Where do the tedious products of $\zeta$’s come from?

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Lamentably, the full analytical content of the $\varepsilon$-expansion of the master two-loop two-point function, with arbitrary self-energy insertions in $4-2\varepsilon$ dimensions, is still unknown. Here we show that multiple zeta values (MZVs) of weights up to 12 suffice through $O(\varepsilon^9)$. Products of primitive MZVs are generated by a processes of “pseudo–exponentiation” whose combinatorics faithfully accord with expectations based on Kreimer’s modified shuffle product and on the Drinfeld–Deligne conjecture. The existence of such a mechanism, relating thousands of complicated rational numbers, enables us to identify precise and simple combinations of MZVs specific to quantum field theories in even numbers of spacetime dimensions.

1. Master two–loop two–point function

The object of study in this contribution is the two–loop integral

$$I = \frac{\hat{P}^2(D/2-\alpha_6)}{\pi^D} \int \frac{d^Dk d^Dl}{P}$$

(1)

with $\alpha_6 \equiv 3D/2-\alpha_1-\alpha_2-\alpha_3-\alpha_4-\alpha_5$ determining the dependence on the number, $D = 4-2\varepsilon$, of spacetime dimensions. It is clearly independent of the norm, $p^2$, of the external momentum $p$. Remarkably, it has a 1440–element symmetry group $[\mathbb{Z}]$, corresponding to all permutations of 6 linear combinations $[\mathbb{Z}]$ of the indices $\alpha_j$, combined with the total reflection $\alpha_j \to D/2-\alpha_j$.

With parameters $\alpha_j = 1+n_j\varepsilon$, resulting from insertions on internal lines, the Taylor expansion of $I = 6\zeta(3) + O(\varepsilon)$ is known $[\mathbb{Z}]$ to involve multiple zeta values.

The MZV $\zeta(5,3) \equiv \sum_{m \geq n > 0} 1/m^5 n^3$, with weight 8 and depth 2, appears in $I$ at order $\varepsilon^5$ and is also present in the six–loop beta function of $\phi^4$ theory $[\mathbb{Z}]$.

Similarly, $\zeta(3,5,3) \equiv \sum_{l \geq m \geq n > 0} 1/l^3 m^5 n^3$, with weight 11 and depth 3, appears at order $\varepsilon^8$ and in $\phi^3$ theory at 7 loops.

In general, we expect $L$–loop counterterms to include MZVs of weights $w \leq 2L-3$, of which the expansion of $I$ through order $\varepsilon^{2L-6}$ is to be taken as a strong diagnostic.

It is one of the many scandals of our limited understanding of the analytical content of perturbative quantum field theory (QFT) that, despite many years of intense effort, we still do not know whether MZVs suffice for even the Taylor expansion of the two–loop integral $[\mathbb{Z}]$.

Here we exhibit remarkable structure in the dependence of the $\sum_{k=0}^9 \left(\frac{k^9}{5^{k}}\right) = 5005$ Taylor coefficients through $O(\varepsilon^9)$ on the

$$1 + 1 + 2 + 2 + 3 + 4 + 5 + 7 + 9 + 12 = 46$$

independent MZV structures from weight 3 to 12. In particular, MZV structures that are imprimitive products will be generated by a process of “pseudo–exponentiation” whose very existence appears to me to be little short of miraculous and whose details resonate strongly both with Dirk Kreimer’s combinatorically modified shuffle product, discussed in these proceedings, and also with the Drinfeld–Deligne conjecture, namely that the Grothendieck–Teichmüller algebra has precisely one generator of each odd degree greater than unity, and none of even degree.

2. Choices of primitive MZVs

As Don Zagier observed, the Drinfeld–Deligne conjecture leads to an enumeration $P(n) = P(n-2) + P(n-3)$ of $\mathbb{Q}$–linearly (i.e. rationally) independent MZV structures of weight $n$, seeded by $P(1) = 0$, $P(2) = P(3) = 1$. This generates the
Padovan numbers $P(3)$ to $P(12)$ in \( [3] \). The filtration of products into primitives then requires

\[
M(w) = \frac{1}{w} \sum_{n|w} \mu(w/n)Q(n)
\]  (4)

primitives to be chosen at weight \( w \), where \( Q(n) = Q(n - 2) + Q(n - 3) \) is the Perrin sequence, seeded by \( Q(1) = 0, Q(2) = 2, Q(3) = 3 \), and the M"obius function \( \mu \) ensures that

\[
\prod_{n>0} (1-x^n)^{-M(n)} = \frac{1}{1-x^2-x^3}.
\]  (5)

At weight \( w = 2 \) we have the primitive \( \pi^2 \) (which mathematicians sometimes relate to \( w = 0 \)) and at each odd weight \( 2n + 1 > 1 \) we have the primitive \( \zeta(2n+1) \). That leaves us with one more primitive MZV to choose at each of the weights 8, 10 and 11. We might take these as \( \zeta(6,2), \zeta(8,2) \) and \( \zeta(8,2,1) \). At weight \( w = 12 \) we need a primitive of depth 2, such as \( \zeta(10,2) \), and one of depth 4, such as \( \zeta(4,2,2,2) \).

From a mathematical point of view, these are entirely adequate choices of primitives, since every MZV of weight \( w \leq 12 \) is expressible as a rational linear combination of products of the filtration.

However, we are concerned here with QFT, where more specific combinations of MZVs are found to occur in counterterms \( [3] \). I shall sketch how I was led, by Kreimer’s fertile ideas \([5,6,7]\), and by the Drinfeld–Deligne conjecture, to the following set of QFT primitives up to weight 12.

1. At weights \( w = 2, 3, 5, 7, 9, 11 \), take \( \zeta(w) \).
2. At \( w = 8 \), take \( \zeta(5,3) \).
3. At \( w = 10 \), take \( \zeta(7,3) + 3\zeta^2(5) \).
4. At \( w = 11 \), take \( \zeta(3,5,3) - \zeta(3)\zeta(5,3) \).
5. At \( w = 12 \), take \( \zeta(7,5) \) and the combination of alternating Euler sums below.

The choice of a second primitive at weight 12 is

\[
Z_2(12) = \zeta(7,5) - \zeta(5,7) + \zeta(5)\zeta(7)
\]  (6)

comprising Euler sums of the form

\[
\zeta(\bar{\pi}, b) = \sum_{m>n>0} \frac{(-1)^m}{m^n} \frac{1}{n^b}
\]  (7)

\[
\zeta(\pi) = \sum_{n>0} \frac{(-1)^n}{n^n} = (2^{1-a} - 1)\zeta(a)
\]  (8)

with alternation of sign notated by a bar above the corresponding index.

With these very specific choices, products in the Taylor expansion of \( [4] \) through order \( \varepsilon^9 \) will be generated by pseudo–exponentiation. The choice of primitives which makes this possible is essentially unique. The existence of such a choice is truly remarkable. For example, the choice of primitive in \( [3] \) was determined by a tiny subset of the available data, whereupon transformation to the appropriate basis reduced a file of many megabytes of tedious products of \( \zeta \)’s to a single line of code.

3. The master function

The key to the expansion of \( [4] \) is the function \( [3] \)

\[
S(a, b, c, d) = \frac{\pi \cot \pi c}{H(a, b, c, d)} - \frac{1}{c} - \frac{b + c}{bc} F(a + c, -b, -c, b + d) \]  (9)

with a hypergeometric series of the form

\[
F(a, b, c, d) = \sum_{n=1}^{\infty} \frac{(-a)_n (-b)_n}{(1 + c)_n (1 + d)_n}, \]  (10)

where \( (a)_n \equiv \Gamma(a + n)/\Gamma(a) \), and with a ratio of products of Gamma functions of the form

\[
H(a, b, c, d) = \frac{G\{a, b, c, d, a + b + c + d\}}{G\{a + c, a + d, b + c, b + d\}} \]  (11)

where \( G(S) \equiv \prod_{a \in S} \Gamma(1 + a) \).

If the propagators in two adjacent internal lines of the master two–loop diagram have unit exponents (i.e. no dressing by self–energy insertions) then the recurrence relations from integration by parts may be solved in terms of two instances \([3]\) of the construct \( [4] \), which solves

\[ aS(a, b, c, d) = 1 + \frac{(a + c)(a + d)}{a + b + c + d} S(a - 1, b, c, d) \]
in the presence of the symmetries
\[ S(a, b, c, d) = S(b, a, c, d) = -S(c, d, a, b). \] (12)

Moreover, the 1440-fold symmetry of the master diagram enables one to reconstruct the 9th-order Taylor expansion of \( I \), with 6 arguments, from the 11th-order expansion of \( S \), with only 4 arguments. If there is any new type of number, beyond the MZVs that are generated by the \( \varepsilon \)–expansions of Pochhammer symbols in \([4]\), then it will show up only at weights greater than 12.

4. Pushdown at weight 12

The technology for developing the Taylor expansion of \( S \) through weight 11 was developed in [3]. At weight 12 we now encounter a remarkable phenomenon: the depth–4 MZV \( \zeta(4, 4, 2, 2) \) is primitive within the confines of the theory of MZVs, but widening the analysis to include alternating Euler sums, one discovers that it may be eliminated in favour of a depth–2 sum, such as
\[ \zeta(\overline{9}, \overline{3}) = \sum_{m>n>0} (-1)^{m+n}/(m^3 n^3). \]
Specifically, the combination \( \zeta(4, 4, 2, 2) - (8/3)^3 \zeta(\overline{9}, \overline{3}) \) is reducible to 11 weight–12 terms in the MZV basis, thus showing that \( \zeta(\overline{9}, \overline{3}) \) can furnish the 12th.

Here one sees another scandal of our limited understanding. This “pushdown” from depth–4 MZVs to depth–2 Euler sums was found empirically using David Bailey’s implementation of Helaman Ferguson’s PSLQ algorithm, which turns high precision numerical evaluations into immensely probable integer relations. In this case, the effort was infinitesimal, in comparison with the PSLQ investigations in [8]. Nevertheless, no-one seems to have any idea of how to prove such pushdowns rigorously, apart from labouring to solve the huge complex of linear relations between \( 3^{12} = 531441 \) words of 12 letters, taken from the alphabet \( A = dx/x, B = dx/(1-x), C = -dx/(1+x) \) for the iterated integrals corresponding to Euler sums.

In terms of CPUtime, it takes but a second of PSLQ work to find the simple coefficient \((8/3)^3\) of \( \zeta(\overline{9}, \overline{3}) \) in the pushdown of \( \zeta(4, 4, 2, 2) \). Yet it would appear to require a huge expense of computer algebra, feasible perhaps only with Jos Vermaseren’s FORM, to obtain this reduction by systematic application of the shuffle algebras of nested sums and iterated integrals in the \( \{A, B, C\} \) alphabet \([\overline{9}, \overline{3}]\).

To develop the Taylor expansion of \( S \) to weight 12, PSLQ was used to find 139 such reductions of MZVs to a basis involving \( \zeta(\overline{9}, \overline{3}) \).

5. Pseudo–exponentiation

After achieving the pushdown to depth 2, one is left with something that seems hugely indigestible, namely the reduction of \( \sum_{k=1}^{11} \binom{\overline{3}+k}{3} = 1364 \) Taylor coefficients of \( S \) to \( \mathbb{Q} \)–linear combinations of \( \sum_{k=1}^{11} P(k+1) = 47 \) terms formed by products of primitives. The data comprises many thousands of rational numbers which are typically the ratios of 10–digit integers. Some reduction of this complexity is achieved by using the symmetries \([4]\). For example the leading term in \( S(a, b, c, d) \) is simply \((a+b+c-d)\zeta(2)\) and this cancels when one combines the two instances of \( S \) in \( I = 6\zeta(3) + O(\varepsilon) \). Even after taking account of such obvious symmetries, several thousand product terms remain to be explained.

Discussion with Dirk Kreimer suggested that perhaps some of the tedious products of primitives might follow a pattern. The basic idea was that some simple structure might be delicately “composed” with an expression relatively free of such products, so that, for example, one might write \( S = E \cap R \), where \( E \) is made of Gamma functions (and hence exponentiates a series of \( \zeta \)'s), \( R \) is far simpler than \( S \), and the rule of composition, denoted by \( \lor \), has the distinctive QFT property of counting like objects and then modifying the ordinary process of multiplication by an appropriate symmetry factor.

There was an obvious candidate for \( E \): the reciprocal of \( H \) in the first term of \([3]\), corresponding to exponentiation of
\[ -\log H(a, b, c, d) = \sum_{s>1} (-1)^s \zeta(s) \frac{N(s) - D(s)}{s}, \]
\[ N(s) = a^s + b^s + c^s + d^s + (a + b + c + d)^s, \]
\[ D(s) = (a + c)^s + (a + d)^s + (b + c)^s + (b + d)^s. \]
However it soon became clear that the powers of \( \pi^2 \) in \( \log H \) can play no role in the composi-
tion \( E \lor R \). This seemed to chime well with the Drinfeld–Deligne conjecture. Hence the Ansatz
\[
E(a, b, c, d) = \left( \frac{H(-a, -b, -c, -d)}{H(a, b, c, d)} \right)^{1/2} \tag{13}
\]
was made, since it exponentiates only odd \( \zeta \)'s.

The challenge was then to find a product–free expansion of the form
\[
R(a, b, c, d) = \sum_{w=2}^{12} \zeta(w) J_w(a, b, c, d) + \sum_{w=8, 10, 11} Z(w) K_w(a, b, c, d) + \sum_{k=1, 2} Z_k(12) K_{12,k}(a, b, c, d) \tag{14}
\]

involving the 11 single sums \( \zeta(w) = \sum_{n \geq 0} 1/n^w \), with \( w \in [2, 12] \), a single additional primitive MZV at each of the weights \( w = 8, 10, 11 \), and two such primitives at \( w = 12 \). Since all 16 of these terms are present in \( S \), and \( E = 1 + O(\varepsilon^3) \) does not exponentiate powers of \( \pi^2 \), this is the minimal product–free Ansatz for \( R \). What was far from clear is that there exists a well–defined procedure \( E \lor R \) that can generate the remaining \( 47 - 16 = 31 \) product structures in \( S \) from the \( 11 + 5 = 16 \) single–sum and primitive terms in \( R \). Bearing in mind that a weight–\( w \) product term in \( S \) entails all \( \binom{w+2}{3} \) monomials of degree \( w - 1 \) in 4 variables, the odds against finding a composition procedure appeared at first so overwhelming as to make such an enterprise foolish.

However, following the well tried maxim that “QFT is far smarter than we are”, I looked to see what happens when one takes the composition to be that of simple multiplication. This faithfully reproduced product terms such as \( \zeta(3) \zeta(2) \) and \( \zeta(3) \zeta(4) \), but to Dirk Kreimer’s great delight gave the wrong result for \( [\zeta(3)]^2 \), whose true dependence on the 56 monomials of 5th order in 4 variables is proportional to \((N(3) - D(3))J_3\) yet has precisely half the coefficient that would be predicted by straightforward multiplication. In other words the composition \( E \lor R \) must take account of symmetry factors: if \( [\zeta(n)]^p/p! \) from the exponential \( E \) is composed with \( \zeta(n) \) from the product–free expansion \( R \), the contribution to \( E \lor R \) must be taken as \([\zeta(n)]^{p+1)/(p+1)!\). Thus to generate the 165 monomials in the \([\zeta(3)]^3 \) term of \( S \) we must modify the result of naive multiplication by the factor \( 2!/3! = 1/3 \). That aspect of pseudo–exponentiation had been eagerly anticipated.

A second aspect came as a surprise, though in retrospect it signals that QFT is in deep accord with the Drinfeld–Deligne conjecture. The first example occurs at weight 8, where we know that we must include a new primitive, such as \( \zeta(5, 3) \), in \( Z(8) \). To a mathematician, such a primitive could include an arbitrary rational multiple of \( \zeta(5) \zeta(3) \). But we seek to generate all monomials found to be multiplying \( \zeta(5) \zeta(3) \) in \( S \), using the composition \( E \lor R \). There are, at most, three sources: \( \zeta(5) \lor \zeta(3), \zeta(3) \lor \zeta(5) \) and, possibly, a multiple of \( \zeta(5) \zeta(3) \) from \( 1 \lor Z(8) \). The functional dependencies on \( a, b, c, d \) of all three contributions are predetermined; we have just three rational numbers at our disposal to fit 120 monomials. A solution exists and it is unique: everything is given by \( \zeta(3) \lor \zeta(5) \).

It appears that the QFT expansion “knows more than we do” about the structure of MZVs. Faced with a choice between \( \zeta(5) \lor \zeta(3) \) and \( \zeta(3) \lor \zeta(5) \) it rejects the former and takes naive multiplication as the composition rule for the latter. For good measure it tells us that the new primitive is \( Z(8) = \zeta(5, 3), \) modulo \( \pi^8 \), with no contribution from \( \zeta(5) \zeta(3) \). Note that we would get an unambiguously wrong answer were we to take the primitive as \( \zeta(3, 5) \).

The situation becomes yet more interesting at weight 10, where \( \zeta(7) \lor \zeta(3) \) is rejected, \( \zeta(3) \lor \zeta(7) \) is accepted, as a plain multiplication, and the primitive is determined to be \( Z(10) = \zeta(7, 3) + 3\zeta^2(5), \) modulo \( \pi^{10} \), with no possibility of \( \zeta(7) \zeta(3) \) appearing in this primitive. Here one sees the monomials in the \([\zeta(5)]^2 \) term of \( S \) generated by the sum of two terms: \((N(5) - D(5))J_5 \) and \( K_{10} \), each of which was predetermined. The former is normalized, as expected, by taking account of the factor of \( 1/2 \) in pseudo–exponentiation; for the latter we have only a single rational number, with which to fit 220 monomials, and the coefficient 3 in \( \zeta(7, 3) + 3\zeta^2(5) \) emerges in every case.
At weight 11, the working out is even more impressive: \( [\zeta(3)]^3 \vee \zeta(5) \) and \( \zeta(3) \vee \zeta(5,3) \) are present, as naive multiplications; \( (\zeta(5) \zeta(3)) \vee \zeta(3) \) is rejected; and the primitive is given for each of the 286 monomials as the combination \( Z(11) = \zeta(3,5,3) - \zeta(3) \zeta(5,3) \), in precise accord with analysis of subdivergence–free 7–loop counterterms [6].

6. Experimentum crucis

Finally, QFT seems to “know more than we do” about pushdown of depth–4 MZVs to depth–2 alternating Euler sums at weight 12. There still remain several hundred rational numbers to be generated by a procedure that is now unambiguous: \( [\zeta(3)]^3 \vee \zeta(3) = [\zeta(3)]^3/4 \) is combinatorically modified, à la Kreimer, and \( \zeta(7) \vee \zeta(5) = 0 \), \( \zeta(9) \vee \zeta(5) = 0 \), are rejected, à la Drinfeld-Deligne, in favour of a pair of primitives. Taking the first as \( Z_1(12) = \zeta(7,5) \) we then determine the second, \( Z_2(12) \), modulo the first, and modulo \( \pi^{12} \). It is forced to contain all 10 of the remaining MZV structures in a basis that includes \( \zeta(4,4,2,2) \). Moreover the coefficients of these terms have numerators of typically 10 digits.

When we push \( \zeta(4,4,2,2) \) down to depth 2, via its empirical PSLQ relation to \( \zeta(9,3) \), some sanity emerges, since the terms in \( Z_2(12) \) now involve only double sums and products of two single sums. Yet still there are apparently grotesque rational coefficients. Finally, we discovered that this seemingly random assortment of terms is simply given by [8], with 3 terms whose coefficients are \( \pm 1 \), though the simplicity of \( \zeta(7) \zeta(5) = 945 \zeta(7) \zeta(5)/1024 \) would have been disguised had we not transformed to a product of alternating sums.

It is as if QFT were taunting us with our ignorance of the mapping between diagrams and numbers that results from the Feynman rules. A vast quantity of data, collected by painfully inadequate methods, collapses to an amazingly simple answer. We are, physicists and mathematicians alike, stumbling on the edge of a structure that is far more refined than the clumsy methods by which we investigate it. In this particular instance, it was the sheer volume of apparently random – yet in fact gracefully proportioned – data, from many numerical instances of self–energy dressings, that led to an answer to the question posed in the title of this contribution.

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