ON MULTIPLE ZETA VALUES

It is a great pleasure, and no small honour, to give this talk on the occasion of Don Zagier’s 60th birthday. I shall report on the recent proof of some conjectures on multiple zeta values, in which Don played a crucial role.

1. INTRODUCTION

Let \( n_1, \ldots, n_r \geq 1, n_r \geq 2 \) be integers. The multiple zeta value is defined by

\[
\zeta(n_1, \ldots, n_r) = \sum_{0 < k_1 < \ldots < k_r} \frac{1}{k_1^{n_1} \cdots k_r^{n_r}} \in \mathbb{R}.
\]

The weight of a tuple \((n_1, \ldots, n_r)\) is the quantity \(n_1 + \ldots + n_r\), its depth is the integer \(r\). These numbers were first defined by Euler for \(r = 2\), and were popularized by Don Zagier in the 90’s, who discovered that they satisfy vast numbers of relations. For example, there are \(a \text{ priori} 2^{13} = 8192\) such numbers in weight 15, but in reality they form a vector space over \(\mathbb{Q}\) of dimension at most 28.

Let \(Z\) denote the \(\mathbb{Q}\)-vector space spanned by the numbers (1.1). It is relatively easy to show that \(Z\) is closed under multiplication. The purpose of this talk is to outline a proof of the following two theorems:

**Theorem 1.** The periods of mixed Tate motives over \(Z\) lie in \(Z[2i\pi^{-1}]\).

An obvious question is whether there is a vector space (or algebra) basis for \(Z\) over \(\mathbb{Q}\), and one can try to write down a conjectural basis in each weight and low depth. There were good reasons for thinking (see \(\S3.2\)) that such a basis might have consisted of the set of \(\zeta(n_1, \ldots, n_r)\pi^{2m}\), where all \(n_i\) are odd.

This approach is quickly scuppered by the existence of exceptional relations such as

\[
28 \zeta(3, 9) + 150 \zeta(5, 7) + 168 \zeta(7, 5) = \frac{5197}{691} \zeta(12).
\]

It is the first in an infinite series of identities amongst double zetas which were discovered by Gangl, Kaneko and Zagier, and are related to the period polynomials for cusp forms of weight \(k\) for \(\text{PSL}(2, \mathbb{Z})\). This is the first inkling of the shadow cast by the world of elliptic motives on the multiple zeta values. In order to circumvent this problem, one can instead try to find a conjectural basis in high depth, and indeed this had previously done by M. Hoffman in 1997, who conjectured the following theorem:

**Theorem 2.** Every multiple zeta value of weight \(N\) is a \(\mathbb{Q}\)-linear combination of

\[\{\zeta(a_1, \ldots, a_r) : \text{where } a_i = 2 \text{ or } 3, \text{ and } a_1 + \ldots + a_r = N\}\]

Theorems 1 and 2 are proved simultaneously using motivic multiple zeta values, which are closely related to the motivic fundamental group of \(\mathbb{P}^1 \setminus \{0, 1, \infty\}\). Deligne has recently proved analogous results for \(\mathbb{P}^1 \setminus \{0, \mu_N, \infty\}\), where \(\mu_N\) is the group of \(N\)th roots of unity and \(N = 2, 3, 4, 6, 8\). The situation is rather different, since for these exceptional values of \(N\), exotic relations such as (1.2) do not arise.

2. MZV’S AS PERIODS

In order to see why multiple zeta values are periods, consider the following example:

\[
\zeta(2) = \int_{0 \leq t_1 \leq t_2 \leq 1} \frac{dt_1}{1-t_2} \frac{dt_2}{t_2} \quad \text{(Leibniz)}
\]

It is a period of the moduli space of genus 0 curves with 5 marked points:

\[\mathcal{M}_{0,5} = (\mathbb{P}^1 \setminus \{0, 1, \infty\} \times \mathbb{P}^1 \setminus \{0, 1, \infty\}) \setminus \Delta\]

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where \( \Delta \) denotes the diagonal. Its real points are pictured here.

Let

\[
\omega = \frac{dt_1}{1-t_1} \frac{dt_2}{t_2} \in \Omega^2(M_{0,5}),
\]

which has singularities contained in \( \mathcal{A} = \bigcup_{i=1}^6 A_i \), and let

\[
X = \{0 \leq t_1 \leq t_2 \leq 1\} \subset \mathbb{P}^1 \times \mathbb{P}^1
\]

whose boundary is contained in \( \mathcal{B} = \bigcup_{i=1}^6 B_i \). They define (co-)homology classes:

\[
[w] \in H^2_D(\mathbb{P}^1 \times \mathbb{P}^1, \mathcal{A}) \\
[X] \in H^2_2(\mathbb{P}^1 \times \mathbb{P}^1, \mathcal{B}) \cong H^2(\mathbb{P}^1 \times \mathbb{P}^1, \mathcal{B}')
\]

As a first approximation, one would like to consider the motive \( H^2(\mathbb{P}^1 \times \mathbb{P}^1, \mathcal{B}', \mathcal{B}' \cap \mathcal{A}'\}) \) which is of mixed Tate type. However, for technical reasons (the boundary of \( X \) meets the boundary of \( \mathcal{A} \) at the points \((0, 0)\) and \((1, 1)\)) this is not the correct object. Instead, one must consider

\[
M = H^2(M_{0,5}', \mathcal{A}', \mathcal{B}', \mathcal{B}' \cap \mathcal{A}')
\]

where \( M_{0,5}' \) is the blow-up of \( \mathbb{P}^1 \times \mathbb{P}^1 \) in \((x, x)\), where \( x = 0, 1, \infty \), and \( \mathcal{A}', \mathcal{B}' \) are slightly larger sets of boundary divisors which include the exceptional divisors. One verifies this time that \([w] \in M_{D,R}\) and \([X] \in M_{D,R}', \mathcal{B}' \cap \mathcal{A}'\). Thus the integral (2.1), and hence the number \( \zeta(2) \), is a period of \( M \).

**Idea 1**: Replace the number \( \zeta(2) \in \mathbb{R} \) with the triple \( \zeta^m(2) \overset{\text{def}}{=} (M, [w], [X]) \), or ‘motivic \( \zeta(2) \)’. The period \( \zeta(2) \) can be retrieved from this data simply by integrating \([w]\) over \([X]\), by (2.1)

2.1. **Generalization.** In general, let \( \varepsilon_1, \ldots, \varepsilon_n \in \{0, 1\} \), where \( \varepsilon_1 = 1 \) and \( \varepsilon_n = 0 \). Let

\[
I(0; \varepsilon_1, \ldots, \varepsilon_n; 1) = \int_{0 \leq t_1 \leq \cdots \leq t_n \leq 1} \frac{dt_1}{t_1 - \varepsilon_1} \cdots \frac{dt_n}{t_n - \varepsilon_n}.
\]

It was observed by Kontsevich that (recall \( n_r \geq 2 \)):

\[
\zeta(n_1, \ldots, n_r) = (-1)^r I(0; 10^{n_1-1}10^{n_2-1} \cdots 10^{n_r-1}; 1)
\]

where \( 0^k \) denotes a sequence of \( k \) consecutive zeros. If \( N = n_1 + \cdots + n_r \), then Goncharov and Manin showed as a consequence that (2.2) is a period of \( H^{N+3}(M_{0,N+3}', \mathcal{A}', \mathcal{B}'(\mathcal{A} \cap \mathcal{B})) \), where \( \mathcal{A}, \mathcal{B} \) are unions of distinct boundary divisors of \( M_{0,N+3}' \), the Deligne-Mumford compactification of \( M_{0,N+3} \), and furthermore that this defines an element in the category \( MT(\mathbb{Z}) \) of mixed Tate motives over \( \mathbb{Z} \).

2.2. **Regularization.** One can define \( I(\varepsilon_0; \varepsilon_1, \ldots, \varepsilon_n; \varepsilon_{n+1}) \) for any \( \varepsilon_i \in \{0, 1\} \), where the integral (2.2) formally diverges. It is easily expressible as a \( \mathbb{Z} \)-linear combination of multiple zeta values (1.1).
3. Mixed Tate motives

3.1. Structure of \( MT(\mathbb{Z}) \). Let \( MT(\mathbb{Z}) \) denote the category of mixed Tate motives over \( \mathbb{Z} \). It is an abelian tensor category whose simple objects are the Tate motives \( \mathbb{Q}(n) \), indexed by \( n \in \mathbb{Z} \), and which have weight \(-2n\). The structure of \( MT(\mathbb{Z}) \) is determined by the data:

\[
\text{Ext}^1_{MT(\mathbb{Z})}(\mathbb{Q}(0), \mathbb{Q}(n)) \cong \begin{cases} \mathbb{Q} & \text{if } n \geq 3 \text{ is odd} \\ 0 & \text{otherwise} \end{cases},
\]

and the fact that the \( \text{Ext}^2 \)'s vanish. The dimensions (3.1) come from Borel’s computation of the ranks of the rational algebraic \( K \)-theory of \( \mathbb{Q} \). A better way to think about it is to observe that \( MT(\mathbb{Z}) \) is a Tannakian category with a canonical fiber functor. Thus \( MT(\mathbb{Z}) \) is equivalent to the category of representations of an affine group scheme \( G_{MT} \) over \( \mathbb{Q} \), which is a semi-direct product

\[
G_{MT} \cong \mathcal{G}_{uf} \rtimes \mathbb{G}_m,
\]

where \( \mathcal{G}_{uf} \) is the prounipotent algebraic group over \( \mathbb{Q} \) whose Lie algebra is the free Lie algebra with one generator \( \sigma_{2n+1} \) in degree \(-2n-1 \). The generators correspond to (3.1), and the freeness follows from the vanishing of the \( \text{Ext}^3 \)'s. A variant of Idea 1 is the following rough statement:

**Idea 2:** A period, e.g. a multiple zeta value, defines a function on \( \mathcal{G}_{uf} \).

3.2. Functions on the motivic Galois group. Let \( A_{MT} \) denote the graded ring of affine functions on \( \mathcal{G}_{uf} \) over \( \mathbb{Q} \). It is a commutative graded Hopf algebra. It follows from the remarks above that \( A_{MT} \) is non-canonically isomorphic to the cofree Hopf algebra on cogenerators \( f_{2r+1} \) in degree \( 2r+1 \geq 3 \):

\[
A_{MT} \cong \mathbb{Q}(f_3, f_5, f_7, \ldots).
\]

This has a basis consisting of non-commutative words in the \( f_{2r+1} \)'s. The multiplication on \( A_{MT} \) is given by the shuffle product, and the coproduct \( \Delta : A_{MT} \to A_{MT} \otimes_{\mathbb{Q}} A_{MT} \) is given by deconcatenation:

\[
\Delta(f_{i_1} \cdots f_{i_n}) = \sum_{k=0}^{r} f_{i_1} \cdots f_{i_k} \otimes f_{i_{k+1}} \cdots f_{i_r}.
\]

Define the following trivial comodule over \( A_{MT} \):

\[
H_{MT}^+ = A_{MT} \otimes_{\mathbb{Q}} \mathbb{Q}[f_2],
\]

where \( f_2 \) is of degree 2, and commutes with the \( f_{2r+1} \)’s. We also write the coaction:

\[
\Delta : H_{MT}^+ \to A_{MT} \otimes_{\mathbb{Q}} H_{MT}^+.
\]

It is determined by its restriction to \( A_{MT} \) and the formula \( \Delta(f_2) = 1 \otimes f_2 \). If we set \( d_k = \dim_{\mathbb{Q}} H_{k,MT} \), then one readily verifies that \( d_0 = 1, d_1 = 0, d_2 = 1 \), and

\[
d_k = d_{k-2} + d_{k-3} \text{ for } k \geq 3.
\]

Here, a subscript (e.g. \( \mathcal{Z}_k, H_k^{MT+} \)) denotes the subspace spanned by elements of weight \( k \).

**Example 3.** \( H_k^{MT+} \) is of dimension 4, spanned by \( f_3, f_5, f_3 f_5, f_3^2 f_2, \) and \( f_2^2 \). Compare the space \( \mathcal{Z}_k \) of MZV’s of weight 8, which is spanned by \( \zeta(3, 5), \zeta(3)\zeta(5), \zeta(3)^2\zeta(2), \) and \( \zeta(8) \).

4. Motivic Multiple Zeta Values

The idea is to lift the multiple zeta values \( \zeta(n_1, \ldots, n_r) \) to motivic versions \( \zeta^m(n_1, \ldots, n_r) \), in such a way that the standard relations hold. Using the theory of the motivic fundamental group of \( \mathbb{P}^1 \setminus \{0, 1, \infty\} \), one can show that there exists a graded algebra \( \mathcal{H} \), generated by elements

\[
I^m(\varepsilon_0; \varepsilon_1, \ldots, \varepsilon_n; \varepsilon_{n+1}) \in \mathcal{H} \quad \text{for all} \quad \varepsilon_0, \ldots, \varepsilon_{n+1} \in \{0, 1\},
\]
which we call motivic iterated integrals, such that all the usual properties of iterated integrals hold (shuffle product, reflection formulae, etc). There is a well-defined map called the period,

\[ \text{per} : \mathcal{H} \to \mathbb{R} \]

\[ I^m(\varepsilon_0; \varepsilon_1, \ldots, \varepsilon_n; \varepsilon_{n+1}) \to I^m(\varepsilon_0; \varepsilon_1, \ldots, \varepsilon_n; \varepsilon_{n+1}) . \]

We define the motivic multiple zeta value to be \( \zeta^m(n_1, \ldots, n_r) = (-1)^r I^m(0; 10^{n_1-1} \ldots 10^{n_r-1}; 1) \). Its period is \( \zeta(n_1, \ldots, n_r) \). The coalgebra \( \mathcal{H} \) admits a coaction of \( A^{MT} \) which we describe in \( \S 5 \).

**Proposition 4.** There is a non-canonical embedding of algebra-comodules over \( A^{MT} \)

\[ \mathcal{H} \hookrightarrow \mathcal{H}^{MT} \]

which maps \( \zeta^m(2) \) to \( f_2 \), and \( \zeta^m(2n + 1) \) to \( f_{2n+1} \) for all \( n \geq 1 \).

The motivic formalism is very powerful. For instance, the proposition immediately implies that

\[ \dim_Q Z_k \leq \dim_Q \mathcal{H}_k \leq \dim_Q \mathcal{H}_k^{MT} = d_k \]

where the numbers \( d_k \) are defined by (3.4). This upper bound was first proved independently by Goncharov and Terasoma, proving one half of Zagier’s conjecture, which states that \( \dim_Q Z_k = d_k \).

5. THE COACTION

What we gain in passing to motivic multiple zeta values is the coaction of \( A^{MT} \). Let \( A = \mathcal{H}/\zeta^m(2) \), and denote the quotient map by \( \pi : \mathcal{H} \to A \). The following formula is a refinement of a formula due to Goncharov and Terasoma, proving one half of Zagier’s conjecture, which states that \( \dim_Q Z_k = d_k \).

**Proposition 5.** The coaction \( \Delta : \mathcal{H} \to A \otimes_Q \mathcal{H} \) can be computed explicitly as follows. For any \( a_0, \ldots, a_{n+1} \in \{0, 1\} \), the image of a generator \( \Delta I^m(a_0; a_1, \ldots, a_n; a_{n+1}) \) is given by

\[ \sum_{i_0 < i_1 < \ldots < i_k < i_{k+1}} \pi \left( \prod_{p=0}^{k} I^m(a_{i_p}; a_{i_p+1}, \ldots, a_{i_{p+1}}-1; a_{i_{p+1}}) \right) \otimes I^m(a_0; a_1, \ldots, a_k; a_{n+1}) \]

where the sum is over indices satisfying \( i_0 = 0 \) and \( i_{k+1} = n + 1 \), and all \( 0 \leq k \leq n \). The left-hand side of the coproduct is viewed modulo \( \zeta^m(2) \). Note that \( I^m(a; b) \) is defined to be 1 for all \( a, b \in \{0, 1\} \).

The following diagram illustrates a typical term in the formula:

![Diagram](image)

\[ \pi \left( I^m(\varepsilon_0; \varepsilon_1; \varepsilon_2) I^m(\varepsilon_3; \varepsilon_4; \varepsilon_5; \varepsilon_6) I^m(\varepsilon_7; \varepsilon_8) \right) \otimes I^m(\varepsilon_0; \varepsilon_3; \varepsilon_6; \varepsilon_8) \]

6. THE HOFFMAN BASIS

**Main Theorem 6.1.** The following elements are linearly independent:

\[ \{ \zeta^m(a_1, \ldots, a_r) \text{ where } a_i = 2 \text{ or } 3 \} \subset \mathcal{H} . \]
Let \( H^{2,3} \) denote the \( \mathbb{Q} \)-linear span of the elements (6.1). We have
\[
(6.2) \quad H^{2,3} \subseteq H \subseteq H^{MT+}
\]
The main theorem implies that
\[
\dim_{\mathbb{Q}} H^{2,3}_N = \# \{ (a_1, \ldots, a_r) : a_i = 2 \text{ or } 3 \text{ and } a_1 + \ldots + a_r = N \}
\]
The number on the right-hand side is clearly equal to the integer \( d_N = \dim_{\mathbb{Q}} H^{MT+}_N \), by (3.4). It follows that \( \dim_{\mathbb{Q}} H^{2,3}_N = \dim_{\mathbb{Q}} H^{MT+}_N \) and we have equalities in (6.2). There are two consequences:

**Corollary 6.** \( H^{2,3} = H \). In other words, every motivic multiple zeta value \( \zeta^m(n_1, \ldots, n_r) \) is a \( \mathbb{Q} \)-linear combination of elements of the form (6.1) with indices 2 or 3.

By taking the period map, this implies that every multiple zeta value is a \( \mathbb{Q} \)-linear combination of Hoffman elements, and hence implies theorem 2.

**Corollary 7.** \( H = H^{MT+} \).

Equivalently, the category of mixed Tate motives over \( \mathbb{Z} \) is spanned by the motivic fundamental group of \( \mathbb{P}^1 \setminus \{0, 1, \infty\} \), as conjectured by Deligne and Ihara. On taking the period map, it implies theorem 1.

7. **Some ideas of the proof of the main theorem**

1. Introduce the level filtration on \( H^{2,3} \), defined by

\[
F_\ell H^{2,3} = \mathbb{Q}(\zeta^m(a_1, \ldots, a_n) : a_i = 2 \text{ or } 3 \text{ and at most } \ell \text{ indices } a_i = 3).
\]

The proof of the independence of (6.1) is by induction on the level.

2. Surprisingly, the subspace \( H^{2,3} \), and the level filtration, are motivic. In other words:

\[
\Delta : F_\ell H^{2,3} \rightarrow A \otimes_{\mathbb{Q}} F_\ell H^{2,3}.
\]

3. The formula (5.1) for the coaction is unwieldy and complicated. It is considerably simplified if one passes to the infinitesimal coaction. For this, let \( \mathcal{L} = A_{>0}/A_{\geq 0}A_{>0} \), and set
\[
D : H \xrightarrow{\Delta} A \otimes_{\mathbb{Q}} H \xrightarrow{\Delta} \mathcal{L} \otimes_{\mathbb{Q}} H
\]

4. Analyze what happens in levels 0 and 1. In level 0, we have \( F_0 H^{2,3} = \{ \zeta^m(2, \ldots, 2) \} \). One shows that \( \zeta^m(2, \ldots, 2) = \frac{\zeta^m}{(n+m)!} \zeta^m(2)^n \) and so maps to 0 in \( A \). In level 1, the elements are

\[
F_1 H^{2,3} = \{ \zeta^m(\underbrace{2, \ldots, 2}_a, 3, \underbrace{2, \ldots, 2}_b) \}
\]

One shows that there exist constants \( c_{a,b} \in \mathbb{Q} \) and \( a_1 \in \mathbb{Q} \) such that

\[
\zeta^m(2, \ldots, 2, 3, 2, \ldots, 2) = c_{a,b} \zeta^m(2a + 2b + 3) + \sum_{i=1}^{a+b} a_1 \zeta^m(2i + 1) \zeta^m(2, \ldots, 2)_{2(a+b+1-i)}
\]

The coefficients \( c_{a,b} \) have to be computed analytically: see §8 for this part of the story.

5. Look at the infinitesimal coaction on the associated graded of \( H^{2,3} \) for the level filtration. In each weight \( N \), and level \( \ell \), (7.1) defines an operator which lowers the level:

\[
D_{N,\ell} : \text{gr}^F_{\ell} H^{2,3}_N \rightarrow \bigoplus_{i \geq 1} \text{gr}^F_{\ell-1} H^{2,3}_{N-2i-1}
\]

The bulk of the work consists in showing that \( D_{N,\ell} \) is injective. This follows from 2-adic properties of the coefficients \( c_{a,b} \), which follow from Zagier’s theorem. Theorem 6.1 follows from the injectivity of the \( D_{N,\ell} \): take a non-trivial relation between the elements (6.1) which is of minimal level. Applying \( D_{N,\ell} \) gives a non-trivial relation of smaller level, which gives a contradiction.
8. Zagier’s theorem

To see why the coaction alone is insufficient to determine the full structure of the motivic multiple zeta values, consider the following example in weight 5. The vector space $H^{MT}_5$ is spanned by two elements: $f_5$ and $f_3f_2$, and likewise $H_5$ is also of dimension two, spanned by $\zeta^m(5)$ and $\zeta^m(3)\zeta^m(2)$. The Hoffman elements of weight 5 are $\zeta^m(2, 3)$ and $\zeta^m(3, 2)$, so we know that

$$\zeta^m(3, 2) = c_{32} \zeta^m(5) + d_{32} \zeta^m(3)\zeta^m(2)$$
$$\zeta^m(2, 3) = c_{23} \zeta^m(5) + d_{23} \zeta^m(3)\zeta^m(2)$$

for some coefficients $c_{23}, c_{32}, d_{23}, d_{32} \in \mathbb{Q}$. The coaction tells us that $d_{23} = 3, d_{32} = -2$ but gives us no information about the coefficients $c_{23}, c_{32}$. They can be computed by taking a regulator map.

Thus to determine $c_{23}$, for example, take the period map, which gives:

$$c_{23} = \frac{\zeta(2, 3) - 3 \zeta(3)\zeta(2)}{\zeta(5)} = \frac{-11}{2}.$$

By a similar computation, one can show that $c_{32} = 9/2$. The injectivity of $D_{5,1}$ in this case is equivalent to the invertibility of the following matrix:

$$\left( \begin{array}{cc} c_{32} & d_{32} \\ c_{23} & d_{23} \end{array} \right) = \left( \begin{array}{cc} 9/2 & -2 \\ 11 & 3 \end{array} \right).$$

8.1. Zagier’s theorem. The missing ingredient is provided by the following theorem.

**Theorem 8.** (Don Zagier 2010). Let $a, b \geq 0$. Then

$$\zeta\left(\overbrace{2, \ldots, 2}^{a}, \overbrace{3, 2, \ldots, 2}^{b}\right) = 2 \sum_{r=1}^{a+b+1} (-1)^r \left( \frac{2r}{2a+2} - (1 - 2^{-2r}) \left( \frac{2r}{2b+1} \right) \right) \zeta(2r+1) \zeta(2, \ldots, 2).$$

His proof is quite remarkable. First he defines the two generating series

$$F(x, y) = \sum_{a, b \geq 0} (-1)^{a+b+1} Z(a, b) x^{2a+2} y^{2b+1}$$
$$F^*(x, y) = \sum_{a, b \geq 0} (-1)^{a+b+1} Z^*(a, b) x^{2a+2} y^{2b+1},$$

where $Z(a, b)$ denotes the left-hand side of the equation in theorem 8, and $Z^*(a, b)$ is the right-hand side. He then shows: first, that the generating function $F(x, y)$ can be expressed as the product of a sine function and the derivative of an $_3F_2$-hypergeometric function, and second, that the generating function $F^*(x, y)$ is a linear combination of fourteen functions which are products of the sine function and a digamma function. These two expressions are seemingly totally unrelated. Nevertheless, he shows that

- $F(x, x) = F^*(x, x)$ for all $x \in \mathbb{C}$
- $F(n, y) = F^*(n, y)$ for all $n \in \mathbb{N}$ and $y \in \mathbb{C}$
- $F(x, n) = F^*(x, n)$ for all $n \in \mathbb{N}$ and $x \in \mathbb{C}$

The last two identities are completely non-trivial. Finally, by bounding the growth of the functions $F(x, y)$ and $F^*(x, y)$, one can show using a variant of the Phragmén-Lindelöf theorem that these properties are enough to conclude that $F(x, y) = F^*(x, y)$ for all $x, y \in \mathbb{C}$, which completes the proof.