

LECTURES ON MULTIPLE ZETA VALUES

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ABSTRACT. These are private lecture notes (i.e. **NOT** intended for publication) for an advanced graduate course on multiple zeta values given at University of Oxford in Trinity term 2019. Its goal is to develop the notion of motivic multiple zeta values from scratch and to present Francis Brown's proof of Hoffman's conjecture for motivic multiple zeta values.

Warning: These are informal lecture notes, so beware of typos and mistakes. If you find any, please let me know under:

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1. INTRODUCTION

1.1. Zeta values. Consider the special values of Riemann's zeta function

$$\zeta(k) = \sum_{n=1}^{\infty} \frac{1}{n^k}, \quad k \geq 2$$

at positive integers. These numbers come up naturally in many seemingly unrelated contexts (e.g., as regulators of K-groups of integers, as volumes of hyperbolic manifolds, in the computation of scattering amplitudes in various physical theories, etc.). A central problem is the following.

Problem 1.1. *Describe all polynomial relations among the $\zeta(k)$.*

The first contribution was made by Euler who computed the values $\zeta(k)$ for even k . To express the result, recall that the Bernoulli numbers B_n are defined by the Taylor expansion

$$\frac{t}{e^t - 1} = \sum_{n=0}^{\infty} B_n \frac{t^n}{n!}.$$

For example, $B_0 = 1$, $B_1 = -\frac{1}{2}$ and $B_2 = \frac{1}{6}$.

Proposition 1.2 (Euler, 1734). *We have*

$$\zeta(2k) = -\frac{B_{2k}(2\pi i)^{2k}}{2(2k)!}.$$

In particular, $\zeta(2k) \in \mathbb{Q}^\times \pi^{2k}$ for every $k \geq 1$.

Proof. We use the partial fraction expansion of the cotangent¹

$$\pi \cot(\pi\alpha) = \frac{1}{\alpha} + \sum_{n>0} \left(\frac{1}{\alpha + n} + \frac{1}{\alpha - n} \right).$$

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¹One way to prove this expansion is to compute the Fourier series of $\cos(\alpha x)$ for $\alpha \in \mathbb{R} \setminus \mathbb{Z}$ and set $x = \pi$. Another one (which is in fact essentially Euler's original argument) is via the product expansion of the sine, $\frac{\sin(\pi\alpha)}{\pi\alpha} = \prod_{n=1}^{\infty} \left(1 - \frac{\alpha^2}{n^2}\right)$.

The right hand side gives, after expanding in a geometric series and collecting terms,

$$\frac{1}{\alpha} - \sum_{k=1}^{\infty} 2\zeta(2k)\alpha^{2k-1},$$

and the left hand side equals

$$\pi i \frac{e^{\pi i \alpha} + e^{-\pi i \alpha}}{e^{\pi i \alpha} - e^{-\pi i \alpha}} = \pi i \left(1 + \frac{2}{e^{2\pi i \alpha} - 1} \right) = \frac{1}{\alpha} + \sum_{k=1}^{\infty} \frac{B_{2k}(2\pi i)^{2k}}{(2k)!} \alpha^{2k-1}.$$

□

Since π is transcendental (Lindemann, 1882), Proposition 1.2 gives the only family of polynomial relations among even zeta values. On the other hand, one does not expect polynomial relations among odd zetas. This is part of the following conjecture.

Conjecture 1.3. *The numbers*

$$\pi, \zeta(3), \zeta(5), \zeta(7), \dots$$

are algebraically independent.

Unfortunately, there is very little evidence for this conjecture, and the best one can do currently are irrationality results. For example, $\zeta(3)$ is known to be irrational (Apéry, 1977), infinitely many odd zetas are irrational (Ball–Rivoal, 2002) and at least one among $\zeta(5), \zeta(7), \zeta(9)$ and $\zeta(11)$ is irrational (Zudilin, 2004).

1.2. Multiple zeta values. Now consider the product of two zeta values,

$$\zeta(k)\zeta(l) = \sum_{m,n>0} \frac{1}{m^k n^l}.$$

Splitting the domain into three parts, Euler observed that

$$\zeta(k)\zeta(l) = \left(\sum_{m>n>0} + \sum_{n>m>0} + \sum_{m=n>0} \right) \frac{1}{m^k n^l}.$$

If one now takes products of zeta values with the above kind of double sums, one obtains triple sums of a similar shape. Iterating this process leads to multiple zeta values.

Definition-Proposition 1.4. Given positive integers k_1, \dots, k_d with $k_1 \geq 2$, the series

$$\zeta(k_1, \dots, k_d) = \sum_{m_1 > \dots > m_d > 0} \frac{1}{m_1^{k_1} \dots m_d^{k_d}}, \quad k_1 \geq 2, k_2, \dots, k_d \geq 1,$$

converges and therefore defines a real number, which is called a *multiple zeta value*. We define the *weight* of $\zeta(k_1, \dots, k_d)$ to be $k_1 + \dots + k_d$ and its *depth* is d .

Proof. It is enough to show convergence of $\zeta(\underbrace{2, 1, \dots, 1}_d)$ for every $d \geq 1$. Using the estimate $\sum_{m=1}^n \frac{1}{m} \leq 1 + \log(n)$, obtained by comparing with the Riemann sum of

the function $x \mapsto 1/x$, we get

$$\zeta(2, 1, \dots, 1) = \sum_{m_1 > \dots > m_d > 0} \frac{1}{m_1^2 m_2 \dots m_d} \leq \sum_{m=1}^{\infty} \frac{(1 + \log(m))^{d-1}}{m^2},$$

and this converges since $(1 + \log(m))^{d-1} \sim o(\sqrt{m})$ as $m \rightarrow \infty$. \square

Remark 1.5. It is convenient to think of the rational number $1 \in \mathbb{Q}$ as a multiple zeta value of weight and depth equal to zero, and we shall tacitly do so in the sequel.

Now let

$$\mathcal{Z} := \text{Span}_{\mathbb{Q}}\{\zeta(k_1, \dots, k_d)\} \subset \mathbb{R}$$

be the \mathbb{Q} -vector space spanned by the multiple zeta values (including 1). In the next section, we will see that \mathcal{Z} is in fact a \mathbb{Q} -subalgebra of \mathbb{R} and that multiplication is compatible with weight and depth. Therefore every algebraic relation between multiple zeta values can be rewritten as a linear relation between other multiple zeta values. In light of Problem 1.1, this suggests the following.

Problem 1.6. *Describe all \mathbb{Q} -linear relations between multiple zeta values.*

Although this problem is of course far from solved, there are several candidates for complete sets of relations, and we will see one of these in the next section.

1.3. Conjectures. The algebraic structure of the \mathbb{Q} -algebra \mathcal{Z} is the subject of various conjectures which have attracted lots of interest, some of which we describe next. For $k \geq 0$, let

$$\mathcal{Z}_k = \{\zeta(k_1, \dots, k_d) \mid k_1 + \dots + k_d = k\} \subset \mathcal{Z}$$

the weight k component of \mathcal{Z} . Clearly $\mathcal{Z} = \sum_k \mathcal{Z}_k$.

Conjecture 1.7. *\mathcal{Z} is graded for the weight, i.e.*

$$\mathcal{Z} = \bigoplus_{k \geq 0} \mathcal{Z}_k.$$

Put differently, there should be no non-trivial \mathbb{Q} -linear relations between different weights. This conjecture is very strong as it readily implies the transcendence of every multiple zeta value of positive weight.

The second conjecture is about the dimensions of the graded pieces of \mathcal{Z} which are a priori finite-dimensional as there are only finitely many multiple zeta values of weight k . To proceed further, let $(d_k)_{k \geq 0}$ be the sequence recursively defined by $d_k = d_{k-2} + d_{k-3}$ for $k \geq 3$ with initial conditions $d_0 = d_2 = 1$, $d_1 = 0$.

Conjecture 1.8 (Zagier, 1994). *We have $\dim_{\mathbb{Q}} \mathcal{Z}_k = d_k$ for every k .*

This conjecture is only known when $d_k \leq 1$ which happens if and only if $k \leq 4$. It would in particular predict the asymptotic $d_k \sim r^k$ as $k \rightarrow \infty$, where $r \approx 1.32$ is the unique real root of $x^3 - x - 1$. Since there are exactly 2^{k-2} multiple zeta values of weight k , there should be many relations among multiple zeta values. For example, in weight 12, there are $2^{10} = 1024$ multiple zeta values but Zagier's conjecture predicts that $\dim_{\mathbb{Q}} \mathcal{Z}_{12} = 12$.

Remark 1.9. There is a refinement of Conjecture 1.8, due to Broadhurst–Kreimer, which also takes the depth into account. Very interestingly, it suggests a relation between multiple zeta values and modular forms which has partially been realized in work of Gangl–Kaneko–Zagier and Brown. We will not touch that conjecture in this lecture.

The final conjecture we present gives an explicit basis for \mathcal{Z} .

Conjecture 1.10 (Hoffman, 1997). *The set*

$$\{\zeta(k_1, \dots, k_d) \mid k_i \in \{2, 3\}\}$$

is a basis for the \mathbb{Q} -vector space \mathcal{Z} .

Multiple zeta values with only 2's and 3's in their index will be called *Hoffman elements* (this includes 1). Counting their number in a fixed weight, we see that Conjecture 1.10 implies Conjecture 1.8.

Here is what's currently known.

- (i) Conjecture 1.7 is nearly completely open. For example, we know that $\mathcal{Z}_0 \cap \mathcal{Z}_2 = \mathcal{Z}_0 \cap \mathcal{Z}_3 = \{0\}$ (by irrationality of π^2 and $\zeta(3)$ respectively) but, for example, whether or not $\mathcal{Z}_2 \cap \mathcal{Z}_3 = \{0\}$ is an open problem.
- (ii)&(iii) In the direction of the conjectures of Hoffman and Zagier, one has the following partial solutions.

Theorem 1.11 (Terasoma (2002), Deligne–Goncharov (2005)). *We have $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq d_k$ for all $k \geq 0$.*

Theorem 1.12 (Brown, 2012). *The Hoffman elements span \mathcal{Z} .*

Perhaps surprisingly, the only known proofs of these results use deep concepts from algebraic geometry, particularly the theory of mixed Tate motives.

1.4. Goals. The key concept in Brown's proof is the notion of *motivic multiple zeta value*. These are elements of a certain \mathbb{Q} -algebra \mathcal{H} which carries important extra structure, most significantly a coaction of a certain "motivic" Hopf algebra \mathcal{A} . Moreover, there is a surjective period map

$$\mathcal{H} \rightarrow \mathcal{Z},$$

which is conjecturally an isomorphism.² Moreover, all conjectures in the last section are known to hold for \mathcal{H} . More precisely:

- (a) There is a notion of weight for motivic multiple zeta values and $\mathcal{H} = \bigoplus_{k \geq 0} \mathcal{H}_k$ is graded for the weight.
- (b) The "motivic Hoffman elements" are a basis for \mathcal{H} (and therefore in particular $\dim_{\mathbb{Q}} \mathcal{H}_k = d_k$).

The statement in (a) is actually a built-in feature of \mathcal{H} . Statement (b), on the other hand, is a deep result and relies crucially on the motivic coaction.

Remark 1.13. In fact, the significance of (b) goes beyond (motivic) multiple zeta values, as it implies important results about the category $MT(\mathbb{Z})$ of mixed Tate motives over \mathbb{Z} , namely the Deligne–Ihara conjecture. It also shows that the periods of $MT(\mathbb{Z})$ are contained in $\mathcal{Z}[(2\pi i)^{-1}]$ (in fact, we have equality).

Goal (of this lecture). *Define motivic multiple zeta values and explain Brown's proof of (b).*

²This would follow from a variant of Grothendieck's period conjecture.

2. THE DOUBLE SHUFFLE RELATIONS

In this section we will see that the \mathbb{Q} -vector space \mathcal{Z} of multiple zeta values is a \mathbb{Q} -algebra. In fact, \mathcal{Z} carries two distinct \mathbb{Q} -algebra structures and the interplay of these two algebra structures is the source of a (conjecturally exhaustive) family of relations.

Notation: For an integer $n \geq 0$ we will denote by $[n] := \{1, 2, 3, \dots, n\}$ the canonical ordered set with n elements (in particular, $[0] := \emptyset$).

For multi-indices $\underline{k} = (k_1, \dots, k_r) \in \mathbb{Z}_{\geq 1}^r$, $\underline{k}' = (k'_1, \dots, k'_s) \in \mathbb{Z}_{\geq 1}^s$, we provisionally denote $\underline{k}'' := (k_1, \dots, k_r, k'_1, \dots, k'_s)$.

2.1. The harmonic product.

Definition 2.1. For positive integers $r, s \geq 1$, define the set of (r, s) -quasishuffles to be

$$QSh(r, s) = \bigcup_{N \geq 1} \{ \sigma : [r+s] \twoheadrightarrow [N] \mid \sigma(1) < \dots < \sigma(r), \\ \sigma(r+1) < \dots < \sigma(r+s) \}.$$

It is straightforward to check that $\#\sigma^{-1}(i) \leq 2$.

Definition 2.2. Define the *harmonic product* of \underline{k} and \underline{k}' to be the following formal sum of multi-indices

$$\underline{k} * \underline{k}' = \sum_{\sigma \in QSh(r, s)} \left(\sum_{\sigma(i)=1} k''_i, \dots, \sum_{\sigma(i)=N} k''_i \right).$$

Example 2.3. For all $k, k', k'' \geq 1$, we have

$$(k) * (k') = (k, k') + (k', k) + (k + k'), \\ (k) * (k', k'') = (k, k', k'') + (k', k, k'') + (k', k'', k) + (k + k', k'') + (k', k + k'').$$

A multi-index $\underline{k} = (k_1, \dots, k_d)$ is called *admissible* if $k_1 \geq 2$. We then have a map

$$\{\text{admissible multi-indices}\} \rightarrow \mathbb{R} \\ \underline{k} \mapsto \zeta(\underline{k}),$$

which admits a unique extension to the set of finite linear combinations of admissible multi-indices which. By slight abuse of notation, we denote this map also by ζ .

Proposition 2.4. For all admissible multi-indices $\underline{k}, \underline{k}'$, we have

$$\zeta(\underline{k})\zeta(\underline{k}') = \zeta(\underline{k} * \underline{k}').$$

In other words, multiple zeta values satisfy the harmonic product.

This is well-defined because the harmonic product of two admissible multi-indices is a finite sum of admissible multi-indices by construction.

Proof. Write $\underline{k} = (k_1, \dots, k_r)$ and $\underline{k}' = (k'_1, \dots, k'_s)$. Then

$$\begin{aligned} \zeta(\underline{k})\zeta(\underline{k}') &= \sum_{\substack{m_1 > \dots > m_r > 0 \\ n_1 > \dots > n_s > 0}} \frac{1}{m_1^{k_1} \dots m_r^{k_r} n_1^{k'_1} \dots n_s^{k'_s}} \\ &= \sum_{\sigma \in QSh(r,s)} \sum_{m_1 > \dots > m_N > 0} \frac{1}{m_1^{\sum_{\sigma(i)=1} k''_i} \dots m_N^{\sum_{\sigma(i)=N} k''_i}} \\ &= \zeta(\underline{k} * \underline{k}'). \end{aligned}$$

□

Corollary 2.5. *The \mathbb{Q} -vector subspace $\mathcal{Z} \subset \mathbb{R}$ is a \mathbb{Q} -subalgebra of \mathbb{R} and the product is compatible with the weight:*

$$\mathcal{Z}_k \cdot \mathcal{Z}_{k'} \subset \mathcal{Z}_{k+k'}, \quad \text{for all } k, k' \geq 0.$$

Proof. This follows from Proposition 2.4 together with the fact that the harmonic product of two multi-indices $\underline{k}, \underline{k}'$ of weights k, k' respectively is a sum of multi-indices of homogeneous weight $k + k'$. □

2.2. The shuffle product. The second product structure on \mathcal{Z} comes from the representation of multiple zeta values as iterated integrals. Consider the following differential one-forms on $\mathbb{P}_{\mathbb{C}}^1$

$$\omega_0(t) = \frac{dt}{t}, \quad \omega_1(t) = \frac{dt}{1-t}.$$

The form ω_0 has simple poles at $t = 0, \infty$ and similarly ω_1 has simple poles at $t = 1, \infty$. We will view $\omega_0(t), \omega_1(t)$ as measures on the open unit interval $(0, 1)$. Likewise, given a multi-index $\underline{k} = (k_1, \dots, k_d)$ of weight $k := k_1 + \dots + k_d$ we consider the following measure on $\Delta^k = \{(t_1, \dots, t_k) \in \mathbb{R}^k \mid 1 > t_1 > \dots > t_k > 0\}$:

$$\omega_{\underline{k}} = \prod_{n=1}^d \omega_0(t_{p_{n-1}+1}) \dots \omega_0(t_{p_n-1}) \omega_1(t_{p_n}), \quad p_n := \sum_{i=1}^n k_i.$$

Proposition 2.6. *For every admissible multi-index \underline{k} of weight k , we have*

$$\zeta(\underline{k}) = \int_{\Delta^k} \omega_{\underline{k}}.$$

To prove the result, we consider the multiple polylogarithm

$$Li_{k_1, \dots, k_d}(z) := \sum_{m_1 > \dots > m_d > 0} \frac{z^{m_1}}{m_1^{k_1} \dots m_d^{k_d}}, \quad |z| < 1,$$

where (k_1, \dots, k_d) is a (not necessarily admissible) multi-index. These are holomorphic functions on the open unit disk which extend continuously to the boundary, except for the point $z = 1$ if $k_1 = 1$.

Proof. We prove more generally that for every real number $0 \leq z < 1$ and every multi-index \underline{k} , we have

$$(2.1) \quad Li_{\underline{k}}(z) = \int_{z > t_1 > \dots > t_k > 0} \omega_{\underline{k}},$$

from which the proposition follows by taking the limit $z \rightarrow 1$ and using Abel's theorem.³ To this end, multiple polylogarithms satisfy the differential equation

$$\frac{d}{dz} Li_{k_1, \dots, k_d}(z) = \begin{cases} \frac{1}{z} Li_{k_1-1, \dots, k_d}(z) & k_1 \geq 2, \\ \frac{1}{1-z} Li_{k_2, \dots, k_d}(z) & k_1 = 1, \end{cases}$$

which follow from differentiating term by term. By the fundamental theorem of calculus, the right hand side of (2.1) satisfies the same (linear, first order) differential equation and since both solutions agree for $z = 0$, we conclude that (2.1) holds. \square

The preceding proposition suggests a different indexation of multiple zeta values using multi-indices $\underline{a} := (a_1, \dots, a_n) \in \{0, 1\}^n$. Such a multi-index is called admissible if $a_1 = 0$ and $a_n = 1$ in which case the associated integral

$$I(0; a_1, \dots, a_n; 1) = \int_{\Delta^n} \omega_{a_1}(t_1) \dots \omega_{a_n}(t_n)$$

converges.

Definition 2.7. Define a map

$$\bigcup_{d \geq 0} \{\underline{k} \in \mathbb{Z}_{\geq 1}^d \mid k_1 + \dots + k_d = k\} \longrightarrow \{\underline{a} \in \{0, 1\}^k \mid a_k = 1\}$$

$$\underline{k} \mapsto \tilde{\underline{k}} = (\tilde{k}_1, \dots, \tilde{k}_k)$$

where

$$\tilde{k}_i = \begin{cases} 1 & i \in \{k_1, k_1 + k_2, \dots, k\} \\ 0 & \text{else} \end{cases}.$$

Proposition 2.8. (i) *The map $\underline{k} \mapsto \tilde{\underline{k}}$ is a bijection which respects the subspaces of admissible indices, i.e. $\tilde{\underline{k}}$ is admissible if and only if \underline{k} is.*

(ii) *We have*

$$\zeta(\underline{k}) = I(0; \tilde{\underline{k}}; 1).$$

The integrals $I(0; a_1, \dots, a_n; 1)$ have a natural product structure which we describe next.

Definition 2.9. For positive integers $r, s \geq 1$, define the set of (r, s) -shuffles to be

$$Sh(r, s) = \{\sigma : [r + s] \rightarrow [r + s] \mid \sigma(1) < \dots < \sigma(r), \sigma(r + 1) < \dots < \sigma(r + s)\}.$$

In other words, an (r, s) -shuffle is a permutation of $[r + s]$ which is increasing on both the first r and the last s numbers.

Proposition 2.10. *For any two admissible multi-indices $\underline{a} = (a_1, \dots, a_r)$, $\underline{a}' = (a'_1, \dots, a'_s)$ as above, we have*

$$I(0; a_1, \dots, a_r; 1) I(0; a'_1, \dots, a'_s; 1) = \sum_{\sigma \in Sh(r, s)} I(0; a''_{\sigma^{-1}(1)}, \dots, a''_{\sigma^{-1}(r+s)}; 1),$$

where $(a''_1, \dots, a''_{r+s}) := (a_1, \dots, a_r, a'_1, \dots, a'_s)$.

³This result extends naturally to complex values of z using the concept of iterated path integral, which will be introduced later.

Proof. Write $\Delta^r = \{(t_1, \dots, t_r) \in \mathbb{R}^r \mid 1 > t_1 > \dots > t_r > 0\}$ and $\Delta^s = \{(t'_1, \dots, t'_s) \in \mathbb{R}^s \mid 1 > t'_1 > \dots > t'_s > 0\}$. By definition and Fubini's theorem, we have

$$I(0; a_1, \dots, a_r; 1)I(0; a'_1, \dots, a'_s; 1) = \int_{\Delta^r \times \Delta^s} \omega_{a_1}(t_1) \dots \omega_{a_r}(t_r) \omega_{a'_1}(t'_1) \dots \omega_{a'_s}(t'_s).$$

The key point is now that the domain of integration can be decomposed
(2.2)

$$\Delta^r \times \Delta^s = \bigcup_{\sigma \in Sh(r,s)} \{(t_1, \dots, t_{r+s}) \in \mathbb{R}^{r+s} \mid 1 > t_{\sigma^{-1}(1)} > \dots > t_{\sigma^{-1}(r+s)} > 0\},$$

where we identified $\Delta^r \times \Delta^s$ as a subset of \mathbb{R}^{r+s} in the canonical way. Note that all non-trivial intersections in (2.2) have dimension $< r + s$, in particular they have measure zero, and we conclude using linearity of the integral. \square

The preceding proposition gives a new proof of Corollary 2.5. Define

$$\underline{k} \sqcup \underline{k}' = \sum_{\sigma \in Sh(r,s)} \underline{k}_\sigma,$$

where \underline{k}_σ is the unique multi-index which satisfies $\widetilde{\underline{k}}_\sigma = (k''_{\sigma^{-1}(1)}, \dots, k''_{\sigma^{-1}(r+s)})$.

Corollary 2.11. *We have*

$$\zeta(\underline{k})\zeta(\underline{k}') = \zeta(\underline{k} \sqcup \underline{k}').$$

Example 2.12.

$$\begin{aligned} \zeta(2)\zeta(2) &= I(0; 0, 1; 1)I(0; 0, 1; 1) = 2I(0; 0, 1, 0, 1; 1) + 4I(0; 0, 0, 1, 1; 1) \\ &= 2\zeta(2, 2) + 4\zeta(3, 1). \end{aligned}$$

2.3. The double shuffle relations and regularization. Equating harmonic and shuffle product gives rise to \mathbb{Q} -linear relations among multiple zeta values, for example

$$\begin{aligned} \zeta(2)\zeta(2) &\stackrel{\text{harm.}}{=} 2\zeta(2, 2) + \zeta(4) \\ &\stackrel{\text{shuffle}}{=} 2\zeta(2, 2) + 4\zeta(3, 1), \end{aligned}$$

which gives $\zeta(3, 1) = \frac{1}{4}\zeta(4)$. These cannot give all relations, however. For example, the relation

$$\zeta(2, 1) = \zeta(3)$$

cannot be proved using double shuffle since the double shuffle relations start in weight 4. In a similar vein, $\zeta(3, 1) = \frac{1}{4}\zeta(4)$ is the only double shuffle relation in weight 4, but we already know that $\dim_{\mathbb{Q}} \mathcal{Z}_4 = 1$, so we are missing two more relations.

It turns out that the solution to this problem is to introduce an auxiliary variable T (which plays the role of “ $\zeta(1)$ ”) and to extend the double shuffle relations from \mathcal{Z} to $\mathcal{Z}[T]$.

Theorem 2.13 (Ihara–Kaneko–Zagier). *For every not necessarily admissible multi-index \underline{k} there exist unique polynomials*

$$\zeta_{\sqcup}(\underline{k}), \zeta_{*}(\underline{k}) \in \mathcal{Z}[T]$$

such that:

(i) We have

$$\zeta_{\sqcup}(\underline{k}) = \zeta_*(\underline{k}) = \zeta(\underline{k})$$

if \underline{k} is admissible,

(ii)

$$\zeta_{\sqcup}(1) = \zeta_*(1) = T,$$

(iii)

$$\zeta_{\sqcup}(\underline{k} \sqcup \underline{k}') = \zeta_{\sqcup}(\underline{k}) \zeta_{\sqcup}(\underline{k}')$$

$$\zeta_*(\underline{k} * \underline{k}') = \zeta_*(\underline{k}) \zeta_*(\underline{k}').$$

Moreover, the two polynomials are related by the equality of generating series

$$\zeta_{\sqcup}(\underline{k}) = \exp \left(\sum_{n=2}^{\infty} (-1)^n \frac{\zeta(n)}{n} \frac{d^n}{dT^n} \right) \zeta_*(\underline{k}).$$

The relations in (iii) above are called *extended double shuffle relations*.

Conjecture 2.14 (Ihara–Kaneko–Zagier). *Every \mathbb{Q} -linear relation between multiple zeta values is a consequence of the relations*

$$\zeta(\underline{k} * \underline{l} - \underline{k} \sqcup \underline{l}) = 0,$$

$$\zeta(\underline{k} * (1) - \underline{k} \sqcup (1)) = 0,$$

where $\underline{k}, \underline{l}$ are admissible.

Remark 2.15 (Euler’s relation). We have

$$(2) \sqcup (1) - (2) * (1) = 2(2, 1) + (1, 2) - (2, 1) - (1, 2) - (3) = (2, 1) - (3),$$

from which $\zeta(2, 1) = \zeta(3)$ follows.

3. PERIODS

Much of the significance of multiple zeta values is due to the fact that they are examples of periods. These are certain complex numbers which arise from the comparison between two cohomology theories naturally associated with algebraic varieties, namely Betti and algebraic de Rham cohomology which we describe next.

Throughout this section, all algebraic varieties will be defined over \mathbb{Q} for simplicity. More generally, we could replace \mathbb{Q} by any subfield $k \subset \mathbb{C}$.

3.1. Betti cohomology. Let M be a topological space. A *singular n -chain* is a continuous map

$$\sigma : \Delta_{\text{st}}^n \rightarrow M,$$

where

$$\Delta_{\text{st}}^n = \{(t_0, \dots, t_n) \in \mathbb{R}^{n+1} \mid \sum_{i=0}^n t_i = 1, t_i \geq 0\},$$

is the standard n -simplex of dimension n . We consider the free abelian group

$$C_n(M) = \bigoplus_{\sigma} \mathbb{Z}\sigma$$

generated by all n -chains. For every $n \geq 1$, there are *boundary* maps

$$\begin{aligned}\partial_n : C_n(M) &\rightarrow C_{n-1}(M) \\ \sigma &\mapsto \sum_{i=0}^n (-1)^i (\sigma \circ \delta_i^n),\end{aligned}$$

where $\delta_i^n : \Delta_{\text{st}}^{n-1} \rightarrow \Delta_{\text{st}}^n$ is the i -th *face map* defined by

$$\delta_i^n(t_0, \dots, t_{n-1}) = (t_0, \dots, t_{i-1}, 0, t_i, \dots, t_{n-1}).$$

The boundary maps verify $\partial_{n-1} \circ \partial_n = 0$ and we therefore obtain a chain complex $(C_\bullet(M), \partial_\bullet)$

$$\dots \longrightarrow C_{n+1}(M) \xrightarrow{\partial_{n+1}} C_n(M) \xrightarrow{\partial_n} C_{n-1}(M) \longrightarrow \dots$$

Definition 3.1. The *singular homology* of M is the homology of $(C_\bullet(M), \partial_\bullet)$:

$$H_n(M, \mathbb{Z}) = \begin{cases} \text{coker}(\partial_1), & n = 0 \\ \ker(\partial_n) / \text{Im}(\partial_{n+1}) & n \geq 1. \end{cases}$$

We denote by $H_*(M, \mathbb{Z}) = \bigoplus_{n \geq 0} H_n(M, \mathbb{Z})$ their formal direct sum.

Elements of $\ker(\partial_n)$ are called n -cycles and elements of $\text{Im}(\partial_{n+1})$ are called n -boundaries.

Example 3.2. Let $M = \mathbb{C}^\times$ with its usual topology. Then $H_0(M, \mathbb{Z}) \cong \mathbb{Z}$, $H_n(M, \mathbb{Z}) \cong \{0\}$ for $n \geq 2$ and

$$H_1(M, \mathbb{Z}) \cong \mathbb{Z} \cdot [\sigma_0],$$

where σ_0 is a loop winding once around 0.

Dually, one has the notion of singular n -cochains defined by

$$C^n(M) := \text{Hom}_{\mathbb{Z}}(C_n(M), \mathbb{Z}),$$

as well as coboundary maps $d^n : C^n(M) \rightarrow C^{n+1}(M)$, and the *singular cohomology* groups are defined by

$$H^n(M, \mathbb{Z}) = \begin{cases} \ker(d^0), & n = 0 \\ \ker(d^n) / \text{Im}(d_{n-1}), & n \geq 1. \end{cases}$$

Again, we denote $H^*(M, \mathbb{Z}) = \bigoplus_{n \geq 0} H^n(M, \mathbb{Z})$.

Remark 3.3. In the definition of $C_n(M)$ (respectively $C^n(M)$), we may replace \mathbb{Z} by any other coefficient ring R and accordingly obtain homology and cohomology R -modules

$$H_*(M, R), H^*(M, R).$$

Usually, we will work with $R = \mathbb{Z}, \mathbb{Q}, \mathbb{R}, \mathbb{C}$.

We shall only be interested in the case where M is the topological space of the complex points $X(\mathbb{C})$ (endowed with the complex topology) of some algebraic variety over k . We give this a special name.

Definition 3.4. Let X/k be an algebraic variety. The *Betti cohomology* $H_B^*(X)$ of X is defined as

$$H_B^*(X) = H^*(X(\mathbb{C}), \mathbb{Q}).$$

3.1.1. *Relative cohomology.* One can also form singular (co-)homology of M relative to a subspace $\iota : N \hookrightarrow M$. More precisely, let $\iota_* : C_\bullet(N) \rightarrow C_\bullet(M)$ be the induced map of complexes which is injective. The *cone* of ι_* is then the complex $(C_\bullet(M, N), \partial_\bullet)$ given by

$$C_\bullet(M, N) = C_{n-1}(N) \oplus C_n(M), \quad C_{-1}(N) := 0$$

in degree n with boundary map

$$(a, b) \mapsto (-\partial_{n-1}a, -\iota_{n-1}(a) + \partial_n b), \quad a \in C_{n-1}(N), b \in C_n(M).$$

The corresponding homology groups are denoted by $H_n(M, N; \mathbb{Z})$ and are called *relative homology* groups. Likewise, one defines relative cohomology groups $H^n(M, N; \mathbb{Z})$ and, in the algebraic case, relative Betti cohomology groups $H_B^n(X, Y; \mathbb{Z})$.

Remark 3.5. It can be shown that the complex $(C_\bullet(M, N), \partial_\bullet)$ is quasi-isomorphic to the quotient complex $(C_\bullet(M)/C_\bullet(N), \partial_\bullet)$ with boundary map induced from the boundary map on $C_\bullet(M)$. Therefore, relative homology classes can be thought of as homology classes on M whose boundary is contained in N .

Example 3.6. Let $M = \mathbb{C}^\times$ and $N = \{1, z\}$ where $z \neq 1$. Then $H_n(M, N; \mathbb{Z}) \cong 0$ for $n \neq 1$ and

$$H_1(M, N; \mathbb{Z}) \cong \mathbb{Z} \cdot [\sigma_0] \oplus \mathbb{Z} \cdot [\gamma_1^z],$$

where γ_1^z is a path from 1 to z .

3.2. **Algebraic de Rham cohomology.** Recall that X/\mathbb{Q} is a smooth variety. To simplify the presentation, we will further assume that $X = \text{Spec}(A)$ is affine. Consider the module Ω_A^1 of Kähler differentials with differential d . Explicitly, if $A = \mathbb{Q}[x_1, \dots, x_n]/(f_1, \dots, f_m)$ for some polynomials f_1, \dots, f_m , then

$$\Omega_A^1 = \left(\bigoplus_{i=1}^n A \cdot dx_i \right) / J,$$

where J is the submodule generated by $df_j = \sum_{i=1}^n \frac{\partial f_j}{\partial x_i} dx_i$, for $j = 1, \dots, m$. We also denote by

$$\Omega_A^p = \Lambda^p \Omega_A^1$$

its p -th exterior power. The differential d naturally extends to Ω_A^p and we obtain a complex

$$A \longrightarrow \Omega_A^1 \longrightarrow \Omega_A^2 \longrightarrow \dots \longrightarrow \Omega_A^n,$$

called the *algebraic de Rham complex* of A . (note that $\Omega_A^p = 0$ if $p > n$).

Definition 3.7. The *algebraic de Rham cohomology* $H_{\text{dR}}^*(X)$ of $X = \text{Spec}(A)$ is the cohomology of the algebraic de Rham complex of A .

Remark 3.8. If X is not necessarily affine, then one defines

$$H_{\text{dR}}^*(X) = \mathbb{H}^*(X, \Omega_X^\bullet),$$

where Ω_X^\bullet is the de Rham complex of X (viewed as a complex of sheaves on X for the Zariski topology) and \mathbb{H}^* denotes hypercohomology.

Example 3.9. Let $X = \mathbb{G}_m := \text{Spec}(\mathbb{Q}[t, t^{-1}])$ which has dimension one. The de Rham complex is given by

$$\mathbb{Q}[t, t^{-1}] \xrightarrow{d} \mathbb{Q}[t, t^{-1}]dt,$$

and therefore $H_{\text{dR}}^0(X) \cong \ker(d)$, $H_{\text{dR}}^1(X) \cong \text{coker}(d)$ and $H_{\text{dR}}^n(X) = 0$ for $n \geq 2$. Clearly $\ker(d) = k$ and since $t^m dt$ is in the image of d if and only if $m \neq -1$, we get

$$\text{coker}(d) \cong \mathbb{Q} \cdot \left[\frac{dt}{t} \right].$$

3.2.1. Relative algebraic de Rham cohomology. Similar to singular cohomology, there is also a relative version of algebraic de Rham cohomology. Let $\iota : Z \hookrightarrow X$ be a smooth closed subscheme over \mathbb{Q} which is affine if X is. There is a restriction map of complexes $\iota^* : \Omega^\bullet(X) \rightarrow \Omega^\bullet(Z)$, and the *relative algebraic de Rham complex* is then given in degree n by

$$\Omega^\bullet(X, Z) = \Omega^n(X) \oplus \Omega^{n-1}(Z),$$

with differential

$$(\alpha, \beta) \mapsto (d\alpha, \iota^*(\alpha) - d\beta).$$

Example 3.10. Let again $X = \mathbb{G}_m$ and $Z = \{p, q\} \subset X$ the closed subscheme defined by two \mathbb{Q} -rational points p and q . Then $\Omega^\bullet(Z) \cong \mathbb{Q} \oplus \mathbb{Q}$, and

$$\iota^* : \Omega^0(X) = \mathbb{Q}[t, t^{-1}] \rightarrow \Omega^0(Z) = \mathbb{Q} \oplus \mathbb{Q}$$

is simply evaluation $f \mapsto (f(p), f(q))$. Therefore the relative de Rham complex is given by

$$\begin{aligned} d : \mathbb{Q}[t, t^{-1}] &\rightarrow \mathbb{Q}[t, t^{-1}]dt \oplus \mathbb{Q} \oplus \mathbb{Q} \\ f &\mapsto (f'(t)dt, f(p), f(q)). \end{aligned}$$

Clearly d is injective and its image is given by

$$\text{Im}(d) = \text{Span}_{\mathbb{Q}}\{(0, 1, 1), (nt^{n-1}, p^n, q^n) \mid n \in \mathbb{Z} \setminus \{0\}\}.$$

It follows that $H_{\text{dR}}^1(X, Z) = \text{Span}_{\mathbb{Q}}\{[(0, 1, 0)], [(dt/t, 0, 0)]\}$. Also, note that $[(0, 1, 0)] = [(1/(q-p)dt, 0, 0)]$.

3.3. Periods of algebraic varieties.

3.3.1. Grothendieck's comparison isomorphism. The fundamental result on the relation between algebraic de Rham and Betti cohomology of algebraic varieties is the following.

Theorem 3.11 (Grothendieck's algebraic de Rham theorem). *Let X/\mathbb{Q} be a smooth algebraic variety. Then there is a canonical comparison isomorphism*

$$\text{comp}_{\text{B,dR}} : H_{\text{dR}}^i(X) \otimes_{\mathbb{Q}} \mathbb{C} \xrightarrow{\cong} H_B^i(X) \otimes_{\mathbb{Q}} \mathbb{C}.$$

If X is affine, then the comparison isomorphism is given by integration, which induces a perfect pairing of \mathbb{Q} -vector spaces

$$\begin{aligned} H_{\text{dR}}^i(X) \otimes_{\mathbb{Q}} H_B^i(X)^\vee &\rightarrow \mathbb{C} \\ \omega \otimes \sigma &\mapsto \int_{\sigma} \omega. \end{aligned}$$

Here, we used the fact that $\int_{\sigma} \omega$ only depends on the classes of ω and σ in (co)-homology by Stokes' theorem.

There is also a relative version which we state in a special case.

Theorem 3.12. *Let X/\mathbb{Q} be a smooth variety, $Z \subset X$ a smooth closed subvariety defined over \mathbb{Q} . Then there is a canonical isomorphism*

$$H_{\text{dR}}^i(X, Z) \otimes_k \mathbb{C} \xrightarrow{\cong} H_B^i(X, Z) \otimes_{\mathbb{Q}} \mathbb{C}.$$

Again, if X (and therefore also Z) is affine, then the comparison isomorphism is given by integration. More precisely, the induced perfect pairing is given by

$$H_{\text{dR}}^i(X, Z) \otimes_{\mathbb{Q}} H_B^i(X, Z)^{\vee} \rightarrow \mathbb{C}$$

$$(\omega_X, \omega_Z) \otimes (\sigma_X, \sigma_Z) \mapsto \int_{\sigma_X} \omega_X + \int_{\sigma_Z} \omega_Z.$$

3.3.2. Periods. Choosing bases of $H_{\text{dR}}^i(X)$ respectively of $H_B^i(X)$, the comparison isomorphism is represented by a certain $\dim H_B^i(X) \times \dim H_B^i(X)$ matrix with coefficients in \mathbb{C} whose entries are called *periods* of X . They depend on the choice of bases, however their k -span does not.

Example 3.13 ($2\pi i$). Again let $X = \mathbb{G}_m$. By Example 3.9, we know that $H_{\text{dR}}^1(X) \cong \mathbb{Q} \cdot [dt/t]$ and by Example 3.2 $H_B^1(X) \cong \mathbb{Q} \cdot [\sigma_0]^{\vee}$ where σ_0 is a loop around 0 in the positive direction. With this choice of basis, the period matrix is simply $(2\pi i)$ since $\int_{\sigma_0} \frac{dt}{t} = 2\pi i$.

Example 3.14 (Logarithms). Here $X = \mathbb{G}_m/\mathbb{Q}$ with $Z = \{1, p\}$, for some $p \in \mathbb{Q}^{\times} \setminus \{1\}$. By Example 3.10, $H_{\text{dR}}^1(X, Z) \cong \mathbb{Q} \cdot [dt/t] \oplus [dt/(p-1)]$ and by Example 3.6, we know $H_B^1(X, Z) \cong \mathbb{Q} \cdot [\sigma]^{\vee} \oplus \mathbb{Q} \cdot [\gamma_1^p]^{\vee}$. The period matrix equals

$$\begin{pmatrix} \int_{\gamma_{1,p}} \frac{dt}{p-1} & \int_{\gamma_{1,p}} \frac{dt}{t} \\ \int_{\sigma_0} \frac{dt}{p-1} & \int_{\sigma_0} \frac{dt}{t} \end{pmatrix} = \begin{pmatrix} 1 & \log(p) \\ 0 & 2\pi i \end{pmatrix}.$$

The most interesting entry is the logarithm in the top right corner.

4. MIXED HODGE STRUCTURES

One drawback of singular cohomology groups $H_B^n(X)$ of an algebraic variety X are by construction topological invariants of X and a priori fail to detect finer information about X . For example, if X, Y are two distinct elliptic curves over \mathbb{Q} , their singular cohomology will be isomorphic.

However, there exists some natural extra linear-algebraic structure which detects the isomorphism class of X as an algebraic variety, namely a Hodge structure on $H_B^n(X)$. This notion is also closely related to the notion of periods, indeed provides a very convenient framework for their study.

We continue to work over the field \mathbb{Q} for simplicity.

4.1. Pure Hodge structures. Let M be a complex projective manifold (or more generally a Kähler manifold). Given a pair of integers (p, q) , let $H^{p,q}(M) \subset H^{p+q}(M, \mathbb{C})$ subspace of classes which locally look like

$$\sum_{I,J} f_{I,J}(z_1, \dots, z_d) dz_{i_1} \wedge \dots \wedge dz_{i_p} \wedge d\bar{z}_{j_1} \wedge \dots \wedge d\bar{z}_{j_q},$$

where $I = \{i_1, \dots, i_p\}$, $J = \{j_1, \dots, j_q\}$ are subsets of $\{1, \dots, d\}$ and $f_{I,J}$ are \mathcal{C}^∞ -functions.

Theorem 4.1 (Hodge). *There is a direct sum decomposition*

$$H^n(M, \mathbb{Q}) \otimes_{\mathbb{Q}} \mathbb{C} = \bigoplus_{p+q=n} H^{p,q}(M),$$

and such that $\overline{H}^{p,q}(M) \cong H^{q,p}(M)$.

The theorem motivates the classical definition of a *Hodge structure* (of weight n) which consists of a finite-dimensional \mathbb{Q} -vector space H together with a bigrading

$$H_{\mathbb{C}} = H \otimes_{\mathbb{Q}} \mathbb{C} = \bigoplus_{p+q=n} H^{p,q}.$$

The following definition will be more convenient for our purposes.

Definition 4.2. A *pure \mathbb{Q} -Hodge structure* of weight n is a triple

$$H = (H_B, (H_{dR}, F^\bullet), \text{comp}_{B,dR}),$$

where H_B, H_{dR} are finite-dimensional \mathbb{Q} -vector spaces, F^\bullet a decreasing, exhaustive Hodge filtration on H_{dR} and $\text{comp}_{B,dR}$ is an isomorphism of complex vector spaces

$$\text{comp}_{B,dR} : H_{dR} \otimes_{\mathbb{Q}} \mathbb{C} \xrightarrow{\cong} H_B \otimes_{\mathbb{Q}} \mathbb{C}.$$

The induced Hodge filtration on $H_{\mathbb{C}} = H_B \otimes_{\mathbb{Q}} \mathbb{C}$, still denoted by F^\bullet , is required to satisfy in addition that

$$H_{\mathbb{C}} = F^p H_{\mathbb{C}} \oplus \overline{F^{n-p+1} H_{\mathbb{C}}}, \quad \text{for all } p.$$

Definition 4.2 is slightly more general than the definition given above. Every Hodge structure as above gives a pure Hodge structure in the sense of Definition 4.2 if one chooses $H = H_B = H_{dR}$, $\text{comp}_{B,dR} = \text{id}$ and

$$F^p H = \bigoplus_{i \geq p} H^{i, n-i}.$$

Conversely, given a pure Hodge structure, one obtains a bigrading on $H_{\mathbb{C}} = H_B \otimes_{\mathbb{Q}} \mathbb{C}$ via

$$H^{p,q} := \text{comp}_{B,dR} \left(F^p (H_{dR} \otimes \mathbb{C}) \cap \overline{F^q (H_{dR} \otimes \mathbb{C})} \right).$$

Definition 4.3. A *morphism of pure \mathbb{Q} -Hodge structures* is a pair (f_B, f_{dR}) of \mathbb{Q} -linear maps $f_B : H_B \rightarrow H'_B$, $f_{dR} : H_{dR} \rightarrow H'_{dR}$ such that $f_{dR}(F^\bullet H_{dR}) \subset F^\bullet H'_{dR}$ and such that the following diagram commutes:

$$\begin{array}{ccc} H_{dR} \otimes_{\mathbb{Q}} \mathbb{C} & \xrightarrow{\text{comp}_{B,dR}} & H_B \otimes_{\mathbb{Q}} \mathbb{C} \\ f_{dR} \otimes \text{id} \downarrow & & \downarrow f_B \otimes \text{id} \\ H'_{dR} \otimes_{\mathbb{Q}} \mathbb{C} & \xrightarrow{\text{comp}'_{B,dR}} & H'_B \otimes_{\mathbb{Q}} \mathbb{C}. \end{array}$$

In particular, it follows from the definition that every morphism between pure Hodge structures of different weights is zero.

Example 4.4 (Hodge structures of Tate type). For an integer $n \in \mathbb{Z}$, define

$$\mathbb{Q}(n) = (\mathbb{Q}, (\mathbb{Q}, F^\bullet), \text{comp}_{B,dR})$$

with Hodge filtration $\mathbb{Q} = F^{-n}\mathbb{Q} \supseteq F^{-n+1}\mathbb{Q} = \{0\}$ and the isomorphism $\text{comp}_{B,dR} : \mathbb{C} \rightarrow \mathbb{C}$ is given by multiplication by $(2\pi i)^{-n}$. The case $n = 1$ is known as the *Tate* Hodge structure. Also, note that $\mathbb{Q}(-1)$ is isomorphic to the triple

$$H^1(\mathbb{G}_m) = (H_B^1(\mathbb{G}_m), (H_{dR}^1(\mathbb{G}_m), F^\bullet), \text{comp}_{B,dR}),$$

where F^\bullet is the trivial filtration concentrated in degree one as above and $\text{comp}_{B,dR}$ is Grothendieck's comparison isomorphism, Theorem 3.11.

The following is essentially a restatement of Hodge's theorem above.

Theorem 4.5. *Let X/\mathbb{Q} be a smooth projective variety. Then the Betti cohomology $H_B^n(X)$ carries a pure Hodge structure of weight n which is functorial in X .*

An important operation on Hodge structures is the Tate twist:

$$H(n) := H \otimes \mathbb{Q}(n).$$

To be precise, for $H = (H_B, (H_{dR}, F^\bullet), \text{comp}_{B,dR})$

$$H(n) = (H_B, (H_{dR}, F^{\bullet+n}), \text{comp}_{B,dR} \cdot (2\pi i)^{-n}),$$

i.e. the Hodge filtration is shifted by n and the comparison isomorphism gets multiplied by $(2\pi i)^{-n}$. From this example, one sees that

$$\mathbb{Q}(n) \cong \mathbb{Q}(1)^{\otimes n}, \quad \mathbb{Q}(-1) \cong \mathbb{Q}(1)^\vee = \text{Hom}_{\mathbb{Q}}(\mathbb{Q}(1), \mathbb{Q}(0)).$$

Example 4.6. We have

$$H^j(\mathbb{P}^n, \mathbb{Q}) \cong \begin{cases} \mathbb{Q}(-j/2), & 0 \leq j \leq 2n \text{ even,} \\ 0 & \text{else.} \end{cases}$$

4.2. Mixed Hodge structures. Mixed Hodge structures appear naturally when one studies the cohomology of varieties which are no longer assumed to be smooth or projective. For example, we have seen that $H^1(\mathbb{G}_m)$ is one-dimensional, but there is no one-dimensional pure Hodge structure of weight one due to Hodge symmetry $\bar{H}^{p,q} \cong H^{q,p}$. Similarly, the relative cohomology groups $H_B^n(X, Z)$ in general do not carry a pure Hodge structure, but rather a mixed Hodge structure.

The “correct” generalization of Hodge's theorem was found by Deligne who proved that the cohomology of a (say quasi-projective) algebraic variety over \mathbb{C} carries a *mixed Hodge structure*.

Definition 4.7. A mixed \mathbb{Q} -Hodge structure is a triple

$$H = ((H_B, W_\bullet^B), (H_{dR}, F^\bullet, W_\bullet^{dR}), \text{comp}_{B,dR})$$

consisting of

- a finite-dimensional \mathbb{Q} -vector space H_B together with an increasing, exhaustive *weight* filtration W_\bullet^B ,
- a finite-dimensional \mathbb{Q} -vector space H_{dR} , together with an increasing, exhaustive *weight* filtration and a decreasing, exhaustive *Hodge* filtration F^\bullet

- an isomorphism of complex vector spaces

$$\text{comp}_{B,dR} : H_{dR} \otimes_{\mathbb{Q}} \mathbb{C} \xrightarrow{\cong} H_B \otimes_{\mathbb{Q}} \mathbb{C}$$

which is strict with respect to W^\bullet , i.e.

$$\text{comp}_{B,dR}(W_{\bullet}^{dR} \otimes \mathbb{C}) = W_{\bullet}^B \otimes \mathbb{C}.$$

These data are required to satisfy that for each integer m , the m -th graded piece

$$\text{gr}_m^W H = (\text{gr}_m^W H_B, (\text{gr}_m^W H_{dR}, F^\bullet), \text{comp}_{B,dR})$$

is a pure \mathbb{Q} -Hodge structure of weight m .

The morphisms between mixed Hodge structures are described as follows.

Definition 4.8. A morphism $f : H \rightarrow H'$ of mixed \mathbb{Q} -Hodge structures is a pair (f_B, f_{dR}) consisting of morphisms of \mathbb{Q} -vector spaces $f_B : H_B \rightarrow H'_B$, $f_{dR} : H_{dR} \rightarrow H'_{dR}$ such that f_B is filtered for W_{\bullet}^B and f_{dR} is filtered for both W_{\bullet}^{dR} and F^\bullet , and such that the following diagram commutes:

$$\begin{array}{ccc} H_{dR} \otimes_{\mathbb{Q}} \mathbb{C} & \xrightarrow{\text{comp}_{B,dR}} & H_B \otimes_{\mathbb{Q}} \mathbb{C} \\ f_{dR} \otimes \text{id} \downarrow & & \downarrow f_B \otimes \text{id} \\ H'_{dR} \otimes_{\mathbb{Q}} \mathbb{C} & \xrightarrow{\text{comp}'_{B,dR}} & H'_B \otimes_{\mathbb{Q}} \mathbb{C}. \end{array}$$

One obtains in this way a category $\mathbf{MHS}(\mathbb{Q})$ of mixed Hodge structures over \mathbb{Q} . A deep result, due to Deligne, is that this category is abelian (even Tannakian, as we shall see later).

Example 4.9. For us, the most important class of mixed \mathbb{Q} -Hodge structures H will be the ones of *Tate type* (also called *mixed \mathbb{Q} -Hodge–Tate structures*). By definition, these are precisely the ones which satisfy $\text{gr}_{2m+1}^W H \cong 0$ and $\text{gr}_{2m}^W H \cong \mathbb{Q}(-m)^{\oplus m_i}$ for some $m_i \geq 0$, for all m . They form an abelian subcategory $\mathbf{MHTS}(\mathbb{Q})$ of $\mathbf{MHS}(\mathbb{Q})$ whose simple objects are precisely the Tate type Hodge structures $\mathbb{Q}(m)$, for $m \in \mathbb{Z}$.

4.3. Some examples of mixed Hodge–Tate structures.

Example 4.10. Consider $X = \mathbb{G}_m$ which is smooth but not projective. Slightly surprisingly, its H_B^1 still carries a pure (rather than a mixed) Hodge structure. This is a consequence of the Mayer–Vietoris sequence

$$\dots \longrightarrow H^1(\mathbb{A}^1) \oplus H^1(\mathbb{A}^1) \longrightarrow H^1(\mathbb{G}_m) \longrightarrow H^2(\mathbb{P}^1) \longrightarrow H^2(\mathbb{A}^1) \oplus H^2(\mathbb{A}^1) \longrightarrow \dots,$$

which exists in either Betti or de Rham cohomology. Since $H_B^n(\mathbb{A}^1) = 0$ for $n \geq 1$, we see that

$$H^1(\mathbb{G}_m) \cong H^2(\mathbb{P}^1),$$

and the latter is isomorphic to $\mathbb{Q}(-1)$.

More generally, if $X = \mathbb{P}^1 \setminus S$ where S is a finite set of points with $|S| \geq 1$, then

$$H^0(X) \cong \mathbb{Q}(0), \quad H^1(X) \cong \mathbb{Q}(-1)^{|S|-1}, \quad H^n(X) = 0, \quad n \geq 2.$$

Example 4.11. Consider $X = \mathbb{G}_m$ and $Z = \{1, p\}$ as in Example 3.14. From the long exact sequence in relative cohomology, we obtain a short exact sequence

$$0 \longrightarrow H^0(\{p\}) \longrightarrow H^1(X, Z) \longrightarrow H^1(X) \longrightarrow 0.$$

Since $H^0(\{p\}) \cong \mathbb{Q}(0)$ and $H^1(X)\mathbb{Q}(-1)$, we can define a mixed Hodge structure on $H^1(X, Z)$ as follows. Take $H_B = H_B^1(X, Z)$ and $H_{dR} = H_{dR}^1(X, Z)$. The weight filtrations on both H_B and H_{dR} are uniquely determined by demanding that the above short exact sequence is a short exact sequence of mixed Hodge structures. More precisely,

$$W_i^B(H_B) \cong W_i^B(\mathbb{Q}(0)_B), i < 2, \quad W_2^B(H_B) = H_B,$$

and similarly for de Rham cohomology. As for the comparison isomorphism, we already know that with respect to suitable bases it is represented by the matrix

$$\begin{pmatrix} 1 & \log(p) \\ 0 & 2\pi i \end{pmatrix},$$

so that it remains to describe the Hodge filtration. By the above short exact sequence, we have

$$F^n(H_{dR}) = H_{dR}, n \leq 0, \quad F^n(H_{dR}) = 0, n \geq 2,$$

so the only variable is $F^1(H_{dR})$ which is a one-dimensional \mathbb{Q} -subspace of H_{dR} . For this, we have

$$F^1(H_{dR}) = \mathbb{Q} \cdot [dt/t].$$

Note that in the last example the weight filtration on H_{dR} is given by $0 \subset \mathbb{Q}[dt] \subset \mathbb{Q}[dt] \oplus \mathbb{Q}[dt/t]$, i.e. by a filtration on the order of poles. In fact, this is how the weight filtration on the mixed Hodge structure of the (relative) cohomology of an arbitrary quasi-projective variety is described in general.

Remark 4.12. For any two integers $m, n \in \mathbb{Z}$, one has

$$\mathrm{Ext}_{\mathbf{MHS}}^1(\mathbb{Q}(m), \mathbb{Q}(n)) \cong \begin{cases} \mathbb{C}/(2\pi i)^{n-m}\mathbb{Q} & m < n \\ 0 & m \geq n \end{cases}.$$

This is a special case of a result of Carlson's which says that

$$\mathrm{Ext}_{\mathbf{MHS}}^1(A, B) \cong \frac{W_0(\mathrm{Hom}(A, B)_{\mathbb{C}})}{W_0 \cap F^0 \mathrm{Hom}(A, B)_{\mathbb{C}} + W_0 \mathrm{Hom}(A, B)}.$$

5. MULTIPLE ZETA VALUES AND $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

The goal of this section is to interpret multiple zeta values as periods associated with $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. This statement requires some explanation, as we have already seen that the periods of the cohomology groups of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ are just rational multiples of $2\pi i$.

Rather, multiple zeta values will be periods of the unipotent fundamental group of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$, a certain completion of the usual topological fundamental group which contains strictly more information than the cohomology groups of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. Important foundational results, due to Chen and Hain respectively, state that there is an analogue of de Rham's theorem in that case and more generally that the unipotent fundamental group carries a (pro-) mixed Hodge structure.

Convention: We choose the algebraic geometer's convention of composing paths, that is from right to left.

5.1. The path space of a manifold. Let M be a smooth manifold which is connected. A continuous map $\gamma : [0, 1] \rightarrow M$ is called a *piecewise smooth path* if there exists a partition $0 = a_0 < a_1 < \dots < a_{n+1} = 1$ such that $\gamma|_{[a_i, a_{i+1}]}$ extends to a smooth function on a neighborhood of $[a_i, a_{i+1}]$, for every i .

Definition 5.1. The *path space* of M is the set

$$\mathcal{P}(M) = \{\gamma : [0, 1] \rightarrow M \mid \gamma \text{ piecewise smooth}\}$$

of all piecewise smooth paths on M . For any two points $x, y \in M$, we denote the subset of paths starting at x and ending at y by

$${}_y\mathcal{P}(M)_x = \{\gamma \in \mathcal{P}(M) \mid \gamma(0) = x, \gamma(1) = y\}.$$

On ${}_y\mathcal{P}(M)_x$, we have the usual equivalence relation \sim given by homotopy of paths (relative to x, y and required to be piecewise smooth in a suitable sense). We denote the quotient set by

$$\pi_1(M; y, x) := {}_y\mathcal{P}(M)_x / \sim.$$

If $x = y$, then $\pi_1(M, x) := \pi_1(M; x, x)$ is called the *fundamental group* of M . More generally, the disjoint union of sets

$$\coprod_{x, y \in M} \pi_1(M; y, x)$$

is a groupoid, called the *fundamental groupoid* of M . This basically just means that for every $x, y, z \in M$, there are maps of sets

$$\pi_1(M; y, x) \times \pi_1(M; z, y) \rightarrow \pi_1(M; z, x)$$

which correspond to composition of paths and which satisfy some natural conditions, such as associativity and existence of an inverse.

5.2. Iterated integrals. A natural question is what are the functions on the fundamental groupoid of a manifold M .

Definition 5.2. A function on $\mathcal{P}(M)$ is called a *homotopy functional* if for every $x, y \in M$ the function restricted to ${}_y\mathcal{P}(M)_x$ descends to $\pi_1(M; y, x)$, i.e. if the value at every $\gamma \in {}_y\mathcal{P}(M)_x$ depends only on the homotopy class of γ .

A simple class of such functions is given by line integrals. Let $k \in \{\mathbb{R}, \mathbb{C}\}$ and consider the k -algebra

$$E^*(M, k) = \bigoplus_{p=0}^{\dim M} E^p(M, k)$$

of smooth k -valued differential forms on M . Given $\omega \in E^1(M, k)$ and $\gamma \in \mathcal{P}(M)$, the line integral of ω along γ is defined by

$$\int_{\gamma} \omega := \int_0^1 \gamma^* \omega.$$

We obtain in this way a functional $\int \omega : \mathcal{P}(M) \rightarrow k$. The following proposition follows basically from Stokes' theorem.

Proposition 5.3. *The function $\int \omega$ is a homotopy functional if and only if the one-form ω is closed.*

A well-known property of line integrals is that given any two composable paths γ_1, γ_2 , i.e. $\gamma_1(1) = \gamma_2(0)$, the line integral $\int \omega$ is additive,

$$\int_{\gamma_1 \gamma_2} = \int_{\gamma_1} \omega + \int_{\gamma_2} \omega.$$

In particular, if $y = x$, then every line integral naturally factors through the commutator $[\pi_1(M, x), \pi_1(M, x)]$. On the other hand, by Hurewicz, we have

$$\pi_1(M, x)/[\pi_1(M, x), \pi_1(M, x)] \cong H_1(M, \mathbb{Z}),$$

so that line integrals are really naturally functions on $H_1(M, \mathbb{Z})$ rather than on the fundamental group.

The notion of iterated integral gets around this problem

Definition 5.4. Let $\omega_1, \dots, \omega_r \in E^1(M, k)$. The iterated integral of $\omega_1, \dots, \omega_r$ is the function

$$\begin{aligned} \int \omega_1 \dots \omega_r : \mathcal{P}(M) &\rightarrow k \\ \gamma &\mapsto \int_{\gamma} \omega_1 \dots \omega_r, \end{aligned}$$

defined as follows:

$$\int_{\gamma} \omega_1 \dots \omega_r = \int_{1 \geq t_1 \dots \geq t_r \geq 0} f_1(t_1) \dots f_r(t_r) dt_1 \dots dt_r,$$

where $\gamma^* \omega_i = f_i(t) dt$ is the pullback of ω_i to $[0, 1]$.

Remark 5.5. It will be convenient to define the empty iterated integral \int to be the constant function 1.

Here is an explanation, due to Deligne, as to why they are called *iterated* integrals. Let S be the operator which maps a one-form $\eta \in E^1([0, 1])$ to the function $S[\eta](t) = \int_0^t \eta$. Then

$$\int_{\gamma} \omega_1 \dots \omega_r = S[\gamma^* \omega_1 \cdot S[\gamma^* \omega_2 \dots S[\gamma^* \omega_r] \dots]](1).$$

Example 5.6. We already know that multiple zeta values are iterated integrals, more precisely

$$\zeta(k_1, \dots, k_d) = \int_{[0,1]} \underbrace{\omega_0 \dots \omega_0 \omega_1}_{k_1} \dots \underbrace{\omega_0 \dots \omega_0 \omega_1}_{k_d},$$

where $\omega_0 = \frac{dz}{z}$ and $\omega_1 = \frac{dz}{1-z}$ the integral is over the straight line path from 0 to 1.

Strictly speaking, this example does not quite fit our definition as the differential one-forms ω_0, ω_1 are not smooth at the boundary of the path of integration. In a similar vein, not every integral along $[0, 1]$ of the forms ω_0, ω_1 will converge. We will later overcome both problems through the systematic use of *tangential base points*.

The following proposition subsumes some basic properties of iterated integrals.

Proposition 5.7. *Iterated integrals satisfy the following properties.*

(i) If $f : N \rightarrow M$ is a smooth map of smooth manifolds, then

$$\int_{\gamma} f^* \omega_1 \dots f^* \omega_r = \int_{f_* \gamma} \omega_1 \dots \omega_r,$$

where $f_* \gamma = f \circ \gamma$. In particular, iterated integrals are invariant under reparametrisation of paths.

(ii) We have the inversion formula

$$\int_{\gamma} \omega_1 \dots \omega_r = (-1)^r \int_{\gamma^{-1}} \omega_r \dots \omega_1.$$

(iii) They satisfy the path deconcatenation formula

$$\int_{\gamma_1 \gamma_2} \omega_1 \dots \omega_r = \sum_{i=0}^n \int_{\gamma_1} \omega_1 \dots \omega_i \int_{\gamma_2} \omega_{i+1} \dots \omega_r,$$

where $\int_{\gamma_1} \omega_1 \dots \omega_i$ is understood to be an empty iterated integral if $i = 0$, and likewise for $\int_{\gamma_2} \omega_{i+1} \dots \omega_r$ if $i = r$ (cf. Remark 5.5).

(iv) One has the shuffle product formula

$$\int_{\gamma} \omega_1 \dots \omega_r \int_{\gamma} \omega_{r+1} \dots \omega_s = \sum_{\sigma \in Sh(r,s)} \int_{\gamma} \omega_{\sigma^{-1}(1)} \dots \omega_{\sigma^{-1}(r+s)}.$$

Proof. (i) is clear from the definition and $(f \circ \gamma)^* = \gamma^* \circ f^*$. As for (ii), using that $(\gamma^{-1})^* \omega_i = -f_i(1-t)dt$ we get

$$\begin{aligned} \int_{\gamma^{-1}} \omega_r \dots \omega_1 &= (-1)^r \int_{1 \geq t_1 \geq \dots \geq t_r \geq 0} f_r(1-t_1) \dots f_1(1-t_1) dt_1 \dots dt_r \\ &= (-1)^r \int_{1 \geq u_1 \geq \dots \geq u_r \geq 0} f_r(u_r) \dots f_1(u_1) du_1 \dots du_r \\ &= (-1)^r \int_{\gamma} \omega_1 \dots \omega_r. \end{aligned}$$

For (iii), write

$$(\gamma_1 \gamma_2)^* \omega_i = f_i(t)dt, \quad \gamma_1^* \omega_i = g_i(t)dt, \quad \gamma_2^* \omega_i = h_i(t)dt.$$

From the definition of composition of paths, one deduces

$$f_i(t) = \begin{cases} 2h_i(2t) & 0 \leq t \leq \frac{1}{2} \\ 2g_i(2t-1) & \frac{1}{2} \leq t \leq 1. \end{cases}$$

Now decompose the domain of integration $\Delta^r = \bigcup_{i=0}^r C_i$ where

$$C_i = \{(t_1, \dots, t_r) \in \mathbb{R}^r \mid 1 \geq t_1 \geq \dots \geq t_i \geq \frac{1}{2} \geq t_{i+1} \geq \dots \geq t_r \geq 0\}.$$

The key point is that $C_i \cong \Delta^i \times \Delta^{r-i}$, and now (iii) follows from linearity of the integral together with

$$\begin{aligned} \int_{C_i} f_1(t_1) \dots f_r(t_r) dt_1 \dots dt_r &= \int_{\substack{1 \geq t_1 \geq \dots \geq t_i \geq \frac{1}{2} \\ \frac{1}{2} \geq t_{i+1} \geq \dots \geq t_r \geq 0}} f_1(t_1) \dots f_r(t_r) dt_1 \dots dt_r \\ &= \frac{2^r}{2^r} \int_{\substack{1 \geq u_1 \geq \dots \geq u_i \geq 0 \\ 1 \geq u_{i+1} \geq \dots \geq u_r \geq 0}} g_1(u_1) \dots g_i(u_i) h_{i+1}(u_{i+1}) \dots h_r(u_r) du_1 \dots du_r \\ &= \int_{\gamma_1} \omega_1 \dots \omega_i \int_{\gamma_2} \omega_{i+1} \dots \omega_r. \end{aligned}$$

which proves (iii), noting that the intersections of the C_i have codimension at least 2, hence measure zero. Finally, (iv) follows similarly to Proposition 2.10. \square

5.3. Which iterated integrals are homotopy functionals? We have seen in Proposition 5.3 that the line integral $\int \omega$ is a homotopy functional if and only if ω is closed. In general, however even if $\omega_1, \dots, \omega_r$ are all closed one-forms, the iterated integral $\int \omega_1 \dots \omega_r$ is not necessarily a homotopy functional as the following example shows.

Example 5.8. Take $M = \mathbb{R}^2$ with coordinate functions x, y . For real numbers $a, b > 0$, consider the path $\gamma_{a,b} : [0, 1] \rightarrow \mathbb{R}^2$ given by $\gamma_{a,b}(t) = (t^a, t^b)$. Let $\omega_1 = dx$ and $\omega_2 = dy$. Clearly ω_1 and ω_2 are both closed. Since $\gamma_{a,b}^* \omega_1 = at^{a-1} dt$, $\gamma_{a,b}^* \omega_2 = bt^{b-1} dt$, a simple calculation shows that

$$\int_{\gamma_{a,b}} = \int_0^1 \left(at_1^{a-1} \int_0^{t_1} bt_2^{b-1} dt_2 \right) dt_1 = \frac{a}{a+b}.$$

In other words, the iterated integral $\int_{\gamma_{a,b}} \omega_1 \omega_2$ depends on the choice of a and b . However, all $\gamma_{a,b}$, for $a, b > 0$, are homotopic.

The solution to the problem of describing all iterated integrals on M which are homotopy functionals is given in terms of the reduced bar construction on the de Rham complex of M .

5.4. The pro-unipotent completion. Let k be a field of characteristic zero. Recall that an affine algebraic group G is called *unipotent* if every non-zero representation V of G has a non-zero fixed vector. The basic example of a unipotent algebraic group is the subgroup $\text{Up}_n \subset \text{GL}_n$ of upper triangular matrices with 1's on the diagonal.

Definition 5.9. Let Γ be an abstract group. The *pro-unipotent completion* Γ^{un} of Γ over k is the universal pro-unipotent affine group scheme G over k endowed with a morphism of abstract groups $\Gamma \rightarrow G(k)$.

More precisely, this means that

- Γ^{un} is a pro-unipotent affine group scheme (i.e. a projective limit of unipotent affine algebraic groups) over k together with a morphism of groups $\rho : \Gamma \rightarrow \Gamma^{\text{un}}(k)$,
- for each morphism $g : \Gamma \rightarrow G(k)$ where G is a pro-unipotent affine algebraic group scheme G over k , there exists a unique morphism $\tilde{g} : \Gamma^{\text{un}} \rightarrow G$ such that $g = \tilde{g}_k \circ \rho$.

If it exists, then Γ^{un} is unique up to unique isomorphism. In some sources Γ^{un} is also called the *Mal'cev completion* of Γ .

Under a certain finiteness assumption on Γ (which is satisfied e.g. if Γ is the fundamental group of $X(\mathbb{C})$ where X/\mathbb{C} is an algebraic variety), one has the following explicit description of Γ^{un} due to Quillen. Let $k[\Gamma] := \{\sum_{g \in \Gamma} a_g g \mid a_g \in k, a_g = 0 \text{ for almost all } g\}$ be the group k -algebra of Γ . Sending each group element $g \mapsto 1$ induces a morphism of \mathbb{Q} -algebras, the *augmentation* of $k[\Gamma]$,

$$\begin{aligned} \varepsilon : k[\Gamma] &\rightarrow k \\ \sum_{g \in \Gamma} a_g g &\mapsto \sum_{g \in \Gamma} a_g, \end{aligned}$$

whose kernel $J := \ker(\varepsilon)$ is called the *augmentation ideal*. The powers of J form a basis of neighborhoods of the zero element $0 \in k[\Gamma]$, and we let

$$k[\Gamma]^\wedge := \varprojlim_N k[\Gamma]/J^{N+1}$$

be the completion of $k[\Gamma]$ with respect to the J -adic topology. Since multiplication in $k[\Gamma]$ is clearly continuous, $k[\Gamma]^\wedge$ is a complete \mathbb{Q} -algebra. It is even a complete Hopf algebra whose coproduct is the unique continuous homomorphism of \mathbb{Q} -algebras

$$\nabla^\vee : k[\Gamma]^\wedge \rightarrow k[\Gamma]^\wedge \hat{\otimes} k[\Gamma]^\wedge$$

which satisfies $\nabla^\vee(g) = g \otimes g$ for all $g \in \Gamma$, and likewise the antipode S^\vee is defined by $g \mapsto g^{-1}$.

As anticipated by the notation above, rather than $k[\Gamma]^\wedge$, the main role will be played by

$$A = (k[\Gamma]^\wedge)^\vee = \varinjlim_N (k[\Gamma]/J^{N+1})^\vee$$

which is the dual Hopf algebra of $k[\Gamma]^\wedge$. More precisely, it is a complete commutative Hopf algebra.

Theorem 5.10 (Quillen). *Let Γ be an abstract group such that the vector space $\Gamma^{\text{ab}} \otimes_{\mathbb{Z}} k$ is finite-dimensional. Then $\Gamma^{\text{un}} \cong \text{Spec}((k[\Gamma]^\wedge)^\vee)$.*

We do not give the proof here but remark that it uses the following alternative characterization of pro-unipotent affine algebraic groups.

5.4.1. An alternative characterization of pro-unipotency. Let $G = \text{Spec}(A)$ be an affine group scheme over k . The group structure on G corresponds to a coalgebra structure on A , therefore its dual A^\vee is a (not necessarily commutative) k -algebra. Also, the unit of G corresponds to an augmentation $\varepsilon : A^\vee \rightarrow k$ and we denote by $J^n \subset A^\vee$ the n -th power of the augmentation ideal. The *conilpotency filtration* is the filtration on A defined by

$$0 \subset C_0 = \text{Ann}_A J \subset C_1 = \text{Ann}_A J^2 \subset \cdots \subset C_i = \text{Ann}_A J^{i+1} \subset \cdots,$$

where $\text{Ann}_A I \subset A$ is the annihilator of the ideal $I \subset A^\vee$.

Proposition 5.11. *The affine group scheme $G = \text{Spec}(A)$ is pro-unipotent if and only if the conilpotency filtration on A is exhaustive, i.e.*

$$A = \bigcup_{i=0}^{\infty} C_i.$$

5.4.2. *The Lie algebra of Γ^{un} .* Under the assumptions of the previous theorem, the pro-unipotent completion Γ^{un} of Γ admits the following alternative description. We first need a definition.

Definition 5.12. An element $g \in k[\Gamma]^\wedge$ is *group-like* if $\nabla^\vee g = g \otimes g$. We denote by $\mathcal{G}(k[\Gamma]^\vee) \subset k[\Gamma]^\wedge$ the subset of group-like elements.

Since ∇^\vee is morphism of \mathbb{Q} -algebras, it follows that $\mathcal{G}(k[\Gamma]^\vee)$ is group. Moreover, the image of every $g \in \Gamma$ is group-like.

Proposition 5.13. *We have $\mathcal{G}(k[\Gamma]^\vee) \cong \Gamma^{\text{un}}(k)$ with structural map given by the natural map $\Gamma \rightarrow \mathcal{G}(k[\Gamma]^\vee) \subset k[\Gamma]^\vee$.*

Using the preceding proposition, it is rather simple to describe the Lie algebra of Γ^{un} .

Definition 5.14. An element $x \in k[\Gamma]^\wedge$ is called *Lie-like* if it satisfies $\nabla^\vee x = x \otimes 1 + 1 \otimes x$. We denote by $\mathcal{L}(k[\Gamma]^\wedge) \subset k[\Gamma]^\wedge$ the subset of Lie-like elements.

Recall that $J \subset k[\Gamma]^\vee$ denotes the augmentation ideal. Since k is of characteristic zero, the usual power series for \exp and \log are well-defined and induce bijections

$$\exp : J \rightarrow 1 + J, \quad \log 1 + J \rightarrow J$$

which are mutually inverse to each other.

Proposition 5.15. *The morphism \exp induces a bijection*

$$\mathcal{G}(k[\Gamma]^\wedge) \cong \mathcal{L}(k[\Gamma]^\wedge)$$

whose inverse is given by the morphism \log .

5.4.3. *An example.* Let $\Gamma = \pi_1(S^1, 1) \simeq \mathbb{Z}$ be the fundamental group of the unit circle $S^1 \subset \mathbb{C}$ and choose a generator γ_0 of Γ . Then $k[\Gamma] \cong k[\gamma_0^{\pm 1}]$, the ring of formal Laurent polynomials in γ_0 . One can show that the augmentation ideal of the group k -algebra $k[\Gamma]$ is generated by $\gamma_0 - 1$, therefore

$$k[\Gamma]^\wedge \cong k[[x]], \quad x := \log(\gamma_0) = \sum_{n \geq 1} (-1)^{n-1} \frac{(\gamma_0 - 1)^n}{n}$$

the k -algebra of formal power series in x which has the structure of complete Hopf algebra by setting $\nabla^\vee x = x \otimes 1 + 1 \otimes x$, since γ_0 is group-like. In order to compute Γ^{un} , it is enough by Proposition 5.13 to determine the group-like elements of $k[[x]]$. Indeed, if $\sum_{n \geq 0} a_n x^n \in \mathcal{G}(k[\Gamma]^\wedge)$, then $a_0 = 1$ and

$$(5.1) \quad \nabla^\vee \left(\sum_{n \geq 0} a_n x^n \right) = \left(\sum_{n \geq 0} a_n x^n \right) \otimes \left(\sum_{n \geq 0} a_n x^n \right).$$

Since $\nabla^\vee x = x \otimes 1 + 1 \otimes x$ and since ∇^\vee is an algebra homomorphism, we have

$$\nabla^\vee x^n = \sum_{k=0}^n \binom{n}{k} x^k \otimes x^{n-k}.$$

Comparing coefficients on both sides of (5.1) now gives the recursive formula

$$a_k a_m = \binom{k+m}{k} a_{k+m}, \quad \text{for all } k, m \geq 0.$$

This implies $a_n = a_1^n/n!$, therefore the projection

$$\begin{aligned} \mathcal{G}(k[\Gamma]^\vee) &\rightarrow k \cong \mathbb{G}_a(k) \\ \sum_{n \geq 0} a_n x^n &\mapsto a_1 \end{aligned}$$

is bijective and induces an isomorphism of group schemes $\Gamma^{\text{un}} \cong \mathbb{G}_a$. We summarize the discussion in the following proposition.

Proposition 5.16. *For $\Gamma = \pi_1(S^1, 1) \simeq$ with generator γ_0 and k a field of characteristic zero, we have a natural isomorphism*

$$\Gamma^{\text{un}} \cong \mathbb{G}_a,$$

where $\mathbb{G}_a := \text{Spec}(k[t])$ is the additive group over k .

As a second example, let $\Gamma = \langle \gamma_0, \gamma_1 \rangle$ be a free group on two generators. As before, we can define elements $\log(\gamma_0), \log(\gamma_1) \in k[\Gamma]^\wedge$. On the other hand, denote by $k\langle e_0, e_1 \rangle$ the k -algebra of formal power series in non-commutative variables e_0, e_1 . It is a complete Hopf algebra with the concatenation product. The coproduct is determined uniquely by $\Delta(e_i) = e_i \otimes 1 + 1 \otimes e_i$ and the antipode is the unique anti-homomorphism such that $S(x_i) = -x_i$.

Now define a morphism of k -algebras

$$k\langle e_0, e_1 \rangle \rightarrow k[\Gamma]^\wedge, \quad e_i \mapsto \log(\gamma_i), \quad i = 0, 1.$$

One verifies that this morphism is bijective and in fact an isomorphism of complete Hopf algebras. Under this isomorphism, the group-like elements $\mathcal{G}(k[\Gamma]^\wedge)$ of $k[\Gamma]^\wedge$ are precisely the formal series f which satisfy $\Delta f = f \otimes f$ whose constant term is 1. Letting $\mathfrak{H} := \mathcal{O}(\Gamma^{\text{un}})$, we have

$$\Gamma^{\text{un}}(k) = \text{Hom}_{\mathbb{Q}\text{-alg}}(\mathfrak{H}, k),$$

and therefore, by duality, that $\mathfrak{H} \cong k\langle e_0^\vee, e_1^\vee \rangle$ is the free shuffle algebra. Its coproduct is given by deconcatenation and the antipode is the same as for $k\langle e_0, e_1 \rangle$.

5.5. The bar complex and Chen's π_1 -de Rham theorem. The goal of this section is to give a cohomological description of homotopy invariant iterated integrals on a smooth manifold M .

To begin with, recall that a *differential graded algebra* (dga for short) over k is a graded k -vector space $A = \bigoplus_{n \in \mathbb{Z}} A^n$ together with

- a graded multiplication $A^n \otimes A^m \rightarrow A^{m+n}$ which is associative and unital,
- a differential $d : A \rightarrow A$ such that $d(A^n) \subset A^{n+1}$ which satisfies Leibniz' rule: $d(ab) = da \cdot b + (-1)^n a \cdot db$ for $a \in A^n$.

We shall mostly consider *commutative* dgas, i.e. which satisfy $ab = (-1)^{mn}ba$ for $a \in A^n, b \in A^m$. Moreover, A is *connected* if $A^n = 0$ for $n < 0$ and $A^0 = k$.

Our main example will be $E^*(M, k)$, the algebra of smooth k -valued differential forms on a smooth manifold M with product \wedge and d the usual exterior derivative. It is commutative but clearly not connected.⁴

⁴The latter fact will pose some difficulties later on which can be worked around by choosing a model $A^* \subset E^*(M, k)$, i.e. a sub-dga which is connected and quasi-isomorphic to $E^*(M, k)$.

Definition 5.17. Let (A^*, \wedge, d) be a commutative connected dga over k , and let $A^+ = \bigoplus_{n \geq 0} A^n$. The *reduced bar complex* associated with A and denoted $B^*(A^*)$ is the total tensor algebra of A^+ :

$$B^*(A^*) = \bigoplus_{n \geq 0} (A^+)^{\otimes n} = k \oplus A^+ \oplus (A^+ \otimes A^+) \oplus \dots$$

We will denote the tensor $x_1 \otimes \dots \otimes x_n$ for $n \geq 1$ using bar notation $[x_1 | \dots | x_n]$ and $1 \in k$ by the empty symbol $[]$.

The reduced bar complex $B^*(A^*)$ of a connected dga has a whole panoply of extra structure:

- A grading by degree

$$\deg[x_1 | \dots | x_n] = \sum_{i=1}^n \deg(x_i) - n.$$

- An increasing length filtration $L_\bullet(B^*(A^*))$ where

$$L_m(B^*(A^*)) = \text{Span}_k\{[x_1 | \dots | x_n] \mid n \leq m\}.$$

- A differential

$$\begin{aligned} d[x_1 | \dots | x_n] &= - \sum_{i=1}^n (-1)^{\sum_{j=1}^{i-1} \deg[x_j]} [x_1 | \dots | dx_i | \dots | x_n] \\ &\quad + \sum_{i=1}^{n-1} (-1)^{\sum_{j=1}^i \deg[x_j]} [x_1 | \dots | x_i \wedge x_{i+1} | \dots | x_n]. \end{aligned}$$

Clearly d increases the degree by one and it satisfies $d \circ d = 0$. We will occasionally write $d = d_I - d_C$ where

$$\begin{aligned} d_I &= - \sum_{i=1}^n (-1)^{\sum_{j=1}^{i-1} \deg[x_j]} [x_1 | \dots | dx_i | \dots | x_n] \\ d_C &= - \sum_{i=1}^{n-1} (-1)^{\sum_{j=1}^i \deg[x_j]} [x_1 | \dots | x_i \wedge x_{i+1} | \dots | x_n]. \end{aligned}$$

- The shuffle product:

$$([x_1 | \dots | x_r] \sqcup [x_{r+1} | \dots | x_{r+s}]) = \sum_{\sigma \in Sh(r,s)} \eta(\sigma) [x_{\sigma^{-1}} | \dots | x_{\sigma^{-1}(r+s)}],$$

where $\eta(\sigma) \in \{\pm 1\}$ is determined by the equation

$$a_1 \wedge \dots \wedge a_{r+s} = \eta(\sigma) a_{\sigma^{-1}} \wedge \dots \wedge a_{\sigma^{-1}(r+s)},$$

where $\deg(a_i) = \deg(x_i) - 1 = \deg[x_i]$.

- A coproduct by deconcatenation

$$\Delta[x_1 | \dots | x_n] = \sum_{i=0}^n [x_1 | \dots | x_i] \otimes [x_{i+1} | \dots | x_n].$$

- An antipode

$$S([x_1 | \dots | x_n]) = (-1)^n \eta(\tau_n) [x_n | \dots | x_1],$$

where $\tau_n(i) = n - i$.

The gist of the extra structure on the reduced bar complex is that it allows us to define a Hopf algebra out of it.

Proposition 5.18. *Let (A^*, \wedge, d) be a connected commutative dga. Then the above operations endow $H^0(B^*(A^*))$, the zeroth cohomology group of the reduced bar complex, with a commutative, filtered Hopf algebra structure.*

Note that since A^* is connected, we have

$$H^0(B^*(A^*)) = \ker(d : B^0(A^*) \rightarrow B^1(A^*)).$$

By definition of the grading, elements of $B^0(A^*)$ are k -linear combinations of $[]$ and $[x_1 | \dots | x_n]$ with $\deg(x_i) = 1$ for all $i = 1, \dots, n$. In particular, when restricted to $B^0(A^*)$, the differential is given by

$$\begin{aligned} d[x_1 | \dots | x_n] &= - \sum_{i=1}^n [x_1 | \dots | dx_i | \dots | x_n] \\ &\quad + \sum_{i=1}^{n-1} [x_1 | \dots | x_i \wedge x_{i+1} | \dots | x_n]. \end{aligned}$$

5.6. The reduced bar complex and iterated integrals. Let M be a connected smooth manifold which is “nice” (for example, $X(\mathbb{C})$ for X an algebraic variety over \mathbb{C})⁵, and let $E^*(M, \mathbb{C})$ be the dga of smooth \mathbb{C} -valued differential forms on M . To simplify the discussion, we will assume existence of a model A^* for $E^*(M, \mathbb{C})$, i.e. a connected dga together with an injection $\varphi : A^* \hookrightarrow E^*(M, \mathbb{C})$ which induces a quasi-isomorphism $H^*(A^*) \cong H^*(E^*(M, \mathbb{C}))$. We will fix such a model and, in the following, we will tacitly identify A^* with a sub-dga of $E^*(M, \mathbb{C})$ using φ .

Given two points $x, y \in M$, let ${}_y\mathcal{P}(M)_x$ be the set of piecewise smooth paths on M from x to y . We then have a pairing

$$(5.2) \quad \langle, \rangle : B^0(A^*) \otimes \mathbb{Q}[{}_y\mathcal{P}(M)_x] \rightarrow \mathbb{C}$$

$$[\eta_1 | \dots | \eta_r] \otimes \gamma \mapsto \int_{\gamma} \eta_1 \dots \eta_r,$$

where $\mathbb{Q}[{}_y\mathcal{P}(M)_x]$ is the free \mathbb{Q} -vector space with basis ${}_y\mathcal{P}(M)_x$. Note that since A^* is connected, the η_i are all in $E^1(M, \mathbb{C})$ and therefore the above pairing is well-defined.

The properties of iterated integrals we encountered in Theorem 5.7 can now be phrased on the level of the pairing \langle, \rangle using the structure on $B^0(A^*)$ as follows.

Theorem 5.19. *Let $\gamma, \gamma_1, \gamma_2 \in \mathcal{P}(M)$ be piecewise smooth paths such that γ_1 and γ_2 are composable, and let $\eta, \eta_1, \eta_2 \in B^0(A^*)$ be elements of degree zero of $B^0(A^*)$. Then we have:*

$$\begin{aligned} \langle S(\eta), \gamma \rangle &= \langle \eta, S(\gamma) \rangle, \\ \langle \eta, \gamma_1 \gamma_2 \rangle &= \langle \Delta \eta, \gamma_1 \otimes \gamma_2 \rangle, \\ \langle \eta_1 \otimes \eta_2, \nabla^\vee \gamma \rangle &= \langle \eta_1 \sqcup \eta_2, \gamma \rangle. \end{aligned}$$

An important consequence of the preceding theorem is the following nilpotence property of iterated integrals which says that the length filtration on iterated integrals is dual to the filtration on the group algebra of paths given by the augmentation ideal.

⁵More generally, one should require that M has the homotopy type of a finite CW complex.

Proposition 5.20. *Let $x, y \in M$, J the augmentation ideal of $\mathbb{Q}[\mathcal{P}(M)_x]$, $N \geq 0$ an integer. Also, let $\gamma \in J^{N+1}\mathbb{Q}[\mathcal{P}(M)_y]$ or $\gamma \in \mathbb{Q}[\mathcal{P}(M)_x]J^{N+1}$. If $\eta \in L_N B^0(A^*)$, then*

$$\langle \eta, \gamma \rangle = 0.$$

Proof. We only do the case $\gamma \in {}_x\mathcal{P}(M)_y$, the other one being analogous.

The proof is by induction on N . The claim is clear for $N = 0$, for then $\gamma = \sum_{i=1}^r q_i \gamma_i$ with $q_i \in \mathbb{Q}$, $\gamma_i \in {}_x\mathcal{P}(M)_y$ with $\sum_{i=1}^r q_i = 0$ and $\eta = \alpha \square$ for some $\alpha \in \mathbb{C}$, and $\langle \square, \gamma_i \rangle = 1$.

Now fix $N > 0$ and assume the statement for all $N' < N$. Write $\gamma = \gamma_1 \gamma_2$ with $\gamma_1 \in J$ and $\gamma_2 \in J^N \mathbb{Q}[\mathcal{P}(M)_y]$ and $\eta = [\omega_1 | \dots | \omega_N]$. Using deconcatenation we get

$$\begin{aligned} \langle \eta, \gamma \rangle &= \langle \Delta \eta, \gamma_1 \otimes \gamma_2 \rangle \\ &= \sum_{i=0}^N \langle [\omega_1 | \dots | \omega_i], \gamma_1 \rangle \langle [\omega_{i+1} | \dots | \omega_N], \gamma_2 \rangle \\ &= \langle \square, \gamma_1 \rangle \langle [\omega_1 | \dots | \omega_N], \gamma_2 \rangle + \sum_{i=1}^N \langle [\omega_1 | \dots | \omega_i], \gamma_1 \rangle \langle [\omega_{i+1} | \dots | \omega_N], \gamma_2 \rangle. \end{aligned}$$

The term $\langle \square, \gamma_1 \rangle$ vanishes since $\gamma_1 \in J$, and all terms in the last sum vanish by induction hypothesis, and this proves the result. \square

So far, we have seen that elements of $B^0(A^*)$ give rise to functions on $\mathbb{Q}[\mathcal{P}(M)_x]$ respecting the respective algebraic structures.

Theorem 5.21. *Let $\eta \in B^0(A^*)$. If $d\eta = 0$, then for all $x, y \in M$, the function $\langle \eta, - \rangle : \mathbb{Q}[\mathcal{P}(M)_x] \rightarrow \mathbb{C}$ is a homotopy functional.*

Sketch. Consider two paths γ_1, γ_2 which are homotopic, and let $F : [0, 1]^2 \rightarrow M$ be a homotopy. Assume for simplicity that F is smooth. For any $\nu = [\nu_1 | \dots | \nu_n] \in B^1(A^*)$, note that every ν_j is a one-form with exactly one exception ν_i which is a two-form. Given such a ν , define its integral along F to be

$$\int_F \nu = (-1)^i \int_{\Delta^n \times [0, 1]} F_1^* \nu_1 \dots F_n^* \nu_n,$$

where $F_i : [0, 1] \times [0, 1]^n \rightarrow M$, $((t_1, \dots, t_n), s) \mapsto F(t_i, s)$ and the second integral is oriented by $ds \wedge dt_1 \wedge \dots \wedge dt_n$.

The heart of the proof is a careful application of Stokes' theorem which shows that

$$\int_F d_I \omega = \int_{\gamma_2} \omega - \int_{\gamma_1} \omega + \int_F d_C \omega$$

for any $\omega = [\omega_1 | \dots | \omega_n] \in B^0(A^*)$. The claim then follows from the definition $d = d_I - d_C$. \square

Using the previous result, we can finally put all the pieces together and state Chen's π_1 -de Rham theorem. As before, let M be a connected, smooth manifold which is "nice" and assume existence of a model A^* for the C^∞ -de Rham complex of M . By what was said so far, the pairing \langle, \rangle given in (5.2) induces a well-defined homomorphism

$$(5.3) \quad H^0(L_N B^*(A^*)) \longrightarrow ((\mathbb{Q}[\pi_1(M; y, x)] / \mathbb{Q}[\pi_1(M; y, x)] J^{N+1}) \otimes \mathbb{C})^\vee,$$

which in the case $x = y$ comes from a homomorphism of filtered Hopf algebras $H^0(B^*(A^*)) \rightarrow \mathcal{O}(\pi_1(M; x)^{\text{un}}) \otimes \mathbb{C}$.

Theorem 5.22. *The morphism (5.3) is an isomorphism.*

5.6.1. *The case $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.* The most important case for us will be $M = \mathbb{P}^1(\mathbb{C}) \setminus \{0, 1, \infty\}$. Its fundamental group is free on two generators γ_0, γ_1 , and we have seen that

$$\mathcal{O}(\pi_1(M; x)^{\text{un}}) \cong \mathbb{Q}\langle e_0, e_1 \rangle$$

where $\pi_1(M; x)^{\text{un}}$ is taken over \mathbb{Q} . We consider the graded \mathbb{Q} -vector space A^* given by

$$A^0 = \mathbb{Q}, \quad A^1 = \mathbb{Q}\omega_0 \oplus \mathbb{Q}\omega_1, \quad A^{\geq 2} = 0,$$

where as before $\omega_0 = dt/t$, $\omega_1 = dt/(1-t)$. It is connected by definition and $A_{\mathbb{C}}^* := A^* \otimes \mathbb{C}$ is a sub-dga of $E^*(M, \mathbb{C})$ in a natural way which is clearly quasi-isomorphic to $E^*(M, \mathbb{C})$.

Let $H^0(B^*(A^*))$ be the zeroth cohomology of the reduced bar complex of A^* . Since $d\omega_0 = d\omega_1 = \omega_0 \wedge \omega_1 = 0$, it follows that

$$H^0(B^*(A^*)) = B^0(A^*),$$

and there is an isomorphism of Hopf algebras

$$\begin{aligned} H^0(B^*(A^*)) &\rightarrow \mathbb{Q}\langle e_0, e_1 \rangle \\ \omega_i &\mapsto e_i, \quad i = 0, 1. \end{aligned}$$

Remark 5.23. Keeping notation as before, let ${}_y A_x^{dR, N} := H^0(L_N B^*(A^*))$, ${}_y A_x^{B, N} := (\mathbb{Q}[\pi_1(M; y, x)]/J^{N+1}\mathbb{Q}[\pi_1(M; y, x)])^\vee$ and $\text{comp}_{dR, B}^N$ the isomorphism (5.3). Hain has shown how to upgrade the triple

$$({}_y A_x^{B, N}, {}_y A_x^{dR, N}, \text{comp}_{dR, B}^N)$$

to a mixed Hodge structure. We only do this in the special case $M = \mathbb{P}^1(\mathbb{C}) \setminus \{0, 1, \infty\}$. On the Betti side, the weight filtration is given by the augmentation filtration:

$$W_{2k}({}_y A_x^{B, N}) = W_{2k+1}({}_y A_x^{B, N}) = (J^{k+1}\mathbb{Q}[\pi_1(M; y, x)]/J^{N+1}\mathbb{Q}[\pi_1(M; y, x)])^\perp,$$

while on the de Rham side it is simply given by the length filtration:

$$W_{2k}({}_y A_x^{dR, N}) = W_{2k+1}({}_y A_x^{dR, N}) = (L_k H^0(B^*(A^*))).$$

Finally, the Hodge filtration is given by defining $F^p({}_y A_x^{dR, N})$ as the subspace generated by words of length ℓ , with $p \leq \ell \leq N$.

6. REGULARIZATION AND TANGENTIAL BASE POINTS

The upshot of the preceding section is that iterated integrals

$$\int_{\gamma} \omega_{i_1} \dots \omega_{i_n}, \quad i_j \in \{0, 1\}$$

over differential forms $\omega_0 = \frac{dt}{t}$, $\omega_1 = \frac{dt}{1-t}$ along a path $\gamma : [0, 1] \rightarrow \mathbb{P}^1(\mathbb{C}) \setminus \{0, 1, \infty\}$ are periods of $\mathcal{O}(\pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}); \gamma(1), \gamma(0))$. Unfortunately, multiple zeta values

do not quite fit into this picture, because in the integral representation

$$\zeta(k_1, \dots, k_d) = \int_{1 \geq t_1 \geq \dots \geq t_k \geq 0} \underbrace{\omega_0 \omega_1 \dots \omega_1}_{k_1} \dots \underbrace{\omega_0 \omega_1 \dots \omega_1}_{k_d}, \quad k := k_1 + \dots + k_d$$

the differential forms ω_0, ω_1 have singularities along the boundary of the integration domain. Another way of putting this is that the straight line path $[0, 1]$ from 0 to 1 is not a path on $\mathbb{P}^1(\mathbb{C}) \setminus \{0, 1, \infty\}$. In order to remedy this, one can use Deligne's formalism of tangential base points.

6.1. Tangent vectors as base points. Throughout this section, we let $M = \mathbb{P}^1(\mathbb{C}) \setminus \{0, 1, \infty\}$. More generally, we could work with $M = X(\mathbb{C})$ where X/\mathbb{C} is a smooth curve.

Definition 6.1. Let $x \in \{0, 1\} \subset \mathbb{P}^1(\mathbb{C})$. A *tangential base point* \vec{v}_x is a non-zero tangent vector at x .

There is a notion of paths between tangential base points as follows.

Definition 6.2. Let \vec{v}_x, \vec{w}_y be tangential base points. A *path from \vec{v}_x to \vec{w}_y* is a piecewise smooth map

$$\gamma : [0, 1] \rightarrow M \cup \{0, 1\}$$

satisfying the following conditions:

$$(1) \quad \begin{aligned} \gamma(0) &= x, & \frac{d\gamma}{dt}(0) &= v \\ \gamma(1) &= y, & \frac{d\gamma}{dt}(1) &= -w \end{aligned} \quad (6.1)$$

$$(2) \quad \gamma(t) \in M \text{ for all } t \in (0, 1).$$

Additional care is needed when one attempts to define composition of paths. One *cannot* use the usual formula

$$\gamma_1 \gamma_2(t) = \begin{cases} \gamma_2(2t) & t \in [0, 1/2] \\ \gamma_1(2t - 1) & t \in [1/2, 1], \end{cases}$$

because the derivative of the parametrizations $t \mapsto 2t, t \mapsto 2t - 1$ is 2 and therefore destroys the condition on the derivatives (6.1). Instead, one requires continuous bijections $\phi_1, \phi_2 : [0, 1] \rightarrow [0, 1]$ such that

$$\begin{aligned} \phi_1(0) &= 0, & \phi_1(1/2) &= 1, & \phi_1'(0) &= 1, \\ \phi_2(1/2) &= 0, & \phi_2(1) &= 1, & \phi_2'(1) &= 1, \\ \phi_1'(1/2) &= \phi_2'(1/2), \end{aligned}$$

and then defines

$$\gamma_1 \gamma_2(t) = \begin{cases} \gamma_2(\phi_1(t)), & t \in [0, 1/2] \\ \gamma_1(\phi_2(t)), & t \in [1/2, 1]. \end{cases}$$

For example, $\phi_1(t) = t + 2t^2$ and $\phi_2(t) = 5t - 2 - 2t^2$ would do the job.

There is also a notion of homotopy for paths between tangential base points which are required to preserve the tangent vectors, and the set of homotopy classes of paths between \vec{v}_x and \vec{v}_y is denoted by

$$\pi_1(M; \vec{w}_y, \vec{v}_x).$$

In a similar way as before, one obtains the fundamental groupoid of M with tangential base points. The only case of interest for us will be the tangential base points $\vec{1}_0, -\vec{1}_1$.

Definition 6.3. We denote by $\text{dch} \in \pi_1(M; -\vec{1}_1, \vec{1}_0)$ the image of the straight line path from 0 to 1.⁶

6.2. Asymptotic expansions. We would like to extend the notion of iterated integral to tangential base points. The main difficulty we need to overcome is that such integrals, when computed naively, may diverge. Consider for example the integral

$$(6.2) \quad \int_{\eta}^1 \frac{dt}{t} = -\log(\eta), \quad 0 < \eta < 1,$$

which diverges as $\eta \rightarrow 0$. We view this as an expansion of the function $\eta \mapsto \int_{\eta} \frac{dt}{t}$ as a polynomial in $\log(\eta)$. The following definition formalizes this.

Definition 6.4. Let $0 < \tau \leq 1$ be a real number and $f : (0, \tau) \rightarrow \mathbb{C}$ a continuous function. We say that f admits a *logarithm asymptotic development* (of degree $\leq r$) if it can be written as

$$f(t) = f_0(t) + \sum_{k=0}^r a_k \log(t)^k,$$

with $|f_0(t)| = O(t^{1-\delta})$ for some $\delta < 1$ and $a_k \in \mathbb{C}$.

One can show that such a development is necessarily unique provided it exists.

Now let $\gamma \in {}_y\mathcal{P}(M)_x$ where x, y are either regular base points $x, y \in M$ or $x, y \in \{\vec{1}_0, -\vec{1}_1\}$. For $0 < \eta < 1/2$, we write

$$\gamma_{\eta}(t) = \gamma(t(1-\eta) + (1-t)\eta),$$

which is a path from $\gamma(\eta)$ to $\eta(1-\eta)$.

Proposition 6.5. Let $(i_1, \dots, i_r) \in \{0, 1\}^r$ be a binary sequence. Then the function

$$I(\eta; i_1, \dots, i_r; 1/2) : (0, 1/2) \rightarrow \mathbb{C}$$

$$\eta \mapsto \int_{\gamma_{\eta}} \omega_{i_1} \dots \omega_{i_r}$$

admits a (necessarily unique) logarithmic asymptotic development of degree $\leq r$.

The key point for the proof is that the forms ω_0, ω_1 have at most simple poles at $t = 0$, and that the integral of a function with a logarithmic asymptotic development has again a logarithmic asymptotic development.

⁶dch=“droit chemin” which translates to “straight path”.

6.3. Regularized iterated integrals. Using the previous proposition, we can now define regularized iterated integrals on M .

Definition 6.6. Let (i_1, \dots, i_r) be a binary sequence and $\gamma \in {}_y\mathcal{P}(M)_x$ be a path. We define

$$\int_{\gamma}^{\text{reg}} \omega_{i_1} \dots \omega_{i_r} = a_0,$$

where a_0 is the constant term in the logarithmic asymptotic expansion:

$$\int_{\gamma_{\eta}} \omega_{i_1} \dots \omega_{i_r} = f_0(\eta) + \sum_{k=0}^r a_k \log(t)^k,$$

whose existence and uniqueness are provided by Proposition 6.5.

Remark 6.7. There is a conceptual interpretation of this definition as a composition of paths formula on the real-oriented blow-up of $\mathbb{P}^1(\mathbb{C})$ at the points 0 and 1, due to Deligne.

One can show that the algebraic properties (ii)-(iv) of iterated integrals given in Proposition 5.7 extend verbatim to the regularized case. A similar statement applies to Theorem 5.19.

6.4. Examples. It follows from (6.2) that

$$\int_{\text{dch}}^{\text{reg}} \omega_0 = 0,$$

and likewise $\int_{\text{dch}}^{\text{reg}} \omega_1 = 0$. On the other hand, we have

$$\int_{\text{dch}}^{\text{reg}} \underbrace{\omega_0 \omega_1 \dots \omega_1}_{k_1} \dots \underbrace{\omega_0 \omega_1 \dots \omega_1}_{k_d} = \zeta(k_1, \dots, k_d),$$

since the corresponding unregularized iterated integral already converges. Together with the shuffle product property of regularized iterated integral, this allows for recursive algebraic computation of all regularized iterated integrals $\int_{\text{dch}}^{\text{reg}} \omega_{i_1} \dots \omega_{i_r}$. For example

$$\int_{\text{dch}}^{\text{reg}} \omega_0 \omega_1 \omega_0 = \int_{\text{dch}}^{\text{reg}} \omega_0 \omega_1 \int_{\text{dch}}^{\text{reg}} \omega_0 - 2 \int_{\text{dch}}^{\text{reg}} \omega_0 \omega_0 \omega_1 = -2\zeta(3).$$

Using this result, one shows likewise that

$$\int_{\text{dch}}^{\text{reg}} \omega_1 \omega_0 \omega_0 = \zeta(3).$$

6.5. Chen's theorem for tangential base points. Another salient feature of the definition of regularized iterated integrals just given is that Chen's π_1 -de Rham theorem carries through without essential change.

Theorem 6.8 (Chen's π_1 -de Rham theorem for tangential base points). *For each integer $N \geq 0$ and each pair of base points x, y (tangential or not), the natural pairing*

$$L_N H^0(B^*(A_{\mathbb{C}}^*)) \otimes \mathbb{Q}[\pi_1(M; y, x)] / J^{N+1} \mathbb{Q}[\pi_1(M; x)] \rightarrow \mathbb{C}$$

$$\langle \eta, \gamma \rangle \mapsto \int_{\gamma}^{\text{reg}} \eta$$

induces an isomorphism

$$L_N H^0(B^*(A_{\mathbb{C}}^*)) \xrightarrow{\cong} \text{Hom}_{\mathbb{Q}}(\mathbb{Q}[\pi_1(M; y, x)]/J^{N+1}\mathbb{Q}[\pi_1(M; x)], \mathbb{C}).$$

Remark 6.9. The last isomorphism is compatible with all extra structure on both sides. Similarly to the case of non-tangential base points, it can be promoted to a comparison isomorphism of a certain (ind)-mixed Hodge structure on $\mathcal{O}(\pi_1(M; y, x)^{\text{un}})$.

7. THE FUNDAMENTAL GROUPOID OF $\mathbb{P}^1 \setminus \{0, 1, \infty\}$

From now on, write $\mathbf{0} := \vec{1}_0$ and $\mathbf{1} := -\vec{1}_1$, and let $x, y \in \{\mathbf{0}, \mathbf{1}\}$. In the preceding sections we have constructed

- (i) The affine pro-algebraic scheme ${}_y\Pi_x^B := \pi_1(\mathbb{P}^1 \setminus \{0, 1, \infty\}; y, x)^{\text{un}}$. Denote its affine ring of functions by ${}_yA_x^B$.
- (ii) The Hopf algebra ${}_yA_x^{dR} := H^0(B^*(A^*))$ where A^* denotes the model of the C^∞ -de Rham complex of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ given in (??). Denote its spectrum by ${}_y\Pi_x^{dR}$.
- (iii) A comparison isomorphism

$$\text{comp}_{B,dR} : {}_yA_x^{dR} \otimes \mathbb{C} \rightarrow {}_yA_x^B \otimes \mathbb{C}.$$

Additionally, the objects in (i) and (ii) are endowed with weight filtrations W_{\bullet}^B , W_{\bullet}^{dR} and (ii) also carries a Hodge filtration F^\bullet which turn the triple

$$({}_yA_x^B, W^B), ({}_yA_x^{dR}, W, F), \text{comp}_{B,dR}$$

into an (ind)-mixed Hodge structure.

Definition 7.1. The diagram consisting of the four schemes ${}_y\Pi_x^?$, for $x, y \in \{\mathbf{0}, \mathbf{1}\}$ with the composition of paths will be called the *tangential fundamental groupoid* of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.

It should be noted that the same constructions work more generally for $\mathbb{P}^1 \setminus S$ where S is any finite set of points. In particular, for $S = \{0, \infty\}$, we have $\mathbb{P}^1 \setminus S = \mathbb{G}_m$ and we likewise get

$$\begin{aligned} {}_y\Pi(\mathbb{G}_m)_x^{dR} &= \mathbb{G}_a \\ {}_yA(\mathbb{G}_m)_x^{dR} &= \mathbb{Q}[x_0] \\ {}_y\Pi(\mathbb{G}_m)_x^B &= \pi_1(\mathbb{G}_m(\mathbb{C}); y, x)^{\text{un}} \\ \text{comp}_{B,dR} : {}_yA(\mathbb{G}_m)_x^{dR} \otimes \mathbb{C} &\xrightarrow{\cong} \mathcal{O}({}_y\Pi(\mathbb{G}_m)_x^B) \otimes \mathbb{C}. \end{aligned}$$

The case \mathbb{G}_m is actually important for us as it gives rise to local monodromy morphisms

$$\begin{aligned} \mathbb{G}_a &\rightarrow {}_{\mathbf{0}}\Pi_{\mathbf{0}}^{dR}, & \mathbb{G}_a &\rightarrow {}_{\mathbf{1}}\Pi_{\mathbf{1}}^{dR} \\ \mathbb{G}_a &\rightarrow {}_{\mathbf{0}}\Pi_{\mathbf{0}}^B, & \mathbb{G}_a &\rightarrow {}_{\mathbf{1}}\Pi_{\mathbf{1}}^B \end{aligned}$$

as follows. The morphism $\mathbb{G}_a \rightarrow {}_{\mathbf{i}}\Pi_{\mathbf{i}}^{dR}$, for $\mathbf{i} \in \{\mathbf{0}, \mathbf{1}\}$, is induced from the unique morphism of \mathbb{Q} -algebras

$$\mathbb{Q}\langle x_0, x_1 \rangle \rightarrow \mathbb{Q}[x_i]$$

which maps $\underbrace{x_i \dots x_i}_n \mapsto \frac{x_i^n}{n!}$ and every other word to zero. On the Betti side, the above morphisms is obtained from the inclusion of a small punctured disk Δ^* around 0 (respectively around 1) into $\mathbb{P}^1 \setminus \{0, 1, \infty\}$.

Definition 7.2. We will denote by D^{dR} the diagram consisting of the four schemes ${}_y\Pi_x^{dR}$ with $x, y \in \{0, 1\}$ whose morphisms are given by composition of paths, together with the scheme \mathbb{G}_a and the two local monodromy morphisms

$$\mathbb{G}_a \rightarrow {}_0\Pi_0^{dR}, \quad \mathbb{G}_a \rightarrow {}_1\Pi_1^{dR}.$$

Likewise, we denote by D^B the diagram consisting of the four schemes ${}_y\Pi_x^B$ with morphisms obtained by composition of paths and the local monodromy maps

$$\mathbb{G}_a \rightarrow {}_0\Pi_0^B, \quad \mathbb{G}_a \rightarrow {}_1\Pi_1^B.$$

7.1. Automorphisms of D^{dR} . Let $\text{Aut}(D^{dR})$ be the automorphism group of the diagram D^{dR} , i.e. collection of automorphisms one for every object of D^{dR} which are compatible with the morphisms (i.e. composition of paths and local monodromy). Also, let $\text{Aut}^0(D^{dR}) \subset \text{Aut}(D^{dR})$ be the subgroup of automorphisms which are the identity on \mathbb{G}_a . The following innocuous lemma will be the key for the study of motivic multiple zeta values.

Lemma 7.3. *There is an isomorphism of schemes*

$$\begin{aligned} \text{Aut}^0(D^{dR}) &\rightarrow \Pi^{dR} \\ f &\mapsto \gamma_f, \end{aligned}$$

where γ_f is determined by the equation $f({}_11_0^{dR}) = {}_11_0^{dR} \cdot \gamma_f$.

Sketch of proof. Identify ${}_0\Pi_0^{dR}(R)$ with the group-like elements of $R\langle\langle e_0, e_1 \rangle\rangle$. Then

$$\begin{aligned} f(\exp(e_0)) &= \exp(e_0) \\ f(\exp(e_1)) &= f({}_11_0^{dR}) \cdot \exp(e_1) \cdot f({}_01_1^{dR}) \end{aligned}$$

since f acts trivially on \mathbb{G}_a . It follows that f is uniquely determined by its value on the trivial de Rham path ${}_11_0^{dR}$. Conversely, given $\gamma \in {}_0\Pi_0^{dR}$, one verifies that

$$f_\gamma(e_0) = e_0, \quad f_\gamma(e_1) = \gamma^{-1} \cdot e_1 \cdot \gamma$$

defines an element of $\text{Aut}^0(D^{dR})$. □

7.2. The Goncharov coproduct. The previous lemma defines, by transport of structure, a new group law on Π^{dR} , called the *Ihara action*. It is defined by

$$(7.1) \quad \gamma \circ \mu = \gamma \cdot \langle \gamma \rangle_0(\mu),$$

where $\langle \gamma \rangle_0$ is the restriction of f_γ to ${}_0\Pi_1^{dR}$. More generally, (7.1) makes sense for μ an arbitrary element of $\mathbb{Q}\langle\langle e_0, e_1 \rangle\rangle$ and is computed for $e = w$ a word in e_0, e_1 explicitly as follows:

- (1) if w starts with e_0 , append γ at the beginning; otherwise append nothing at the beginning
- (2) if w ends with e_1 , append γ at the end; otherwise append nothing
- (3) between e_0 and e_1 , insert γ^{-1} and between e_1 and e_0 insert γ
- (4) between two consecutive appearances of either e_0 or e_1 , insert nothing

Example 7.4. As an example, consider the word $w = e_0 e_0 e_1 e_0 e_1 e_1$. For an arbitrary $\gamma \in {}_{\mathbf{o}}\Pi_0^{dR}$, we have

$$\gamma \circ w = \gamma e_0 e_0 \gamma^{-1} e_1 \gamma e_0 \gamma^{-1} e_1 e_1 \gamma.$$

Of particular interest will be the coproduct

$$\Delta^\Gamma : \mathbb{Q}\langle x_0, x_1 \rangle \rightarrow \mathbb{Q}\langle x_0, x_1 \rangle \otimes \mathbb{Q}\langle x_0, x_1 \rangle$$

which is called the *Goncharov coproduct*. It is determined uniquely by the equation

$$\Delta^\Gamma(x)(\gamma \otimes \mu) = x(\gamma \circ \mu) = x(\gamma \cdot \langle \gamma \rangle_0(\mu)), \quad \gamma, \mu \in {}_{\mathbf{o}}\Pi_0^{dR}.$$

Our next goal is to give an explicit formula for Δ^Γ . For this, we associate to a binary sequence $\alpha = (\varepsilon_1, \dots, \varepsilon_n) \in \{0, 1\}^n$ the word

$$x_\alpha = x_{\varepsilon_1} \dots x_{\varepsilon_n}.$$

We will also denote $x_\alpha^* := S(x_\alpha) = (-1)^n x_{\varepsilon_n} \dots x_{\varepsilon_1}$. It will further be customary to introduce the notation

$$\begin{aligned} I(1; \alpha; 0) &= x_\alpha, & I(0; \alpha; 1) &= x_\alpha^* \\ I(0; \alpha; 0) &= I(1; \alpha; 1) = 1, & \text{if } \alpha &= \emptyset \\ I(0; \alpha; 0) &= I(1; \alpha; 1) = 0, & \text{if } \alpha &\neq \emptyset. \end{aligned}$$

which is reminiscent of iterated integrals.

Proposition 7.5. *The Goncharov coproduct is given by the following formula. Letting $\varepsilon_0, \dots, \varepsilon_{n+1}$ be a binary sequence, we have*

$$\begin{aligned} \Delta^\Gamma I(\varepsilon_0; \varepsilon_1 \dots \varepsilon_n; \varepsilon_{n+1}) &= \sum_{0=i_0 < i_1 < \dots < i_{k+1}=n+1} \prod_{p=0}^k I(\varepsilon_{i_p}; \varepsilon_{i_{p+1}} \dots \varepsilon_{i_{p+1}-1}; \varepsilon_{i_{p+1}}) \\ &\quad \otimes I(\varepsilon_0; \varepsilon_{i_1} \dots \varepsilon_{i_k}; \varepsilon_{n+1}). \end{aligned}$$

Remark 7.6. This formula has a pictorial description by thinking of the ε_i on a semi-circle. The sum is then over all polygons linking the end points $\varepsilon_0, \varepsilon_{n+1}$ and possibly linking intermediate entries ε_i . The linked points are put on the right of the tensor product while the skipped points comprise the factors in the product on the left of \otimes .

Example 7.7. (i) In the case $n = 1$, we have

$$\Delta^\Gamma I(\varepsilon_0; \varepsilon_1; \varepsilon_2) = I(\varepsilon_0; \varepsilon_1; \varepsilon_2) \otimes 1 + 1 \otimes I(\varepsilon_0; \varepsilon_1; \varepsilon_2).$$

(ii) For $n = 2$, the general formula is

$$\begin{aligned} \Delta^\Gamma I(\varepsilon_0; \varepsilon_1 \varepsilon_2; \varepsilon_3) &= I(\varepsilon_0; \varepsilon_1 \varepsilon_2; \varepsilon_3) \otimes 1 + I(\varepsilon_1; \varepsilon_2; \varepsilon_3) \otimes I(\varepsilon_0; \varepsilon_1; \varepsilon_3) \\ &\quad + I(\varepsilon_0; \varepsilon_1; \varepsilon_2) \otimes I(\varepsilon_0; \varepsilon_2; \varepsilon_3) \\ &\quad + 1 \otimes I(\varepsilon_0; \varepsilon_1 \varepsilon_2 \varepsilon_3). \end{aligned}$$

8. MOTIVIC MULTIPLE ZETA VALUES

8.1. Tannakian categories. Let k be a field.

Definition 8.1. A *neutral Tannakian category* over k is a rigid k -linear abelian tensor category \mathcal{C} such that $\text{End}(\mathbf{1}) = k$ and such that there exists an exact, faithful k -linear tensor functor $\omega : \mathcal{C} \rightarrow \mathbf{Vec}_k$ (called a *fibre functor*).

Example 8.2. The following are examples of (neutral) Tannakian categories.

- (i) The category \mathbf{Vec}_k of k -vector spaces.
- (ii) The category \mathbf{GrVec}_k of graded k -vector spaces.
- (iii) The category $\mathbf{Rep}_k(G)$ of finite-dimensional k -representations of an abstract group G .
- (iv) The category $\mathbf{MHS}(\mathbb{Q})$ of mixed Hodge structures over \mathbb{Q} .

The fundamental fact about Tannakian categories is that each of them is equivalent to the category of representations of a certain affine group scheme determined by the fibre functor $\omega : \mathcal{C} \rightarrow \mathbf{Vec}_k$. To be precise, for a k -algebra R , let $\underline{\mathbf{Aut}}^\otimes(\omega)(R)$ be the set of natural tensor automorphisms of the functor $X \mapsto \omega(X) \otimes R$. In the case $R = k$, we simply write $\mathbf{Aut}^\otimes(\omega)$ instead of $\underline{\mathbf{Aut}}^\otimes(\omega)(k)$.

Theorem 8.3 (Tannakian reconstruction theorem). *Let \mathcal{C} be a Tannakian category with fibre functor ω . Then*

- *the functor $R \mapsto \underline{\mathbf{Aut}}^\otimes(\omega)(R)$ is representable by an affine group scheme over k that we denote by $\underline{\mathbf{Aut}}^\otimes(\omega)$.*
- *for every $X \in \mathbf{Ob}(\mathcal{C})$, the group scheme $\underline{\mathbf{Aut}}^\otimes(\omega)$ acts naturally on $\omega(X)$ and the functor*

$$\mathcal{C} \rightarrow \mathbf{Rep}_k(\underline{\mathbf{Aut}}^\otimes(\omega))$$

sending X to $\omega(X)$ together with the above action of $\underline{\mathbf{Aut}}^\otimes(\omega)$ is an equivalence of categories.

Definition 8.4. The affine group scheme $\underline{\mathbf{Aut}}^\otimes(\omega)$ is called the *Tannakian group* of (\mathcal{C}, ω) .

Example 8.5. In the examples (i)-(iii) above, there is a canonical fibre functor given by mapping an object of the respective category to the underlying k -vector space. The Tannakian groups are then, respectively, the trivial group, \mathbb{G}_m and G viewed as a constant group scheme.

8.2. The Tannakian category of mixed Tate motives over \mathbb{Z} . Instead of constructing the category of mixed Tate motives, we subsume its basic properties in the following theorem which represents the joint efforts of several mathematicians (notably Voevodsky, Bloch, Deligne, Beilinson, Goncharov, Levine,...) over a course of about 40 years.

Theorem 8.6. *There exists a Tannakian category $\mathbf{MT}(\mathbb{Z})$ of mixed Tate motives over \mathbb{Z} with the following properties.*

- (i) *There is an exact tensor functor*

$$\mathbf{MT}(\mathbb{Z}) \rightarrow \mathbf{MHTS}(\mathbb{Q}),$$

called the Hodge realization which is fully faithful.

- (ii) *The simple objects are the Tate motives $\mathbb{Q}(n)$ whose Hodge realization is precisely the Tate Hodge structure $\mathbb{Q}(n)$. Moreover, every object M of $\mathbf{MT}(\mathbb{Z})$ is endowed with an increasing, finite weight filtration*

$$\dots \subset W_{2n}M \subset W_{2n+2}M \subset \dots,$$

such that $\mathrm{gr}_{2n}^W M \cong \mathbb{Q}(-n)^{r_n}$ for some $r_n \geq 0$.

- (iii) *There is a canonical fibre functor $\omega : \mathbf{MT}(\mathbb{Z}) \rightarrow \mathbf{Vec}_{\mathbb{Q}}$ which is graded $\omega = \bigoplus_{n \in \mathbb{Z}} \omega_n$ and given explicitly by*

$$\omega_n(M) = \mathrm{Hom}_{\mathbf{MT}(\mathbb{Z})}(\mathbb{Q}(n), \mathrm{gr}_{-2n}^W(M)).$$

Moreover, it equals the functor

$$\mathbf{MT}(\mathbb{Z}) \rightarrow \mathbf{MHTS}(\mathbb{Q}) \xrightarrow{\omega_{dR}} \mathbf{Vec}_{\mathbb{Q}},$$

where the first arrow is the Hodge realization and the second one the functor $(V_B, V_{dR}, \mathrm{comp}_{B,dR}) \mapsto V_{dR}$.

- (iv) *The extension groups between the simple objects $\mathbb{Q}(n)$ are given by:*

$$\mathrm{Ext}_{\mathbf{MT}(\mathbb{Z})}^0(\mathbb{Q}(m), \mathbb{Q}(n)) = \mathrm{Hom}(\mathbb{Q}(m), \mathbb{Q}(n)) \cong \begin{cases} \mathbb{Q} & m = n \\ 0 & m \neq n \end{cases}$$

$$\mathrm{Ext}_{\mathbf{MT}(\mathbb{Z})}^1(\mathbb{Q}(m), \mathbb{Q}(n)) \cong \begin{cases} \mathbb{Q} & n - m \geq 3 \text{ odd} \\ 0 & \text{else} \end{cases}$$

and $\mathrm{Ext}_{\mathbf{MT}(\mathbb{Z})}^n(\mathbb{Q}(m), \mathbb{Q}(n)) \cong 0$ for $n \geq 2$.

- (v) *The Tannakian group of $(\mathbf{MT}(\mathbb{Z}), \omega)$, denoted by G_{dR} , is a semi-direct product*

$$G_{dR} \cong U_{dR} \rtimes \mathbb{G}_m,$$

where U_{dR} is pro-unipotent. The graded Lie algebra $\mathfrak{u}_{dR}^{\mathrm{gr}}$ of U_{dR} is (non-canonically) isomorphic to the free Lie algebra with one generator σ_{2n+1} in each degree $-(2n+1)$ for all $n \geq 1$.

The key fact which relates $\mathbf{MT}(\mathbb{Z})$ to multiple zeta values is given by the following theorem.

Theorem 8.7. *The diagram D^{dR} is the de Rham realization of a diagram of mixed Tate motives over \mathbb{Z} .*

Therefore we obtain a commutative diagram

$$\begin{array}{ccccccc} 0 & \longrightarrow & U_{dR} & \longrightarrow & G_{dR} & \longrightarrow & \mathbb{G}_m \longrightarrow 0 \\ & & \downarrow & & \downarrow & & \parallel \\ 0 & \longrightarrow & \Pi & \longrightarrow & \mathrm{Aut}(D^{dR}) & \longrightarrow & \mathbb{G}_m \longrightarrow 0 \end{array}$$

where $\Pi = {}_1\Pi_0^{dR}$ is viewed as a group scheme under the Ihara action \circ via Lemma 7.3. In particular, G_{dR} acts on ${}_1\Pi_0^{dR}$.

8.3. The algebra of motivic multiple zeta values. Recall that we have a canonical comparison isomorphism

$$\mathrm{comp}_{dR,B} : {}_1\Pi_0^B(\mathbb{C}) \rightarrow {}_1\Pi_0^{dR}(\mathbb{C})$$

given by (regularized) iterated integration of differential forms on $\mathbb{P}^1 \setminus \{0, 1, \infty\}$. Explicitly, if $\mathrm{dch} \in {}_1\Pi_0^B(\mathbb{Q})$ denotes the image of the straight line path from 0 to 1, then

$$\mathrm{dch}^{dR} := \mathrm{comp}_{dR,B}(\mathrm{dch}) = \sum_{w=w_{i_1} \dots w_{i_n} \in \langle e_0, e_1 \rangle} \int_{\mathrm{dch}}^{\mathrm{reg}} \omega_{i_1} \dots \omega_{i_n} \cdot w \in {}_1\Pi_0^{dR}(\mathbb{C}).$$

In fact, the coefficients of dch^{dR} are given by linear combinations of multiple zeta values which are real numbers, and therefore $\text{dch}^{dR} \in {}_1\Pi_0^{dR}(\mathbb{R})$.

Evaluation at dch^{dR} gives a \mathbb{Q} -linear map

$$(8.1) \quad \begin{aligned} \mathcal{O}({}_1\Pi_0^{dR}) &\cong \mathbb{Q}\langle x_0, x_1 \rangle \rightarrow \mathbb{R} \\ f &\mapsto f(\text{dch}^{dR}), \end{aligned}$$

i.e. a word $w^\vee = x_{i_1} \dots x_{i_n}$ is mapped to the coefficient of the dual word $w = e_{i_1} \dots e_{i_n}$ in dch^{dR} .

Definition 8.8. Define the algebra of motivic multiple zeta values \mathcal{H} to be

$$\mathcal{H} := \mathcal{O}(\mathcal{Y}),$$

where \mathcal{Y} is the Zariski-closure of the G_{dR} -orbit of dch^{dR} :

$$\mathcal{Y} := \overline{G_{\text{dR}} \cdot \text{dch}^{dR}} \subset {}_1\Pi_0^{dR}.$$

By definition, elements of \mathcal{H} are linear combinations of equivalence classes of words in x_0, x_1 . Moreover, since \mathcal{Y} is defined over \mathbb{Q} , it follows that \mathcal{H} is a \mathbb{Q} -algebra. In addition, \mathcal{H} has the following extra structure.

- (i) A grading induced by the action of \mathbb{G}_m on \mathcal{Y} .
- (ii) A surjection of \mathbb{Q} -algebras

$$\text{per} : \mathcal{H} \rightarrow \mathbb{R},$$

which is called the *period map*, and which is given by evaluation at $\text{dch}^{dR} \in \mathcal{Y}$. It maps \mathcal{H}_k surjectively onto \mathcal{Z}_k , the \mathbb{Q} -span of all multiple zeta values of weight k .

Remark 8.9. The raison d'être of the definition of \mathcal{H} is as follows. Let $I \subset \mathcal{O}({}_1\Pi_0^{dR})$ be the kernel of (8.1). By definition, it encodes all \mathbb{Q} -algebraic relations among the coefficients of dch^{dR} . Since the image of (8.1) is precisely the algebra \mathcal{Z} of multiple zeta values, we have

$$\mathcal{O}({}_1\Pi_0^{dR})/I \cong \mathcal{Z}.$$

Now the defining ideal J of the closed subscheme \mathcal{Y} is contained in I and admits the following alternative definition: $J \subset I$ is the largest graded sub-ideal which is stable under the motivic coaction $\Delta : \mathcal{O}({}_1\Pi_0^{dR}) \rightarrow \mathcal{O}({}_1\Pi_0^{dR}) \otimes \mathcal{O}(G_{\text{dR}})$, i.e. $\Delta(J) \subset J \otimes \mathcal{O}(G_{\text{dR}})$ where the coaction is dual to the action of G_{dR} on ${}_1\Pi_0^{dR}$.

Remark 8.10. The definition of \mathcal{H} given here is rather cumbersome in practice. A better definition can be given using the formalism of motivic periods but we do not go into this here.

8.4. Motivic decomposition and Zagier's conjecture. We next relate motivic multiple zeta values to the affine ring of functions on the Tannakian fundamental group G_{dR} of $\mathbf{MT}(\mathbb{Z})$. Let IU_{dR} be the quotient of U_{dR} which acts on ${}_1\Pi_0^{dR}$. It is the largest quotient of U_{dR} which acts faithfully on ${}_1\Pi_0^{dR}$ and is naturally graded. Let

$$\mathcal{A} := \mathcal{O}(IU_{\text{dR}})$$

be the graded affine ring of functions on IU_{dR} .

Proposition 8.11. *There is a non-canonical isomorphism of graded \mathbb{Q} -algebras*

$$\mathcal{H} \cong \mathcal{A} \otimes \mathbb{Q}[t],$$

where t sits in degree 2.

Remark 8.12. The element t corresponds to the motivic version of $\zeta(2)$.

This result implies Theorem 1.11 of Deligne–Goncharov and Terasoma. To see this, let

$$\mathcal{A}^{\mathbf{MT}} := \mathcal{O}(U_{\mathrm{dR}})$$

which is a graded Hopf algebra with coproduct Δ , and consider the following trivial Hopf comodule

$$\mathcal{H}^{\mathbf{MT}} := \mathcal{A}^{\mathbf{MT}} \otimes \mathbb{Q}[f_2], \quad \Delta(f_2) = 1 \otimes f_2.$$

It is a graded \mathbb{Q} -vector space where f_2 has degree 2.

Proposition 8.13. *The Hilbert–Poincaré series*

$$H_{\mathcal{H}^{\mathbf{MT}}}(t) := \sum_{k \geq 0} \dim_{\mathbb{Q}}(\mathcal{H}_k^{\mathbf{MT}}) t^k$$

of $\mathcal{H}^{\mathbf{MT}}$ is given by

$$H_{\mathcal{H}^{\mathbf{MT}}}(t) = \frac{1}{1 - t^2 - t^3}.$$

In particular, we have $\dim_{\mathbb{Q}} \mathcal{H}_k^{\mathbf{MT}} = d_k$ for all k , with d_k as in Conjecture 1.8.

On the other hand, by Proposition 8.11, \mathcal{H} is a subalgebra of $\mathcal{H}^{\mathbf{MT}}$ since \mathcal{A} is a subalgebra of $\mathcal{A}^{\mathbf{MT}}$. Therefore, $\dim_{\mathbb{Q}} \mathcal{H}_k \leq d_k$ for all k . Applying the period map, we see that $\dim_{\mathbb{Q}} \mathcal{Z}_k \leq \dim_{\mathbb{Q}} \mathcal{H}_k$ and we obtain Theorem 1.11.

9. THE PROOF OF BROWN’S THEOREM

9.1. Summary of motivic multiple zeta values. Recall that we defined the \mathbb{Q} -algebra of motivic multiple zeta values to be

$$\mathcal{H} := \mathcal{O}(\mathcal{Y})$$

where $\mathcal{Y} := \overline{\mathcal{G}_{\mathrm{dR}} \cdot \mathrm{dch}^{dR}} \subset {}_1\Pi_0^{dR}$, and dch^{dR} denotes the Drinfeld associator. More concretely, since

$$\mathcal{O}({}_1\Pi_0^{dR}) \cong \mathbb{Q}\langle x_0, x_1 \rangle,$$

the \mathbb{Q} -algebra \mathcal{H} is a quotient of the shuffle algebra $\mathbb{Q}\langle x_0, x_1 \rangle$.

Definition 9.1. For a binary sequence α , define the *motivic iterated integral* $I^{\mathbf{m}}(1; \alpha; 0)$ to be the class

$$[x_{\alpha}] \in \mathcal{H},$$

of the word $x_{\alpha} \in \mathbb{Q}\langle x_0, x_1 \rangle$ associated to α . Also, define

$$I^{\mathbf{m}}(0; \alpha; 1) = x_{\alpha}^*|_{\mathcal{Y}}$$

and

$$I^{\mathbf{m}}(0; \alpha; 0) = I^{\mathbf{m}}(1; \alpha; 1) = \begin{cases} 1 & \alpha = \emptyset \\ 0 & \alpha \neq \emptyset. \end{cases}$$

Remark 9.2. The motivic iterated integrals have several further algebraic properties, for example they satisfy the shuffle product. We do not go into this here but point out in the text whenever we use these.

Definition 9.3. For positive integers k_1, \dots, k_d , denote the associated *motivic multiple zeta value* by

$$\zeta^{\mathfrak{m}}(k_1, \dots, k_d) = I^{\mathfrak{m}}(1; 0^{k_1-1}1 \dots 0^{k_d-1}1; 0).$$

Also, recall the following properties of motivic multiple zeta values.

- (i) The \mathbb{Q} -algebra \mathcal{H} is graded for the weight

$$\mathcal{H} = \bigoplus_{k \geq 0} \mathcal{H}_k,$$

and each weight-graded component satisfies $\dim_{\mathbb{Q}} \mathcal{H}_k \leq d_k$ where d_k are the dimensions occurring in Conjecture 1.8.

- (ii) There is a morphism of \mathbb{Q} -algebras

$$\text{per} : \mathcal{H} \rightarrow \mathcal{Z}, \quad \zeta^{\mathfrak{m}}(k_1, \dots, k_d) \mapsto \zeta_{\sqcup}(k_1, \dots, k_d)$$

called the *period map*. It is surjective and respects the weight.

- (iii) There is a coaction due to Goncharov

$$\Delta : \mathcal{H} \rightarrow \mathcal{A} \otimes_{\mathbb{Q}} \mathcal{H}$$

given explicitly by

$$\Delta I^{\mathfrak{m}}(\varepsilon_0; \varepsilon_1 \dots \varepsilon_n; \varepsilon_{n+1}) = \sum_{0=i_0 < i_1 < \dots < i_{k+1}=n+1} \pi \left(\prod_{p=0}^k I^{\mathfrak{m}}(\varepsilon_{i_p}; \varepsilon_{i_{p+1}} \dots \varepsilon_{i_{p+1}-1}; \varepsilon_{i_{p+1}}) \right) \otimes I^{\mathfrak{m}}(\varepsilon_0; \varepsilon_{i_1} \dots \varepsilon_{i_k}; \varepsilon_{n+1}),$$

where $\pi : \mathcal{H} \rightarrow \mathcal{A} \cong \mathcal{H}/\zeta^{\mathfrak{m}}(2)\mathcal{H}$ denotes the canonical projection.

9.2. The main theorem and outline of proof. The main theorem about motivic multiple zeta values is the following.

Theorem 9.4 (Brown). *The motivic Hoffman elements*

$$\{\zeta^{\mathfrak{m}}(k_1, \dots, k_d) \mid k_i \in \{2, 3\}\}$$

are \mathbb{Q} -linearly independent.

Roughly speaking, the key steps in the proof are as follows.

- (i) The formula for the coaction above is too complicated to compute with, so one needs to pass to a suitable linearization. This will lead to certain derivations D_n , for $n \geq 1$ an odd integer which will be easier to study.
- (ii) Let $\mathcal{H}^{2,3}$ be the \mathbb{Q} -span of the motivic Hoffman elements. It carries a natural ascending filtration $F_l \mathcal{H}^{2,3}$ by number of 3's which is called the *level*.
- (iii) Using the motivic derivations D_n , one then defines level-lowering operators

$$\partial_{N,l} : \text{gr}_l^F \mathcal{H}_N^{2,3} \rightarrow \bigoplus_{3 \leq 2r+1 \leq N} \text{gr}_{l-1}^F \mathcal{H}_{N-2r-1}^{2,3}.$$

The crucial fact is that these operators are injective which uses as input a deep arithmetic theorem of Zagier's.

- (iv) The proof of Theorem 9.4 then proceeds by induction on the level. In level 0, one only has

$$\zeta^{\mathfrak{m}}(2^{\{n\}}) = \frac{6^n}{(2n+1)!} \zeta^{\mathfrak{m}}(2)^n$$

and these are linearly independent since $\zeta(2)$ is transcendental (Lindemann). This settles the base case. For the general case, assume given a \mathbb{Q} -linear combination of motivic Hoffman elements of homogeneous weight N and level l (the general case can be reduced to this) which is zero. Applying $\partial_{N,l}$, one obtains another \mathbb{Q} -linear relation of strictly smaller level which therefore has to be identically zero, and one concludes since $\partial_{N,l}$ is injective.

9.3. Linearized coaction. Let $\mathcal{A}_{>0} \subset \mathcal{A}$ be the ideal of elements of positive weight, and denote $\mathcal{L} = \mathcal{A}_{>0}/(\mathcal{A}_{>0})^2$. It is also graded for the weight, $\mathcal{L} = \bigoplus_{N \geq 1} \mathcal{L}_N$.

Definition 9.5. for $r \geq 1$, define a map

$$D_{2r+1} : \mathcal{H} \rightarrow \mathcal{L}_{2r+1} \otimes \mathcal{H}$$

as the composition

$$\mathcal{H} \xrightarrow{\Delta - 1 \otimes \text{id}} \mathcal{A}_{>0} \otimes \mathcal{H} \xrightarrow{q \otimes \text{id}} \mathcal{L} \otimes \mathcal{H} \xrightarrow{p_{2r+1} \otimes \text{id}} \mathcal{L}_{2r+1} \otimes \mathcal{H},$$

where $q : \mathcal{A}_{>0} \rightarrow \mathcal{L}$ is the natural projection and p_{2r+1} is projection onto the weight $2r+1$ component. We also put

$$D_{<N} = \bigoplus_{3 \leq 2r+1 < N} D_{2r+1}.$$

The following proposition gives an explicit formula for D_n . Let $\varpi_n : \mathcal{H} \rightarrow \mathcal{L}_n$ be the composition $p_n \circ q \circ \pi$.

Proposition 9.6. *For $n < N$ odd, we have*

$$D_n I^{\mathfrak{m}}(\varepsilon_0; \varepsilon_1, \dots, \varepsilon_N; \varepsilon_{N+1}) = \sum_{p=0}^{N-n} \varpi_n(I^{\mathfrak{m}}(\varepsilon_p; \varepsilon_{p+1}, \dots, \varepsilon_{p+n}; \varepsilon_{p+n+1})) \otimes I^{\mathfrak{m}}(\varepsilon_0; \varepsilon_1, \dots, \varepsilon_p, \varepsilon_{p+n+1}, \dots, \varepsilon_N; \varepsilon_{N+1}).$$

An important fact about the operators D_n is that we can explicitly determine their kernel. More precisely.

Theorem 9.7. *Let $N \geq 2$. Then*

$$\ker D_{<N} \cap \mathcal{H}_N = \mathbb{Q} \zeta^{\mathfrak{m}}(N).$$

This result will be used via its corollary below.

Corollary 9.8. *Let $N \geq 2$ and let $a^{\mathfrak{m}} \in \mathcal{H}_N$. If $D_{<N}(a^{\mathfrak{m}}) = 0$ and $\text{per}(a^{\mathfrak{m}}) = \alpha \zeta(N)$ for some rational number α , then $a^{\mathfrak{m}} = \alpha \zeta^{\mathfrak{m}}(N)$.*

As a simple example, we have the following result already alluded to above which for multiple zeta values is a classical result of Euler.

Proposition 9.9. *For each $n \geq 1$, the following equality holds:*

$$\zeta^{\mathfrak{m}}(2^{\{n\}}) = \frac{6^n}{(2n+1)!} \zeta^{\mathfrak{m}}(2)^n.$$

Sketch of proof. By definition, we have $\zeta^{\mathfrak{m}}(2^{\{n\}}) = I^{\mathfrak{m}}(1; 01 \dots 01; 0)$. From this it is not hard to see that $D_{2r+1}\zeta^{\mathfrak{m}}(2^{\{n\}}) = 0$ for every $3 \leq 2r+1 < 2n$, and therefore $\zeta^{\mathfrak{m}}(2^{\{n\}}) \in \mathbb{Q}\zeta^{\mathfrak{m}}(2n) = \mathbb{Q}\zeta^{\mathfrak{m}}(2)^n$. The precise rational multiple is obtained by applying the period map and referring to the analogous result for multiple zeta values due to Euler. \square

9.4. Zagier's theorem. In the preceding subsection, we have seen an explicit formula for motivic multiple zeta values with only 2's. The following, much deeper, result gives a similar explicit formula for motivic multiple zeta values with many 2's and exactly one 3.

To state it, define for each $a, b, r \geq 0$ rational numbers

$$A_{a,b}^r = \binom{2r}{2a+2}, \quad B_{a,b}^r = (1 - 2^{-2r}) \binom{2r}{2b+1}.$$

Theorem 9.10 (Brown–Zagier). *Let $a, b \geq 0$ and $n := a + b + 1$. Then we have*

$$\zeta^{\mathfrak{m}}(2^{\{b\}}, 3, 2^{\{a\}}) = 2 \sum_{r=1}^n (-1)^r (A_{a,b}^r - B_{a,b}^r) \zeta^{\mathfrak{m}}(2r+1) \zeta^{\mathfrak{m}}(2^{\{n-r\}}).$$

Idea of proof. The hardest part is the corresponding result for multiple zeta values which is due to Zagier. Using Corollary 9.8, one then shows that Zagier's result can be lifted to motivic multiple zeta values. \square

9.5. The level filtration. Recall that $\mathcal{H}^{2,3} \subset \mathcal{H}$ denotes the \mathbb{Q} -linear span of the Hoffman elements. Instead of studying $\mathcal{H}^{2,3}$, it will be customary to consider a “formal” version of $\mathcal{H}^{2,3}$ as follows.

Definition 9.11. We denote by $\tilde{\mathcal{H}}^{2,3} \subset \mathcal{O}(\Pi)$ the subspace generated by functions $I(1; \alpha; 0)$ where α is a binary sequence associated with an admissible multi-index containing only 2's and 3's as entries.

By definition, $\mathcal{H}^{2,3}$ is then the image of $\tilde{\mathcal{H}}^{2,3}$ under the restriction map $\text{res} : \mathcal{O}(\Pi) \rightarrow \mathcal{H}$.

One then defines an ascending *level filtration*

$$\dots \subset F_{l-1} \tilde{\mathcal{H}}^{2,3} \subset F_l \tilde{\mathcal{H}}^{2,3} \subset F_{l+1} \tilde{\mathcal{H}}^{2,3} \subset \dots$$

where $F_l \tilde{\mathcal{H}}^{2,3} \subset \tilde{\mathcal{H}}^{2,3}$ is defined to be the subspace spanned by $I(1; \alpha; 0)$ such that the multi-index corresponding to α has at most l occurrences of the number 3. Under res , the filtration F_\bullet is given explicitly by

$$F_l \mathcal{H}^{2,3} = \langle \zeta^{\mathfrak{m}}(k_1, \dots, k_d) \mid \text{number of } k_i = 3 \leq l \rangle_{\mathbb{Q}}.$$

9.6. Level-lowering. A key fact is that the operators D_n are in a strong sense compatible with the level filtration. To make this precise, for every $r \geq 1$, define an operator

$$\tilde{D}_{2r+1} : \mathcal{O}(\Pi) \rightarrow \mathcal{L}_{2r+1} \otimes \mathcal{O}(\Pi)$$

analogously to the definition of D_{2r+1} .

Lemma 9.12. *For every $r \geq 1$, the operator \tilde{D}_{2r+1} decreases the level, i.e. restricts to an operator*

$$\tilde{D}_{2r+1} : F_l \tilde{\mathcal{H}}^{2,3} \rightarrow \mathcal{L}_{2r+1} \otimes F_{l-1} \tilde{\mathcal{H}}^{2,3}.$$

Passing to the associated graded, we obtain morphisms

$$\mathrm{gr}_l^F \tilde{D}_{2r+1} : \mathrm{gr}_l^F \tilde{\mathcal{H}}^{2,3} \rightarrow \mathcal{L}_{2r+1} \otimes \mathrm{gr}_{l-1}^F \tilde{\mathcal{H}}^{2,3}.$$

A careful study of the coaction together with algebraic properties of the $I(1; \alpha; 0)$ yields the next lemma.

Lemma 9.13. *For all $r, l \geq 1$, one has*

$$\mathrm{gr}_l^F \tilde{D}_{2r+1}(\mathrm{gr}_l^F \tilde{\mathcal{H}}^{2,3}) \subset \mathbb{Q}\varpi(\zeta^{\mathfrak{m}}(2r+1)) \otimes \mathrm{gr}_{l-1}^F \tilde{\mathcal{H}}^{2,3}.$$

We can now make the key definition.

Definition 9.14. For all $N, l \geq 1$, the *level-lowering operator* $\tilde{\partial}_{N,l}$ is the \mathbb{Q} -linear map

$$\tilde{\partial}_{N,l} : \mathrm{gr}_l^F \tilde{\mathcal{H}}_N^{2,3} \rightarrow \bigoplus_{3 \leq 2r+1 \leq N} \mathrm{gr}_{l-1}^F \tilde{\mathcal{H}}_{2r+1}^{2,3}$$

obtained by first applying $\bigoplus_{3 \leq 2r+1 \leq N} \mathrm{gr}_l^F \tilde{D}_{2r+1}|_{\mathrm{gr}_l^F \tilde{\mathcal{H}}^{2,3}}$ and then sending $\varpi_{2r+1}(\zeta^{\mathfrak{m}}(2r+1))$ to 1.

9.7. Injectivity and end of proof.

Lemma 9.15. *For all $N, l \geq 1$, the level-lowering operator $\tilde{\partial}_{N,l}$ is an isomorphism of \mathbb{Q} -vector spaces.*

Idea of proof. Employing the explicit formula for the \tilde{D}_{2r+1} and using Theorem 9.10, the matrix of $\tilde{\partial}_{N,l}$ in the standard basis of $\tilde{\mathcal{H}}^{2,3}$ is upper triangular modulo 2 upper diagonal entries are essentially the coefficients appearing in Theorem 9.10. Using 2-adic properties of these coefficients, one shows that the matrix representing $\tilde{\partial}_{N,l}$ is invertible modulo 2, hence invertible. \square

Using the preceding lemma and induction on the level, one proves the following result which ends the proof of Theorem 9.4.

Lemma 9.16. *The natural map $\tilde{\mathcal{H}}^{2,3} \rightarrow \mathcal{H}^{2,3}$ is an isomorphism of \mathbb{Q} -vector spaces.*

9.8. Some consequences. As already alluded to in Remark 1.13, Theorem 9.4 has consequences for the structure of the category $\mathbf{MT}(\mathbb{Z})$.

Let $\mathbf{MT}'(\mathbb{Z})$ be the full Tannakian subcategory of $\mathbf{MT}(\mathbb{Z})$ generated by the objects ${}_{\mathbf{x}}U_{\mathbf{y}}^{Mot,N}$ for $N \geq 0$ and $\mathbf{x}, \mathbf{y} \in \{\vec{1}_0, -\vec{1}_1\}$ and let ω'_{dR} be the restriction of the de Rham fibre functor ω_{dR} to $\mathbf{MT}'(\mathbb{Z})$.

Corollary 9.17. *The canonical projection*

$$\underline{\mathrm{Aut}}_{\mathbf{MT}(\mathbb{Z})}^{\otimes}(\omega_{dR}) \rightarrow \underline{\mathrm{Aut}}_{\mathbf{MT}'(\mathbb{Z})}^{\otimes}(\omega'_{dR})$$

is an isomorphism of affine group schemes. In particular, the inclusion $\mathbf{MT}'(\mathbb{Z}) \rightarrow \mathbf{MT}(\mathbb{Z})$ is an equivalence of Tannakian categories.

Essentially, the preceding corollary says that every mixed Tate motive over \mathbb{Z} can be obtained from the motivic fundamental groupoid of $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ by using some standard operations in Tannakian categories, (quotients, tensor products, direct sums...).

Another consequence is the following result on periods.

Corollary 9.18. *The ring of periods of the category $\mathbf{MT}(\mathbb{Z})$ equals $\mathbb{Z}[(2\pi i)^{-1}]$.*

This corollary may be viewed as explaining the importance of multiple zeta values: up to powers of $2\pi i$, they are precisely the periods of mixed Tate motives over \mathbb{Z} , one of the simplest classes of mixed motives.

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