \dots f_{i_{2n}}) = 0$$

for words of even weight  $\geq 2$ , and confirms that single-valued motivic multiple zeta values in even weight are decomposable in  $\mathcal{A}_{>0}^{\text{sv}}$ .

**7.3. Hoffman-type generators for  $\mathcal{H}^{\text{sv}}$ .** Let  $V$  be a finite ordered set. A Lyndon word in the elements of  $V$  is a word which is smaller in the lexicographic ordering than its strict right factors: if  $w = uv$ , then  $w < v$  whenever  $u, v$  are nonempty.

In [9, Section 8], the following theorem was proved.

**THEOREM 7.2.** *The ring of motivic multiple zeta values  $\mathcal{H}$  is generated by the Hoffman–Lyndon elements  $\zeta^{\text{m}}(w)$ , where  $w$  is a Lyndon word in the alphabet  $\{2, 3\}$ , for the ordering  $3 < 2$ .*

We immediately have the following corollary of Proposition 6.5.

**COROLLARY 7.3.** *The ring of single-valued motivic multiple zeta values  $\mathcal{H}^{\text{sv}}$  is generated by the single-valued Hoffman–Lyndon elements*

$$\zeta_{\text{sv}}^m(w),$$

where  $w$  is a Lyndon word of odd weight in the alphabet  $\{2, 3\}$ , where  $3 < 2$ .

A Hoffman–Lyndon word of odd weight necessarily has an odd number of 3s. It follows from Theorem 7.2 that the Poincaré series of  $\mathcal{H}$  is given by

$$\sum_{n \geq 0} \dim \mathcal{H}_n t^n = \frac{1}{1 - t^2 - t^3}.$$

The dimensions  $\ell_n = \dim \mathcal{L}_n$  of the Lie coalgebra  $\mathcal{L}$  are determined by

$$\prod_{n \geq 1} (1 - t^n)^{-\ell_n} = \frac{1}{1 - t^2 - t^3}.$$

The numbers  $\ell_n$  can be interpreted either as the number of Lyndon words of weight  $n$  in  $\{2, 3\}$ , where  $3 < 2$ , or as the number of Lyndon words of weight  $n$  in the alphabet  $\{f_3 < f_5 < f_7, \dots\}$ , via the isomorphism (7.2). By Proposition 6.5, we have the following.

**COROLLARY 7.4.** *The Poincaré series of  $\mathcal{H}^{\text{sv}}$  is given by*

$$\sum_{n \geq 0} \dim \mathcal{H}_n^{\text{sv}} t^n = \prod_{n \text{ odd} \geq 1} (1 - t^n)^{-\ell_n}.$$

**7.4. Examples.** For the convenience of the reader, we list the dimensions of the space of motivic multiple zeta values  $\mathcal{H}$  and its version modulo products  $\mathcal{L}$ :

$N$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
$\dim \mathcal{L}_N$	0	1	1	0	1	0	1	1	1	1	2	2	3	3	4	5	7	8	11	13
$\dim \mathcal{H}_N$	1	1	1	1	2	2	3	4	5	7	9	12	16	21	28	37	49	65	86	114

Next, their single-valued versions  $\mathcal{H}^{\text{sv}}$  and  $\mathcal{L}^{\text{sv}}$ :

$N$	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
$\dim \mathcal{L}_N^{\text{sv}}$	0	0	1	0	1	0	1	0	1	0	2	0	3	0	4	0	7	0	11	0
$\dim \mathcal{H}_N^{\text{sv}}$	1	0	1	0	1	1	1	1	2	2	3	3	5	5	8	8	13	14	21	23

Note that  $\dim_{\mathbb{Q}} \mathcal{H}_N^{\text{sv}}$  happens to equal  $\dim_{\mathbb{Q}} \mathcal{L}_{N+2}$  for  $1 \leq N \leq 12$ , which adds to the large supply of evidence for exercising caution when identifying integer sequences!

Below, we list algebra generators for  $\mathcal{H}_N^{sv}$  for  $1 \leq N \leq 14$ . They were calculated by Oliver Schnetz using [27], which gives a very efficient way to compute (5.2) [28].

$N$	3	5	7	9	11	13
Generators of $\mathcal{H}_{sv}$	$\zeta_{sv}^m(3)$	$\zeta_{sv}^m(5)$	$\zeta_{sv}^m(7)$	$\zeta_{sv}^m(9)$	$\zeta_{sv}^m(11)$ $\zeta_{sv}^m(3, 5, 3)$	$\zeta_{sv}^m(13)$ $\zeta_{sv}^m(5, 3, 5)$ $\zeta_{sv}^m(3, 7, 3)$

Here,  $\zeta_{sv}^m(2n + 1) = 2\zeta^m(2n + 1)$  for all  $n \geq 1$ , and

$$\begin{aligned} \zeta_{sv}^m(3, 5, 3) &= 2\zeta^m(3, 5, 3) - 2\zeta^m(3)\zeta^m(3, 5) - 10\zeta^m(3)^2\zeta^m(5) & (7.4) \\ \zeta_{sv}^m(5, 3, 5) &= 2\zeta^m(5, 3, 5) - 22\zeta^m(5)\zeta^m(3, 5) - 120\zeta^m(5)^2\zeta^m(3) \\ &\quad - 10\zeta^m(5)\zeta^m(8) \\ \zeta_{sv}^m(3, 7, 3) &= 2\zeta^m(3, 7, 3) - 2\zeta^m(3)\zeta^m(3, 7) - 28\zeta^m(3)^2\zeta^m(7) \\ &\quad - 24\zeta^m(5)\zeta^m(3, 5) - 144\zeta^m(5)^2\zeta^m(3) - 12\zeta^m(5)\zeta^m(8). \end{aligned}$$

To obtain formulas for the numbers  $\zeta_{sv}$ , simply drop the superscripts  $m$ .

REMARK 7.5. Let us denote the commutative generating series of *unipotent de Rham* multiple zeta values in depth  $r$  by

$$Z_r(x_1, \dots, x_r) = \sum_{n_1, \dots, n_r \geq 1} \zeta^u(n_1, \dots, n_r) x_1^{n_1-1} \dots x_r^{n_r-1}. \quad (7.5)$$

The operator  $\sigma$  acts by multiplying  $\zeta^u(n_1, \dots, n_r)$  by  $(-1)^{n_1 + \dots + n_r}$ . Let  $Z_r^{sv}$  denote the corresponding single-valued version. Using the methods of [12], we can verify that

$$\begin{aligned} Z_1^{sv} &= Z_1 - \sigma Z_1 \\ Z_2^{sv} &\equiv Z_2 - \sigma Z_2 - 2Z_1 \circlearrowleft Z_1 \\ Z_3^{sv} &\equiv Z_3 - \sigma Z_3 - 2Z_1 \circlearrowleft Z_2 - 2Z_1 \circlearrowleft (Z_1 \circlearrowleft Z_1), \end{aligned}$$

where the equivalence sign means modulo  $\zeta^m(2)$  and modulo terms of lower depth, and where  $\circlearrowleft$  is the linearized Ihara operator defined in [12, Section 6]. For example,

$$\begin{aligned} f(x_1) \circlearrowleft g(x_1) &= f(x_1)g(x_2) + f(x_2 - x_1)(g(x_1) - g(x_2)) \\ f(x_1) \circlearrowleft g(x_1, x_2) &= f(x_1)g(x_2, x_3) + f(x_2 - x_1)(g(x_1, x_3) - g(x_2, x_3)) \\ &\quad + f(x_3 - x_2)(g(x_1, x_2) - g(x_1, x_3)). \end{aligned}$$

In particular, this confirms the formulas (7.4) in odd weights, modulo  $\zeta^m(2)$ .

It is likely that David Broadhurst's knot numbers (see for example [8], Equations (9) and (10)) are further examples of single-valued multiple zeta values in depth 3. If true, this could certainly be verified with the coaction, but I did not check this.

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