Feynman integrals and multiple polylogarithms

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Abstract

In this talk I review the connections between Feynman integrals and multiple polylogarithms. After an introductory section on loop integrals I discuss the Mellin-Barnes transformation and shuffle algebras. In a subsequent section multiple polylogarithms are introduced. Finally, I discuss how certain Feynman integrals evaluate to multiple polylogarithms.
1 Introduction

In this talk I will discuss techniques for the computation of loop integrals, which occur in perturbative calculations in quantum field theory. Particle physics has become a field where precision measurements have become possible. Of course, the increase in experimental precision has to be matched with more accurate calculations from the theoretical side. This is the “raison d’être” for loop calculations: A higher accuracy is reached by including more terms in the perturbative expansion. The complexity of a calculation increases obviously with the number of loops, but also with the number of external particles or the number of non-zero internal masses associated to propagators. To give an idea of the state of the art, specific quantities which are just pure numbers have been computed up to an impressive fourth or third order. Examples are the calculation of the 4-loop contribution to the QCD β-function [1], the calculation of the anomalous magnetic moment of the electron up to three loops [2], and the calculation of the ratio of the total cross section for hadron production to the total cross section for the production of a μ^+ μ^- pair in electron-positron annihilation to order $O \alpha_s^3$ [3]. Quantities which depend on a single variable are known at the best to the third order. Outstanding examples are the computation of the three-loop Altarelli-Parisi splitting functions [4, 5] or the calculation of the two-loop amplitudes for the most interesting $2 \to 2$ processes [6–16]. For the calculation of these amplitudes, the knowledge of certain highly non-trivial two-loop integrals has been essential [17–19]. The complexity of a two-loop computation increases, if the result depends on more than one variable. An example for a two-loop calculation whose result depends on two variables is the computation of the two-loop amplitudes for $e^+ e^- \to 3$ jets [20–22]. But in general, if more than one variable is involved, we have to content ourselves with next-to-leading order calculations. An example for the state of the art is here the computation of the electro-weak corrections to the process $e^+ e^- \to 4$ fermions [23, 24].

From a mathematical point of view loop calculations reveal interesting algebraic structures. Multiple polylogarithms play an important role to express the results of loop calculations. The mathematical aspects will be discussed in this talk. Additional material related to loop calculations can found in the reviews [25–28] and the book [29].

This paper is organised as follows: In the next section I review basic facts about Feynman integrals. Section 3 is devoted to the Mellin-Barnes transformation. In section 4 algebraic structures like shuffle algebras are introduced. Section 5 deals with multiple polylogarithms. Section 6 combines the various aspects and shows, how certain Feynman integrals evaluate to multiple polylogarithms. Finally, section 7 contains a summary.

2 Feynman integrals

To set the scene let us consider a scalar Feynman graph $G$. Fig. 1 shows an example. In this example there are three external lines and six internal lines. The momenta flowing in or out through the external lines are labelled $p_1$, $p_2$ and $p_3$ and can be taken as fixed vectors. They are constrained by momentum conservation: If all momenta are taken to flow outwards, momentum...
conservation requires that

$$p_1 + p_2 + p_3 = 0.$$ \hfill (1)

At each vertex of a graph we have again momentum conservation: The sum of all momenta flowing into the vertex equals the sum of all momenta flowing out of the vertex. A graph, where the external momenta determine uniquely all internal momenta, is called a tree graph. It can be shown that such a graph does not contain any closed circuit.

In contrast, graphs which do contain one or more closed circuits are called loop graphs. If we have to specify besides the external momenta in addition $l$ internal momenta in order to determine uniquely all internal momenta we say that the graph contains $l$ loops. In this sense, a tree graph is a graph with zero loops and the graph in fig. 1 contains two loops. Let us agree that we label the $l$ additional internal momenta by $k_1$ to $k_l$.

Feynman rules allow us to translate a Feynman graph into a mathematical formula. For a scalar graph we have substitute for each internal line $j$ a propagator

$$\frac{i}{q_j^2 + m_j^2 + \delta}.$$ \hfill (2)

Here, $q_j$ is the momentum flowing through line $j$. It is a linear combination of the external momenta $p$ and the loop momenta $k$:

$$q_j = q_j(p; k):$$ \hfill (3)

$m_j$ is the mass of the particle of line $j$. The propagator would have a pole for $p_j^2 = m_j^2$, or phrased differently $E_j = \sqrt{p_j^2 + m_j^2}$. When integrating over $E$, the integration contour has to be deformed to avoid these two poles. Causality dictates into which directions the contour has to be deformed. The pole on the negative real axis is avoided by escaping into the lower complex half-plane, the pole at the positive real axis is avoided by a deformation into the upper complex half-plane. Feynman invented the trick to add a small imaginary part $\delta$ to the denominator, which keeps track of the directions into which the contour has to be deformed. In the following the $\delta$-term is omitted in order to keep the notation compact.

The Feynman rules tell us also to integrate for each loop over the loop momentum:

$$\int \frac{d^4 k_r}{(2\pi)^4}.$$ \hfill (4)
However, there is a complication: If we proceed naively and write down for each loop an integral over four-dimensional Minkowski space, we end up with ill-defined integrals, since these integrals may contain ultraviolet or infrared divergences! Therefore the first step is to make these integrals well-defined by introducing a regulator. There are several possibilities how this can be done, but the method of dimensional regularisation [30–32] has almost become a standard, as the calculations in this regularisation scheme turn out to be the simplest. Within dimensional regularisation one replaces the four-dimensional integral over the loop momentum by a $D$-dimensional integral, where $D$ is now an additional parameter, which can be a non-integer or even a complex number. We consider the result of the integration as a function of $D$ and we are interested in the behaviour of this function as $D$ approaches 4. It is common practice to parameterise the deviation of $D$ from 4 by

$$D = 4 - 2\varepsilon :$$

The divergences in loop integrals will manifest themselves in poles in $1/\varepsilon$. In an $l$-loop integral ultraviolet divergences will lead to poles $1/\varepsilon^l$ at the worst, whereas infrared divergences can lead to poles up to $1/\varepsilon^{2l}$. We will also encounter integrals, where the dimension is shifted by units of two. In these cases we often write

$$D = 2m - 2\varepsilon ;$$

where $m$ is an integer, and we are again interested in the Laurent series in $\varepsilon$. 

Let us now consider a generic scalar $l$-loop integral $I_G$ in $D = 2m - 2\varepsilon$ dimensions with $n$ propagators, corresponding to a graph $G$. Let us further make a slight generalisation: For each internal line $j$ the corresponding propagator in the integrand can be raised to a power $\nu_j$. Therefore the integral will depend also on the numbers $\nu_1,..,\nu_n$. We define the Feynman integral by

$$I_G = e^{\nu_1 \mu^2} \cdot \mu^{2\varepsilon} \cdot \int \frac{d^{2m} k}{i \pi^{D/2}} \prod_{j=1}^{n} \frac{1}{(q_j^2 + m_j^2)^{\nu_j}} :$$

The momenta $q_j$ of the propagators are linear combinations of the external momenta and the loop momenta. In eq. (7) there are some overall factors, which I inserted for convenience: $\mu$ is an arbitrary mass scale and the factor $\mu^{2\varepsilon}$ ensures that the mass dimension of eq. (7) is an integer. The factor $e^{\nu_1 \mu^2}$ avoids a proliferation of Euler’s constant

$$\gamma_E = \lim_{n!} \sum_{j=1}^{n} \frac{1}{j} \ln n = 0.5772156649 \cdots ;$$

in the final result. The integral measure is now $d^D k = i \pi^{D-2}$ instead of $d^D k = (2\pi)^D$, and each propagator is multiplied by $i$. The small imaginary parts $i\delta$ in the propagators are not written explicitly.

How to perform the $D$-dimensional loop integrals? The first step is to convert the products of propagators into a sum. This can be done with the Feynman parameter technique. In its full
generality it is also applicable to cases, where each factor in the denominator is raised to some power \( \nu \). The formula reads:

\[
\prod_{i=1}^{n} \frac{1}{p_i^{\nu_i}} = \frac{\Gamma(\nu)}{\prod_{i=1}^{n} \Gamma(\nu_i)} \int_0^1 \prod_{i=1}^{n} dx_i x_i^{\nu_i} \delta \left( \sum_{i=1}^{n} x_i \right) \frac{1}{\sum_{i=1}^{n} x_i P_i} ; \quad \nu = \sum_{i=1}^{n} \nu_i ; \tag{9}
\]

Applied to eq. (7) we have

\[
\sum_{i=1}^{n} x_i P_i = \sum_{i=1}^{n} x_i (q_i^2 + m_i^2) ; \tag{10}
\]

One can now use translational invariance of the \( D \)-dimensional loop integrals and shift each loop momentum \( k_r \) to complete the square, such that the integrand depends only on \( k_r^2 \). Then all \( D \)-dimensional loop integrals can be performed. As the integrals over the Feynman parameters still remain, this allows us to treat the \( D \)-dimensional loop integrals for Feynman parameter integrals. One arrives at the following Feynman parameter integral [33]:

\[
I_G = e^{\epsilon e \mu} \mu^2 \frac{l \Gamma(\nu)}{\prod_{j=1}^{n} \Gamma(\nu_j)} \int_0^1 \prod_{j=1}^{n} dx_j x_j^{\nu_j} \delta \left( \sum_{i=1}^{n} x_i \right) \frac{1}{\sum_{i=1}^{n} x_i P_i} \frac{n!}{\prod_{r=1}^{l} M_{rs}k_s + \sum_{r=1}^{l} 2k_r} Q J ; \tag{11}
\]

The functions \( \mathcal{U} \) and \( \mathcal{F} \) depend on the Feynman parameters. If one expresses

\[
\sum_{j=1}^{n} x_j (q_j^2 + m_j^2) = \sum_{r=1}^{l} \sum_{s=1}^{l} k_r M_{rs}k_s + \sum_{r=1}^{l} 2k_r \quad Q \quad J ; \tag{12}
\]

where \( M \) is a \( l \times l \) matrix with scalar entries and \( Q \) is a \( l \)-vector with fourvectors as entries, one obtains

\[
\mathcal{U} = \det (M) ; \quad \mathcal{F} = \det (M) \quad J + QM^{-1}Q ; \tag{13}
\]

Alternatively, the functions \( \mathcal{U} \) and \( \mathcal{F} \) can be derived from the topology of the corresponding Feynman graph \( G \). Cutting \( l \) lines of a given connected \( l \)-loop graph such that it becomes a connected tree graph \( T \) defines a chord \( C(T,G) \) as being the set of lines not belonging to this tree. The Feynman parameters associated with each chord define a monomial of degree \( l \). The set of all such trees (or 1-trees) is denoted by \( T_1 \). The 1-trees \( T_2 \) define \( \mathcal{U} \) as being the sum over all monomials corresponding to the chords \( C(T,G) \). Cutting one more line of a 1-tree leads to two disconnected trees \( (T_1,T_2) \), or a 2-tree. \( T_2 \) is the set of all such pairs. The corresponding chords define monomials of degree \( l + 1 \). Each 2-tree of a graph corresponds to a cut defined by cutting the lines which connected the two now disconnected trees in the original graph. The square of the sum of momenta through the cut lines of one of the two disconnected trees \( T_1 \) or \( T_2 \) defines a Lorentz invariant

\[
S_T = \sum_{j \in C(T,G)} p_j ; \tag{14}
\]
The function $F_0$ is the sum over all such monomials times minus the corresponding invariant. The function $F$ is then given by $F_0$ plus an additional piece involving the internal masses $m_j$. In summary, the functions $U$ and $F$ are obtained from the graph as follows:

$$
U = \sum_{T_2 \in \mathcal{T}_1} \prod_{j \in \mathcal{C}(T_2 \mathcal{G})} x_j ;
$$

$$
F_0 = \sum_{(T_1 T_2) \in \mathcal{T}_2 \mathcal{C}(T_1 \mathcal{G})} \prod_{j \in s_{T_1}} x_j (s_{T_1}) ;
$$

$$
F = F_0 + U \sum_{j=1}^{n} x_j m_j^2 ;
$$

In general, $U$ is a positive semi-definite function. Its vanishing is related to the UV sub-divergences of the graph. Overall UV divergences, if present, will always be contained in the prefactor $\Gamma(\nu_{\text{LD}=2})$. In the Euclidean region, $F$ is also a positive semi-definite function of the Feynman parameters $x_j$.

As an example we consider the graph in fig. 1. For simplicity we assume that all internal propagators are massless. Then the functions $U$ and $F$ read:

$$
U = x_{15}x_{23} + x_{15}x_{46} + x_{23}x_{46} ;
$$

$$
F = (x_1x_3x_4 + x_5x_2x_6 + x_1x_5x_{2346}) \ p_1^2
+ (x_6x_3x_5 + x_4x_1x_2 + x_4x_6x_{1235}) \ p_2^2
+ (x_2x_4x_5 + x_3x_1x_6 + x_2x_3x_{1456}) \ p_3^2 ;
$$

(15)

Here we used the notation that $x_{ij::r} = x_i + x_j + \cdots + x_r$.

Finally let us remark, that in eq. (7) we restricted ourselves to scalar integrals, where the numerator of the integrand is independent of the loop momentum. A priori more complicated cases, where the loop momentum appears in the numerator might occur. However, there is a general reduction algorithm, which reduces these tensor integrals to scalar integrals [34,35]. The price we have to pay is that these scalar integrals involve higher powers of the propagators and/or have shifted dimensions. Therefore we considered in eq. (6) shifted dimensions and in eq. (7) arbitrary powers of the propagators. In conclusion, the integrals of the form as in eq. (7) are the most general loop integrals we have to solve.

### 3 The Mellin-Barnes transformation

In sect. 2 we saw that the Feynman parameter integrals depend on two graph polynomials $U$ and $F$, which are homogeneous functions of the Feynman parameters. In this section we will continue the discussion how these integrals can be performed and exchanged against a (multiple) sum over residues. The case, where the two polynomials are absent is particular simple:

$$
\int_0^1 \prod_{j=1}^{n} dx_j \ x_j^{\nu_j} \delta(1 - \sum_{j=1}^{n} x_j) = \frac{\prod_{j=1}^{n} \Gamma(\nu_j)}{\Gamma(\nu_1 + \cdots + \nu_n)} ;
$$

(17)
With the help of the Mellin-Barnes transformation we now reduce the general case to eq. \((17)\). The Mellin-Barnes transformation reads
\[
(A_1 + A_2 + \cdots + A_n)^c = \frac{1}{\Gamma(c)} \frac{1}{(2\pi i)^{n-1}} \int_{i\infty}^{i\infty} d\sigma_1 \cdots \int_{i\infty}^{i\infty} d\sigma_n \Gamma(\sigma_1) \cdots \Gamma(c + \sigma_n) A_1^{\sigma_1} \cdots A_n^{\sigma_n} \Gamma(c).
\]
(18)

Each contour is such that the poles of \(\Gamma(\sigma)\) are to the right and the poles of \(\Gamma(\sigma + c)\) are to the left. This transformation can be used to convert the sum of monomials of the polynomials \(U\) and \(F\) into a product, such that all Feynman parameter integrals are of the form of eq. \((17)\). As this transformation converts sums into products it is the “inverse” of Feynman parametrisation.

Eq. \((18)\) is derived from the theory of Mellin transformations: Let \(h(x)\) be a function which is bounded by a power law for \(x \to 0\) and \(x \to \infty\), e.g.
\[
\begin{align*}
  h(x) & \propto x^{\gamma_0} \quad \text{for } x \to 0; \\
  h(x) & \propto x^c \quad \text{for } x \to \infty.
\end{align*}
\]
(19)

Then the Mellin transform is defined for \(c_0 < \text{Re } \sigma < c_1\) by
\[
h_M(\sigma) = \int_0^\infty dx \, h(x) x^{\sigma - 1};
\]
(20)

The inverse Mellin transform is given by
\[
h(x) = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} d\sigma \, h_M(\sigma) x^{-\sigma};
\]
(21)

The integration contour is parallel to the imaginary axis and \(c_0 < \text{Re } \gamma < c_1\). As an example for the Mellin transform we consider the function
\[
h(x) = \frac{x^c}{(1 + x)^c}.
\]
(22)

with Mellin transform \(h_M(\sigma) = \Gamma(\sigma) \Gamma(\sigma + c) = \Gamma(c)\). For \(\text{Re } c < \text{Re } \gamma < 0\) we have
\[
\frac{x^c}{(1 + x)^c} = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} d\sigma \, \frac{\Gamma(\sigma) \Gamma(\sigma + c)}{\Gamma(c)} x^{-\sigma};
\]
(23)

From eq. \((23)\) one obtains with \(x = B = A\) the Mellin-Barnes formula
\[
(A + B)^c = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} d\sigma \, \frac{\Gamma(\sigma) \Gamma(\sigma + c)}{\Gamma(c)} A^\sigma B^{-\sigma - c};
\]
(24)
Eq. (18) is then obtained by repeated use of eq. (24).

With the help of eq. (17) and eq. (18) we may exchange the Feynman parameter integrals against multiple contour integrals. A single contour integral is of the form

\[ I = \frac{1}{2\pi i} \int_{\gamma} \frac{\Gamma(\sigma + a_1) \cdots \Gamma(\sigma + a_m) \Gamma(\sigma + b_1) \cdots \Gamma(\sigma + b_n)}{\Gamma(\sigma + c_1) \cdots \Gamma(\sigma + c_p) \Gamma(\sigma + d_1) \cdots \Gamma(\sigma + d_q)} \, x^\sigma \, d\sigma \]  

(25)

If \( \max(\text{Re}(a_1); \cdots; \text{Re}(a_m)) < \min(\text{Re}(b_1); \cdots; \text{Re}(b_n)) \) the contour can be chosen as a straight line parallel to the imaginary axis with

\[ \max(\text{Re}(a_1); \cdots; \text{Re}(a_m)) < \text{Re} \gamma < \min(\text{Re}(b_1); \cdots; \text{Re}(b_n)) ; \]  

(26)

otherwise the contour is indented, such that the residues of \( \Gamma(\sigma + a_1), \ldots, \Gamma(\sigma + a_m) \) are to the right of the contour, whereas the residues of \( \Gamma(\sigma + b_1), \ldots, \Gamma(\sigma + b_n) \) are to the left of the contour. We further set

\[ \alpha = m + n \quad p \cdot q ; \]
\[ \beta = m \quad n \quad p \quad q ; \]
\[ \lambda = \text{Re} \left( \sum_{j=1}^{m} a_j + \sum_{j=1}^{n} b_j \right) \quad \sum_{j=1}^{p} c_j \quad \sum_{j=1}^{q} d_j \quad \frac{1}{2} (m + n \quad p \quad q) : \]  

(27)

Then the integral eq. (25) converges absolutely for \( \alpha > 0 \) \[36\] and defines an analytic function in

\[ \exists \arg x \gamma < \min \pi \frac{\alpha}{2} : \]

(28)

The integral eq. (25) is most conveniently evaluated with the help of the residuum theorem by closing the contour to the left or to the right. Therefore we need to know under which conditions the semi-circle at infinity used to close the contour gives a vanishing contribution. This is obviously the case for \( \exists \gamma < 1 \) if we close the contour to the left, and for \( \exists \gamma > 1 \), if we close the contour to the right. The case \( \exists \gamma = 1 \) deserves some special attention. One can show that in the case \( \beta = 0 \) the semi-circle gives a vanishing contribution, provided

\[ \lambda < 1 ; \]  

(29)

To sum up all residues which lie inside the contour it is useful to know the residues of the Gamma function:

\[ \text{res } (\Gamma(\sigma + a) ; \sigma = a + n) = \frac{(\frac{1}{n})!}{n!} ; \quad \text{res } (\Gamma(\sigma + a) ; \sigma = a + n) = \frac{(\frac{1}{n})!}{n!} : \]  

(30)

In general, one obtains (multiple) sum over residues. In particular simple cases the contour integrals can be performed in closed form with the help of two lemmas of Barnes. Barnes first
lemma states that

\[ \frac{1}{2\pi i} \int_{i\infty}^{i\infty} d\sigma \, \Gamma(a + \sigma) \Gamma(b + \sigma) \Gamma(c + \sigma) \Gamma(d + \sigma) = \frac{\Gamma(a + c) \Gamma(a + d) \Gamma(b + c) \Gamma(b + d)}{\Gamma(a + b + c + d)} ; \]

(31)

if none of the poles of \( \Gamma(a + \sigma) \Gamma(b + \sigma) \) coincides with the ones from \( \Gamma(c + \sigma) \Gamma(d + \sigma) \). Barnes second lemma reads

\[ \frac{1}{2\pi i} \int_{i\infty}^{i\infty} d\sigma \, \frac{\Gamma(a + \sigma) \Gamma(b + \sigma) \Gamma(c + \sigma) \Gamma(d + \sigma) \Gamma(e + \sigma)}{\Gamma(a + b + c + d + e + \sigma)} = \frac{\Gamma(a + d) \Gamma(b + d) \Gamma(c + d) \Gamma(a + e) \Gamma(b + e) \Gamma(c + e)}{\Gamma(a + b + d + e) \Gamma(a + c + d + e) \Gamma(b + c + d + e)} ; \]

(32)

Although the Mellin-Barnes transformation has been known for a long time, the method has seen a revival in applications in recent years [17–19, 37–49].

4 Shuffle algebras

Before we continue the discussion of loop integrals, it is useful to discuss first shuffle algebras and generalisations thereof from an algebraic viewpoint. Consider a set of letters \( A \). The set \( A \) is called the alphabet. A word is an ordered sequence of letters:

\[ w = l_1 l_2 : : : l_k \]  

(33)

The word of length zero is denoted by \( e \). Let \( K \) be a field and consider the vector space of words over \( K \). A shuffle algebra \( \mathcal{A} \) on the vector space of words is defined by

\[ (l_1 l_2 : : : l_k) \cdot (l_{k+1} : : : l_r) = \sum_{\sigma \in \text{shuffles}} l_{\sigma(1)} l_{\sigma(2)} : : : l_{\sigma(r)} ; \]

(34)

where the sum runs over all permutations \( \sigma \), which preserve the relative order of \( 1 ; 2 ; : : : ; k \) and of \( k + 1 ; : : : ; r \). The name “shuffle algebra” is related to the analogy of shuffling cards: If a deck of cards is split into two parts and then shuffled, the relative order within the two individual parts is conserved. The empty word \( e \) is the unit in this algebra:

\[ e \cdot w = w = e \cdot w ; \]

(35)

A recursive definition of the shuffle product is given by

\[ (l_1 l_2 : : : l_k) \cdot (l_{k+1} : : : l_r) = l_1 [(l_2 : : : l_k) \cdot (l_{k+1} : : : l_r)] + l_{k+1} [(l_1 l_2 : : : l_k) \cdot (l_{k+1} : : : l_r)] \]

(36)

It is well known fact that the shuffle algebra is actually a (non-cocommutative) Hopf algebra [50]. In this context let us briefly review the definitions of a coalgebra, a bialgebra and a Hopf algebra,
which are closely related: First note that the unit in an algebra can be viewed as a map from $K$ to $A$ and that the multiplication can be viewed as a map from the tensor product $A \otimes A$ to $A$ (e.g. one takes two elements from $A$, multiplies them and gets one element out).

A coalgebra has instead of multiplication and unit the dual structures: a comultiplication $\Delta$ and a counit $\bar{e}$. The counit is a map from $A$ to $K$, whereas comultiplication is a map from $A$ to $A \otimes A$. Note that comultiplication and counit go in the reverse direction compared to multiplication and unit. We will always assume that the comultiplication is coassociative. The general form of the coproduct is

$$\Delta(a) = \sum_i a_i^{(1)} a_i^{(2)};$$

where $a_i^{(1)}$ denotes an element of $A$ appearing in the first slot of $A \otimes A$ and $a_i^{(2)}$ correspondingly denotes an element of $A$ appearing in the second slot. Sweedler’s notation [51] consists in dropping the dummy index $i$ and the summation symbol:

$$\Delta(a) = a^{(1)} a^{(2)}$$

The sum is implicitly understood. This is similar to Einstein’s summation convention, except that the dummy summation index $i$ is also dropped. The superscripts $^{(1)}$ and $^{(2)}$ indicate that a sum is involved.

A bialgebra is an algebra and a coalgebra at the same time, such that the two structures are compatible with each other. Using Sweedler’s notation, the compatibility between the multiplication and comultiplication is expressed as

$$\Delta(ab) = a^{(1)} b^{(1)} a^{(2)} b^{(2)};$$

A Hopf algebra is a bialgebra with an additional map from $A$ to $A$, called the antipode $S$, which fulfils

$$a^{(1)} S a^{(2)} = S a^{(1)} a^{(2)} = 0 \quad \text{for } a \in e;$$

With this background at hand we can now state the coproduct, the counit and the antipode for the shuffle algebra: The counit $\bar{e}$ is given by:

$$\bar{e}(e) = 1; \quad \bar{e}(l_1 l_2 \cdots l_n) = 0;$$

The coproduct $\Delta$ is given by:

$$\Delta(l_1 l_2 \cdots l_k) = \sum_{j=0}^k l_{j+1} \cdots l_k \otimes l_1 \cdots l_j;$$

The antipode $S$ is given by:

$$S(l_1 l_2 \cdots l_k) = (1^k l_{k-1} \cdots l_2 l_1);$$
The shuffle algebra is generated by the Lyndon words. If one introduces a lexicographic ordering on the letters of the alphabet $A$, a Lyndon word is defined by the property

$$w < v$$

for any sub-words $u$ and $v$ such that $w = uv$.

An important example for a shuffle algebra are iterated integrals. Let $[a;b]$ be a segment of the real line and $f_1, f_2, \ldots$ functions on this interval. Let us define the following iterated integrals:

$$I (f_1; f_2; \ldots; f_k; a; b) = \int_a^b f_1 (t_1) dt_1 \int_a^{t_1} f_2 (t_2) dt_2 \cdots \int_a^{t_{k-1}} f_k (t_k) dt_k$$

For fixed $a$ and $b$ we have a shuffle algebra:

$$I (f_1; f_2; \ldots; f_k; a; b) \cdot I (f_{k+1}; f_{k+2}; \ldots; f_r; a; b) = \sum_{\text{shuffles } \sigma} I (f_{\sigma(1)}; f_{\sigma(2)}; \ldots; f_{\sigma(r)}; a; b);$$

where the sum runs over all permutations $\sigma$, which preserve the relative order of $1; 2; \cdots; k$ and of $k + 1; \cdots; r$. The proof is sketched in fig. 2. The two outermost integrations are recursively replaced by integrations over the upper and lower triangle.

We now consider generalisations of shuffle algebras. Assume that for the set of letters we have an additional operation

$$(;): \quad A \rightarrow A ! A; \quad l_1 \quad l_2 \rightarrow (l_1 l_2);$$

which is commutative and associative. Then we can define a new product of words recursively through

$$(l_1 l_2; \ldots; l_k) \cdot (l_{k+1}; \ldots; l_r) = l_1 [l_2; \ldots; l_k] \cdot (l_{k+1}; \ldots; l_r) + \sum_{\text{shuffles } \sigma} \left[ I (f_{\sigma(1)}; \ldots; f_{\sigma(k)}; a; b) \cdot I (f_{\sigma(k+1)}; \ldots; f_{\sigma(r)}; a; b); \right]$$

This product is a generalisation of the shuffle product and differs from the recursive definition of the shuffle product in eq. (36) through the extra term in the last line. This modified product is known under the names quasi-shuffle product [52], mixable shuffle product [53] or stuffle.
product \[54\]. Quasi-shuffle algebras are Hopf algebras. Comultiplication and counit are defined as for the shuffle algebras. The counit \( \bar{e} \) is given by:

\[
\bar{e}(e) = 1; \quad \bar{e}(l_1 l_2 \cdots l_n) = 0:
\]

(49)

The coproduct \( \Delta \) is given by:

\[
\Delta(l_1 l_2 \cdots l_k) = \sum_{j=0}^{k} l_{j+1} \cdots l_k l_1 \cdots l_j
\]

(50)

The antipode \( S \) is recursively defined through

\[
S(l_1 l_2 \cdots l_k) = l_1 l_2 \cdots l_k \sum_{j=1}^{k-1} S(l_{j+1} \cdots l_k) l_1 \cdots l_j
\]

(51)

An example for a quasi-shuffle algebra are nested sums. Let \( n_a \) and \( n_b \) be integers with \( n_a < n_b \) and let \( f_1, f_2, \ldots \) be functions defined on the integers. We consider the following nested sums:

\[
S(f_1 ; f_2 ; \cdots ; f_k ; n_a , n_b) = \sum_{i_1 = n_a}^{n_b} f_1(i_1) \sum_{i_2 = n_a}^{n_b} f_2(i_2) \cdots \sum_{i_k = n_a}^{n_b} f_k(i_k)
\]

(52)

For fixed \( n_a \) and \( n_b \) we have a quasi-shuffle algebra:

\[
S(f_1 ; f_2 ; \cdots ; f_k ; n_a , n_b) =
\sum_{i_1 = n_a}^{n_b} f_1(i_1) S(f_2 ; \cdots ; f_k ; n_a , i_1, 1) S(f_1 ; \cdots ; f_r ; n_a , i_1, 1)
\]

\[
+ \sum_{j_1 = n_a}^{n_b} f_k(j_1) S(f_1 ; f_2 ; \cdots ; f_k ; n_a , j_1, 1) S(f_1 ; \cdots ; f_r ; n_a , j_1, 1)
\]

\[
+ \sum_{i = n_a}^{n_b} f_1(i) f_k(i) S(f_2 ; \cdots ; f_k ; n_a , i, 1) S(f_1 ; \cdots ; f_r ; n_a , i, 1)
\]

(53)

Note that the product of two letters corresponds to the point-wise product of the two functions:

\[
(f_i ; f_j)(n) = f_i(n) f_j(n):
\]

(54)

The proof that nested sums obey the quasi-shuffle algebra is sketched in Fig. 3. The outermost sums of the nested sums on the l.h.s of (53) are split into the three regions indicated in Fig. 3.
5 Multiple polylogarithms

In the previous section we have seen that iterated integrals form a shuffle algebra, while nested sums form a quasi-shuffle algebra. In this context multiple polylogarithms form an interesting class of functions. They have a representation as iterated integrals as well as nested sums. Therefore multiple polylogarithms form a shuffle algebra as well as a quasi-shuffle algebra. The two algebra structures are independent. Let us start with the representation as nested sums. The multiple polylogarithms are defined by

\[ \text{Li}_{m_1, \ldots, m_k}(x_1; \ldots; x_k) = \sum_{i_1 > i_2 > \cdots > i_k > 0} \frac{x_1^{i_1}}{i_1^{m_1}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}} \]  \hspace{1cm} (55)

The multiple polylogarithms are generalisations of the classical polylogarithms \( \text{Li}_n(x) \) [55], whose most prominent examples are

\[ \text{Li}_1(x) = \sum_{i_1=1}^{\infty} \frac{x^{i_1}}{i_1} = \ln(1-x); \quad \text{Li}_2(x) = \sum_{i_1=1}^{\infty} \frac{x^{i_1}}{i_1^2} \]  \hspace{1cm} (56)

as well as Nielsen’s generalised polylogarithms [56]

\[ S_{n;p}(x) = \text{Li}_{n+1, \ldots; m; \ldots; p; \ldots, 1}(x; \ldots; \frac{1}{\ldots; 1}) \]  \hspace{1cm} (57)

and the harmonic polylogarithms [57]

\[ H_{m_1, \ldots; m_k}(x) = \text{Li}_{m_1, \ldots; m_k}(x; \ldots; \frac{1}{\ldots; 1}) \]  \hspace{1cm} (58)

Multiple polylogarithms have been studied extensively in the literature by physicists [57–70] and mathematicians [54, 71–81].

In addition, multiple polylogarithms have an integral representation. To discuss the integral representation it is convenient to introduce for \( z_k \neq 0 \) the following functions

\[ G(z_1; \ldots; z_k; y) = \int_0^y \int_{t_1}^{t_1} \int_{z_1}^{z_1} \cdots \int_{z_2}^{z_2} \frac{dt_1}{t_1} \frac{dt_2}{z_2} \cdots \frac{dt_k}{z_k} \]  \hspace{1cm} (59)

In this definition one variable is redundant due to the following scaling relation:

\[ G(z_1; \ldots; z_k; y) = G(xz_1; \ldots; xz_k; xy) \]  \hspace{1cm} (60)

If one further defines

\[ g(z; y) = \frac{1}{y \cdot z} \]  \hspace{1cm} (61)
then one has
\[
\frac{d}{dy} G(z_1; \ldots; z_k; y) = g(z_1; y) G(z_2; \ldots; z_k; y)
\]
(62)
and
\[
G(z_1; z_2; \ldots; z_k; y) = \int_0^y dt \, g(z_1; t) G(z_2; \ldots; z_k; t).
\]
(63)
One can slightly enlarge the set and define \(G(0; \ldots; 0; y)\) with \(k\) zeros for \(z_1\) to \(z_k\) to be
\[
G(0; \ldots; 0; y) = \frac{1}{k!} (\ln y)^k.
\]
(64)
This permits us to allow trailing zeros in the sequence \((z_1; \ldots; z_k)\) by defining the function \(G\) with trailing zeros via (63) and (64). To relate the multiple polylogarithms to the functions \(G\) it is convenient to introduce the following short-hand notation:
\[
G_{m_1; \ldots; m_k}(z_1; \ldots; z_k; y) = G(0; \ldots; 0; z_1; \ldots; z_k; y)
\]
(65)
Here, all \(z_j\) for \(j = 1; \ldots; k\) are assumed to be non-zero. One then finds
\[
\text{Li}_{m_1; \ldots; m_k}(x_1; \ldots; x_k) = (1)^k G_{m_1; \ldots; m_k} \frac{1}{x_1}; \frac{1}{x_1 x_2}; \ldots; \frac{1}{x_1 \ldots x_k}; 1.
\]
(66)
The inverse formula reads
\[
G_{m_1; \ldots; m_k}(z_1; \ldots; z_k; y) = (1)^k \text{Li}_{m_1; \ldots; m_k} \frac{y}{z_1}; \frac{z_1}{z_2}; \ldots; \frac{z_k}{z_k}; 1.
\]
(67)
Eq. (66) together with (65) and (59) defines an integral representation for the multiple polylogarithms. To make this more explicit I first introduce some notation for iterated integrals
\[
\int_0^\Lambda \frac{dt}{t} \frac{dt}{a_n} \cdots \frac{dt}{a_1} = \int_0^{\Lambda_{n-1}} \frac{dt_n}{t_n} \cdots \int_0^{\Lambda_1} \frac{dt_1}{t_1} \frac{dt}{a_1}
\]
(68)
and the short hand notation:
\[
\int_0^\Lambda \frac{dt}{t} \frac{m \, dt}{t} \frac{dt}{a} = \int_0^{\Lambda} \frac{dt}{\underline{\frac{m \, dt}{t}} a}.
\]
(69)
The integral representation for \( \text{Li}_{m_1; \ldots; m_k} (x_1; \ldots; x_k) \) reads then

\[
\text{Li}_{m_1; \ldots; m_k} (x_1; \ldots; x_k) = \frac{1}{b_1} \int_0^1 \frac{dt}{t} \frac{m_1}{b_1} \frac{dt}{b_2} \frac{m_2}{b_2} \cdots \frac{dt}{b_k} \frac{m_k}{b_k};
\]

where the \( b_j \)'s are related to the \( x_j \)'s

\[
b_j = \frac{1}{x_1 x_2 \cdots x_j};
\]

Up to now we treated multiple polylogarithms from an algebraic point of view. Equally important are the analytical properties, which are needed for an efficient numerical evaluation. As an example I first discuss the numerical evaluation of the dilogarithm [82]:

\[
\text{Li}_2 (x) = \int_0^x \frac{dt}{t} \frac{\ln(1/t)}{t} = \sum_{n=1}^{\infty} \frac{x^n}{n^2};
\]

The power series expansion can be evaluated numerically, provided \( |x| < 1 \). Using the functional equations

\[
\text{Li}_2 (x) = \text{Li}_2 (1/x) + \frac{\pi^2}{6} \ln(x) \ln(1/x); \quad \text{Li}_2 (1/x) = \text{Li}_2 (1) - \frac{\pi^2}{6} \ln(x) \ln(1/x);
\]

any argument of the dilogarithm can be mapped into the region \( |x| < 1 \) and \( \text{Re}(x) = 1 \). The numerical computation can be accelerated by using an expansion in \( \ln(1/x) \) and the Bernoulli numbers \( B_i \):

\[
\text{Li}_2 (x) = \sum_{i=0}^{\infty} \frac{B_i}{(i+1)!} \left( \ln(1/x) \right)^{i+1};
\]

The generalisation to multiple polylogarithms proceeds along the same lines [67]: Using the integral representation

\[
G_{m_1; \ldots; m_k} (z_1; \ldots; z_k; y) =
\int_0^y \frac{dt}{t} \frac{m_1}{z_1} \frac{dt}{z_1} \frac{m_2}{z_2} \cdots \frac{dt}{z_k} \frac{m_k}{z_k};
\]
one transforms all arguments into a region, where one has a converging power series expansion:
\[ G_{m_1, \ldots, m_k}(z_1; \ldots; z_k; y) = \sum_{j_1=1}^{\infty} \cdots \sum_{j_k=1}^{\infty} \frac{1}{(j_1 + \cdots + j_k)^{m_1}} \frac{y^{j_1}}{z_1} \cdots \frac{1}{(j_2 + \cdots + j_k)^{m_2}} \frac{y^{j_2}}{z_2} \cdots \frac{1}{(j_k)^{m_k}} \frac{y^{j_k}}{z_k} : \] (76)

The multiple polylogarithms satisfy the Hölder convolution [54]. For \( z_1 \neq 1 \) and \( z_w \neq 0 \) this identity reads
\[ G(z_1; \ldots; z_w; 1) = \sum_{j=0}^{w} (1)^j G(z_j; 1; z_j; \ldots; 1; z_1; 1) \frac{1}{p} G(z_{j+1}; \ldots; z_w; 1) \] (77)

The Hölder convolution can be used to accelerate the convergence for the series representation of the multiple polylogarithms.

6 Laurent expansion of Feynman integrals

Let us return to the question on how to compute Feynman integrals. In section 3 we saw how to obtain from the Mellin-Barnes transformation (multiple) sums by closing the integration contours and summing up the residues. As a simple example let us consider that the sum of residues is equal to
\[ \sum_{i=0}^{\infty} \frac{\Gamma(i+a_1+t_1 \varepsilon) \Gamma(i+a_2+t_2 \varepsilon)}{\Gamma(i+1) \Gamma(i+a_3+t_3 \varepsilon)} x^i \] (78)

Here \( a_1, a_2 \) and \( a_3 \) are assumed to be integers. Up to prefactors the expression in eq. (78) is a hyper-geometric function \( {}_2F_1 \). We are interested in the Laurent expansion of this expression in the small parameter \( \varepsilon \). The basic formula for the expansion of Gamma functions reads
\[ \Gamma(n+\varepsilon) = \Gamma(1+\varepsilon) \Gamma(n) 1 + \varepsilon Z_1(n+1) + \varepsilon^2 Z_{11}(n+1) + \cdots + \sum_{i=1}^{n} \varepsilon^i Z_{11\cdots i}(n+1) ; \] (79)

where \( Z_{m_1;\ldots;m_k}(n) \) are Euler-Zagier sums defined by
\[ Z_{m_1;\ldots;m_k}(n) = \sum_{i_1 > i_2 > \cdots > i_k > 0} \frac{1}{i_1^{m_1} \cdots i_k^{m_k}} ; \] (80)

This motivates the following definition of a special form of nested sums, called Z-sums:
\[ Z(n;m_1;\ldots;m_k;x_1;\ldots;x_k) = \sum_{i_1 > i_2 > \cdots > i_k > 0} \frac{x_1^{i_1}}{i_1^{m_1}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}} ; \] (81)
k is called the depth of the Z-sum and \( w = m_1 + \cdots + m_k \) is called the weight. If the sums go to infinity \( (n = \infty) \) the Z-sums are multiple polylogarithms:

\[
Z(\infty; m_1; \cdots; m_k; x_1; \cdots; x_k) = \lim_{m \to \infty} \, (x_1; \cdots; x_k).
\]

(82)

For \( x_1 = \cdots = x_k = 1 \) the definition reduces to the Euler-Zagier sums [83, 84]:

\[
Z(n; m_1; \cdots; m_k; 1; \cdots; 1) = Z_{m_1; \cdots; m_k}(n).
\]

(83)

For \( n = \infty \) and \( x_1 = \cdots = x_k = 1 \) the sum is a multiple \( \zeta \)-value [54]:

\[
Z(\infty; m_1; \cdots; m_k; 1; \cdots; 1) = \zeta_{m_1; \cdots; m_k}.
\]

(84)

The usefulness of the Z-sums lies in the fact, that they interpolate between multiple polylogarithms and Euler-Zagier sums. The Z-sums form a quasi-shuffle algebra.

Using \( \Gamma(x + 1) = x \Gamma(x) \), partial fractioning and an adjustment of the summation index one can transform eq. (78) into terms of the form

\[
\sum_{i=1}^{\infty} \frac{\Gamma(i + t_1 \varepsilon) \Gamma(i + t_2 \varepsilon) \Gamma(i + t_3 \varepsilon) \Gamma(i + t_4 \varepsilon) \cdots \Gamma(i + t_n \varepsilon)}{\Gamma(i) \Gamma(i + t_1 \varepsilon) \cdots \Gamma(i + t_n \varepsilon)} \frac{x^i}{p^m};
\]

(85)

where \( m \) is an integer. Now using eq. (79) one obtains

\[
\Gamma(1 + \varepsilon) \sum_{i=1}^{\infty} \frac{(1 + \varepsilon t_1 Z_1(i, 1) + \cdots) (1 + \varepsilon t_2 Z_1(i, 1) + \cdots) \cdots}{(1 + \varepsilon t_3 Z_1(i, 1) + \cdots)} \frac{x^i}{p^m};
\]

(86)

Inverting the power series in the denominator and truncating in \( \varepsilon \) one obtains in each order in \( \varepsilon \) terms of the form

\[
\sum_{i=1}^{\infty} \frac{x^i}{p^m} Z_{m_1; \cdots; m_k}(i, 1); Z_{m_1; \cdots; m_k}^0(i, 1); Z_{m_1; \cdots; m_k}^{0,0}(i, 1);
\]

(87)

Using the quasi-shuffle product for Z-sums the three Euler-Zagier sums can be reduced to single Euler-Zagier sums and one finally arrives at terms of the form

\[
\sum_{i=1}^{\infty} \frac{x^i}{p^m} Z_{m_1; \cdots; m_k}(i, 1);
\]

(88)

which are special cases of multiple polylogarithms, called harmonic polylogarithms \( H_{m_1; \cdots; m_k}(x) \).

This completes the algorithm for the expansion in \( \varepsilon \) for sums of the form as in eq. (78).

The Hopf algebra of Z-sums has additional structures if we allow expressions of the form

\[
\frac{x^n}{n^{m_0}} Z(n; m_1; \cdots; m_k; x_1; \cdots; x_k);
\]

(89)

e.g. Z-sums multiplied by a letter. Then the following convolution product

\[
\sum_{i=1}^{n} \frac{x^i}{i^{m_0}} Z(i, 1; \cdots) \frac{y^n}{n^{m_0}} Z(n, i, 1; \cdots);
\]

(90)
can again be expressed in terms of expressions of the form (89). In addition there is a conjugation, e.g. sums of the form
\[ \sum_{i=1}^{n} n_i \left( \frac{1}{i} \right) = 1 \]
\[ \vdots \]
\[ \sum_{i=1}^{n} \left( \frac{1}{i} \right) + 1 \delta \]
\[ = (91) \]

The name conjugation stems from the following fact: To any function \( f(n) \) of an integer variable \( n \) one can define a conjugated function \( C \ f(n) \) as the following sum
\[ C \ f(n) = \sum_{i=1}^{n} n_i \left( \frac{1}{i} \right) f(i) : \]
\[ (92) \]

Then conjugation satisfies the following two properties:
\[ C \ 1 = 1 ; \]
\[ C \ C \ f(n) = f(n) ; \]
\[ (93) \]

Finally there is the combination of conjugation and convolution, e.g. sums of the form
\[ \sum_{i=1}^{n} \left( \frac{1}{i} \right) \frac{x_i}{i^m} Z(i ; \vdots) = \frac{y^n}{i^m} Z(n \ i ; \vdots) \]
\[ (94) \]

These properties can be used to expand more complicated transcendental functions like
\[ \sum_{i=0}^{\infty} \frac{n}{j=0} \frac{\Gamma(i+a_1)}{\Gamma(i+a_k)} \frac{\Gamma(j+b_1)}{\Gamma(j+b_0)} \frac{\Gamma(i+j+c_1)}{\Gamma(i+j+c_0)} \frac{\Gamma(i+j+c_m)}{\Gamma(i+j+c_m^0)} x_i y_j \]
\[ (95) \]
or
\[ \sum_{i=0}^{\infty} \frac{n}{j=0} \frac{\Gamma(i+a_1)}{\Gamma(i+a_k)} \frac{\Gamma(j+b_1)}{\Gamma(j+b_0)} \frac{\Gamma(i+j+c_1)}{\Gamma(i+j+c_0)} \frac{\Gamma(i+j+c_m)}{\Gamma(i+j+c_m^0)} x_i y_j \]
\[ (96) \]

Examples for functions of this type are the first and second Appell function \( F_1 \) and \( F_2 \). Note that in these examples there are always as many Gamma functions in the numerator as in the denominator. We assume that all \( a_n, a_0, b_n, b_0, c_n \) and \( c_0 \) are of the form “integer + const \( \varepsilon \)”. The first type can be generalised to the form “rational number + const \( \varepsilon \)”, if the Gamma functions always occur in ratios of the form
\[ \frac{\Gamma(n+a)}{\Gamma(n+c)} = \frac{\frac{p}{q} + b \varepsilon}{\frac{p}{q} + d \varepsilon} \]
\[ (97) \]
where the same rational number \( p = q \) occurs in the numerator and in the denominator [66]. In this case we have to replace eq. (79) by

\[
\Gamma \left[ n + 1 \right] \frac{p}{q} + \varepsilon = \frac{\Gamma \left[ 1 \right] \frac{p}{q} + \varepsilon}{\Gamma \left[ 1 \right] \frac{p}{q}} \frac{\Gamma \left[ n + 1 \right] \frac{p}{q}}{\Gamma \left[ n + 1 \right] \frac{p}{q}} \exp \left[ \frac{1}{q} \sum_{l=0}^{q-1} r_{q}^{l} \sum_{k=1}^{\infty} \varepsilon^{k} \left( \frac{q}{k} \right) Z(q, n; k; q) \right] ;
\]

which introduces the \( q \)-th roots of unity

\[
r_{q}^{p} = \exp \frac{2\pi ip}{q} ;
\]

In summary these techniques allow a systematic procedure for the computation of Feynman integrals, if certain conditions are met. These conditions require that factors of Gamma functions are balanced like in eq. (95) or eq. (96) [63, 66]. The algebraic properties of nested sums and iterated integrals discussed here are well-suited for an implementation into a computer algebra system and several packages for these manipulations exist [58, 85–88].

7 Conclusions

In this article I discussed the mathematical structures underlying the computation of Feynman loop integrals. One encounters iterated structures as nested sums or iterated integrals, which form a Hopf algebra with a shuffle or quasi-shuffle product. Of particular importance are multiple polylogarithms. The algebraic properties of these functions are very rich: They form at the same time a shuffle algebra as well as a quasi-shuffle algebra. Based on these algebraic structures I discussed algorithms which evaluate Feynman integrals to multiple polylogarithms.

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