

# ITERATED INTEGRALS IN QUANTUM FIELD THEORY

ABSTRACT. These notes are based on a series of lectures given to a mixed audience of mathematics and physics students at Villa de Leyva in Colombia. The first half is an introduction to iterated integrals and polylogarithms, with emphasis on the case  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . The second half gives an overview of some recent results connecting them with Feynman diagrams in perturbative quantum field theory.

## 1. INTRODUCTION

The theory of iterated integrals was first invented by K. T. Chen in order to construct functions on the (infinite-dimensional) space of paths on a manifold, and has since become an important tool in various branches of algebraic geometry, topology and number theory. It turns out that this theory makes contact with physics in (at least) the following ways:

- (1) The theory of Dyson series
- (2) Conformal field theory and the KZ equation
- (3) The Feynman path integral and calculus of variations
- (4) Feynman diagram computations in perturbative QFT

The relation between Dyson series and Chen's iterated integrals is more or less tautological. The relationship with conformal field theory is well-documented, and we discuss a special case of the KZ equation in these notes. The relationship with the Feynman path integral is perhaps the deepest and most mysterious, and we say nothing about it here. Our belief is that a complete understanding of the path integral will only be possible via the perturbative approach, and by first understanding the relationship with (2) and (4). Thus the first goal of these notes is to try to explain why iterated integrals should occur in perturbative quantum field theory.

Our main example is the thrice punctured Riemann sphere  $M = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ . The iterated integrals on  $M$  can be written in terms of multiple polylogarithms, which are functions which go back to Poincaré and Lappo-Danilevsky and defined for integers  $n_1, \dots, n_r \in \mathbb{N}$  by

$$(1.1) \quad \text{Li}_{n_1, \dots, n_r}(z) = \sum_{0 < k_1 < \dots < k_r} \frac{z^{k_r}}{k_1^{n_1} \dots k_r^{n_r}}.$$

This sum converges for  $|z| < 1$  and has an analytic continuation to a multivalued function on  $\mathbb{C} \setminus \{0, 1\}$ . The monodromy of these functions can be expressed in terms of multiple zeta values, which were first discovered by Euler, and given by

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

where now  $n_r \geq 2$  to ensure convergence of the sum. Polylogarithms, and especially multiple zeta values, have undergone a huge renewal of interest in recent years due to their appearance in many branches of geometry and number theory, but especially in particle physics. The remarkable fact is that (1.1) and (1.2) suffice to express the Feynman amplitudes for a huge number of different processes at low loop orders, and

the particle physics literature is filled with complicated expressions involving them. One can therefore say that the iterated integrals on the *single space*  $M$  generates a class of numbers and functions which are sufficient to express almost all perturbative quantum field theory at low loop orders.

It is unfortunate, (perhaps owing to a lack of communication) that various subclasses and variants of the functions (1.1) were rediscovered in their own right by physicists in an ad hoc manner, and go by the name of classical, Nielsen or harmonic polylogarithms, amongst others. However, the general theory of iterated integrals gives a single class of functions which are universal in a certain sense (the salient property is having unipotent monodromy), contains all these classes, and has better properties. Thus the second goal of these notes is to present a systematic treatment of polylogarithms from this more general viewpoint, which we hope may be of use to working physicists.

In the second half of these notes, we give an overview of the mysterious appearance of multiple zeta values in calculations in perturbative quantum field theory, and suggest that the reason for this, at least at low loop orders, comes from this same unipotency property. However, the general number-theoretic content of perturbative quantum field theories is very far from being understood, and we hope that an account of this might also be of interest to mathematicians.

Finally, it is important to mention that we have made very little use of cohomology or the theory of motives, for reasons of space. A more sophisticated approach would require a detailed explanation of the theory of mixed Tate motives, and also the close relation between algebraic geometry and Feynman integrals as in [2]. However, it turns out a posteriori that the mixed Tate motives only occur insofar as they are the motives of the fundamental group of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ , so in fact they can be cut out of the story altogether in a first approximation.

**1.1. Overview of the lectures.** The first five sections §2 – §6 approximately correspond to one lecture each and give a standard and purely mathematical account of iterated integrals. Since it is almost certainly impossible to improve on the many excellent survey articles (e.g. [8], [9], [12],[13]) on this topic, we have tried to shift the emphasis to the specific example of the punctured Riemann sphere  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  and relate the general structures to the theory of polylogarithms. Another reason for this is that the iterated integrals on punctured Riemann surfaces of higher genus are still not known, and the genus 0 case is one of the very few examples of manifolds where all the constructions can be made explicit.

The final section §7 is an expanded version of various talks on numbers and periods in quantum field theory given at Villa de Leyva, Durham, Berlin and Paris and is more or less independent from the previous lectures. Owing to the rapidly expanding nature of this topic, a complete survey is both inappropriate at this point in time and probably impossible, so the presentation is very biased by our own recent work in this direction.

## 2. DEFINITION AND FIRST PROPERTIES OF ITERATED INTEGRALS

We motivate the definition of iterated integrals by recalling Picard's method for solving a system of ordinary linear differential equations by successive approximation. We then state some first properties of iterated integrals.

**2.1. Picard integration.** Let  $A(t)$  be a  $n \times n$  matrix of continuous functions defined on an open subset  $U$  of  $\mathbb{R}$ , and consider the system of linear differential equations:

$$(2.1) \quad \frac{d}{dt}X(t) = A(t)X(t), \quad t \in U,$$

with some initial condition  $X(t_0) = X_0$ , where  $t_0 \in U$ , and  $X_0$  is some  $n \times n$  matrix. The differential equation (2.1) is equivalent to the integral equation

$$(2.2) \quad X(t) - X_0 = \int_{t_0}^t A(s)X(s)ds.$$

Picard's method for solving this differential system is by successive approximation. We denote by  $X_0(t)$  the constant function  $t \mapsto X_0$ , and define

$$X_{n+1}(t) = X_0(t) + \int_{t_0}^t A(s)X_n(s)ds \quad \text{for } n \geq 0.$$

If the limit  $\lim_{n \rightarrow \infty} X_n(t)$  were to exist, then it would give a solution to the original problem (2.1). The first couple of terms are:

$$\begin{aligned} X_1(t) &= X_0 + \int_{t_0}^t A(s)ds X_0, \\ X_2(t) &= X_0 + \int_{t_0}^t A(s)ds X_0 + \int_{t_0}^t A(s) \int_{t_0}^s A(s')ds' X_0 \end{aligned}$$

Assuming  $t_0 < t$ , the second term in the previous equation can be written as

$$\int_{t_0 \leq s_1 \leq s_2 \leq t} A(s_2)A(s_1)ds_1ds_2 X_0.$$

Continuing in the same way, we can formally write the limit  $X(t) = \lim_{n \rightarrow \infty} X_n(t)$  as  $X(t) = T(t, t_0)X_0$ , where  $T(t, t_0)$  is given explicitly by:

$$(2.3) \quad T(t, t_0) = 1_n + \sum_{n \geq 1} \int_{t_0 \leq s_1 \leq \dots \leq s_n \leq t} A(s_n)A(s_{n-1}) \dots A(s_1) ds_1 \dots ds_n$$

and  $1_n$  is the identity  $n \times n$  matrix. The right hand side is an infinite sum of what are nowadays called iterated integrals (see below), and the quantity  $T(t, t_0)$  is known as the transport of the equation (2.1).

Now the sum (2.3) converges absolutely on compacta  $K \subset U$  by the bound

$$\left| \int_{t_0 \leq s_1 \leq \dots \leq s_n \leq t} A(s_n) \dots A(s_1) ds_1 \dots ds_n \right| \leq \sup_{s \in K} \|A(s)\|^n \frac{(t - t_0)^n}{n!}$$

where the second factor is the volume of the bounded simplex

$$\Delta_n(t_0, t) = \{(s_1, \dots, s_n) \in \mathbb{R}^n : t_0 \leq s_1 \leq \dots \leq s_n \leq t\}.$$

between  $t_0 < t$ . Therefore setting  $X(t) = T(t, t_0)X_0$  where  $T(t, t_0)$  is given by (2.3) does indeed define the desired solution to (2.1) on  $U$ .

There are two special cases which are of interest. Suppose first of all that the matrices  $A(s), A(s')$  commute for all  $s, s'$ . Then we can rearrange the order of integration in each integrand of (2.3) and rewrite it as an exponential series

$$T(t, t_0) = \sum_{n \geq 0} \frac{1}{n!} \int_{[t_0, t]^n} A(t_1)A(t_2) \dots A(t_n) dt_1 \dots dt_n = \sum_{n \geq 0} \frac{1}{n!} \left( \int_{t_0}^t A(t) dt \right)^n .$$

This also follows from a special case of the shuffle product formula, which we discuss below. In this case we can write the full solution in the form:

$$X(t) = e^{\int_{t_0}^t A(s) ds} X_0$$

This formula should be familiar to physicists under the name of Dyson series, and is the first point of contact between iterated integrals and quantum field theory.

The second case of interest is when any product  $A(s_1) \dots A(s_N)$  vanishes for sufficiently large  $N$ . This occurs, for example, when  $A(t)$  is strictly upper triangular. In this case the series (2.3) and hence  $X(t)$  is a finite sum of iterated integrals, and the solution  $X(t)$  is simply called an iterated integral. Thus we should expect iterated integrals to appear whenever there are differential equations of this type (the condition is that they should have unipotent monodromy, as we shall discuss below).

**2.2. Iterated integrals.** Let  $k$  be the real or complex numbers, and let  $M$  be a smooth manifold over  $k$ . Let  $\gamma : [0, 1] \rightarrow M$  be a piecewise smooth path on  $M$ , and let  $\omega_1, \dots, \omega_n$  be smooth  $k$ -valued 1-forms on  $M$ . Let us write

$$\gamma^*(\omega_i) = f_i(t) dt ,$$

for the pull-back of the forms  $\omega_i$  to the interval  $[0, 1]$ . Recall that the ordinary line integral is given by

$$\int_{\gamma} \omega_1 = \int_{[0, 1]} \gamma^*(\omega_1) = \int_0^1 f_1(t_1) dt_1 ,$$

and does not depend on the choice of parameterization of  $\gamma$ .

**Definition 2.1.** The iterated integral of  $\omega_1, \dots, \omega_n$  along  $\gamma$  is defined by

$$\int_{\gamma} \omega_1 \dots \omega_n = \int_{0 \leq t_1 \leq \dots \leq t_n \leq 1} f_1(t_1) dt_1 \dots f_n(t_n) dt_n .$$

More generally, an iterated integral is any  $k$ -linear combination of such integrals. The empty iterated integral (when  $n = 0$ ) is defined to be the constant function 1.

**Proposition 2.2.** *Iterated integrals satisfy the following first properties:*

*i). The iterated integral  $\int_{\gamma} \omega_1 \dots \omega_n$  does not depend on the choice of parameterization of the path  $\gamma$ .*

*ii). If  $\gamma^{-1}(t) = \gamma(1 - t)$  denotes the reversal of the path  $\gamma$ , then*

$$\int_{\gamma^{-1}} \omega_1 \dots \omega_n = (-1)^n \int_{\gamma} \omega_n \dots \omega_1$$

*iii). If  $\alpha, \beta : I \rightarrow M$  are two paths such that  $\beta(0) = \alpha(1)$ , then let  $\alpha\beta$  denote the composed path obtained by traversing first  $\beta$  and then  $\alpha$ . Then*

$$\int_{\alpha\beta} \omega_1 \dots \omega_n = \sum_{i=0}^n \int_{\alpha} \omega_1 \dots \omega_i \int_{\beta} \omega_{i+1} \dots \omega_n .$$

where we recall that the empty iterated integral ( $n = 0$ ) is just the constant function 1.

iv). There is the shuffle product formula

$$\int_{\gamma} \omega_1 \dots \omega_r \int_{\gamma} \omega_{r+1} \dots \omega_{r+s} = \sum_{\sigma \in \Sigma(r,s)} \int_{\gamma} \omega_{\sigma(1)} \dots \omega_{\sigma(r+s)} ,$$

where  $\Sigma(r,s)$  is the set  $(r,s)$ -shuffles:

$$\Sigma(r,s) = \{ \sigma \in \Sigma(n) : \sigma(1) < \dots < \sigma(r) \text{ and } \sigma(r+1) < \dots < \sigma(r+s) \} .$$

*Proof.* i) and ii) are left as exercises. The identities (iii) and (iv) for  $n = 2$  can be seen from the following two pictures:



which show that  $[0,1] \times [0,1] = \{0 \leq t_1 \leq t_2 \leq 1\} \cup \{0 \leq t_2 \leq t_1 \leq 1\}$  (right) and  $\{0 \leq t_1 \leq t_2 \leq 1\} = \{0 \leq t_1 \leq t_2 \leq \frac{1}{2}\} \cup \{0 \leq t_1 \leq \frac{1}{2} \leq t_2 \leq 1\} \cup \{\frac{1}{2} \leq t_1 \leq t_2 \leq 1\}$  (left). In general (iii) follows from the formula:

$$\Delta_n(0,1) \cong \bigcup_{i=0}^n \Delta_i(0, \frac{1}{2}) \times \Delta_{n-i}(\frac{1}{2}, 1)$$

plus the fact that all overlaps are of codimension at least 2, and do not contribute to the integral. Likewise, (iv) follows from the formula for the decomposition of a product of simplices into smaller simplices:

$$\Delta_m(0,1) \times \Delta_n(0,1) = \bigcup_{\sigma \in \Sigma(m,n)} \sigma_* \Delta_{m+n}(0,1) ,$$

where all overlaps again do not contribute to the integral.  $\square$

One way to see the iterated integral as an ordinary integral is to notice that a smooth path  $\gamma : [0,1] \rightarrow M$  gives rise to a map

$$\gamma_n = \underbrace{\gamma \times \dots \times \gamma}_n : [0,1]^n \longrightarrow \underbrace{M \times \dots \times M}_n .$$

The product  $\Omega = \omega_1 \wedge \dots \wedge \omega_n$  defines a differential form on  $M^{\times n}$  which is pulled back to the hypercube  $[0,1]^n$  by this map. The iterated integral is just the integral of  $\gamma_n^*(\Omega)$  over the simplex  $\{0 \leq t_1 \leq \dots \leq t_n \leq 1\} \subset [0,1]^n$ , and all the above properties follow from purely combinatorial properties of such simplices.

**2.3. Homotopy functionals.** Two continuous paths  $\gamma_0, \gamma_1 : [0,1] \rightarrow M$  such that  $\gamma_0(0) = \gamma_1(0) = x_0$  and  $\gamma_0(1) = \gamma_1(1) = x_1$  are said to be homotopic relative to their endpoints  $x_0, x_1$  if there exists a continuous map  $\phi : [0,1] \times [0,1] \rightarrow M$  such that

$$\begin{aligned} \phi(0,t) &= \gamma_0(t) \\ \phi(1,t) &= \gamma_1(t) \end{aligned}$$

for all  $0 \leq t \leq 1$ , and  $\phi(s,0) = x_0$ ,  $\phi(s,1) = x_1$  for all  $0 \leq s \leq 1$ . This defines an equivalence relation on paths, and we write  $\gamma_0 \sim \gamma_1$  to denote two homotopic paths (rel. to their endpoints). We pass freely between piecewise continuous and smooth paths, since one can show that any piecewise continuous path is homotopic to a smooth one.

**Definition 2.3.** Let  $PM$  denote the set of piecewise smooth paths  $\gamma : [0, 1] \rightarrow M$ . A function  $F : PM \rightarrow k$  is called a homotopy functional if

$$\gamma_0 \sim \gamma_1 \quad \Rightarrow \quad F(\gamma_0) = F(\gamma_1) .$$

**Example 2.4.** Let  $M = \mathbb{R}^2$ , and for any  $r, s > 0$ , let  $\gamma_{r,s} : [0, 1] \rightarrow M$  be the path defined by  $\gamma(t) = (t^r, t^s)$ , whose endpoints are  $(0, 0)$  and  $(1, 1)$ . All such paths are homotopic relative to their endpoints. Let  $x, y$  be the standard coordinates on  $\mathbb{R}^2$ , and consider the exact one-forms  $\omega_1 = dx, \omega_2 = dy$ . Then the iterated integral

$$\int_{\gamma} \omega_1 \omega_2 = \int_{0 \leq t_1 \leq t_2 \leq 1} r t_1^{r-1} dt_1 s t_2^{s-1} dt_2 = \frac{s}{r+s} ,$$

clearly depends on the paths  $\gamma_{r,s}$ . Thus the general iterated integral is *not* a homotopy functional. The reason for this, as we shall see later, is that the form  $\omega_1 \wedge \omega_2$  is non-zero.

*Remark 2.5.* It is a general fact [10] that if  $\omega_1, \dots, \omega_k$  are one forms on  $M$  which span the cotangent bundle at every point of  $M$ , then

$$\int_{\gamma_1} \omega_{i_1} \dots \omega_{i_n} = \int_{\gamma_2} \omega_{i_1} \dots \omega_{i_n}$$

for all  $n \geq 1$ , and  $i_1, \dots, i_n \in \{1, \dots, k\}$ , if and only if  $\gamma_1$  and  $\gamma_2$  are two different parametrizations of the same path. In other words, iterated integrals define functions on the infinite-dimensional space of paths on a manifold, and are sufficient to separate points on it. This is perhaps the first hint that iterated integrals should be related to the Feynman path integral.

From now on, we will only be interested in iterated integrals which do give rise to homotopy functionals. We will give necessary and sufficient conditions for an iterated integral to be a homotopy functional in §6.

**2.4. Multivalued functions and monodromy.** Let  $M$  be a connected and locally simply connected topological space and let  $\pi : \widetilde{M} \rightarrow M$  be a universal covering. A multivalued function on  $M$  will refer to a continuous function  $f$  on  $\widetilde{M}$ . If, on some simply connected open set  $U \subset M$ , one chooses a continuous section  $s : U \rightarrow \widetilde{M}$  of  $\pi$ , then the function  $f \circ s$  defines a local branch of the multivalued function  $f$ .

Suppose that  $F$  is a homotopy functional on  $M$ . Let us fix a point  $x_0 \in M$  and allow  $x_1 \in M$  to move around. Then we can consider

$$F(x_1) := F(\gamma, \text{ for any piecewise smooth } \gamma \text{ such that } \gamma(0) = x_0, \gamma(1) = x_1)$$

Thus any homotopy functional defines a multivalued function on  $M$ .

**Example 2.6.** Let  $M = \mathbb{C} \setminus \{0\}$ , and let  $x_0 \in M$ . Let  $\omega_0 = \frac{dz}{z}$ , and let  $\gamma : [0, 1] \rightarrow M$  be a smooth path such that  $\gamma(0) = x_0$  and  $\gamma(1) = z$ . We have

$$\int_{\gamma} \omega_0 = \log(z) - \log(x_0) .$$

It follows from the shuffle product formula that the iterated integral of  $\omega_0$  can be expressed in terms of the logarithm:

$$\int_{\gamma} \underbrace{\omega_0 \dots \omega_0}_n = \frac{1}{n!} \left( \int_{\gamma} \omega_0 \right)^n = \frac{1}{n!} (\log(z) - \log(x_0))^n ,$$

and therefore clearly only depends on the homotopy class of  $\gamma$ , and the endpoints  $x_0, z$ .

We will often take the base-point  $x_0$  to be 0 by formally defining:

$$\int_{\gamma} \underbrace{\omega_0 \dots \omega_0}_n = \frac{1}{n!} \log^n(z),$$

as multivalued functions, where  $\gamma$  is a path from 0 to  $z$ . If one must specify a branch, then we take the simply connected open subset  $U = \mathbb{C} \setminus (-\infty, 0] \subset M$ , and define  $\log(z)$  to be the principal branch which vanishes at  $z = 1$ .

**Example 2.7.** Let  $M = \mathbb{C} \setminus \{0, 1\}$ , and let  $x_0 \in M$ . Consider the closed 1-forms:

$$\omega_0 = \frac{dz}{z}, \quad \omega_1 = \frac{dz}{z-1},$$

whose cohomology classes give a basis for the de Rham cohomology  $H^1(M; \mathbb{C})$ . Let  $\gamma : I \rightarrow M$  be a smooth path such that  $\gamma(0) = x_0$  and  $\gamma(1) = z$ , and consider the family of iterated integrals

$$I(\omega_{i_1} \dots \omega_{i_n}, \gamma) = \int_{\gamma} \omega_{i_1} \dots \omega_{i_n}$$

where  $i_k \in \{0, 1\}$ . We shall see in §3 that these integrals only depend on the homotopy class of  $\gamma$  and the endpoints  $x_0, z$ , and write down branches of the corresponding multivalued functions explicitly. As in the previous example, we can also take  $x_0 = 0$ , giving

$$(2.4) \quad \int_{\gamma} \underbrace{\omega_0 \dots \omega_0}_n = \frac{1}{n!} \log^n(z),$$

for a path  $\gamma$  satisfying  $\gamma(0) = 0$  and  $\gamma(1) = z$ , by definition. One can verify that for all other iterated integrals we have

$$(2.5) \quad \lim_{\varepsilon \rightarrow 0} \int_{\gamma_{\varepsilon}} \omega_{i_1} \dots \omega_{i_n} < \infty$$

if at least one  $i_k \neq 0$ , and where  $\gamma(0) = \varepsilon, \gamma(1) = z$ . Thus, although the point 0 is not actually in the space  $M$ , we can define iterated integrals with 0 as a basepoint if one takes care to separate the two different cases where the  $i_k$  are all equal to 0 (equation (2.4)) or not (equation (2.5)). This will be discussed in §3.

3. THE CASE  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  AND POLYLOGARITHMS

In this lecture and the next, we study of the set of iterated integrals on  $\mathbb{C} \setminus \{0, 1\}$  and relate them to polylogarithms. Because of their historical and mathematical importance, we first consider the special case of the classical polylogarithms.

**3.1. The classical polylogarithms.** Let  $n \geq 1$ . The classical polylogarithms were first defined by Leibniz in a letter to Bernoulli (?) by the series

$$(3.1) \quad \text{Li}_n(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^n},$$

which converges absolutely for  $|z| < 1$ , and therefore defines a holomorphic function in a neighbourhood of the origin. These functions are generalizations of the logarithm  $\text{Li}_1(z) = -\log(1-z)$ , and satisfy the differential equations

$$\frac{d}{dz} \text{Li}_n(z) = \frac{1}{z} \text{Li}_{n-1}(z)$$

for all  $n \geq 2$ . It follows that for  $n \geq 2$ , we can also define

$$(3.2) \quad \text{Li}_n(z) = \int_{\gamma} \text{Li}_{n-1}(t) \frac{dt}{t},$$

where  $\gamma$  is a smooth path from 0 to  $z$  in  $\mathbb{C} \setminus \{0, 1\}$ . This integral formula proves by induction that  $\text{Li}_n(z)$  has an analytic continuation to a multivalued function on  $M = \mathbb{C} \setminus \{0, 1\}$ . Recall that we had one forms  $\omega_0 = \frac{dz}{z}$  and  $\omega_1 = \frac{dz}{1-z}$  on  $M$ . It follows from (3.2) and the definition of iterated integrals that  $\text{Li}_n(z)$  is

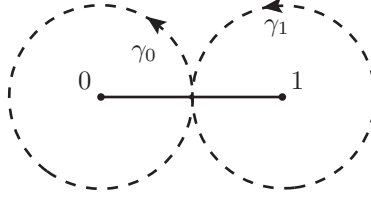
$$\int_{\gamma} \omega_1 \underbrace{\omega_0 \dots \omega_0}_n = \int_{0 \leq t_1 \leq \dots \leq t_n \leq 1} \frac{z dt_1}{1-zt_1} \frac{dt_2}{t_2} \dots \frac{dt_n}{t_n}.$$

Note that the lower bound of integration 0 is not in the space  $M$ , but this in fact poses no problem here, since  $\omega_1$  has no pole at 0 and so the integral converges. The representation as functions also shows that these iterated integrals are homotopy functionals. This will follow from the general results of §6 as a consequence of the fact that  $d\omega_0 = d\omega_1 = \omega_0 \wedge \omega_1 = 0$ .

Thus we see that the classical polylogarithms are special cases of iterated integrals on  $M$ . For an exposition of some their numerous applications in number theory and geometry see the survey paper [18].

**3.2. Monodromy.** To describe the monodromy of the classical polylogarithms, we need a basepoint  $x$  on  $M$ . If one wishes, one can take  $x = \frac{1}{2}$  throughout this section, but since this choice is not canonical, we prefer to take the real interval  $x = (0, 1)$  as a base point. One can verify that all the usual properties one requires of a basepoint are satisfied, because  $(0, 1)$  is contractible. From this point of view, there are three canonical basepoints given by the three connected components  $(-\infty, 0)$ ,  $(0, 1)$  and  $(1, \infty)$  of the set of real points  $\mathbb{R} \setminus \{0, 1\}$ . The fundamental group  $\pi_1(M, x)$  is then the free group generated by the homotopy classes of two loops  $\gamma_0, \gamma_1$  which wind once around 0, 1, respectively:





For  $i = 0, 1$ , let  $\mathcal{M}_i$  (monodromy around the point  $i$ ) denote the operator which associates to a local branch of a multivalued function  $f(z)$  on  $M$  its analytic continuation along the path  $\gamma_i$ . It follows from the properties of analytic continuation that  $\mathcal{M}_i$  are multiplicative and commute with differentiation: i.e., for any multivalued functions  $f, g$  on  $\mathbb{C} \setminus \{0, 1\}$ , and  $i \in \{0, 1\}$ ,

$$(3.3) \quad \begin{aligned} \mathcal{M}_i\left(\frac{d}{dz}f(z)\right) &= \frac{d}{dz}(\mathcal{M}_if(z)) \\ \mathcal{M}_i(f(z)g(z)) &= (\mathcal{M}_if(z))(\mathcal{M}_ig(z)) . \end{aligned}$$

We will show in §4.2 that:

$$(3.4) \quad \begin{aligned} \mathcal{M}_0\text{Li}_n(z) &= \text{Li}_n(z) \\ \mathcal{M}_1\text{Li}_n(z) &= \text{Li}_n(z) + \frac{2i\pi}{(n-1)!} \log^{n-1}(z) . \end{aligned}$$

Note that the local branch of  $\text{Li}_n(z)$  defined by (3.1) is holomorphic at the origin, but its Riemann surface is ramified there, because after doing an analytic continuation around the point 1 it acquires a term  $\log^{n-1}(z)$  which has a singularity at the origin.

**3.3. Digression: matrix representation for the monodromy.** Before passing to more general iterated integrals on  $M$ , we relate the above, in the case of the dilogarithm  $\text{Li}_2(z)$ , to Picard's method §2.1. Let  $U \subset M$  and define

$$(3.5) \quad A(z) = \begin{pmatrix} 0 & 0 & 0 \\ \frac{1}{z} & 0 & 0 \\ 0 & \frac{1}{1-z} & 0 \end{pmatrix} \quad \text{and} \quad \Omega(z) = A(z)dz = \begin{pmatrix} 0 & 0 & 0 \\ \omega_0 & 0 & 0 \\ 0 & \omega_1 & 0 \end{pmatrix}$$

Since  $A(z)$  is nilpotent, applying Picard's method to the equation  $X'(z) = A(z)X(z)$  with initial condition  $X(z_0) = 1_2$ , where  $1_2$  is the identity  $2 \times 2$  matrix, on  $U$  gives a finite expansion in terms of iterated integrals

$$X(z) = \begin{pmatrix} 1 & 0 & 0 \\ \int_{\gamma} \omega_0 & 1 & 0 \\ \int_{\gamma} \omega_1 \omega_0 & \int_{\gamma} \omega_1 & 1 \end{pmatrix}$$

It is customary to rescale this integral by multiplying the  $n^{\text{th}}$  column by  $(2\pi i)^n$ . Equivalently, consider the trivial bundle  $\mathbb{C}^3 \times M \rightarrow M$ . On it we have a connection  $d + \Omega : \mathbb{C}^3 \rightarrow \Omega^1(M) \otimes \mathbb{C}^3$ . It extends via the map  $M \hookrightarrow \mathbb{C}$  to a connection on  $\mathbb{C}^3 \times \mathbb{C} \rightarrow \mathbb{C}$  which has regular singularities at  $z = 0$  and  $z = 1$ . In other words,  $dV(z) = \Omega V(z)$  is a Fuchsian differential equation and has the solution:

$$V_2 = \begin{pmatrix} 1 & 0 & 0 \\ \text{Li}_1(z) & 2i\pi & 0 \\ \text{Li}_2(z) & 2i\pi \log(z) & (2i\pi)^2 \end{pmatrix}$$

The monodromy of the dilogarithm  $\text{Li}_2(z)$  given by (3.4) can be conveniently encoded as follows. We have  $\mathcal{M}_0 V_2 = V_2 M_0$  and  $\mathcal{M}_1 V_2 = V_2 M_1$ , where

$$M_0 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \quad \text{and} \quad M_1 = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Consider, therefore, the unipotent group

$$G = \begin{pmatrix} 1 & 0 & 0 \\ * & 1 & 0 \\ * & * & 1 \end{pmatrix}$$

of lower triangular matrices. Let  $G(R)$  denote the corresponding group with its entries  $*$  in any ring  $R$ . The monodromy gives a representation

$$\begin{aligned} \rho : \pi_1(M, x) &\longrightarrow G(\mathbb{Z}) \\ \gamma_0, \gamma_1 &\mapsto M_0, M_1 \end{aligned}$$

Thus we obtain a commutative diagram:

$$(3.6) \quad \begin{array}{ccc} \widetilde{M} & \longrightarrow & G(\mathbb{C}) \\ \downarrow & & \downarrow \\ M & \longrightarrow & G(\mathbb{C})/G(\mathbb{Z}) \end{array}$$

where the horizontal map along the top associates the matrix  $V_2(z)$  to a point  $z \in \widetilde{M}$ , and the lower horizontal map takes a point  $z \in M$  to  $V_2(z) \bmod G(\mathbb{Z})$ . In this sense, the dilogarithm has unipotent monodromy.

One can write down similar matrices  $A_n$  for each of the classical polylogarithms  $\text{Li}_n(z)$  (exercise), and we shall see later how to generalize this picture to include all the iterated integrals on  $M$ , using an infinite-dimensional bundle.

**3.4. Multiple polylogarithms in one variable.** We now describe all the iterated integrals on  $\mathbb{C} \setminus \{0, 1\}$  by writing down the functions which they represent. These are known as multiple polylogarithms (in one variable), which were studied in great detail by Lappo-Danilevsky, and partly rediscovered by physicists more recently.

**Definition 3.1.** Let  $n_1, \dots, n_r \in \mathbb{N}$  and define the multiple polylogarithm in one variable (these are also frequently called hyperlogarithms)

$$\text{Li}_{n_1, \dots, n_r}(z) = \sum_{1 \leq k_1 < \dots < k_r} \frac{z^{k_r}}{k_1^{n_1} \dots k_r^{n_r}}$$

This converges absolutely for  $|z| < 1$  and defines a germ of a holomorphic function in the neighbourhood of the origin.

It follows immediately from the definitions that

$$(3.7) \quad \frac{d}{dz} \text{Li}_{n_1, \dots, n_r}(z) = \begin{cases} \frac{1}{z} \text{Li}_{n_1, \dots, n_r-1}(z), & \text{if } n_r > 1, \\ \frac{1}{1-z} \text{Li}_{n_1, \dots, n_r-1}(z), & \text{if } n_r = 1. \end{cases}$$

As in the case of the classical polylogarithms it follows from these equations that we have an iterated integral representation

$$(3.8) \quad \text{Li}_{n_1, \dots, n_r}(z) = \int_{\gamma} \omega_1 \omega_0^{n_1-1} \omega_1 \dots \omega_0^{n_r-1}$$

where  $\gamma : [0, 1] \rightarrow \mathbb{C} \setminus \{0, 1\}$  is a smooth path such that  $\gamma(1) = z$ . This formula also defines an analytic continuation to the whole of  $M$ , and thus the multiple polylogarithms are multivalued functions on  $M$ . All these iterated integrals begin with  $\omega_1$ .

It remains to describe the iterated integrals which consist of words in  $\omega_0, \omega_1$  which begin with  $\omega_0$ . One way to do this is to use the regularization at 0 defined in example 2.6 and use the shuffle product. It turns out that all remaining iterated integrals can be obtained from the ones we have already along with  $\int_\gamma \omega_0$ , which is defined to be  $\log z$ . For example, we have from proposition 2.2 *iii*) that

$$\int_\gamma \omega_0 \int_\gamma \omega_1 = \int_\gamma \omega_0 \omega_1 + \int_\gamma \omega_1 \omega_0$$

and so we are obliged to define  $\int_\gamma \omega_0 \omega_1 := \int_\gamma \omega_1 \omega_0 - \int_\gamma \omega_0 \int_\gamma \omega_1 = \text{Li}_2(z) - \log(z) \text{Li}_1(z)$ . Therefore if we fix the value of  $\int_\gamma \omega_0$  then the shuffle product determines all the iterated integrals uniquely. We can formalize this in a slightly more algebraic setting below.

**3.5. Algebraic representation.** Let  $X = \{x_0, x_1\}$  denote an alphabet in two letters, and let  $X^\times$  denote the free monoid generated by  $X$ , i.e., the set of words in the letters  $x_0, x_1$  along with the empty word  $e$ . Let  $\mathbb{Q}\langle x_0, x_1 \rangle$  denote the vector space generated by the words in  $X$ , equipped with the shuffle product:

$$x_{i_1} \dots x_{i_r} \amalg x_{i_{r+1}} \dots x_{i_{r+s}} = \sum_{\sigma \in \Sigma(r,s)} x_{\sigma(1)} \dots x_{\sigma(r+s)},$$

and where  $e \amalg w = w \amalg e = w$  for all  $w \in X^*$ . To every word  $w \in X^*$  we associate a multivalued function  $\text{Li}_w(z)$ , as follows:

i). Firstly, if  $w \in X^\times x_1$ , then we can write  $w = x_0^{n_1-1} x_1 \dots x_0^{n_r-1} x_1$ , and we set

$$\text{Li}_w(z) = \int_0^z \omega_1 \omega_0^{n_1-1} \omega_1 \dots \omega_0^{n_r-1} = \text{Li}_{n_1, \dots, n_k}(z)$$

Note the reversal of the letters in the iterated integral. By the shuffle product formula (proposition 2.2 *iii*), we have

$$(3.9) \quad \text{Li}_w(z) \text{Li}_{w'}(z) = \text{Li}_{w \amalg w'}(z)$$

where the notation  $\text{Li}$  is extended by linearity:  $\text{Li}_{\sum w_i}(z) := \sum \text{Li}_{w_i}(z)$ .

ii). We can extend the definition of  $\text{Li}_w(z)$  to all words  $w \in X^\times$  by setting:

$$(3.10) \quad \text{Li}_{x_0^n}(z) = \int_\gamma \underbrace{\omega_0 \dots \omega_0}_n = \frac{1}{n!} \log^n(z)$$

**Exercise 3.2.** Every word  $w \in X^\times$  is a unique sum of shuffles

$$w = \sum_{i=0}^k x_0^i \amalg w_i$$

where  $w_i \in X^* x_1$  are convergent.

Setting  $\text{Li}_w(z) = \sum_{i=0}^k \text{Li}_{x_0^i}(z) \text{Li}_{w_i}(z)$  completes the definition of the functions  $\text{Li}_w(z)$ . With this definition, the shuffle relations (3.9) are valid for all words  $w \in X^*$ .

## 4. THE KZ EQUATION AND THE MONODROMY OF POLYLOGARITHMS

Recall that we defined multiple polylogarithm functions  $\text{Li}_w(z)$ , indexed by the set of words in  $X$ , as multivalued functions on  $M = \mathbb{C} \setminus \{0, 1\}$  which satisfy:

$$(4.1) \quad d\text{Li}_{x_i w}(z) = \omega_i \text{Li}_w(z) \quad \text{for} \quad i = 0, 1 ,$$

where  $\omega_0 = dz/z$  and  $\omega_1 = dz/(1-z)$ . Furthermore, we had

$$(4.2) \quad \begin{aligned} \lim_{z \rightarrow 0} \text{Li}_w(z) &= 0 \text{ for all words } w \neq x_0^n , \\ \text{Li}_{x_0^n}(z) &= \frac{1}{n!} \log(z) \end{aligned}$$

Since the properties (4.2) fix all the constants of integration in the differential equations (4.1), this determines the functions  $\text{Li}_w(z)$  uniquely. Recall also that the general shuffle product formula for iterated integrals implied also the shuffle product for multiple polylogarithms:  $\text{Li}_w(z)\text{Li}_{w'}(z) = \text{Li}_{w \amalg w'}(z)$ .

In order to study the monodromy of the functions  $\text{Li}_w(z)$  it is helpful to consider their generating series:

$$L(z) = \sum_{w \in X^*} w \text{Li}_w(z) .$$

Formally, let

$$\mathbb{C}\langle\langle X \rangle\rangle = \left\{ \sum_{w \in X^*} S_w w : S_w \in \mathbb{C} \right\}$$

denote the ring of non-commutative formal power series in the words  $X^*$ , equipped with the concatenation product ( $w.w' = ww'$ ). The function  $L(z)$  defines a multivalued function on  $M$  taking values in  $\mathbb{C}\langle\langle X \rangle\rangle$ , and satisfies the differential equation:

$$(4.3) \quad \frac{d}{dz} L(z) = \left( \frac{x_0}{z} + \frac{x_1}{z-1} \right) L(z) .$$

Thus  $L(z)$  should be viewed as a flat section of the corresponding connection on the infinite-dimensional trivial bundle  $\mathbb{C}\langle\langle X \rangle\rangle \times M \rightarrow M$ . Term by term, (4.3) is equivalent to the differential equations (4.1). This equation is known as the Knizhnik and Zamolodchikov equation (in the one-dimensional case). The conditions (4.2) can be written

$$L(z) \sim \exp(x_0 \log z) \quad \text{as } z \rightarrow 0$$

This notation means that there exists a  $\mathbb{C}\langle\langle X \rangle\rangle$ -valued function  $h(z)$ , which is holomorphic in the neighbourhood of the origin, such that

$$(4.4) \quad L(z) = h(z) \exp(x_0 \log z) \quad \text{for } z \text{ near } 0 ,$$

and  $h(0)$  is the constant series  $1 \in \mathbb{C}\langle\langle X \rangle\rangle$ . As before, the condition (4.4) uniquely determines the solution  $L(z)$  to (4.3).

**4.1. Drinfel'd associator and multiple zeta values.** By the same argument, there exists another solution  $L^1(z)$  to (4.3) which satisfies:

$$(4.5) \quad L^1(z) \sim \exp(x_1 \log(1-z)) \text{ as } z \rightarrow 1 .$$

In this situation, it is usual to consider the parallel transport:

$$(4.6) \quad \Phi(z) = (L^1(z))^{-1} L(z) ,$$

which relates the two solutions. It follows from differentiating  $L^1(z)\Phi(z) = L(z)$  and equation (4.3), that  $L^1(z)d\Phi(z) = 0$ . Since the leading term of  $L^1(z)$  is 1, it is invertible in  $\mathbb{C}\langle\langle X \rangle\rangle$ , and therefore  $d\Phi(z) = 0$ . It follows that  $\Phi(z)$  is a constant series

denoted  $\Phi(x_0, x_1) \in \mathbb{C}\langle\langle X \rangle\rangle$ , and known as Drinfel'd's associator. It follows from the asymptotics of the solution  $L^1(z)$  near 1 (equations (4.5) and (4.6)) that we can write:

$$(4.7) \quad \Phi(x_0, x_1) = \lim_{z \rightarrow 1^-} (\exp(-x_1 \log(1-z))L(z)) .$$

In this sense,  $\Phi(x_0, x_1)$  is a regularized limit of  $L(z)$  as  $z \rightarrow 1^-$  along the real axis. More precisely, it follows from (4.5) that every multiple polylogarithm  $\text{Li}_w(z)$  has a canonical branch for  $z \in (0, 1)$  which can be written in the form

$$\text{Li}_w(z) = a_0(z) + a_1(z) \log(1-z) + \dots + a_{|w|}(z) \log^{|w|}(1-z)$$

where  $a_i(z)$  is holomorphic in a neighbourhood of  $z = 1$ . The regularized value at  $z = 1$  can therefore be defined as

$$\text{Reg}_{z=1} \text{Li}_w(z) = a_0(1) ,$$

and  $\Phi(x_0, x_1)$  is the generating series of these regularized values. In particular, it has real coefficients, i.e.,  $\Phi(x_0, x_1) \in \mathbb{R}\langle\langle X \rangle\rangle$ . One can determine the coefficients completely in terms of multiple zeta values.

**Definition 4.1.** Let  $n_1, \dots, n_r \in \mathbb{N}$ , such that  $n_r \geq 2$ . The multiple zeta value is defined by the absolutely convergent sum:

$$\zeta(n_1, \dots, n_r) = \sum_{0 < k_1 < \dots < k_r} \frac{1}{k_1^{n_1} \dots k_r^{n_r}} \in \mathbb{R}$$

**Lemma 4.2.** *There is a unique function  $\zeta : \mathbb{Q}\langle X \rangle \rightarrow \mathbb{R}$  such that*

$$\begin{aligned} \zeta(x_0) &= \zeta(x_1) = 0 \\ \zeta(x_0^{n_r-1} x_1 \dots x_0^{n_1-1} x_1) &= \zeta(n_1, \dots, n_r) \\ \zeta(w)\zeta(w') &= \zeta(w \amalg w') \end{aligned}$$

*The coefficients of  $\Phi(x_0, x_1)$  are exactly the  $\zeta(w)$ , i.e.,*

$$\Phi(x_0, x_1) = \sum_{w \in X^*} w \zeta(w)$$

*Proof.* First of all, for all words  $w \in x_0 X^* x_1$ ,  $\text{Li}_w(z)$  converges at the point  $z = 1$ , and we have  $\zeta(w) = \text{Li}_w(1)$ . The definition of the series  $\text{Li}_w(z)$  gives the formula for  $\zeta(w)$  as a nested sum. Furthermore, the shuffle product for the functions  $\text{Li}_w(z)$  implies the corresponding formula  $\zeta(w)\zeta(w') = \zeta(w \amalg w')$  for all words  $w, w' \in x_0 X^* x_1$ . It is then an exercise to show that every word  $w \in X$  can be uniquely written as a sum of shuffles of words of the form  $x_0^i x_1^j$  and  $w \in x_0 X^* x_1$ . It follows that there is a unique way to extend  $\zeta$  by linearity to all words  $w \in X^*$  after fixing the values of  $\zeta(x_0)$  and  $\zeta(x_1)$  such that the three properties are satisfied. This proves the first part. To prove that the coefficients of  $\Phi(x_0, x_1)$  are given by the  $\zeta(w)$ , one verifies from (4.7) that the coefficient of  $w$  is  $\text{Reg}_{z=1} \text{Li}_w(z)$ , which satisfies the shuffle relations for convergent  $w$ , and vanishes for  $w = x_0, x_1$ , since  $\text{Li}_{x_0}(z) = \log z$  and  $\text{Li}_{x_1}(z) = -\log(1-z)$ .  $\square$

The fact that the coefficients of  $\Phi(x_0, x_1)$  are multiple zeta values was first observed by Kontsevich. Explicitly, one can write

$$\Phi(x_0, x_1) = 1 + \zeta(2)[x_0, x_1] + \zeta(3)([x_0, [x_0, x_1]] - [[x_0, x_1], x_1]) + \dots$$

**4.2. Monodromy.** We can now proceed with the calculation of the monodromy of the multiple polylogarithms. In this section we write  $\Phi$  instead of  $\Phi(x_0, x_1)$ .

**Proposition 4.3.** *The action of the monodromy operators  $\mathcal{M}_i$ ,  $i = 0, 1$  on the generating series  $L(z)$  is given by:*

$$(4.8) \quad \begin{aligned} \mathcal{M}_0 L(z) &= L(z) \exp(2i\pi x_0) \\ \mathcal{M}_1 L(z) &= L(z) \Phi^{-1} \exp(2i\pi x_1) \Phi \end{aligned}$$

*Proof.* The first line follows immediately from the asymptotics of  $L(z)$  (4.4). Using the fact that  $L^1(z)\Phi = L(z)$ , and that the series  $\Phi$  is invertible in  $\mathbb{C}\langle\langle X \rangle\rangle$ ,

$$\mathcal{M}_1 L(z) = \mathcal{M}_1 L^1(z)\Phi = L^1(z) \exp(2i\pi x_1)\Phi = L(z) \Phi^{-1} \exp(2i\pi x_1)\Phi .$$

□

**Corollary 4.4.** *The monodromy (or holonomy) of  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  can be expressed in terms of multiple zeta values and  $2i\pi$ .*

We can easily deduce the monodromy of the classical polylogarithms from (4.8). Since  $\text{Li}_n(z)$  corresponds to  $\text{Li}_{x_0^{n-1}x_1}(z)$ , it suffices to compute the coefficient of  $x_0^{n-1}x_1$  in  $\mathcal{M}_1 L(z)$ . Since words which contain two or more  $x_1$ 's do not contribute:

$$L(z)\Phi^{-1} \exp(2i\pi x_1)\Phi = L(z)(1 + \Phi^{-1}2i\pi x_1\Phi + \dots) ,$$

which is

$$\text{Li}_{x_0^{n-1}x_1}(z) + \sum_{i+j=n-1} \text{Li}_{x_0^i}(z)\Phi_{x_0^j}^{-1}2i\pi$$

where  $\Phi_{x_0^j}^{-1}$  is the coefficient of  $x_0^j$  in  $\Phi^{-1}$ . But the coefficient of  $x_0^j$ , for  $j \geq 1$  in  $\Phi$  is just  $\zeta(x_0^j) = 0$ , and this implies that the coefficient of  $x_0^j$  in  $\Phi^{-1}$  is also 0. The previous formula therefore reduces to  $\text{Li}_n(z) + \frac{2i\pi}{(n-1)!} \log^{n-1}(z)$ , as promised.

**4.3. A (pro-)unipotent group.** Now consider the non-commutative algebra  $\mathbb{C}\langle X \rangle$  equipped with the concatenation product. For  $n \geq 1$ , the set  $I_n$  of words of length  $\geq n$  is a (two-sided) ideal in  $\mathbb{C}\langle X \rangle$ , and the quotient  $W_n = \mathbb{C}\langle X \rangle / I_n$  is isomorphic as a vector space to the  $\mathbb{C}$ -vector space spanned by the set of all words of length  $< n$ . There are two nilpotent operators,  $X_0, X_1 : W_n \rightarrow W_n$  given by left multiplication by  $x_0, x_1$ , respectively.

By passing to the quotient  $\mathbb{C}\langle X \rangle \rightarrow W_n$ , (4.3) defines a connection on  $W_n$  for all  $n$ , which are compatible with the quotient maps  $W_n \rightarrow W_{n-1}$ . The monodromy of this connection is unipotent (i.e., can be written as a lower-triangular matrix in a suitable basis of  $W_n$ ), and is given explicitly by (4.8). This is the promised generalization of the dilogarithm variation of §3.3.

**4.4. Structure of iterated integrals on  $\mathbb{C} \setminus \{0, 1\}$ .** In summary, we have the following description of the iterated integrals on  $\mathbb{C} \setminus \{0, 1\}$ .

**Theorem 4.5.** *The map*

$$(4.9) \quad \begin{aligned} (\mathbb{C}\langle X \rangle, \mathfrak{M}) &\longrightarrow \{\text{homotopy invariant iterated integrals on } \mathbb{C} \setminus \{0, 1\}\} \\ w &\longmapsto \text{Li}_w(z) \end{aligned}$$

*is an isomorphism. In other words, every homotopy-invariant iterated integral on  $\mathbb{C} \setminus \{0, 1\}$  is a linear combination of the  $\text{Li}_w(z)$ , and the  $\text{Li}_w(z)$  are linearly independent.*

In fact, one can show more: every multivalued function on  $\mathbb{C} \setminus \{0, 1\}$  with unipotent monodromy and satisfying a polynomial growth condition at  $0, 1$  and  $\infty$  is a linear combination of  $\text{Li}_w(z)$  with coefficients in  $\mathbb{C}(z)$ , and furthermore, the only algebraic relations between the  $\text{Li}_w(z)$  over  $\mathbb{C}(z)$  are given by the shuffle product. Thus the multiple polylogarithms are the universal unipotent functions on the thrice punctured projective line.

The multiple polylogarithms also inherit a Hopf algebra structure from the previous theorem. This is because the shuffle algebra  $\mathbb{Q}\langle X \rangle$  is itself a graded commutative Hopf algebra for the deconcatenation coproduct defined by:

$$\Delta : \mathbb{Q}\langle X \rangle \longrightarrow \mathbb{Q}\langle X \rangle \otimes_{\mathbb{Q}} \mathbb{Q}\langle X \rangle$$

$$\Delta(x_{i_1} \dots x_{i_n}) = \sum_{k=1}^n x_{i_1} \dots x_{i_r} \otimes x_{i_{r+1}} \dots x_{i_n}$$

where the grading is given by the number of letters. As we shall see in §6, this is a general feature of iterated integrals.

A different way to state the universality of the multiple polylogarithms as a class of functions on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  is as follows. Let  $\mathcal{O} = \mathbb{Q}[z, \frac{1}{z}, \frac{1}{1-z}]$  denote the ring of regular functions on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$ . It is a differential algebra with respect to the operator  $\frac{\partial}{\partial z}$ . Consider the algebra

$$L = \mathcal{O}\langle \text{Li}_w(z) : w \in X^* \rangle$$

consisting of linear combinations of  $\text{Li}_w(z)$  with coefficients in  $\mathcal{O}$ . It too is a differential algebra with respect to the operator  $\frac{\partial}{\partial z}$ .

**Theorem 4.6.** *Every element in  $L$  has a primitive, which is unique up to a constant.*

In other words, for every  $f \in L$ , there exists  $F \in L$  such that  $\frac{\partial F}{\partial z} = f$ , and  $L$  is the smallest extension of  $\mathcal{O}$  with this property. Thus  $L$  is the smallest class of polylogarithm functions on  $\mathbb{P}^1 \setminus \{0, 1, \infty\}$  which are stable under multiplication and taking primitives. This is the key property which will be used in §7 in relation to Feynman integrals.

## 5. A BRIEF OVERVIEW OF MULTIPLE ZETA VALUES

**5.1. Single zeta values.** First consider the values of the Riemann zeta function  $\zeta(n)$ , for  $n$  an integer  $n \geq 2$ . It was shown by Euler in 1735 that  $\zeta(2) = \frac{\pi^2}{6}$  (this had been conjectured by Mengoli in 1644), and subsequently that

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

where the Bernoulli numbers  $B_m$  are given by the generating series

$$\frac{x}{1 - e^{-x}} = \sum_{m=0}^{\infty} B_m \frac{x^m}{m!}.$$

In particular,  $\zeta(2n)$  is an explicit rational multiple of  $\pi^{2n}$ . It is expected that no such formula should exist for the odd zeta values.

**Conjecture 1.** The numbers  $\pi, \zeta(3), \zeta(5), \dots$ , are algebraically independent over  $\mathbb{Q}$ .

Surprisingly little is known about this conjecture. What is known is that  $\pi$  is transcendental (Lindemann 1882), that  $\zeta(3)$  is irrational (Apéry 1978), and that infinitely many values of  $\zeta(2n+1)$  are irrational (Ball-Rivoal 2000), and various refinements in this direction. However, it is still not known whether  $\zeta(5)$  is irrational or not.

**5.2. Multiple zeta values.** Multiple zeta values, on the other hand, satisfy a huge number of algebraic relations over  $\mathbb{Q}$ . The so-called ‘standard relations’ or ‘double shuffle relations’ are linear and quadratic relations between them which we briefly summarize below. Recall that  $X = \{x_0, x_1\}$  is an alphabet on two letters, and let  $\mathbb{Q}\langle X \rangle$  denote the free non-commutative algebra on the symbols  $x_0$  and  $x_1$  with the concatenation product, i.e., the vector space generated by all words in  $X$  including the empty word 1. We already defined a map  $\zeta : x_0 X^* x_1 \rightarrow \mathbb{R}$

$$\zeta(x_0^{n_r-1} x_1 \dots x_0^{n_0-1} x_1) = \zeta(n_1, \dots, n_r),$$

which we can extend by linearity to the subspace  $x_0 \mathbb{Q}\langle X \rangle x_1 \subset \mathbb{Q}\langle X \rangle$  of convergent words. The weight of  $\zeta(n_1, \dots, n_r)$  is defined to be the quantity  $n_1 + \dots + n_r$ . This defines a filtration on the vector space of multiple zeta values. The standard relations can be described in terms of two different product structures on  $x_0 \mathbb{Q}\langle X \rangle x_1$ .

- *Shuffle product.* Recall that we had a commutative and associative product

$$\mathfrak{m} : \mathbb{Q}\langle X \rangle \times \mathbb{Q}\langle X \rangle \rightarrow \mathbb{Q}\langle X \rangle$$

which is uniquely determined by the properties (exercise)

$$w \mathfrak{m} 1 = w \quad 1 \mathfrak{m} w = w \quad \text{for all } w \in X^*$$

$$x_i w \mathfrak{m} x_j w' = x_i (w \mathfrak{m} x_j w') + x_j (x_i w \mathfrak{m} w')$$

for all  $x_i, x_j \in X, w, w' \in X^*$ . The subspace  $\mathbb{Q}1 \oplus x_0 \mathbb{Q}\langle X \rangle x_1$  of convergent words is a subalgebra of  $\mathbb{Q}\langle X \rangle$  with respect to  $\mathfrak{m}$ . It follows immediately from the corresponding shuffle product formula for the functions  $\text{Li}_w(z)$  that

$$\zeta(w)\zeta(w') = \zeta(w \mathfrak{m} w') \quad \text{for all } w, w' \in x_0 X^* x_1.$$

This gives, for example,  $\zeta(x_0 x_1)\zeta(x_0 x_1) = 2\zeta(x_0 x_1 x_0 x_1) + 4\zeta(x_0 x_0 x_1 x_1)$ , that is  $\zeta(2)\zeta(2) = 2\zeta(2, 2) + 4\zeta(1, 3)$ .



- *The stuffle (or quasi-shuffle) product.* The stuffle product comes from the representation of multiple zetas as nested sums. We will not prove the general case (see e.g. [25, 27]), but only illustrate in the simplest case. Decomposing the domain  $\mathbb{N} \times \mathbb{N}$  of summation into 3 regions in the following gives:

$$\sum_{k \geq 1} \frac{1}{k^m} \sum_{\ell \geq 1} \frac{1}{\ell^n} = \left( \sum_{k < \ell} + \sum_{\ell < k} + \sum_{k = \ell} \right) \frac{1}{k^m \ell^n}$$

$$\zeta(m)\zeta(n) = \zeta(m, n) + \zeta(n, m) + \zeta(m + n)$$

The general case is similar and gives a formula relating the product of any multiple zetas as a linear combination of other multiple zetas of the same weight. This product can also be encoded symbolically with words as follows. For each  $i \geq 1$ , we write  $y_i = x_0^{i-1} x_1$ . Then  $\mathbb{Q}1 \oplus \mathbb{Q}\langle X \rangle x_1 \cong \mathbb{Q}\langle Y \rangle$ , where  $Y = \{y_n, n \in \mathbb{N}\}$ . The stuffle product, written

$$\star : \mathbb{Q}\langle Y \rangle \times \mathbb{Q}\langle Y \rangle \rightarrow \mathbb{Q}\langle Y \rangle ,$$

is defined inductively as follows:

$$w \star 1 = w \quad 1 \star w = w \quad \text{for all } w \in Y^*$$

$$y_i w \star y_j w' = y_i (w \star y_j w') + y_j (y_i w \star w') + y_{i+j} (w \star w') ,$$

for all  $i, j \geq 1$  and  $w, w' \in Y^*$ . The stuffle relation is then:

$$\zeta(w)\zeta(w') = \zeta(w \star w') \quad \text{for all } w, w' \in x_0 X^* x_1 .$$

For example, the relation we derived earlier by decomposing the domain of summation corresponds to  $y_m \star y_n = y_m y_n + y_n y_m + y_{m+n}$ .

- *Regularization relation.* Let  $w \in x_0 X^* x_1$  be a convergent word. One can prove that  $x_1 \star w - x_1 \text{III} w \in x_0 X^* x_1$  is also a linear combination of convergent words. The regularization, or Hoffman, relation is given by:

$$\zeta(x_1 \star w - x_1 \text{III} w) = 0 .$$

Applying this identity to  $w = x_0 x_1$ , for example, yields the relation

$$(5.1) \quad \zeta(3) = \zeta(1, 2)$$

which was first proved by Euler.

It is conjectured that all algebraic relations over  $\mathbb{Q}$  satisfied by the multiple zeta values are generated by the previous three identities (to get a sense of this, prove that  $\zeta(4)$  is a multiple of  $\zeta(2)^2$  using the standard identities only).

One can then try to write down a minimal basis for the multiple zeta values in each weight by solving these equations. What one finds is the following table, to weight 8:

Weight	1	2	3	4	5	6	7	8
		$\zeta(2)$	$\zeta(3)$	$\zeta(4)$	$\zeta(5)$	$\zeta(6)$	$\zeta(7)$	$\zeta(8)$
					$\zeta(2)\zeta(3)$	$\zeta(3)^2$	$\zeta(2)\zeta(5)$	$\zeta(3)\zeta(5)$
							$\zeta(3)\zeta(4)$	$\zeta(3)^2\zeta(2)$
								$\zeta(3, 5)$
dim	0	1	1	1	2	2	3	4

For example, in depth 3 there are *a priori* two multiple zeta values,  $\zeta(3)$  and  $\zeta(1, 2)$ , but the identity (5.1) tells us that they coincide. So  $\dim_{\mathbb{Q}}(\mathbb{Q}\zeta(3) + \mathbb{Q}\zeta(1, 2)) = 1$ . We could have replaced  $\zeta(2n)$  with  $\zeta(2)^n$  in the table by Euler's theorem. Note that up to weight 7, all multiple zeta values are spanned by products of ordinary zeta values

$\zeta(n)$ . In weight 8, something interesting happens for the first time, and there is a new quantity  $\zeta(3, 5)$  which is irreducible, in the sense that it (conjecturally, at least) cannot be expressed as a polynomial in the  $\zeta(n)$ .

The dimensions at the bottom, which we denote by  $d_k$  in weight  $k$ , mean the following. Take the  $\mathbb{Q}$ -vector space spanned by the symbols  $\zeta(w)$ , where  $w$  ranges over the set of convergent words of length  $k$ , and take the quotient by all linear relations  $\zeta(\eta \sqcap \eta') - \zeta(\eta \star \eta')$  deduced from the standard relations. This gives an upper bound for the dimension of the vector space spanned by the actual values  $\zeta(w) \in \mathbb{R}$ .

**Conjecture 2.** (Zagier)  $d_k = d_{k-2} + d_{k-3}$ .

This conjecture is purely algebraic, but in fact Zagier also conjectured that the dimension of the *actual* zeta values in weight  $k$  should be  $d_k$ . This, transcendental part of the conjecture, is already completely unknown in weight 5 and is equivalent to

$$\frac{\zeta(5)}{\zeta(2)\zeta(3)} \notin \mathbb{Q}.$$

What is known in the algebraic direction is the following:

**Theorem 5.1.** (Goncharov, Terasoma). *Let  $D_1 = 0, D_2 = 1$ , and define  $D_k$  for  $k \geq 2$  by  $D_k = D_{k-2} + D_{k-3}$ . Then*

$$\dim_{\mathbb{Q}}\langle \zeta(k) \text{ of weight } k \rangle \leq D_k.$$

The proof of this theorem is one of the most striking applications of the theory of mixed Tate motives. What is not known, however, is whether the standard relations are enough to span all  $\mathbb{Q}$ -relations satisfied by the multiple zeta values, and there is no known algorithm to reduce a given multiple zeta value into a given basis using the above relations.

There is also a more precise conjecture for the number of zeta values of given weight and depth (the depth of  $\zeta(n_1, \dots, n_r)$  being the number  $r$ ) which is due to Broadhurst and Kreimer [3].

**5.3. Hopf algebra interpretation.** Some of the previous conjectures can be reformulated in terms of a certain Hopf algebra. Let  $\mathcal{L} = \mathbb{Q}[e_3, e_5, \dots]$  denote the free Lie algebra generated by one element  $e_{2n+1}$  in every odd degree. Consider the Lie algebra

$$\mathcal{F} = \mathbb{Q}[e_2] \oplus \mathcal{L},$$

in which the new generator  $e_2$  in degree 2 commutes with all the others. The underlying graded vector space is generated by, in increasing weight:

$$e_2, e_3, e_5, e_7, [e_3, e_5], e_9, [e_3, e_7], e_{11}, [e_3, [e_5, e_3]], \dots$$

Let  $\mathcal{UF}$  be its universal enveloping algebra, and let  $\mathbb{M}$  be its graded dual, which is a commutative Hopf algebra. Concretely,  $\mathbb{M}$  is the set of all non-commutative words in letters  $f_{2n+1}$  dual to  $e_{2n+1}$ , equipped with the shuffle product  $\sqcap$ :

$$\mathbb{M} = \mathbb{Q}[f_2] \otimes_{\mathbb{Q}} (\mathbb{Q}\langle f_3, f_5, f_7 \rangle \dots, \sqcap)$$

The generators in each weight up to 8 are precisely:

$$f_2 ; f_3 ; f_2^2 ; f_5, f_2 f_3 ; f_3^2, f_2^3 ; f_7, f_2 f_5, f_2^2 f_3 ; f_2^4, f_2 f_3^2, f_3 \sqcap f_5, f_3 f_5,$$

which matches the table for MZVs above. In weight 8 the basis can be written  $f_3 f_5, f_5 f_3, f_2^4, f_2 f_3^2$ . The following conjecture, due to Goncharov [11], is a more precise version of conjecture 2.

**Conjecture 3.** The algebra spanned by the multiple zetas over  $\mathbb{Q}$  is isomorphic to  $\mathbb{M}$ .

This conjecture comes from the theory of mixed Tate motives (over  $\mathbb{Z}$ ) and has several consequences.

- Firstly, since  $\mathbb{M}$  is graded by the weight, it implies that there should exist no algebraic relations between any multiple zeta values of different weights.
- Secondly, it implies conjecture 2. To see this, let  $V = \bigoplus_{k \geq 0} V_k$  be any graded vector space such that the  $V_k$  are finite-dimensional, and let

$$\chi(V)(t) = \sum_k \dim_k(V_k) t^k$$

denote the generating series of its graded dimensions. For any two such graded vector spaces  $V, V'$  we have  $\chi(V \otimes_{\mathbb{Q}} V') = \chi(V)\chi(V')$ . Then

$$\chi(\mathbb{Q}\langle f_3, f_5, \dots \rangle)(t) = \frac{1}{1 - t^3 - t^5 - t^7 - \dots} = \frac{1 - t^2}{1 - t^2 - t^3}$$

and since  $\mathbb{M} = \mathbb{Q}\langle f_2 \rangle \otimes_{\mathbb{Q}} \mathbb{Q}\langle f_3, f_5, \dots \rangle$  we deduce that

$$\chi(\mathbb{M})(t) = \left( \frac{1}{1 - t^2} \right) \left( \frac{1 - t^2}{1 - t^2 - t^3} \right) = \frac{1}{1 - t^2 - t^3} = \sum_{k \geq 0} D_k t^k,$$

where the numbers  $D_k$  satisfy  $D_k = D_{k-2} + D_{k-3}$ .

- Since  $\mathbb{M}$  is a Hopf algebra, it implies that the coproduct  $\Delta : \mathbb{M} \rightarrow \mathbb{M} \otimes \mathbb{M}$  should also exist on the level of multiple zeta values. The coproduct on  $\mathbb{M}$  is induced by the deconcatenation coproduct

$$\begin{aligned} \Delta(f_{2i_1+1} \dots f_{2i_r+1}) &= f_{2i_1+1} \dots f_{2i_r+1} \otimes 1 + 1 \otimes f_{2i_1+1} \dots f_{2i_r+1} \\ &+ \sum_{k=1}^{r-1} f_{2i_1+1} \dots f_{2i_k+1} \otimes f_{2i_{k+1}+1} \dots f_{2i_r+1}. \end{aligned}$$

It makes no sense to define a coproduct on the level of the numbers  $\zeta(w)$  because of the inaccessibility of the transcendence conjectures. However, one can lift the ordinary zeta values to ‘motivic multiple zeta values’  $\zeta^M(w)$ , which generate a sub-Hopf algebra  $\mathbb{M}' \subset \mathbb{M}$  (conjecturally,  $\mathbb{M}' = \mathbb{M}$ ). The objects  $\zeta^M(w)$  satisfy the standard relations, and the period map takes each  $\zeta^M(w)$  to the number  $\zeta(w)$ . On the level of the motivic multiple zetas, the restriction of  $\Delta$  to  $\mathbb{M}'$  does make sense, and for example, gives [11]:

$$\begin{aligned} \Delta \zeta^M(n) &= 1 \otimes \zeta^M(n) + \zeta^M(n) \otimes 1 \\ \Delta \zeta^M(3, 5) &= 1 \otimes \zeta^M(3, 5) - 5 \zeta^M(3) \otimes \zeta^M(5) + \zeta^M(3, 5) \otimes 1 \end{aligned}$$

Note, however, that the coproduct on the motivic multiple zeta values is very complicated in general and shows that  $\zeta^M(n_1, \dots, n_r)$  does not correspond to an element of  $\mathbb{M}$  (i.e. word in the  $f$ ’s) in any straightforward way.

*Remark 5.2.* The (conjectural) existence of a coproduct on the multiple zeta values is a genuinely new feature given by the motivic theory, and it seems, has not yet been exploited by physicists. We believe that it should have much relevance to perturbative quantum field theories: many Feynman amplitudes should be certain linear combinations of MVZs which are ‘simple’ with respect to the coproduct  $\Delta$  (in other words, they should be filtered in an interesting way by the coradical filtration).

## 6. ITERATED INTEGRALS AND HOMOTOPY INVARIANCE

We now return to the general theory of iterated integrals and state necessary and sufficient conditions for an iterated integral to be a homotopy functional. We then state Chen's  $\pi_1$ -de Rham theorem, and relate it to the previous talks.

**6.1. Homotopy functionals.** For motivation we begin by constructing some simple examples of homotopy-invariant iterated integrals. Let  $M$  be a smooth manifold,  $\omega$  a smooth 1-form on  $M$ , and  $\gamma : [0, 1] \rightarrow M$  a smooth path.

**Lemma 6.1.** *The line integral  $\int_\gamma \omega$  is a homotopy functional if and only if  $\omega$  is closed.*

*Proof.* Since the result is well known, we only sketch the argument. Suppose that the integral is a homotopy functional. Then for every closed loop  $\gamma : [0, 1] \rightarrow M$  which bounds a small disk  $D \subset M$ , the integral of  $\omega$  along  $\gamma$  is zero. By Stokes' theorem

$$\oint_\gamma \omega = \int_D d\omega .$$

Since this vanishes for all small disks centered at every point of  $M$ , we conclude that  $d\omega = 0$ . In the converse direction, by the Poincaré lemma, a closed form is locally exact, and so  $d\omega = 0$  implies that the integral around any small loop is zero.  $\square$

Now suppose that  $\omega_1, \omega_2$  are closed one-forms. By the previous lemma, the line integrals  $\int \omega_i$ , for  $i = 1, 2$  are homotopy functionals. Therefore if  $\gamma : [0, 1] \rightarrow M$  is a smooth path with fixed initial point  $\gamma(0)$  but variable endpoint  $z = \gamma(1)$  then  $F_2(z) = \int_\gamma \omega_2$  defines a multivalued function on  $M$  which satisfies  $dF_2(z) = \omega_2$  by the fundamental theorem of calculus. Consider the iterated integral

$$I = \int_\gamma \omega_1 \omega_2 + \omega_{12}$$

Recall from the definition of the iterated integrals that  $I = \int_\gamma \omega_1 \wedge F_2(z) + \omega_{12}$ . By the lemma, it is a homotopy functional if and only if the integrand is closed, i.e.,

$$d(\omega_1 \wedge F_2(z) + \omega_{12}) = 0 .$$

By Leibniz' rule, this gives:  $d\omega_1 \wedge F_2(z) + \omega_1 \wedge \omega_2 + d\omega_{12} = 0$ . Thus  $I$  defines a homotopy functional if and only if

$$(6.1) \quad \omega_1 \wedge \omega_2 + d\omega_{12} = 0 .$$

More generally, suppose that  $\omega_i$  are closed one-forms. A similar calculation shows that

$$\int \sum_{i,j} \omega_i \omega_j + \omega_k$$

is a homotopy functional if and only if  $\sum_{i,j} \omega_i \wedge \omega_j + d\omega_k = 0$ .

**Example 6.2.** Let  $\omega_1, \omega_2, \omega_3$  be closed one-forms on  $M$ , and suppose that  $\omega_1 \wedge \omega_2$  and  $\omega_2 \wedge \omega_3$  are exact. Then we can find  $\omega_{12}, \omega_{13}$  such that  $d\omega_{12} = -\omega_1 \wedge \omega_2$  and  $d\omega_{13} = -\omega_2 \wedge \omega_3$ . It follows that  $\omega_1 \wedge \omega_{23} + \omega_{12} \wedge \omega_3$  is closed. Now suppose that there is a one-form  $\omega_{123}$  (known as a Massey triple product of  $\omega_1, \omega_2, \omega_3$ ) such that

$$d\omega_{123} = \omega_1 \wedge \omega_{23} + \omega_{12} \wedge \omega_3 .$$

Then  $\int \omega_1 \omega_2 \omega_3 + \omega_{12} \omega_3 + \omega_{123}$  is a homotopy functional.

**Exercise 6.3.** Consider the trivial bundle  $k^3 \times M \rightarrow M$ . The following matrix of 1-forms

$$\Omega = \begin{pmatrix} 0 & 0 & 0 \\ \omega_1 & 0 & 0 \\ \omega_{12} & \omega_2 & 0 \end{pmatrix}$$

defines a connection on it which is integrable if and only if  $d\Omega = \Omega \wedge \Omega$ , which is exactly the requirement  $d\omega_{12} = \omega_1 \wedge \omega_2$  (6.1).

**6.2. The bar construction.** The general condition for the homotopy invariance of iterated integrals can be stated in terms of the bar construction. Let  $\mathcal{A}^*(M)$  be the complex of  $C^\infty$  forms on  $M$ , and let us suppose that  $X \subset \mathcal{A}^*(M)$  is a connected model for  $M$ , i.e, such that  $X^0 \cong k$  and the map

$$(6.2) \quad X \longrightarrow \mathcal{A}^*(M)$$

induces an isomorphism  $H^*(X) \rightarrow H^*(\mathcal{A}^*(M)) = H^*(M)$  (in fact it suffices to be an isomorphism on  $H^1$  and injective on  $H^2$ ). When considering the tensor product  $(X^1)^{\otimes n}$ , it is customary in this context to use the bar notation and write  $[\omega_1 | \dots | \omega_n]$  for  $\omega_1 \otimes \dots \otimes \omega_n$ . Consider the map:

$$D : (X^1)^{\otimes n} \rightarrow (\mathcal{A}^\bullet(M))^{\otimes n}$$

$$D([\omega_1 | \dots | \omega_n]) = \sum_{i=1}^n [\omega_1 | \dots | \omega_{i-1} | d\omega_i | \omega_{i+1} | \dots | \omega_n] + \sum_{i=1}^{n-1} [\omega_1 | \dots | \omega_{i-1} | \omega_i \wedge \omega_{i+1} | \dots | \omega_n]$$

Let us define

$$B_n(M) = \{ \xi = \sum_{\ell=0}^n \sum_{i_1, \dots, i_\ell} [\omega_{i_1} | \dots | \omega_{i_\ell}] \text{ such that } D\xi = 0, \text{ where } \omega_{i_j} \in X^1 \}$$

We call such an element  $\xi$  satisfying  $D\xi = 0$  an integrable word in  $X^1$ . The union  $B(M) = \cup_{n \geq 0} B_n(M)$  is a vector space over  $k$ , and the index  $n$  defines a filtration on it which is called the length filtration. One verifies that  $B(M)$  is a commutative algebra for the shuffle product

$$\sharp : B(M) \otimes_k B(M) \longrightarrow B(M)$$

(for this, one must check that  $D$  defined above satisfies the Leibniz rule with respect to the shuffle product on  $X^{\otimes n}$ ) and is in fact a commutative Hopf algebra for the deconcatenation coproduct:

$$\Delta : B(M) \longrightarrow B(M) \otimes_k B(M)$$

$$(6.3) \quad [\omega_{i_1} | \dots | \omega_{i_\ell}] \mapsto \sum_{r=0}^{\ell} [\omega_{i_1} | \dots | \omega_{i_r}] \otimes [\omega_{i_{r+1}} | \dots | \omega_{i_\ell}]$$

In conclusion,  $B(M)$  is a filtered, commutative Hopf algebra. It follows from the definition of  $D$  and (6.2) that in length one, we have:

$$B_1(M) \cong k \oplus H^1(M; k).$$

To any element  $\xi$  in  $B_n(M)$ , we can associate the corresponding iterated integral

$$(6.4) \quad \sum_{\ell=0}^n \sum_{i_1, \dots, i_\ell} [\omega_{i_1} | \dots | \omega_{i_\ell}] \mapsto \sum_{\ell=0}^n \sum_{i_1, \dots, i_\ell} \int_{\gamma} \omega_{i_1} \dots \omega_{i_\ell}$$

where  $\gamma : [0, 1] \rightarrow M$  is a smooth path in  $M$ . Chen's theorem states that this iterated integral is a homotopy functional, and furthermore, that all such homotopy functionals arise in this way.

**Theorem 6.4.** (Chen). *The integration map (6.4) gives an isomorphism:*

$$B_n(M) \longrightarrow \{\text{homotopy invariant iterated integrals of length } \leq n\}$$

In particular, if we consider paths with fixed  $\gamma(0) = z_0$  and let  $\gamma(1) = z$ , then the iterated integrals of elements  $\xi \in B_n(M)$  along  $\gamma$  define multivalued functions on  $M$ . One can check that their differential is given by

$$d\left(\sum_{\ell=0}^n \sum_{i_1, \dots, i_\ell} \int_{\gamma} \omega_{i_1} \cdots \omega_{i_\ell}\right) = \sum_{\ell=0}^n \sum_{i_1, \dots, i_\ell} \omega_{i_\ell} \int_{\gamma} \omega_{i_1} \cdots \omega_{i_{\ell-1}},$$

which is induced from the  $(\ell - 1, 1)$ -part of the coproduct  $\Delta$ .

*Remark 6.5.*  $B_n(M)$  is usually written  $H_0(\overline{B}_n(\mathcal{A}^\bullet(M)))$ , where  $\overline{B}_n$  denotes Chen's reduced bar construction.

One can generalize the definition of iterated integrals for forms of any degree. Such an iterated integral defines a form on the space of paths of  $M$ . The  $H_0$  refers to locally constant functions on the space of paths, i.e., the homotopy invariant functions on  $M$ .

**6.3. Chen's theorem.** Let  $M$  be a smooth manifold, and let  $\pi_1(M, x)$  be the fundamental group of  $M$  based at a point  $x \in M$ . One can extend the definition of iterated integrals by linearity to the group ring

$$\mathbb{Q}[\pi_1(M, x)]$$

as follows. For any combination of paths  $g = \sum_{i=1}^n a_i \gamma_i \in \mathbb{Q}[\pi_1(M, x)]$ , and any one forms  $\omega_1, \dots, \omega_r$  on  $M$ , one can define the iterated integral along  $g$  by:

$$\int_g \omega_1 \cdots \omega_r = \sum_{i=1}^n a_i \int_{\gamma_i} \omega_1 \cdots \omega_r.$$

Recall that for ordinary line integrals, we have the formula

$$\int_{(\gamma_1-1)(\gamma_2-1)} \omega = 0$$

where 1 is the constant path at  $x$ . By expanding  $(\gamma_1 - 1)(\gamma_2 - 1)$ , this is equivalent to the composition of paths formula (proposition 2.2 (iii)):

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

The generalization for iterated integrals is the following.

**Lemma 6.6.** *Let  $\omega_1, \dots, \omega_r$  be smooth 1-forms on  $M$ , and let  $\gamma_1, \dots, \gamma_s$  be loops on  $M$  based at  $x$ . If  $s > r$  then*

$$\int_{(\gamma_1-1)\dots(\gamma_s-1)} \omega_1 \dots \omega_r = 0$$

*Proof.* The formula for the composition of paths (proposition 2.2 (iii)), remains valid for linear combinations of paths. Recall that, in that formula, the empty iterated integral ( $r = 0$ ) over a path  $\gamma$  is just the constant function 1. It follows that the empty iterated integral over  $(\gamma_1 - 1)$  is zero. The general case follows by induction. Setting  $\beta = (\gamma_2 - 1) \dots (\gamma_s - 1) \in \mathbb{Q}[\pi_1(M, x)]$ , we can write  $(\gamma_1 - 1) \dots (\gamma_s - 1) = \gamma_1 \beta - \beta$ . Therefore by the composition of paths formula,

$$\int_{(\gamma_1-1)\beta} \omega_1 \dots \omega_r = \sum_{i=0}^r \int_{\gamma_1} \omega_1 \dots \omega_i \int_{\beta} \omega_{i+1} \dots \omega_r - \int_{\beta} \omega_1 \dots \omega_r$$

$$= \sum_{i=1}^r \int_{\gamma_1} \omega_1 \dots \omega_i \int_{\beta} \omega_{i+1} \dots \omega_r$$

But the second term in the last line is an integral of at most  $r - 1$  forms over a composition  $\beta = (\gamma_2 - 1) \dots (\gamma_s - 1)$ , which vanishes by induction since  $s - 1 > r - 1$ .  $\square$

Consider the augmentation map:

$$\begin{aligned} \varepsilon : \mathbb{Q}[\pi(M, x)] &\longrightarrow \mathbb{Q} \\ \gamma &\longmapsto 1 \end{aligned}$$

and let  $J = \ker \varepsilon \subset \mathbb{Q}[\pi_1(M, x)]$  be the augmentation ideal. It is generated by the elements of the form  $\gamma - 1$ , with  $\gamma \in \pi_1(M, x)$ . The truncated group ring is defined by:

$$V_n = \mathbb{Q}\pi_1(M, x)/J^{n+1}.$$

Recall that the integration map gives a pairing

$$(6.5) \quad \begin{aligned} \mathbb{Q}[\pi_1(M, x)] \otimes_{\mathbb{Q}} B_n(M) &\longrightarrow \mathbb{C} \\ g \otimes [\omega_1 | \dots | \omega_n] &\longmapsto \int_g \omega_1 \dots \omega_n \end{aligned}$$

The previous lemma states that this map vanishes on  $J^m$  if  $m \geq n + 1$ . From this we deduce a map

$$(6.6) \quad \begin{aligned} B_n(M) &\xrightarrow{\phi} \text{Hom}_{\mathbb{Q}}(V_{n+1}, \mathbb{C}) \\ \xi &\longmapsto \left( g \mapsto \int_g \xi \right) \end{aligned}$$

**Theorem 6.7.** (*Chen's  $\pi_1$ -de Rham theorem*). *The map  $\phi$  is an isomorphism.*

References for the proofs of the above theorems can be found in [13], [10], [12].

**Example 6.8.** Recall that we had  $B_1(M) \cong H_{DR}^1(M) \oplus k$ . On the other hand

$$V_2 = \mathbb{Q}[\pi_1(M, x)]/J^2 \cong H_1(M) \oplus \mathbb{Q}$$

by Hurwitz' theorem. Therefore in the case  $n = 1$ , Chen's theorem is equivalent to saying that the integration map

$$H_{DR}^1(M) \longrightarrow \text{Hom}(H_1(M), \mathbb{C})$$

is an isomorphism. This is exactly de Rham's theorem in degree one.

**6.4. Example: multiple polylogarithms in one variable.** Let  $M = \mathbb{P}^1 \setminus \{0, 1, \infty\}$ . In this case we can take  $X \subset \mathcal{A}^1(M)$  to be the  $\mathbb{C}$ -vector space spanned by  $\omega_0 = \frac{dz}{z}$  and  $\omega_1 = \frac{dz}{1-z}$  since these form a basis for  $H^1(M)$ . Since  $\omega_0, \omega_1$  are closed and satisfy  $\omega_i \wedge \omega_j = 0$  for all  $i, j \in \{0, 1\}$  ( $M$  is one-dimensional) the integrability condition  $D\xi = 0$  is trivially satisfied for any word  $\xi$  in the forms  $\omega_0, \omega_1$ . Thus

$$B_n(M) = \{[\omega_{i_1} | \dots | \omega_{i_k}] : i_j \in \{0, 1\} \quad k \leq n\}$$

is the set of words in  $\{\omega_0, \omega_1\}^*$  with at most  $n$  letters, and the bar construction is isomorphic to the shuffle algebra:

$$B(M) \cong \mathbb{C}\langle\{\omega_0, \omega_1\}\rangle$$

equipped with the deconcatenation coproduct, and Chen's theorem boils down to theorem 4.5. In this case, it follows from the fact that  $M$  is defined over  $\mathbb{Q}$  that  $B(M)$  can also be defined over  $\mathbb{Q}$ , simply by taking  $\mathbb{Q}$ -linear combinations of words in  $\omega_0, \omega_1$ . Note that it is this  $\mathbb{Q}$ -structure that defines the  $\mathbb{Q}$ -algebra of multiple zeta values.

**6.5. Example: multiple polylogarithms in several variables.** The previous example generalizes to the family of manifolds  $M = \mathfrak{M}_{0,n+3}$ , where  $n \geq 1$ , defined by the complement of hyperplanes

$$\mathfrak{M}_{0,n+3}(\mathbb{C}) = \{(t_1, \dots, t_n) \in \mathbb{C}^n : t_i \neq t_j, \quad t_i \neq 0, 1\}.$$

The notation  $\mathfrak{M}_{0,n+3}$  comes from the fact that these are isomorphic to the moduli spaces of curves of genus 0 with  $n+3$  ordered marked points. The previous example concerns the iterated integrals on  $\mathfrak{M}_{0,4}(\mathbb{C}) \cong \mathbb{C} \setminus \{0, 1\}$ . In order to write down the bar construction, we need a model for the de Rham complex on  $\mathfrak{M}_{0,n}$ . Therefore consider the set of differential forms

$$\Omega = \left\{ \frac{dt_i - dt_j}{t_i - t_j}, \frac{dt_i}{t_i}, \frac{dt_i}{1 - t_i} \right\}$$

and denote its elements by  $\omega_1, \dots, \omega_N$ , where  $N = n(n-3)/2$ . Let  $X = \bigoplus_{n \geq 0} X^n$  denote the  $\mathbb{Q}$ -subalgebra of regular differential forms on  $\mathfrak{M}_{0,n}$  spanned by  $\Omega$  and graded by the degree. It is connected, i.e.,  $X^0 \cong \mathbb{Q}$ .

**Theorem 6.9.** (Arnold) *The map  $X_{\otimes \mathbb{Q}} \mathbb{C} \rightarrow A^*(\mathfrak{M}_{0,n+3})$  is a quasi-isomorphism, i.e., induces an isomorphism on cohomology.*

This means that the space  $\mathfrak{M}_{0,n+3}$  is formal and implies that there are no Massey products in this case. Furthermore,  $X$  has a natural  $\mathbb{Q}$  structure and so we henceforth work over  $\mathbb{Q}$ . The set of integrable words of length  $n$  in  $B(\Omega)$  can be written

$$\xi = \sum_{I=(i_1, \dots, i_n)} c_I [\omega_{i_1} | \dots | \omega_{i_n}] \quad c_I \in \mathbb{Q}$$

such that

$$\omega_{i_1} \otimes \dots \otimes \omega_{i_k} \wedge \omega_{i_{k+1}} \otimes \dots \otimes \omega_{i_n} = 0 \quad \in \quad (\Omega^1)^{\otimes k-1} \otimes \Omega^2 \otimes (\Omega^1)^{\otimes n-k-1}.$$

In particular, the bar construction  $B(\mathfrak{M}_{0,n+3})$  is graded by the length.

The description of the iterated integrals on  $\mathfrak{M}_{0,n+3}$  requires the definition of multiple polylogarithms in several variables.

**Definition 6.10.** (Goncharov) Let  $n_1, \dots, n_r \in \mathbb{N}$  and define the multiple polylogarithm in several variables by the nested sum

$$\text{Li}_{n_1, \dots, n_r}(x_1, \dots, x_r) = \sum_{0 < k_1 < \dots < k_r} \frac{x_1^{k_1} \dots x_r^{k_r}}{k_1^{n_1} \dots k_r^{n_r}}$$

which converges absolutely on compacta in the polydisc  $|x_i| < 1$ .

In order to make the connection with  $\mathfrak{M}_{0,n+3}$  consider the functions

$$I_{n_1, \dots, n_r}(t_1, \dots, t_n) = \text{Li}_{n_1, \dots, n_r} \left( \frac{t_1}{t_2}, \dots, \frac{t_{r-1}}{t_r}, t_r \right)$$

which can be shown to have an analytic continuation as multivalued functions on the whole of  $\mathfrak{M}_{0,r+3}$ , and have unipotent monodromy. The converse is also true:

**Theorem 6.11.** *Every (homotopy-invariant) iterated integral on  $\mathfrak{M}_{0,n+3}$  can be expressed (non-uniquely) as a sum of products of the functions  $\log(t_i)$ ,  $1 \leq i \leq n$ , and the multiple polylogarithms  $I_{n_1, \dots, n_r}(\frac{s_1}{s_2}, \dots, \frac{s_{r-1}}{s_r}, s_r)$  where  $s_i \in \{1, t_1, \dots, t_n\}$ .*

A basis for the iterated integrals on  $\mathfrak{M}_{0,n+3}$  is given in [4].



**Example 6.12.** Consider the function  $I_{1,1}(t_1, t_2)$ . It follows from the definition as a nested sum that it satisfies a differential equation of the form:

$$dI_{1,1}(t_1, t_2) = dI_1\left(\frac{t_1}{t_2}\right)I_1(t_2) + dI_1(t_2)I_1(t_1) - dI_1\left(\frac{t_2}{t_1}\right)I_1(t_1)$$

Since  $I_1(t) = -\log(1-t)$ , one deduces that the following word

$$\xi = [d\log(1 - \frac{t_1}{t_2})|d\log(1 - t_2)] + [d\log(1 - t_2)|d\log(1 - t_1)] - [\log(1 - \frac{t_2}{t_1})|\log(1 - t_1)]$$

is integrable, and  $I_{1,1}(t_1, t_2)$  is the iterated integral:

$$I_{1,1}(t_1, t_2) = \int_{\gamma} \xi$$

where  $\gamma$  is a path from  $(0,0)$  to  $(t_1, t_2)$ . In particular, the expression for  $\xi$  gives a formula for the coproduct of  $I_{1,1}(t_1, t_2)$ .

*Remark 6.13.* By computing the integrable word for  $I_{n_1, \dots, n_r}(t_1, \dots, t_r)$ , and then taking the appropriate limit of its coproduct as  $t_1, \dots, t_r \rightarrow 1$ , one can retrieve the correct expression for the motivic coproduct for  $\zeta^M(n_1, \dots, n_r)$  mentioned earlier (§5.2).

The multivariable analogue of theorem 4.6 is the following. Let  $\mathcal{O}(\mathfrak{M}_{0,n+3}) = \mathbb{Q}[t_1, \dots, t_n, t_i^{-1}, (1-t_i)^{-1}, (t_i-t_j)^{-1}]$  denote the ring of regular functions on  $\mathfrak{M}_{0,n+3}$  and let  $L$  denote the  $\mathcal{O}(\mathfrak{M}_{0,n+3})$ -algebra spanned by the functions in theorem 6.11.

**Theorem 6.14.** *The following complex*

$$0 \rightarrow L \rightarrow L \otimes_{\mathbb{Q}} X^1 \rightarrow L \otimes_{\mathbb{Q}} X^2 \rightarrow \dots \rightarrow L \otimes_{\mathbb{Q}} X^n \rightarrow 0,$$

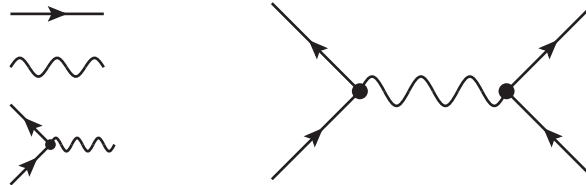
*is exact in all degrees  $\geq 1$ .*

In other words, every closed form of degree  $\geq 1$  on  $\mathfrak{M}_{0,n+3}$  with coefficients in  $L$  is exact. Concretely, any differential form of degree  $\geq 1$  whose coefficients are multiple polylogarithms and rational functions in  $\mathcal{O}(\mathfrak{M}_{0,n+3})$  always has a primitive of the same form. As in the single-variable case  $\mathfrak{M}_{0,4}$ , it is this property which provides the connection with Feynman diagram computations (see §7).

*Remark 6.15.* Even though the picture in genus 0 is quite complete, the analogous numbers and functions are not known in the case of curves of higher genus.

## 7. FEYNMAN INTEGRALS

**7.1. Very short introduction to perturbative quantum field theory.** A quantum field theory can be represented by certain families of vertices and edges of different types. By putting them together, one obtains Feynman diagrams, such as on the right:



The graph elements on the left are taken from quantum electrodynamics: the solid line represents an electron moving in the direction of the arrow (or a positron moving in the opposite direction), the wiggly line represents a photon, and the three-valent vertex represents their interaction. A graph such as on the right represents a process involving these elementary particles; in this case, the exchange of a photon between two electrons. The same diagram has other interpretations, depending on the direction of the time axis (if the time axis goes from left to right, it shows an electron and positron annihilating to give a photon, which in turn decays into an electron and positron). To this graph one associates a ‘probability’ or Feynman amplitude, which is an integral determined from the graph by the Feynman rules. From the mathematician’s point of view, a Feynman graph can be thought of as a compact way to encode an integral. In order to obtain a physical prediction for a process, one must then sum over all possible Feynman amplitudes which contribute to the given process. The diagrams with higher numbers of loops represent successive approximations - the higher the loop order diagrams one can calculate, the more accurate the theoretical prediction. But this comes at great cost, since the number of diagrams grows very fast at increasing loop orders, and the integrals themselves become extremely hard to compute. Indeed, a vast amount of effort in the modern physics literature is devoted to the calculation of Feynman integrals, and this is the main way in which theoretical predictions for particle collider experiments are currently obtained.

In the next paragraph, we try to justify the (rather arduous, but well-understood [15],[22]) passage from realistic quantum field theories to the simplified scalar Feynman diagrams we shall consider in the sequel. The reader only interested in the connection with number theory can skip straight to §7.3.

**7.2. Parametric forms for scalar integrals.** The reduction of (momentum space) Feynman integrals down to a convenient convergent parametric form, is a long and involved process involving several steps, which are well documented, and which we do not wish to reproduce here. Roughly speaking, there are three main stages:

- (1) Reduction to scalar integrals
- (2) Change of variables to parametric form (via the Schwinger or Feynman trick)
- (3) Regularization and renormalization of divergent subgraphs (e.g., BPHZ)

Here follow some comments on each step. In this talk we shall only consider scalar integrals. The general effect of tensor structures only affects the numerators of the resulting parametric integrals, so it follows that the mathematical structure, and number theory content, of the general case is very similar. It also turns out that the parametric form of Feynman integrals (2), which goes back to the early days of quantum field theory, is not the most frequently used by practitioners at present, but turns out to be the closest to algebraic geometry, and hence most convenient for our purposes. It is likely

that much of what follows could also be translated to the coordinate space setting. The renormalization of (ultra-violet) divergences (3) is the most delicate point. In recent calculations, a common approach appears to be the following: first, one regularizes divergent integrals using dimensional regularization (working in dimensions  $D = 4 - 2\varepsilon$ , and expanding integrals as Laurent series in  $\varepsilon$ ); secondly, counter-terms are subtracted according to the BPHZ formula to retrieve the finite convergent part. In this talk, we shall mainly consider subdivergence-free graphs for which no renormalization is required. However, the methods surely carry over to the general case. For this, one must completely reconsider the approach to step (3), and perform the subtraction of counter-terms directly on the level of the parametric integral. At the end one can write the renormalized Feynman integral as a single absolutely convergent parametric integral, and apply the methods below. Again, the mathematics is not so dissimilar from the subdivergence-free case (this will be discussed in a forthcoming paper with D. Kreimer). In conclusion, the reduction to scalar, subdivergence-free parametric integrals, does not forfeit much and the mathematical structure we consider below captures much of the general case.

**7.3. The first and second Symanzik polynomials.** A Feynman graph  $G$  is a collection of *corollas* of degree  $n \geq 3$  (a single vertex  $v$  surrounded by  $n$  half-edges  $v_1, \dots, v_n$ ), and a collection of *internal edges*  $E_{int}$  which are unordered pairs  $e = \{v_i, w_j\}$  of half-edges, where  $v, w$  are (possibly the same) corolla. A half-edge may occur in at most one internal edge, and the set of half-edges  $E_{ext}$  which occur in no internal edge are called *external edges*. An internal edge  $\{v_i, v_j\}$  which consists of two half-edges from the same corolla is called a *tadpole*. Each internal edge  $e \in E_{int}$  has associated to it a mass  $m_e$ , and each external edge  $e \in E_{ext}$  has a momentum  $q_e$ , which is a vector in  $\mathbb{R}^4$ . We shall always assume that  $G$  is connected. Finally, we also require that the total momentum entering  $G$  adds up to zero (conservation of momentum). For example, consider the figure below on the right, with edges numbered 1–4, which is obtained from the three corollas of degree 4 on the left:

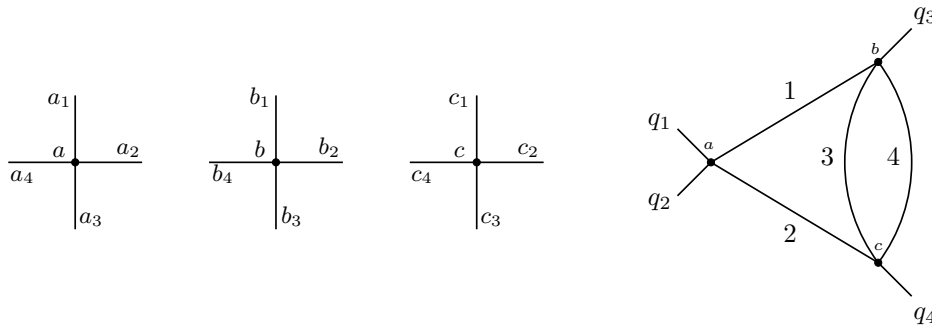


FIGURE 1. The dunce's cap, with edges 1, 2, 3, 4 and external momenta  $q_1, \dots, q_4$ . Conservation of momentum gives  $q_1 + q_2 = q_3 + q_4$ . It is obtained from the three corollas on the left by gluing the half-edges  $1 = \{a_3, b_4\}$ ,  $2 = \{a_4, c_3\}$ ,  $3 = \{b_1, c_1\}$ ,  $4 = \{b_2, c_2\}$ . The external edges  $\{a_1, a_2, b_3, c_4\}$  carry momenta  $q_1, q_2, q_3, q_4$  respectively.

To such a Feynman graph  $G$ , one associates two polynomials as follows. For each internal edge  $e \in E_{int}$ , we associate a variable  $\alpha_e$  known as the Schwinger parameter. The *graph polynomial*, or first Symanzik polynomial, of  $G$  does not depend in any way

on the external edges and is the polynomial defined by

$$\Psi_G = \sum_{T \subset G} \prod_{e \notin E_T} \alpha_e$$

where the sum is over all spanning trees  $T$  of  $G$  and the product is over all internal edges of  $G$  which are not in  $T$ . A spanning tree is a subgraph of  $G$  which is connected, has no loops, and passes through every vertex of  $G$ . In the example above, the set of spanning trees are  $\{1, 2\}$ ,  $\{1, 3\}$ ,  $\{1, 4\}$ ,  $\{2, 3\}$ ,  $\{3, 4\}$ , so it follows that

$$\Psi_G = \alpha_3 \alpha_4 + \alpha_2 \alpha_4 + \alpha_2 \alpha_3 + \alpha_1 \alpha_4 + \alpha_1 \alpha_2 .$$

The degree of  $\Psi_G$  is equal to  $h_G$ , the loop number (or first Betti number) of  $G$ .

The second Symanzik polynomial of  $G$  (which we will not actually require in the sequel) is a function of the external momenta and is defined by

$$\Phi_G = \sum_S \prod_{e \notin S} \alpha_e (q^S)^2$$

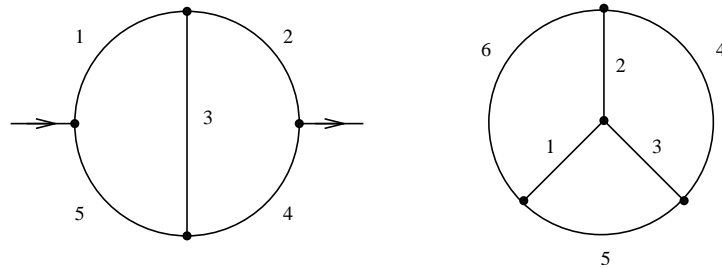
where the sum is over spanning 2-trees  $S = T_1 \cup T_2$  and  $q^S$  is the total momentum entering either  $T_1$  or  $T_2$  (which is the same, by conservation of momentum). A spanning 2-tree is defined to be a subgraph  $S$  with exactly two connected components  $T_1, T_2$ , each of which is a tree (which can reduce to a single vertex), and such that  $S$  contains every vertex of  $G$ . In the example above, the spanning 2-trees are  $\{\{1\}, \{c\}\}$ ,  $\{\{2\}, \{b\}\}$ ,  $\{\{a\}, \{3\}\}$  and  $\{\{a\}, \{4\}\}$ , so

$$\Phi_G = q_4^2 \alpha_2 \alpha_3 \alpha_4 + q_3^2 \alpha_1 \alpha_3 \alpha_4 + (q_1 + q_2)^2 (\alpha_1 \alpha_2 \alpha_4 + \alpha_1 \alpha_2 \alpha_3) ,$$

where we recall that  $(q_1 + q_2)^2 = (q_3 + q_4)^2$ . Up to (omitted)  $\Gamma$ -factors, the general shape of the unregularized (divergent) parametric Feynman integral of  $G$  in  $d$  space-time dimensions is:

$$(7.1) \quad I_G(m, q) = \int_{[0, \infty]^{E_{int}}} \frac{\Psi_G^{N_G - (h_G + 1)d/2}}{(\Psi_G \sum_{e \in E_{int}} m_e^2 \alpha_e - \Phi_G)^{N_G - h_G d/2}} \delta(\sum_e \alpha_e - 1)$$

which is a function of the masses  $m_e$  and external momenta  $q_i$ . Here we only consider the case when all masses are equal to zero, there is a single external momentum  $q$ , and the momentum dependence is trivial, i.e., the momentum dependence factors out of the integral (7.1). This is the case, for example, for the graph below on the left, known as the master 2-loop diagram, which has an external particle entering on the left with momentum  $q$ :



For such graphs, one can show from an identity between the two Symanzik polynomials  $\Phi_G$  and  $\Psi_G$  that (7.1) reduces, up to trivial factors, to the Feynman integral of the graph on the right given by closing up the external edges:

$$(7.2) \quad I_G = \int_{[0, \infty]^{E_{int}}} \frac{1}{\Psi_G^{d/2}} \delta(\sum_e \alpha_e - 1)$$

In summary, one can reduce massless Feynman integrals with trivial momentum dependence by a series of tricks to the apparently unphysical-looking graphs such as the wheel with 3 spokes graph above on the right, which have no external edges. In so doing, the second Symanzik polynomial drops out altogether, and one obtains a single number, the *residue* of  $G$  which we study below. Although these graphs now bear little resemblance to the bona-fide Feynman integrals of realistic quantum field theories, they will capture much of their number-theoretic content, and indeed most of the difficulty in practical Feynman diagram computations reduces to the problem of computing such master integrals, as they are known.

**7.4. Massless  $\phi^4$  theory.** Having performed all the above reductions, we can simply restrict ourselves to looking at graphs  $G$  with no external edges. We work in  $d = 4$  spacetime dimensions. In order to ensure convergence, one says that a graph  $G$  is *primitively divergent*<sup>1</sup> if

- $N_G = 2h_G$
- $N_\gamma > 2h_\gamma$  for all strict subgraphs  $\gamma \subset G$ .

Furthermore, we say that  $G$  is in  $\phi^4$  theory if the valency of every vertex is at most 4. The dunce's cap graph pictured above is not primitively divergent, since it contains a subgraph  $\{3, 4\}$  which has one loop and two edges, and therefore violates the second condition of primitive divergence. A convenient way to remove the  $\delta$ -function in (7.2) is simply to write it as an affine integral:

$$I_G = \int_{[0, \infty]^{N-1}} \frac{d\alpha_1 \dots d\alpha_{N-1}}{\Psi_G^2|_{\alpha_N=1}}$$

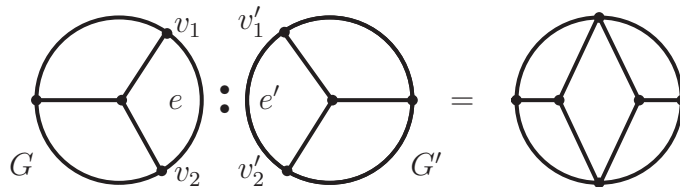
which does not depend on which choice of variable  $\alpha_N$  is set to 1. When  $G$  is primitively divergent the integral converges absolutely and defines a real number known as the residue of the graph  $G$ . Thus we have a well-defined map

$$I : \{\text{Primitive divergent } G\} \longrightarrow \mathbb{R}$$

which is entirely determined by the combinatorics of each graph. Unfortunately, the map  $I$  is very difficult to evaluate at present, and is known analytically in only a handful of cases. We give a brief survey of known results below.

**7.4.1. Numerology of massless  $\phi^4$ .** We first state the main operations on massless primitively-divergent graphs and their effect on the residue, before giving a brief list of some known residue computations.

*Two vertex join.* Let  $G, G'$  be two primitively divergent graphs and choose edges  $e, e'$  with endpoints  $v_1, v_2$  and  $v'_1, v'_2$ , in  $G, G'$  respectively. The *two vertex join*  $G \bullet G'$  of  $G, G'$ , is the graph obtained by gluing  $G \setminus e$  and  $G' \setminus e'$  by identifying the vertices  $v_i$  with  $v'_i$ ,  $i = 1, 2$ :



<sup>1</sup>It is important to note that the residues of the primitively divergent graphs give contributions to the  $\beta$ -function of  $\phi^4$  theory which are renormalization-scheme independent

The two vertex join is also primitively divergent. One can show that

$$(7.3) \quad I_{G \bullet G'} = I_G I_{G'} ,$$

*i.e.*, the residue is multiplicative with respect to the two-vertex join.

*Completion.* Let  $G$  be a primitive-divergent graph in  $\phi^4$  theory with at least 2 loops. It is easy to show from the definition of primitive divergence that there are exactly four vertices which have valency three. Let  $\widehat{G}$  denote the completed graph obtained by adding a new vertex to  $G$ , which is joined to each of the four 3-valent vertices in  $G$ . The graph  $\widehat{G}$  is 4-regular, *i.e.*, every vertex has valency exactly four. Now it can happen that two distinct primitive-divergent graphs  $G, G'$  have the same completion (see below). In this case, they have the same residue:

$$(7.4) \quad I_G = I_{G'} \quad \text{if} \quad \widehat{G} = \widehat{G}' .$$

This identity is a well-known consequence of conformal symmetries of Feynman integrals, but this elegant combinatorial interpretation is due to O. Schnetz.

*Planar duality.* Let  $G$  be a planar graph. Then for every planar embedding of  $G$  there is a well-defined dual graph  $G'$  obtained by placing a vertex in the interior of each face of  $G$  and connecting any two vertices by an edge whenever the corresponding faces are neighbouring. Then one shows that the residues coincide:

$$(7.5) \quad I_G = I_{G'} .$$

There are more sophisticated identities between residues obtained by more complex operations on graphs (see [20]). Note also that a sequence of the above operations can take one outside the class of  $\phi^4$  graphs (or primitive divergent graphs, or even graphs altogether), but result in an identity between actual primitive-divergent graphs. There is currently no conjectural complete explanation to determine when  $I_G = I_{G'}$  for non-isomorphic graphs  $G, G'$ , let alone when  $\sum_i n_i I_{G_i} = 0$ , where  $n_i \in \mathbb{Z}$ .

**7.5. Numerology.** First consider the two families of graphs depicted below: the wheels with  $n$  spokes  $W_n$ , and the zig-zag graphs  $Z_n$  ( $n \geq 3$ ). The index  $n$  refers to the number of loops of the graph. Both families  $W_n$  and  $Z_n$  are primitive divergent, but only  $W_3, W_4$  and the family  $Z_n$  is in  $\phi^4$ , since  $W_n$  has a vertex of valency  $n$ . One expects that the corresponding residues satisfy ([3],[20]):

$$I_{W_n} = \binom{2n-2}{n-1} \zeta(2n-3) \quad , \quad I_{Z_n} = 4 \frac{(2n-2)!}{n!(n-1)!} \left(1 - \frac{1 - (-1)^n}{2^{2n-3}}\right) \zeta(2n-3)$$

The statement on the left for  $I_{W_n}$  can be proved by Gegenbauer polynomial techniques, but no ‘parametric’ or algebro-geometric proof is known for general  $n$ . The statement on the right is a conjecture, and is proved for small values of  $n$  only.

The smallest non-trivial primitively divergent graph is the wheel with 3 spokes  $W_3$ , and it is the unique such graph at this loop order. At four loops, the unique primitively divergent graph is  $W_4$ . Next, there are only 3 primitive-divergent graphs at 5 loops, shown below. The one on the far left is the two-vertex join of  $W_3$ , and so its residue is the product  $I_{W_3}^2$ . One can check that the non-planar graph on the right satisfies

$$\widehat{NP}_5 \cong \widehat{W_3 \bullet W_3}$$

so this implies that its residue is also equal to  $I_{W_3}^2$ . At higher loop orders, the number of primitively divergent graphs grows very fast, and the exact analytic results peter

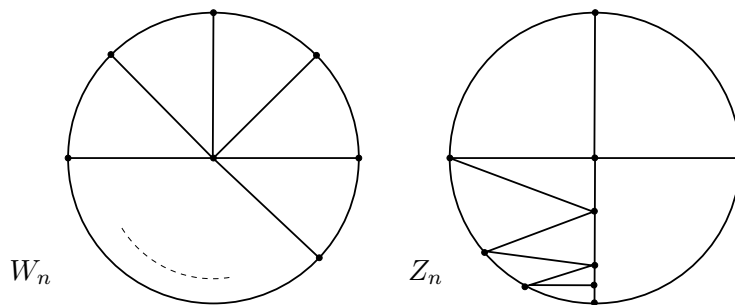
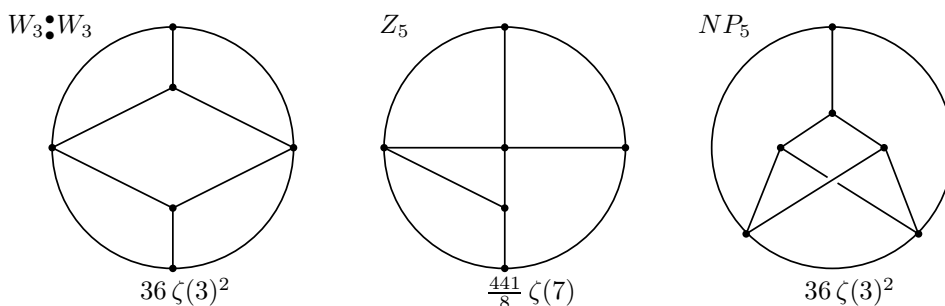


FIGURE 2. The wheels with spokes (left), and zig-zags (right) are the only two families of primitively divergent graphs for which a conjectural formula for the residue exists.



out very quickly. Indeed, at seven and higher loops, there remain graphs whose residue cannot be determined to a single significant digit. The census [20] gives an excellent survey of what is known on this topic. There are a few remarks which need to be made in this context:

- (1) As first observed by Broadhurst and Kreimer [3], the single zeta values do not suffice to express the residues  $I_G$  starting from 6 loops. The complete bipartite graph  $K_{3,4}$ , for example, is primitive divergent with 6 loops and its residue involves  $\zeta(3, 5)$ , which is conjecturally irreducible. There are also several examples which are known (numerically) to evaluate to multiple zeta values of depth 3, so it is likely that multiple zeta values of all depths occur.
- (2) As discussed earlier, the multiple zeta values are filtered (conjecturally, graded) by their weight, so it makes sense to ask what the transcendental weight of a Feynman diagram is. One can show that the generic weight, for a primitively divergent graph  $G$  with  $\ell$  loops which evaluates to multiple zeta values, is  $2\ell - 3$ . However, for many graphs the transcendental weight drops (at five loops, for example the graphs  $W_3 \bullet W_3$  and  $NP_5$  but not  $Z_5$  have a drop in the weight). Some combinatorial criteria for a weight drop to occur are given in [6], but a complete answer to the weight problem is not known.
- (3) The holy grail of the motivic approach to Feynman integrals would be to compute the motivic coproduct for the residue  $I_G$  in terms of the combinatorics of  $G$ , but it is not known how to do this for a single non-trivial  $G$ . Were such a formula available, one could intuit the value of a Feynman graph just by looking at its combinatorics, a dream first expressed by Kreimer.

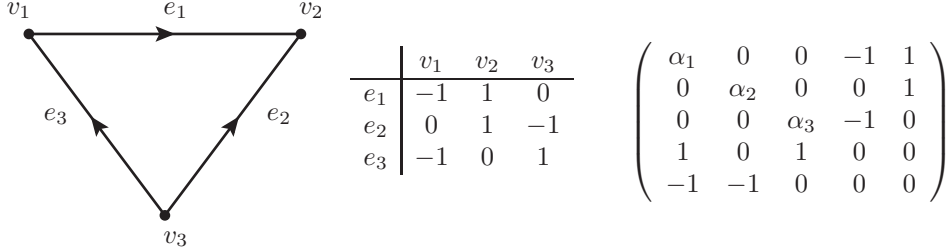
**7.6. Properties of Graph Polynomials.** In order to give some idea why multiple zeta values and polylogarithms should occur in massless scalar quantum field theories, we must look at some properties of graph polynomials.

*Matrix representation for  $\Psi_G$ .* Let  $G$  be a graph with no tadpoles, and let  $\mathcal{E}_G$  be its reduced incidence matrix, obtained as follows. Choose an orientation on  $G$ , and a numbering on its edges and vertices. Define the  $e_G \times v_G$  matrix  $\mathcal{E}'_G(e_i, v_j)$  to be  $-1$  if  $e_i$  is the source of  $v_j$  for the chosen orientation,  $+1$  if it is the target, and  $0$  otherwise, and let  $\mathcal{E}_G$  denote the matrix obtained from  $\mathcal{E}'_G$  by removing one of its columns. Its entries are  $0, 1, -1$  and depends on these choices. Let

$$M_G = \left( \begin{array}{ccc|c} \alpha_1 & & & \mathcal{E}_G \\ & \ddots & & \\ & & \alpha_{e_G} & \\ \hline & -{}^T\mathcal{E}_G & & 0 \end{array} \right)$$

It follows from the Matrix-Tree theorem that  $\Psi_G = \det M_G$ .

**Example 7.1.** Consider the following oriented graph  $G$ . In the middle is its incidence matrix  $\mathcal{E}'_G$ , and on the right the matrix  $M_G$  obtained by deleting column  $v_3$ .



We have  $\Psi_G = \det(M_G) = \alpha_1 + \alpha_2 + \alpha_3$  in this case.

*Dodgson polynomials.* For a graph  $G$  as above, let us fix a choice of matrix  $M_G$ . For any subsets of edges  $I, J, K \subset \{1, \dots, N\}$  of  $G$  such that  $|I| = |J|$ ,

$$\Psi_{G,K}^{I,J} = \det M_G(I, J) \Big|_{\alpha_k=0, k \in K}$$

where  $M_G(I, J)$  denotes the matrix  $M_G$  with rows  $I$  and columns  $J$  removed. We call  $\Psi_{G,K}^{I,J}$  the Dodgson polynomials of  $G$ . There also exists a formula for  $\Psi_{G,K}^{I,J}$  in terms of spanning trees, which shows that it is a sum of monomials in the  $\alpha_i$  with a coefficient of  $+1$  or  $-1$ . Changing the choice of  $M_G$  only modifies all the  $\Psi_{G,K}^{I,J}$  by a sign.

*Algebraic relations.* The key to computing the Feynman integrals is to exploit the many identities between the polynomials  $\Psi_{G,K}^{I,J}$ . We have:

- The *contraction-deletion formula*. For any edge  $e \notin I \cup J \cup K$ , it follows from the shape of the matrix  $M_G$  that the polynomial  $\Psi_{G,K}^{I,J}$  is of degree at most one in the Schwinger variable  $\alpha_e$ . We can therefore write:

$$\Psi_{G,K}^{I,J} = \Psi_{G,K}^{Ie,Je} \alpha_e + \Psi_{G,Ke}^{I,J}$$

The contraction-deletion relations state that  $\Psi_{G,K}^{Ie,Je} = \Psi_{G \setminus e, K}^{I,J}$  where  $G \setminus e$  denotes the graph obtained by deleting the edge  $e$  and identifying its endpoints, and  $\Psi_{G,Ke}^{I,J} = \Psi_{G/e, K}^{I,J}$ , where  $G/e$  denotes the graph obtained by contracting the edge  $e$ . Note that if deleting the edge  $e$  disconnects the graph  $G$ , then  $\Psi_{G \setminus e, K}^{I,J} = 0$  and if  $e$  is a tadpole (a self-edge) then  $\Psi_{G/e, K}^{I,J} = 0$ .



- Generally, the minors of a matrix satisfy *determinantal identities*. This yields quadratic identities such as the following:

$$\Psi_{G,Kabx}^{I,J} \Psi_{G,K}^{Iax,Jbx} - \Psi_{G,Kab}^{Ix,Jx} \Psi_{G,Kx}^{Ia,Jb} = \Psi_{G,Kb}^{Ia,Jx} \Psi_{G,Ka}^{Ix,Jb}$$

or linear Plücker-type identities such as:

$$\Psi_{G,K}^{ij,kl} - \Psi_{G,K}^{ik,jl} + \Psi_{G,K}^{il,jk} = 0$$

This class of identities hold for any symmetric matrix, and hold irrespective of the particular combinatorics of the graph  $G$ .

- *Graph-specific identities*. If, for example,  $K$  contains a loop, then  $\Psi_{G,K}^{I,J} = 0$ . Likewise, one can show that if  $E$  is the set of all edges which meets a given vertex of  $G$ , then  $\Psi_{G,K}^{I,J} = 0$  whenever  $E \subset I$  or  $E \subset J$ . In general, the local structure of the graph can cause certain Dodgson polynomials to vanish, which will in turn induce new relations between other Dodgson polynomials via the quadratic equations mentioned above.

**7.7. A naive integration method.** A basic idea is to try to compute the Feynman integral in parametric form by integrating out one variable at a time.

To illustrate this we can attempt to compute the residue:

$$I_G = \int_{[0,\infty]^{N-1}} \frac{d\alpha_1 \dots d\alpha_{N-1}}{\Psi_G^2 \Big|_{\alpha_N=1}}$$

For more general Feynman diagrams, the numerator will be a polynomial in  $\alpha_i$ ,  $\log \alpha_i$  and  $\log \Psi_G$ . This won't affect the method significantly.

By the contraction-deletion formula, we can write  $\Psi = \Psi^{1,1}\alpha_1 + \Psi_1$ . We will henceforth drop the  $G$ 's from the notation. Therefore

$$I_G = \int_0^\infty \frac{d\alpha_1 \dots d\alpha_{N-1}}{\Psi^2}$$

can be written

$$\int_0^\infty \frac{d\alpha_1 \dots d\alpha_{N-1}}{(\Psi^{1,1}\alpha_1 + \Psi_1)^2} = \int_0^\infty \frac{d\alpha_2 \dots d\alpha_{N-1}}{\Psi^{1,1}\Psi_1}$$

By contraction-deletion, the polynomials  $\Psi^{1,1}$  and  $\Psi_1$  are linear in the variable  $\alpha_2$ :

$$\begin{aligned} \Psi^{1,1} &= \Psi^{12,12}\alpha_2 + \Psi_2^{1,1}, \\ \Psi_1 &= \Psi_1^{2,2}\alpha_2 + \Psi_{12} \end{aligned}$$

We can write the previous integral as

$$\int \frac{1}{\Psi^{1,1}\Psi_1} = \int_0^\infty \frac{d\alpha_2 \dots d\alpha_{N-1}}{(\Psi^{12,12}\alpha_2 + \Psi_2^{1,1})(\Psi_1^{2,2}\alpha_2 + \Psi_{12})}$$

By decomposing into partial fractions, one can then integrate out  $\alpha_2$ . This leaves an integrand of the form

$$\frac{\log \Psi_2^{1,1} + \log \Psi_1^{2,2} - \log \Psi^{12,12} - \log \Psi_{12}}{\Psi_2^{1,1}\Psi_1^{2,2} - \Psi^{12,12}\Psi_{12}}$$

At this point, we should be stuck since the denominator is quadratic in every variable. One would expect to have to take a square root at the next stage of integration, but miraculously, we can use the quadratic identities between Dodgson polynomials to get a factorization:

$$\Psi_2^{1,1}\Psi_1^{2,2} - \Psi^{12,12}\Psi_{12} = (\Psi^{1,2})^2$$

So after two integrations we have

$$\int \frac{d\alpha_1 d\alpha_2}{\Psi^2} = \frac{\log \Psi_2^{1,1} + \log \Psi_1^{2,2} - \log \Psi^{12,12} - \log \Psi_{12}}{(\Psi^{1,2})^2}$$

We can then write  $\Psi^{1,2} = \Psi^{13,23}\alpha_3 + \Psi_3^{1,2}$  and keep integrating out the variables  $\alpha_3, \alpha_4, \dots$  successively.

As long as we can find a Schwinger coordinate  $\alpha_i$  in which all the terms in the integrand are *linear*, then we can always perform the next integration using iterated integrals (this is theorem 6.14). This requires choosing a good order on the edges of  $G$ ; it can be the case that for some choices of orderings the integration process terminates, but for others, one is blocked by polynomials which are of degree  $> 1$  in every remaining variable.

In this case, the integral is expressible as multiple polylogarithms:

$$\text{Li}_{n_1, \dots, n_r}(x_1, \dots, x_r) = \sum_{1 \leq k_1 < \dots < k_r} \frac{x_1^{k_1} \dots x_r^{k_r}}{k_1^{n_1} \dots k_r^{n_r}}$$

where the arguments are quotients of Dodgson polynomials  $\Psi_{G,K}^{I,J}$  (this follows from the explicit description of iterated integrals on the moduli spaces  $\mathfrak{M}_{0,n}$  in §6). When this process terminates, the Feynman integral is expressed as values of multiple polylogarithms evaluated at 1 (or roots of unity).

We say that  $G$  is *linearly reducible* if this integration process terminates, i.e., we can find a variable with respect to which all the arguments are linear. The conclusion is that if  $G$  is linearly reducible, the residue of  $G$  is computable in terms of multiple zeta values, or similar numbers. Likewise, when there are masses or momenta in the integrand, one would in this case obtain multiple polylogarithms in certain rational functions of the kinematic variables.

**7.8. The five-invariant.** Most of the terms which occur are of the form  $\Psi_{G,K}^{I,J}$  which are linear in every variable. However, this is not always the case. The first obstruction which can occur is the *five invariant*, defined for any five edges  $i, j, k, l, m$  in  $G$ :

$${}^5\Psi(i, j, k, l, m) = \pm \det \begin{pmatrix} \Psi_m^{ij,kl} & \Psi_m^{ijm,klm} \\ \Psi_m^{ik,jl} & \Psi_m^{ikm,jlm} \end{pmatrix}$$

It is not obvious that this is well-defined, but one can show that if one permutes the five indices  $i, j, k, l, m$  in the definition, the five-invariant only changes by a sign. Thus it does give an invariant of the set of edges  $\{i, j, k, l, m\} \subset G$ . In the general case, the five-invariant is of degree  $> 1$  in its variables and does not factorize. In other words, we run out of identities in the generic case.

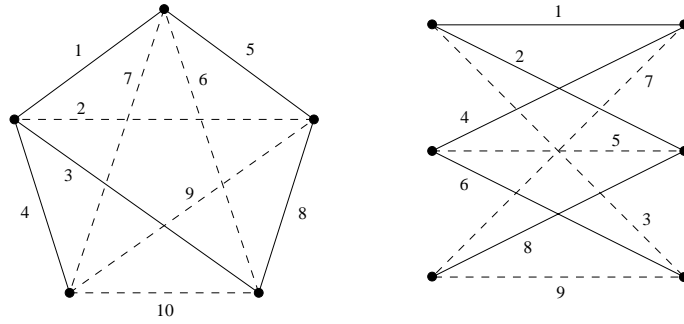
But if, for example,  $i, j, k, l, m$  contains a triangle (or if three of the edges meet at a 3-valent vertex) then one of the matrix entries, say  $\Psi_m^{ik,jl}$  vanishes, and  ${}^5\Psi(i, j, k, l, m)$  factorizes into a product of Dodgson polynomials

$$\Psi_m^{ijm,klm} \Psi_m^{ik,jl},$$

which are linear in each variable, and so we can keep on going. Thus the *generic* graph is not at all linearly reducible - it is the local combinatorial structure of the graph which generates sufficiently many identities of type to ensure linear reducibility. One can ask which are the smallest graphs which have a non-trivial 5-invariant at all. These are the non-planar graphs  $K_5$  (fewest vertices, left) and  $K_{3,3}$  (fewest edges, right):

For example, the 5-invariant  ${}^5\Psi_{K_{3,3}}(1, 2, 4, 6, 8)$  for the graph on the right is given by:

$$\alpha_5 \alpha_9^2 + \alpha_3 \alpha_5 \alpha_9 + \alpha_5 \alpha_7 \alpha_9 + \alpha_3 \alpha_5 \alpha_7 - \alpha_3 \alpha_7 \alpha_9$$



One can see that this polynomial is in fact of degree one in all its variables except  $\alpha_9$ ; it turns out that these two graphs are still linearly reducible; one must only choose a more intelligent order in which to integrate out the edges.

The first *serious* obstructions to the integration method §7.7 occur at 8 loops.

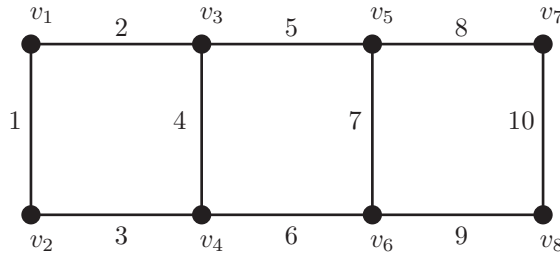
**7.9. General results on the periods.** One can ask if there is a simple combinatorial criterion to ensure linear reducibility, and this requires the following definition.

**Definition 7.2.** Let  $\mathcal{O}$  be an ordering on the edges of  $G$ . It gives rise to a filtration

$$\emptyset = G_0 \subset G_1 \dots \subset G_{N-1} \subset G_N = G$$

of subgraphs of  $G$ , where  $G_i$  has exactly  $i$  edges. To any such sequence we obtain a sequence of integers  $v_i^{\mathcal{O}}$  = number of vertices of  $G_i \cap (G \setminus G_i)$ . We say that  $G$  has *vertex-width* at most  $n$  if there exists an ordering  $\mathcal{O}$  such that  $v_i^{\mathcal{O}} \leq n$  for all  $i$ .

**Example 7.3.** Consider the following graph, with the ordering on its edges as shown. Set  $G_i = \{1, \dots, i\}$ , and let  $W_i$  be the set of vertices in  $G_i \cap (G \setminus G_i)$ .



We have  $W_1 = \{v_1, v_2\}$ ,  $W_2 = \{v_2, v_3\}$ ,  $W_3 = \{v_3, v_4\}$ ,  $W_4 = \{v_3, v_4\}$ ,  $W_5 = \{v_4, v_5\}$  and so on. This shows that the vertex width is at most 2.

Bounding the vertex width is a very strong constraint on a graph: the set of planar graphs have arbitrarily high vertex width.

**Theorem 7.4.** *If  $G$  has vertex width at most 3, then  $G$  is linearly reducible.*

In particular, one can prove that for such graphs, the residue  $I_G$  evaluates to multiple zeta values (or perhaps alternating sums, which are values of multiple polylogarithms evaluated at  $x_i = \pm 1$ ). The zig-zags and wheels are examples of families of graphs with vertex width 3.

**7.10. Counting points over finite fields.** Let us now consider the (at first sight) unrelated problem of counting the points of graph hypersurfaces over finite fields. Let  $G$  be a graph, and consider the graph hypersurface

$$X_G = \{(\alpha_1, \dots, \alpha_N) \in \mathbb{A}^N : \Psi_G(\alpha_1, \dots, \alpha_N) = 0\}$$

defined to be the zero locus of the polynomial  $\Psi_G$ , viewed in affine space  $\mathbb{A}^N$ . Since  $\Psi_G$  has integer coefficients, it makes sense to reduce the equation modulo  $q$ , where  $q$  is any power of a prime  $p$ . This gives a function:

$$(7.6) \quad [X_G] : \{\text{Prime powers } q\} \longrightarrow \mathbb{N} \\ q \longmapsto |X_G(\mathbb{F}_q)|$$

which to  $q$  associates the number of solutions of  $\Psi_G = 0$  in  $\mathbb{F}_q^N$ . Indeed such a counting function exists for any polynomial, or system of polynomials, defined over  $\mathbb{Z}$ . The question, first asked by Kontsevich in 1997, is whether  $[X_G]$  is a polynomial in  $q$ .

**Example 7.5.** Consider the primitive-divergent graphs in  $\phi^4$  theory up to 5 loops. They are the wheels  $W_3, W_4$ , and at 5 loops we have the zig-zag graph  $Z_5$ , the two-vertex join  $W_3 \bullet W_3$ , and the non-planar graph  $NP_5$ . One can compute:

$$\begin{aligned} [W_3] &= q^2(q^3 + q - 1) \\ [W_4] &= q^2(q^5 + 3q^3 - 6q^2 + 4q - 1) \\ [Z_5] &= q^2(q^7 + 5q^5 - 10q^4 + 7q^3 - 4q^2 + 3q - 1) \\ [W_3 \bullet W_3] &= q^3(q^6 + q^5 + q^4 - 3q^3 - q^2 + 3q - 1) \\ [NP_5] &= q^5(q^4 + 4q^2 - 7q + 3) \end{aligned}$$

One way to prove that a given function  $[X_G]$  is polynomial in  $q$  is to use the following inductive argument, due to Stembridge [24]. For any set of polynomials  $f_1, \dots, f_k$  in  $\mathbb{Z}[\alpha_1, \dots, \alpha_N]$ , denote the point count of the intersection  $\cap_k \{f_k = 0\}$  by

$$[f_1, \dots, f_k] = |\{(\alpha_1, \dots, \alpha_N) \in \mathbb{F}_q^N : f_1 = \dots = f_k = 0\}|$$

Consider a polynomial  $f = f^1 \alpha_1 + f_1$  which is linear in  $\alpha_1$ , where  $f^1, f_1 \in \mathbb{Z}[\alpha_2, \dots, \alpha_N]$ . For  $f$  to vanish, either  $f^1$  is invertible in  $\mathbb{F}_q$  (in which case we can solve for  $\alpha_1$ ), or both  $f^1$  and  $f_1$  vanish (in which case  $\alpha_1$  can take any value in  $\mathbb{F}_q$ ). Hence

$$(7.7) \quad [f^1 \alpha_1 + f_1] = q[f^1, f_1] + q^{N-1} - [f_1].$$

Similarly, if we have two polynomials  $f, g$  linear in  $\alpha_1$ , one checks in a similar way that

$$(7.8) \quad [f^1 \alpha_1 + f_1, g^1 \alpha_1 + g_1] = q[f_1, g_1, f^1, g^1] + [f^1 g_1 - g^1 f_1] - [f^1, g^1]$$

By a computer implementation of this method, Stembridge proved that for all graphs  $G$  with at most 12 edges, the point counts  $[X_G]$  are polynomials in  $q$ . Previously, Stanley had showed that certain graphs obtained by deleting edges from complete graphs have this property, and gave explicit formulae for the point counts in these cases.

A landmark result due to Belkale and Brosnan showed that this is false in general.

**Theorem 7.6.** [1] *The point-counting functions  $[X_G]$  are of general type, as  $G$  ranges over the set of all graphs.*

Concretely, this means that given any set of polynomials  $f_1, \dots, f_n$  with integer coefficients as above, one can construct a set of graphs  $G_1, \dots, G_M$  such that

$$[f_1, \dots, f_n] = \sum_{i=1}^M p_i(q)[G_i]$$

where  $p_i(q) \in \mathbb{Z}[q, q^{-1}, (q-1)^{-1}]$ . In other words, graph hypersurfaces are universal in the sense of motives. However, until recently no explicit non-polynomial example was known, and the method seems to produce counter-examples with very large numbers of edges. It is also not clear in this approach if the conditions of physicality, e.g., being primitive-divergent and in  $\phi^4$  theory, are enough to ensure polynomiality, since the graphs  $G_i$  are hard to control.

Now, by applying Stembridge's method to the graph polynomial  $\Psi_G$ , one sees at the first stage that there are terms  $\Psi^1, \Psi_1$  and at the second stage that we obtain a term  $\Psi^{12}\Psi_{12} - \Psi_2^1\Psi_1^2 = (\Psi^{1,2})^2$ . In general, one obtains iterated resultants of Dodgson polynomials  $\Psi_{G,K}^{I,J}$ , as in the previous integration method. One can show that

**Theorem 7.7.** *If  $G$  has vertex width 3 then there exists a polynomial  $P_G$  such that  $[X_G](q) = P_G(q)$  for all  $q$  not divisible by 2.*

It is possible that the condition that  $q$  be divisible by 2 can be dropped. This is the case for the wheels and zig-zags, whose polynomials can be computed explicitly [7]. It was recently shown independently by D. Doryn and O. Schnetz that some primitive-divergent graphs in  $\phi^4$  at seven loops have 'quasi-polynomial' point counts, (more precisely, are given by more than one polynomial according to whether small primes divide  $q$  or not). At 8 loops, one finds that:

**Theorem 7.8.** [7] *There exists a primitive-divergent graph  $G$  in  $\phi^4$  theory such that*

$$[X_G](q) \equiv a_q^2 q^2 \pmod{q^3}$$

for all prime powers  $q$ , where  $q+1-a_q$  is the number of points over  $\mathbb{F}_q$  of the (complex multiplication) elliptic curve defined by the equation

$$(7.9) \quad y^2 + xy = x^3 - x^2 - 2x + 1 .$$

This graph has vertex-width 4.

The  $a_q$  are given by the coefficients of a certain modular form, and the theorem proves in particular that  $[X_G]$  is not a quasi-polynomial. There is another interpretation of the term  $[X_G](q) \pmod{q^3}$  in terms of the denominator in the integration method of the previous section. This strongly suggests that the residue  $I_G$  of this graph should not be a multiple zeta value, but a period of the fundamental group of the elliptic curve (7.9) with punctures.

**7.11. Geometric interpretation.** Consider the graph hypersurface  $X_G \subset \mathbb{A}^N$ , and let  $B = \bigcup_{i=1}^N \{\alpha_i = 0\}$  denote the union of the coordinate axes. Consider the projection

$$(7.10) \quad \begin{aligned} \pi_i : \mathbb{A}^N &\longrightarrow \mathbb{A}^{N-i} \\ (\alpha_1, \dots, \alpha_N) &\mapsto (\alpha_{i+1}, \dots, \alpha_N) \end{aligned}$$

For each  $i$ , one can show that there exists an algebraic subvariety  $L_i \subset \mathbb{A}^{N-i}$  (the discriminant), where  $L_i$  is a union of irreducible hypersurfaces, such that

$$(7.11) \quad \pi_i : \mathbb{A}^N \setminus (X_G \cup B \cup \pi_i^{-1}(L_i)) \longrightarrow \mathbb{A}^{N-i} \setminus L_i$$

is locally trivial in the sense of stratified varieties: in other words, the fibers over every complex point of  $\mathbb{C}^N \setminus L_i(\mathbb{C})$  are topologically constant. In this situation, the partial Feynman integral

$$(7.12) \quad I_G^i(\alpha_{i+1}, \dots, \alpha_n) = \int_{[0, \infty]^i} \frac{d\alpha_1 \dots d\alpha_i}{\Psi_G^2}$$

obtained by integrating in the fiber is a multi-valued function of the parameters  $\alpha_{i+1}, \dots, \alpha_n$ , and has singularities contained in  $L_i$ . Thus the variety  $L_i$  corresponds to what physicists refer to as a Landau variety.

The main result of [5] is that when  $G$  is of vertex width  $\leq 3$ , then with the natural numbering of its edges, one can compute the  $L_i$  inductively and show that

$$L_i \subseteq \{\Psi_{G,K}^{I,J} = 0 : I \cup J \cup K = \{1, \dots, i\}\}$$

This involves an inductive argument using the fact that discriminants of one-dimensional projections can be written as resultants, and the fact that the local topology of the graph  $G$  generates enough identities to ensure that these resultants always factorize into products of polynomials  $\Psi_{G,K}^{I,J}$ . Since each polynomial  $\Psi_{G,K}^{I,J}$  is of degree  $\leq 1$  in each variable, one can show that the partial integral  $I_G^i(\alpha_{i+1}, \dots, \alpha_n)$  has unipotent monodromy. By the universality of multiple polylogarithms, we conclude that (7.12) is expressible in terms of multiple polylogarithms with singularities along the  $\Psi_{G,K}^{I,J} = 0$  only. This ultimately explains the appearance of multiple zeta values (or alternating sums) in the Feynman integral calculations.

On the other hand, the fibrations (7.11) can also be used to count points over finite fields. For example, the map  $\pi_1 : \mathbb{A}^N \setminus (X_G \cup B \cup \pi_1^{-1}(L_1)) \rightarrow \mathbb{A}^{N-1} \setminus L_1$  is a fibration, whose fibers are a complement of a finite number of points in  $\mathbb{A}^1$ . Since  $L_1 = \{\Psi_G^{1,1} \Psi_{G,1} = 0\}$  we can use the fibration to count points over  $\mathbb{F}_q$ , which yields a version of (7.7), since for a locally trivial fibration the number of points in the total space is simply the number of points in the base multiplied by the number of points in the fiber. Continuing in this way yields all the terms in the Stembridge reduction algorithm, and ultimately theorem 7.7.

**7.12. Conclusion.** The appearance of multiple zeta values in massless  $\phi^4$  theory at low loop orders can be explained as follows. For certain classes of graphs, the particular algebraic properties of graph polynomials imply that the partial Feynman integrals 7.12 have unipotent monodromy, which by Chen's theory can be expressed in terms of iterated integrals. The explicit description of iterated integrals on moduli spaces of curves of genus 0 allows one to express these functions in terms of multiple polylogarithms. The multiple zeta values or Euler sums then appear as the special values (or holonomy) of these functions. This argument works for all graphs up to seven or eight loops, and a similar argument should certainly also work for a suitable class of Feynman graphs with subdivergences, and non-trivial kinematic variables. Instead of obtaining numbers, the amplitudes will be now expressible as multiple polylogarithm functions whose arguments depend on the masses and momenta.

At higher loop orders, the presence of an elliptic curve strongly suggests that the Feynman integrals will fail to be multiple zeta values. Together with the work of Belkale and Brosnan, this points to the fact that  $\phi^4$  theory is mathematically far richer than previously thought, and confirms David Broadhurst's philosophy that one should expect totally new phenomena to occur in quantum field theories at every new loop order.

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