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Nested Sums, Expansion of Transcendental Functions and Multi-Scale Multi-Loop Integrals

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Abstract

Expansion of higher transcendental functions in a small parameter are needed in many areas of science. For certain classes of functions this can be achieved by algebraic means. These algebraic tools are based on nested sums and can be formulated as algorithms suitable for an implementation on a computer. Examples, such as expansions of generalized hypergeometric functions or Appell functions are discussed. As a further application, we give the general solution of a two-loop integral, the so-called C-topology, in terms of multiple nested sums. In addition, we discuss some important properties of nested sums, in particular we show that they satisfy a Hopf algebra.

1 Introduction

The expansion of higher transcendental functions [1, 2] is a common problem occuring in many areas of science. It is of particular interest in particle physics in the calculation of higher order radiative corrections to scattering amplitudes. There, higher transcendental functions occur frequently in formal solutions for specific loop integrals. The necessary expansions of these functions are in general a highly non-trivial task. This is particularly true, if the expansions are required to a very high order.

In calculations of higher order radiative corrections classical polylogarithms [3], as well as Nielsen's generalized polylogarithms [4] appear. However, this set of functions will not suffice, if the number of loops grows, or if several different scales are involved in the problem. Several extensions of this class of functions to multiple polylogarithms have been discussed recently [5] - [8] .

It is the aim of this paper to perform a systematic study of multiple nested sums appearing in the expansion of higher transcendental functions around integer values of their indices. To that end, we define so called Z-sums, study their algebraic properties and discuss their relation to the multiple polylogarithms introduced in the literature [5] - [8] . We give algorithms to solve these multiple nested sums to any order in the expansion parameter ε in terms of a given basis in Z-sums. All algorithms can be readily implemented on a computer. The Z-sums can be considered as certain generalizations of Euler-Zagier sums [9, 10] or of harmonic sums [11] - [13] involving multiple ratios of scales. The latter are known in physics since the calculation of higher order Mellin moments of the deep-inelastic structure functions [11], [14] - [16] .

At the same time, our results allow us to investigate higher loop multi-scale integrals occuring for instance in pertubative corrections to four-particle scattering amplitudes. These integrals have received great attention in recent years, mainly motivated by calculations of the next-to-next-to-leading order corrections to amplitudes for Bhabha scattering [17], for $pp \to 2$ jets [18] - [20] , for $pp \to \gamma\gamma$ [21] and for light-by-light scattering [22].

The relevant master integrals at two loops with four external legs have been calculated using a variety of techniques. Analytic results were obtained either with the help of Mellin-Barnes representations [23, 24] or with differential equations [8, 25]. Numerical results were obtained by a numerical evaluation of the coefficients of the ε-expansion [26, 27] . Here, we want to advocate a different point of view based on multiple nested sums. As a new result and to illustrate our approach, we discuss a specific two-loop integral, the so-called C-topology with one leg offshell, which can be reduced for arbitrary powers of the propagators and arbitrary dimensions to the aforementioned sums. This is useful for the calculation of the two-loop amplitude for $e^+e^- \to$ 3 jets. Some of the techniques presented here have already been used in a recent calculation with massive fermions [28]. In addition, there exists a wide variety of related literature on higher transcendental functions occuring in loop integrals and we can only mention a few of them here [29] - [35] .

This papers is organized as follows. In the next section we introduce nested sums, show that they satisfy an algebra and summarize some important special cases of our definitions. Section 3 contains the main results of this paper, in particular the algorithms for solving certain classes of nested sums. In sec. 4 we give some examples for expansions of generalized hypergeometric functions, Appell functions and the Kampé de Fériet function. As an application to higher loop multi-scale integrals, we discuss the C-topology in sec. 4.4. In Appendix A we show that the algebraic structure of nested sums forms a Hopf algebra [36, 37]. In Appendix B we briefly review the multiple polylogarithms of Goncharov [5].

2 Definition and properties of nested sums

We define the Z-sums by

$$
\begin{aligned}
Z(n) &= \begin{cases} 1, & n \geq 0, \\ 0, & n < 0, \end{cases} \\
Z(n; m_1, ..., m_k; x_1, ..., x_k) &= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} Z(i-1; m_2, ..., m_k; x_2, ..., x_k), \qquad (1)
\end{aligned}
$$

k is called the depth, $w = m_1 + ... + m_k$ the weight. An equivalent definition is given by

$$
Z(n; m_1, ..., m_k; x_1, ..., x_k) = \sum_{n \geq i_1 > i_2 > ... > i_k > 0} \frac{x_1^{i_1}}{{i_1}^{m_1}} \cdots \frac{x_k^{i_k}}{{i_k}^{m_k}}. \qquad (2)
$$

In a similar way we define the S-sums by

$$
\begin{aligned}
S(n) &= \begin{cases} 1, & n > 0, \\ 0, & n \leq 0, \end{cases} \\
S(n; m_1, ..., m_k; x_1, ..., x_k) &= \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} S(i; m_2, ..., m_k; x_2, ..., x_k). \qquad (3)
\end{aligned}
$$

Once again an equivalent representation is given by:

$$
S(n; m_1, ..., m_k; x_1, ..., x_k) = \sum_{n \geq i_1 \geq i_2 \geq ... \geq i_k \geq 1} \frac{x_1^{i_1}}{{i_1}^{m_1}} \cdots \frac{x_k^{i_k}}{{i_k}^{m_k}}. \qquad (4)
$$

The S-sums are closely related to the Z-sums, the difference being the upper summation boundary for the nested sums: $(i-1)$ for Z-sums, i for S-sums. We introduce both Z-sums and S-sums, since some properties are more naturally expressed in terms of Z-sums while others are more naturally expressed in terms of S-sums. We can easily convert from the notation with Z-sums to the notation with S-sums and vice versa:

$$
\begin{aligned}
S(n; m_1, ...; x_1, ...) &= \sum_{i_1=1}^{n} \frac{x_1^{i_1}}{{i_1}^{m_1}} \sum_{i_2=1}^{i_1-1} \frac{x_2^{i_2}}{{i_2}^{m_2}} S(i_2; m_3, ...; x_3, ...) \\
&\quad + S(n; m_1 + m_2, m_3, ...; x_1 x_2, x_3, ...), \\
Z(n; m_1, ...; x_1, ...) &= \sum_{i_1=1}^{n} \frac{x_1^{i_1}}{{i_1}^{m_1}} \sum_{i_2=1}^{i_1} \frac{x_2^{i_2}}{{i_2}^{m_2}} Z(i_2 - 1; m_3, ...; x_3, ...) \\
&\quad - Z(n; m_1 + m_2, m_3, ...; x_1 x_2, x_3, ...). \qquad (5)
\end{aligned}
$$

The first formula allows to convert recursively a S-sum into a Z-sum. The second formula yields the conversion from a Z-sum to a S-sum. For example in terms of S-sums the Z-sum $Z(n; m_1, m_2, m_3, x_1, x_2, x_3)$ reads

$$
\begin{aligned}
Z(n; m_1, m_2, m_3, x_1, x_2, x_3) &= S(n; m_1, m_2, m_3, x_1, x_2, x_3) - S(n; m_1 + m_2, m_3, x_1 x_2, x_3) \\
&\quad - S(n; m_1, m_2 + m_3, x_1, x_2 x_3) + S(n; m_1 + m_2 + m_3, x_1 x_2 x_3). \qquad (6)
\end{aligned}
$$

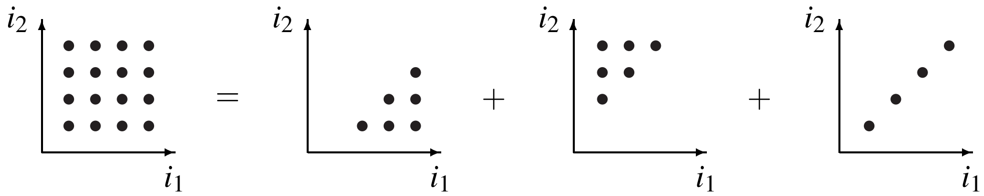


Figure 1: Sketch of the proof for the multiplication of Z-sums. The sum over the square is replaced by the sum over the three regions on the r.h.s.

Furthermore the Z-sums and the S-sums obey an algebra. A product of two Z-sums with the same upper summation limit can be written in terms of single Z-sums. A straightforward generalization of the results given by Vermaseren on the multiplication of harmonic sums yields [12]:

$$\begin{aligned}
& Z(n;m_1,...,m_k;x_1,...,x_k) \times Z(n;m_1',...,m_l';x_1',...,x_l') \\
= & \sum_{i_1=1}^{n} \frac{x_1^{i_1}}{i_1^{m_1}} Z(i_1-1;m_2,...,m_k;x_2,...,x_k) Z(i_1-1;m_1',...,m_l';x_1',...,x_l') \\
& + \sum_{i_2=1}^{n} \frac{x_1'^{i_2}}{i_2^{m_1'}} Z(i_2-1;m_1,...,m_k;x_1,...,x_k) Z(i_2-1;m_2',...,m_l';x_2',...,x_l') \\
& + \sum_{i=1}^{n} \frac{(x_1 x_1')^i}{i^{m_1+m_1'}} Z(i-1;m_2,...,m_k;x_2,...,x_k) Z(i-1;m_2',...,m_l';x_2',...,x_l'). \qquad (7)
\end{aligned}$$

Recursive application of eq. (7) leads to single Z-sums. The proof of eq. (7) follows immediately from the relation

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij} = \sum_{i=1}^{n}\sum_{j=1}^{i-1} a_{ij} + \sum_{j=1}^{n}\sum_{i=1}^{j-1} a_{ij} + \sum_{i=1}^{n} a_{ii}, \qquad (8)$$

which is sketched in fig. 1. Note that eq. (7) directly translates into an algorithm for the multiplication of two Z-sums. Details on the implementation of this algorithms on a computer can be found for example in [12]. We give an example for the product of two Z-sums:

$$\begin{aligned}
Z(n;m_1,m_2;x_1,x_2) \times Z(n;m_3;x_3) = & \; Z(n;m_1,m_2,m_3;x_1,x_2,x_3) + Z(n;m_1,m_3,m_2;x_1,x_3,x_2) \\
& + Z(n;m_3,m_1,m_2;x_3,x_1,x_2) + Z(n;m_1,m_2+m_3;x_1,x_2x_3) \\
& + Z(n;m_1+m_3,m_2;x_1x_3,x_2). \qquad (9)
\end{aligned}$$

Note that the product conserves the weight. The Z-sums form actually a Hopf algebra. More details can be found in appendix A.

The S-sums also obey an algebra. The basic formula reads

$$\begin{aligned}
& S(n;m_1,...,m_k;x_1,...,x_k) \times S(n;m_1',...,m_l';x_1',...,x_l') \\
= & \sum_{i_1=1}^{n} \frac{x_1^{i_1}}{i_1^{m_1}} S(i_1;m_2,...,m_k;x_2,...,x_k) S(i_1;m_1',...,m_l';x_1',...,x_l')
\end{aligned}$$

$$+\sum_{i_2=1}^{n} \frac{x_1'^{i_2}}{i_2^{m_1'}} S(i_2;m_1,...,m_k;x_1,...,x_k) S(i_2;m_2',...,m_l';x_2',...,x_l')$$
$$-\sum_{i=1}^{n} \frac{(x_1 x_1')^i}{i^{m_1+m_1'}} S(i;m_2,...,m_k;x_2,...,x_k) S(i;m_2',...,m_l';x_2',...,x_l'). \quad (10)$$

Note the minus sign in front of the last term compared to the corresponding formula for Z-sums.

2.1 Special cases

Z-sums and S-sums are generalizations of more known objects. We give here an overview of the most important special cases.

For $n = \infty$ the Z-sums are the multiple polylogarithms of Goncharov [5]:

$$Z(\infty;m_1,...,m_k;x_1,...,x_k) = \mathrm{Li}_{m_k,...,m_1}(x_k,...,x_1). \quad (11)$$

For $x_1 = ... = x_k = 1$ the definition reduces to the Euler-Zagier sums [9, 10]:

$$Z(n;m_1,...,m_k;1,...,1) = Z_{m_1,...,m_k}(n). \quad (12)$$

For $n = \infty$ and $x_1 = ... = x_k = 1$ the sum is a multiple ζ-value [6]:

$$Z(\infty;m_1,...,m_k;1,...,1) = \zeta(m_k,...,m_1). \quad (13)$$

The S-sums reduce for $x_1 = ... = x_k = 1$ (and positive m_i) to harmonic sums [12]:

$$S(n;m_1,...,m_k;1,...,1) = S_{m_1,...,m_k}(n). \quad (14)$$

The multiple polylogarithms of Goncharov contain as the notation already suggests as subsets the classical polylogarithms $\mathrm{Li}_n(x)$ [3], as well as Nielsen's generalized polylogarithms [4]

$$S_{n,p}(x) = \mathrm{Li}_{1,...,1,n+1}(\underbrace{1,...,1}_{p-1},x), \quad (15)$$

the harmonic polylogarithms of Remiddi and Vermaseren [7]

$$H_{m_1,...,m_k}(x) = \mathrm{Li}_{m_k,...,m_1}(\underbrace{1,...,1}_{k-1},x) \quad (16)$$

and the two-dimensional harmonic polylogarithms introduced recently by Gehrmann and Remiddi [8]. The exact connection to the two-dimensional harmonic polylogarithms is shown in appendix B together with a brief review of the multiple polylogarithms of Goncharov. Euler-Zagier sums and harmonic sums occur in the expansion of Gamma functions: For positive integers n we have on the positive side

$$\Gamma(n+\varepsilon) = \Gamma(1+\varepsilon)\Gamma(n) \times \left(1+\varepsilon Z_1(n-1)+\varepsilon^2 Z_{11}(n-1)+\varepsilon^3 Z_{111}(n-1)+...+\varepsilon^{n-1} Z_{11...1}(n-1)\right). \quad (17)$$

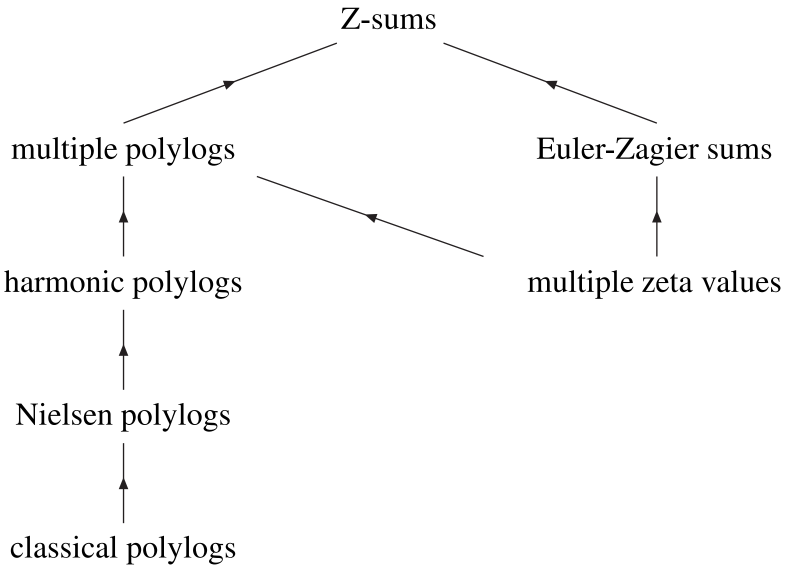


Figure 2: The inheritance diagram for Z-sums shows the relations between the various special cases.

On the negative side (again $n > 0$) we have

$$\begin{aligned} & \Gamma(-n+1+\varepsilon) \\ = & \frac{\Gamma(1+\varepsilon)}{\varepsilon} \frac{(-1)^{n-1}}{\Gamma(n)} \left(1+\varepsilon S_1(n-1)+\varepsilon^2 S_{11}(n-1)+\varepsilon^3 S_{111}(n-1)+...\right). \end{aligned} \tag{18}$$

The usefulness of the Z-sums lies in the fact, that they interpolate between Goncharov's multiple polylogarithms and Euler-Zagier sums. In addition, the interpolation is compatible with the algebra structure. Fig. 2 summarizes the relations between the various special cases.

3 Algorithms

In this section we give the detailed algorithms which allow to solve the ε-expansion of nested transcendental sums in terms of Z-sums or S-sums defined in eq.(1) and eq.(3), respectively. By a transcendental sum we mean a sum over i of finite or infinite summation range involving the following objects:

1. Fractions of the form
$$\frac{x^i}{(i+c)^m}, \tag{19}$$
where m is an integer, c a non-negative integer and x a real number.

2. Ratios of two Gamma functions
$$\frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+a_2+b_2\varepsilon)}, \tag{20}$$

where a_1 and a_2 are integers.

3. Z- and S-sums are also allowed to appear as subsums:

$$Z(i+c-1;m_1,...;x_1,...) \quad \text{or} \quad S(i+c';m_1,...;x_1,...). \tag{21}$$

The offsets c and c' are integers.

4. We further allow these building blocks to occur also with index $(n-i)$, for example as in

$$S(n-i;m_1',...;x_1',...). \tag{22}$$

Here n denotes the upper summation limit.

5. In addition binomials

$$\left(\begin{array}{c} n \\ i \end{array} \right) = \frac{n!}{i!(n-i)!} \tag{23}$$

may occur.

Some examples of sums which can be constructed from these building blocks are

$$\sum_{i=1}^{n} \frac{x^i}{(i+4)^3} \frac{y^i}{(i+2)^8} \frac{\Gamma(i+1+\varepsilon)}{\Gamma(i+2+3\varepsilon)} \quad \text{and} \quad \sum_{i=1}^{\infty} x^i \frac{\Gamma(i+a\varepsilon)}{\Gamma(i+1-c\varepsilon)} \frac{\Gamma(i+b\varepsilon)}{\Gamma(i+1)}. \tag{24}$$

There are some simplifications, which can be done immediately: Partial fractioning is used to reduce a product for $c_1 \neq c_2$

$$\frac{x_1^i}{(i+c_1)^{m_1}} \frac{x_2^i}{(i+c_2)^{m_2}} = \frac{1}{c_2-c_1} \left[\frac{x_1^i}{(i+c_1)^{m_1}} \frac{x_2^i}{(i+c_2)^{m_2-1}} - \frac{x_1^i}{(i+c_1)^{m_1-1}} \frac{x_2^i}{(i+c_2)^{m_2}} \right], \tag{25}$$

to terms which involve only the first factor or only the second one, but not both.

Ratios of two Gamma functions as in eq. (20) are first reduced to the form $\Gamma(i+b_1\varepsilon)/\Gamma(i+b_2\varepsilon)$ with the help of the identity $\Gamma(x+1) = x\,\Gamma(x)$. They are then expanded in ε using eq. (17). To invert the power series which is obtained in the denominator the formula

$$\begin{aligned} & \left(1+\varepsilon Z_1(n-1)+\varepsilon^2 Z_{11}(n-1)+\varepsilon^3 Z_{111}(n-1)+...+\varepsilon^{n-1} Z_{11...1}(n-1)\right)^{-1} \\ & = 1-\varepsilon S_1(n-1)+\varepsilon^2 S_{11}(n-1)-\varepsilon^3 S_{111}(n-1)+... \end{aligned} \tag{26}$$

is useful to speed up the computation on a computer.

There are also some basic operations involving Z- or S-sums. First of all we can easily convert between the two notations, using eq. (5). Furthermore we would like to be able to relate the Z-sum $Z(n+c-1,...)$ to $Z(n-1,...)$ or the S-sum $S(n+c,...)$ to $S(n,...)$, where $c>0$ is a fixed number. This can easily be done with the help of the following formulae:

$$\begin{aligned} & Z(n+c-1;m_1,...;x_1,...) \\ & = Z(n-1;m_1,...;x_1,...) + \sum_{j=0}^{c-1} x_1^j \frac{x_1^n}{(n+j)^{m_1}} Z(n-1+j;m_2,...;x_2,...), \\ & S(n+c;m_1,...;x_1,...) \\ & = S(n;m_1,...;x_1,...) + \sum_{j=1}^{c} x_1^j \frac{x_1^n}{(n+j)^{m_1}} S(n+j;m_2,...;x_2,...). \end{aligned} \tag{27}$$

The Z- or S-sums appearing in the last term have a reduced depth and the problem can be solved recursively.
Another situation which appears quite often is the product of two sums. If the upper summation limits of the two sums differ by some integer c we first synchronize them with the help of eq. (27). For sums with equal upper summation limit one may use the algebra eq. (7) or eq. (10) to convert the product into single sums of higher weight.
Furthermore we can bring Z-sums and S-sums to a standard form by eliminating letters with negative degrees, that is positive powers of i. In general, these cases are easy to handle. We illustrate this for S-sums. We consider $S(n;-m_1,m_2,...;x_1,x_2,...)$, write out the outermost sum of the S-function and then interchange the order of summation:

$$S(n;-m_1,m_2,...;x_1,x_2,...) = \sum_{i_2=1}^{n} \frac{x_2^{i_2}}{i_2^{m_2}} S(i_2;m_3,...) \sum_{i_1=i_2}^{n} i_1^{m_1} x_1^{i_1}. \tag{28}$$

The inner sum can be evaluated for any given weight analytically. Subsequently the outer sum can be done with eq. (3). If a negative weight occurs inside a sum, eq. (28) is applied to the subsum starting from the negative weight.

If a binomial appears in the sum, this sum may be written as a conjugation. To any function $f(n)$ of an integer variable n one defines the conjugated function $C \circ f(n)$ as the following sum [12]

$$C \circ f(n) = -\sum_{i=1}^{n} \left(\begin{array}{c} n \\ i \end{array} \right) (-1)^i f(i). \tag{29}$$

Conjugation satisfies the following two properties

$$C \circ 1 = 1, \tag{30}$$
$$C \circ C \circ f(n) = f(n), \tag{31}$$

which can be easily verified.

We classify four types of transcendental sums, which are dealt with in the algorithms A to D.

1. Sum over i involving only $Z(i-1;...)$ (type A).
2. Sum over i involving both $Z(i-1;...)$ and $Z(n-i-1;...)$ (type B).
3. Sum over i involving $S(i;...)$ and a binomial (type C).
4. Sum over i involving both $S(i;...)$, $S(n-i;...)$ and a binomial (type D).

Many of the algorithms use a recursion. They relate a given problem to a simpler one, either with a reduced depth or weight of the Z-sums or S-sums involved. In these cases we only give one step in the recursion.
The algorithms presented in this paper are all suited for programming in a computer algebra system like GiNaC [38], FORM [39] or the commercial ones like Mathematica or Maple. Implementations within the GiNaC framework [40] and in FORM along the lines of ref. [12] are in preparation and will be published elsewhere.

3.1 Algorithm A

Here we consider sums of the form

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} \frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+c_1+d_1\varepsilon)} ... \frac{\Gamma(i+a_k+b_k\varepsilon)}{\Gamma(i+c_k+d_k\varepsilon)} Z(i+o-1, m_1, ..., m_l, x_1, ..., x_l) \quad (32)$$

and show how to reduce them to Z-sums. We assume that all a_j and c_j are integers, c is assumed to be a nonnegative integer and o should be an integer. The upper summation limit is allowed to be infinity.

After expanding the Gamma functions and synchronizing the subsum $Z(i+o-1, m_1, ...)$ the problem is reduced to sums of the form

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} Z(i-1, ...) \quad (33)$$

with $c \geq 0$. It remains to reduce the offset c to zero. If the depth of the subsum is zero, we have

$$\sum_{i=1}^{n} \frac{x^i}{(i+c)^m} = \frac{1}{x} \sum_{i=1}^{n} \frac{x^i}{(i+c-1)^m} - \frac{1}{c^m} + \frac{x^n}{(n+c)^m}. \quad (34)$$

The last term contributes only if n is not equal to infinity. If the depth of the subsum is not equal to zero, we have

$$\begin{aligned} \sum_{i=1}^{n} \frac{x^i}{(i+c)^m} Z(i-1, ...) &= \frac{1}{x} \sum_{i=1}^{n} \frac{x^i}{(i+c-1)^m} Z(i-1, ...) \\ &- \sum_{i=1}^{n} \frac{x^i}{(i+c)^m} \frac{x_1^i}{i^{m_1}} Z(i-1, m_2, ...) + \frac{x^n}{(n+c)^m} Z(n-1, ...). \end{aligned} \quad (35)$$

Note that the third term only contributes if n is not equal to infinity. Finally we arrive at

$$\sum_{i=1}^{n} \frac{x^i}{i^m} Z(i-1, ...), \quad (36)$$

which is again a Z-sum. If the upper summation limit n equals infinity this sum yields immediately a multiple polylogarithm according to eq. (11). In the special case where n equals infinity and the subsum is an Euler-Zagier sum we obtain a harmonic polylogarithm according to eq. (16).

3.2 Algorithm B

Here we consider sums of the form

$$\begin{aligned} &\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} \frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+c_1+d_1\varepsilon)} ... \frac{\Gamma(i+a_k+b_k\varepsilon)}{\Gamma(i+c_k+d_k\varepsilon)} Z(i+o-1, m_1, ..., m_l, x_1, ..., x_l) \\ &\quad \times \frac{y^{n-i}}{(n-i+c')^{m'}} \frac{\Gamma(n-i+a_1'+b_1'\varepsilon)}{\Gamma(n-i+c_1'+d_1'\varepsilon)} ... \frac{\Gamma(n-i+a_{k'}'+b_{k'}'\varepsilon)}{\Gamma(n-i+c_{k'}'+d_{k'}'\varepsilon)} \\ &\qquad \times Z(n-i+o'-1, m_1', ..., m_{l'}', x_1', ..., x_{l'}') \end{aligned} \quad (37)$$

and show how to reduce them to Z-sums. Here, all a_j, a'_j, c_j and c'_j should be integers, c, c' should be nonnegative integers and o, o' should be integers. Note that the upper summation limit is $(n-1)$. The upper summation limit should not be infinity.

Using the expansion of the Gamma functions and the synchronization of the subsums, we immediately obtain sums of the form

$$\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,...) \frac{y^{n-i}}{(n-i+c')^{m'}} Z(n-i-1,m'_1,....). \tag{38}$$

Partial fractioning (and a change of the summation index $i \to n-i$ in sums involving the fraction with $(n-i+c')$) reduces these sums further to sums of the type

$$\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,...) Z(n-i-1,m'_1,....). \tag{39}$$

If the depth of $Z(n-i-1,m'_1,....)$ is zero, we have a sum of type A with upper summation index $(n-1)$:

$$\sum_{i=1}^{n-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,...). \tag{40}$$

Otherwise we can rewrite eq. (39) as

$$\sum_{j=1}^{n-1} \left[\sum_{i=1}^{j-1} \frac{x^i}{(i+c)^m} Z(i-1,m_1,...) \frac{x_1'^{\,j-i}}{(j-i)^{m'_1}} Z(j-i-1,m'_2,....) \right] \tag{41}$$

and use recursion. The inner sum is again of type B, but with a reduced depth, such that the recursion will finally terminate.

3.3 Algorithm C

Here we consider sums of the form

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} \frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+c_1+d_1\varepsilon)} \cdots \frac{\Gamma(i+a_k+b_k\varepsilon)}{\Gamma(i+c_k+d_k\varepsilon)}$$
$$\times S(i+o,m_1,...,m_l,x_1,...,x_l), \tag{42}$$

where a_j and c_j are integers, c is a nonnegative integer and o is an integer. The upper summation limit should not be infinity. These sums cannot be reduced to Z-sums with upper summation limit n alone. However, they can be reduced to Z-sums with upper summation limit n and multiple polylogarithms (which are Z-sums to infinity).

Again, we expand the Gamma functions and synchronize the subsum. It is therefore sufficient to consider sums of the form

$$-\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} S(i,...) \tag{43}$$

with $c \geq 0$. To reduce the offset c to zero we rewrite the sum as

$$\left(-\frac{1}{x}\right)\frac{1}{n+1}(-1)\sum_{i=1}^{n+1}\left(\begin{array}{c} n+1 \\ i \end{array}\right)(-1)^i \frac{x^i}{(i+c-1)^m} i S(i-1,...). \tag{44}$$

Repeated application of the above relation yields sums of the form

$$-\sum_{i=1}^{n}\left(\begin{array}{c} n \\ i \end{array}\right)(-1)^i \frac{x^i}{i^m} S(i,...). \tag{45}$$

If m is negative we rewrite eq. (45) as

$$-nx(-1)\sum_{i=1}^{n-1}\left(\begin{array}{c} n-1 \\ i \end{array}\right)(-1)^i \frac{x^i}{(i+1)^{m+1}} S(i+1,...)+nxS(1,...). \tag{46}$$

We can therefore assume that m is a non-negative number. Furthermore, due to eq. (28) we may assume that in the S-sum $S(i;m_1,...;x_1,...)$ no m_j is negative and that if some m_j is zero, then the corresponding x_j is not equal to 1. The sum $S(i,...)$ is then rewritten as

$$\begin{aligned}
S(i;m_1,...,m_k;x_1,...,x_k) &= S(N;m_1,...,m_k;x_1,...,x_k) \\
& - S(N;m_2,...,m_k;x_2,...,x_k) \times \left(\sum_{i_1=i+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}}\right) \\
& + S(N;m_3,...,m_k;x_3,...,x_k) \times \left(\sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}\right) \\
& - ... + (-1)^k \left(\sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N} ... \sum_{i_k=i_{k-1}+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}...\frac{x_k^{i_k}}{i_k^{m_k}}\right).
\end{aligned} \tag{47}$$

The proof of eq. (47) is not too complicated and consists in repeated application of the identity

$$\sum_{i=1}^{n}\sum_{j=1}^{i} a_{ij} = \sum_{i=1}^{N}\sum_{j=1}^{i} a_{ij} - \sum_{i=n+1}^{N}\sum_{j=1}^{N} a_{ij} + \sum_{i=n+1}^{N}\sum_{j=i+1}^{N} a_{ij}. \tag{48}$$

Eq. (47) holds for any N and in particular we may take $N=\infty$ in the end. Each term is then a product of a S-sum at infinity and a sum of a new type. The S-sum at infinity is converted to a Z-sum at infinity and expressed in terms of multiple polylogarithms. We now deal with sums of the form

$$-\sum_{i=1}^{n}\left(\begin{array}{c} n \\ i \end{array}\right)(-1)^i \frac{x_0^i}{i^{m_0}} \sum_{i_1=i+1}^{N}\sum_{i_2=i_1+1}^{N} ... \sum_{i_k=i_{k-1}+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}...\frac{x_k^{i_k}}{i_k^{m_k}}. \tag{49}$$

We introduce raising and lowering operators as follows:

$$\begin{aligned}
\left(\mathbf{x}^+\right)^m \cdot 1 &= \frac{1}{m!}\ln^m(x), \\
\mathbf{x}^+ \cdot f(x) &= \int\limits_0^x \frac{dx'}{x'} f(x'), \\
\mathbf{x}^- \cdot f(x) &= x\frac{d}{dx} f(x).
\end{aligned} \tag{50}$$

It is understood that in the second line only functions which are integrable at $x=0$ are considered. We see that $\mathbf{x}^-$ is the inverse to $\mathbf{x}^+$, e.g. $\mathbf{x}^-\mathbf{x}^+ = \mathrm{id}$. However $\mathbf{x}^+\mathbf{x}^- = \mathrm{id}$ holds only if applied to non-trivial sums. For the trivial sum we have $\mathbf{x}^+\mathbf{x}^- Z(n) = 0$.
With the help of the raising operators eq. (49) may be rewritten as

$$\left(\mathbf{x_k}^+\right)^{m_k} \left(\mathbf{x_{k-1}}^+\right)^{m_{k-1}} \ldots \left(\mathbf{x_1}^+\right)^{m_1} \left(\mathbf{x_0}^+\right)^{m_0} (-1) \sum\limits_{i=1}^{n} \left(\begin{array}{c} n \\ i \end{array} \right) (-x_0)^i$$
$$\times \sum\limits_{i_1=i+1}^{N} \sum\limits_{i_2=i_1+1}^{N} \ldots \sum\limits_{i_k=i_{k-1}+1}^{N} x_1^{i_1} x_2^{i_2} \ldots x_k^{i_k}. \quad (51)$$

It may happen that some x_i's are equal to one. In this case we first calculate the sum for arbitrary x_i's and take then the limit $x_i \to 1$. Some care has to be taken for the double limit $x \to 1$ and $N \to \infty$. The order is as follows: First all limits $x \to 1$ are taken, then the limit $N \to \infty$ in eq. (47) is performed.

The sums in eq. (51) can be performed with the help of the geometric series

$$\sum\limits_{i=n+1}^{N} x^i = \frac{x}{1-x} x^n - \frac{x}{1-x} x^N. \quad (52)$$

It is evident that if we don't have to take the limit $x \to 1$ we can immediately neglect the second term. Also in the case $x = 1$ the second term can be neglected. It gives rise to terms of the form

$$\left(\mathbf{x}^+\right)^m \frac{x}{1-x} x^N = \sum\limits_{i=N+1}^{\infty} \frac{x^i}{i^m}. \quad (53)$$

On the r.h.s the limit $x \to 1$ may safely be performed and the resulting sum gives a vanishing contribution in the limit $N \to \infty$.

Performing the sums in eq. (51) we therefore only have to consider expressions of the form

$$\left(\mathbf{x_k}^+\right)^{m_k} \left(\mathbf{x_{k-1}}^+\right)^{m_{k-1}} \ldots \left(\mathbf{x_1}^+\right)^{m_1} \left(\mathbf{x_0}^+\right)^{m_0} \frac{x_k}{1-x_k} \frac{x_{k-1}x_k}{1-x_{k-1}x_k} \ldots \frac{x_1 \ldots x_k}{1-x_1 \ldots x_k}$$
$$\times \left[1 - (1 - x_0 x_1 \ldots x_k)^n\right]. \quad (54)$$

We then perform succesivly the integrations corresponding to the raising operators. The basic formulae are:

$$\begin{aligned}
\mathbf{x_1^+} \left[1-(1-x_1x_2)^n\right] &= \sum\limits_{i=1}^{n} \frac{1}{i} \left[1-(1-x_1x_2)^i\right], \\
\mathbf{x_1^+} \frac{x_1x_2}{1-x_1x_2} \left[1-(1-x_0x_1x_2)^n\right] &= -\left[1-(1-x_0)^n\right] \sum\limits_{i=1}^{\infty} \frac{1}{i} \left(\frac{1}{1-x_0}\right)^i \left[1-(1-x_0x_1x_2)^i\right] \\
&\quad - (1-x_0)^n \sum\limits_{i=1}^{n} \frac{1}{i} \left(\frac{1}{1-x_0}\right)^i \left[1-(1-x_0x_1x_2)^i\right], \\
\mathbf{x_1^+} \frac{x_1x_2}{1-x_1x_2} \left[1-(1-x_1x_2)^n\right] &= -\frac{1}{n} \left[1-(1-x_1x_2)^n\right] + \sum\limits_{i=1}^{N} \frac{(x_1x_2)^i}{i} \\
&\quad + \left(\mathbf{x_1^+}\right) \frac{x_1x_2}{1-x_1x_2} (x_1x_2)^N. \quad (55)
\end{aligned}$$

We use the first formula to reduce m_0 in eq. (54) to zero:

$$\sum_{i=1}^{n} \frac{1}{i} \left(x_k^+\right)^{m_k} ... \left(x_1^+\right)^{m_1} \left(x_0^+\right)^{m_0-1} \frac{x_k}{1-x_k} \frac{x_{k-1}x_k}{1-x_{k-1}x_k} ... \frac{x_1...x_k}{1-x_1...x_k} \left[1-(1-x_0x_1...x_k)^i\right]. \tag{56}$$

In the following we may therefore assume $m_0 = 0$ in eq. (54). If $m_0 = 0$, $m_1 > 0$ and $x_0 \neq 1$ we obtain for eq. (54)

$$\begin{aligned}
&-\sum_{i=1}^{\infty} \frac{1}{i} \left(\frac{1}{1-x_0}\right)^i \left(x_k^+\right)^{m_k} ... \left((x_0x_1)^+\right)^{m_1-1} \frac{x_k}{1-x_k} \frac{x_{k-1}x_k}{1-x_{k-1}x_k} ... \frac{x_2...x_k}{1-x_2...x_k} \\
&\quad \times \left[1-(1-(x_0x_1)...x_k)^i\right] \\
&\quad +(1-x_0)^n \sum_{i=1}^{\infty} \frac{1}{i} \left(\frac{1}{1-x_0}\right)^i \left(x_k^+\right)^{m_k} ... \left((x_0x_1)^+\right)^{m_1-1} \frac{x_k}{1-x_k} \frac{x_{k-1}x_k}{1-x_{k-1}x_k} ... \frac{x_2...x_k}{1-x_2...x_k} \\
&\quad \times \left[1-(1-(x_0x_1)...x_k)^i\right] \\
&\quad -(1-x_0)^n \sum_{i=1}^{n} \frac{1}{i} \left(\frac{1}{1-x_0}\right)^i \left(x_k^+\right)^{m_k} ... \left((x_0x_1)^+\right)^{m_1-1} \frac{x_k}{1-x_k} \frac{x_{k-1}x_k}{1-x_{k-1}x_k} ... \frac{x_2...x_k}{1-x_2...x_k} \\
&\quad \times \left[1-(1-(x_0x_1)...x_k)^i\right].
\end{aligned} \tag{57}$$

In the case $m_0 = 0$, $m_1 > 0$ and $x_0 = 1$ we use the third formula of eq. (55). Again we may neglect contributions of the form eq. (53). Doing so we obtain

$$\begin{aligned}
&-\frac{1}{n} \left(x_k^+\right)^{m_k} ... \left(x_1^+\right)^{m_1-1} \frac{x_k}{1-x_k} \frac{x_{k-1}x_k}{1-x_{k-1}x_k} ... \frac{x_2...x_k}{1-x_2...x_k} \left[1-(1-x_1...x_k)^n\right] \\
&+\sum_{i=1}^{N} \frac{x_1^i}{i^{m_1}} \sum_{i_2=i+1}^{N} ... \sum_{i_k=i_{k-1}+1}^{N} \frac{x_2^{i_2}}{i_2^{m_2}} ... \frac{x_k^{i_k}}{i_k^{m_k}}.
\end{aligned} \tag{58}$$

It remains to treat the last term to complete the recursion. The last term introduces a sum of the type

$$\sum_{i_1=n+1}^{N} ... \sum_{i_k=i_{k-1}+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}} ... \frac{x_k^{i_k}}{i_k^{m_k}}. \tag{59}$$

Using the inverse formula to eq. (47)

$$\begin{aligned}
&\sum_{i_1=n+1}^{N} ... \sum_{i_k=i_{k-1}+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}} ... \frac{x_k^{i_k}}{i_k^{m_k}} \\
&= (-1)^k S(n;m_1,...m_k;x_1,...,x_k) - (-1)^k S(N;m_1,...m_k;x_1,...,x_k) \\
&\quad +(-1)^k S(N;m_2,...m_k;x_2,...,x_k) \sum_{i_1=n+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}} - ... \\
&\quad +(-1)^k S(N;m_k;x_k) \sum_{i_1=n+1}^{N} ... \sum_{i_{k-1}=i_{k-2}+1}^{N} \frac{x_1^{i_1}}{i_1^{m_1}} ... \frac{x_{k-1}^{i_{k-1}}}{i_{k-1}^{m_{k-1}}}
\end{aligned} \tag{60}$$

this sum is easily related to S-sums with upper summation limit n and (after taking the limit $N \to \infty$) to multiple polylogarithms.

If $m_0 = 0$, $m_1 = 0$ and $x_1 \neq 1$ we rewrite eq. (54) as

$$
\begin{aligned}
& -\frac{1}{1-x_1}\left(x_k^+\right)^{m_k} ... \left(x_3^+\right)^{m_3}\left(\left(x_2 x_1\right)^+\right)^{m_2} \frac{x_k}{1-x_k} ... \frac{x_3 ... x_k}{1-x_3 ... x_k} \frac{(x_1 x_2) x_3 ... x_k}{1-(x_1 x_2) x_3 ... x_k} \\
& \quad \times \left[1-\left(1-x_0 (x_1 x_2) x_3 ... x_k\right)^i\right] \\
& \quad + \frac{x_1}{1-x_1}\left(x_k^+\right)^{m_k} ... \left(x_2^+\right)^{m_2} \frac{x_k}{1-x_k} ... \frac{x_2 x_3 ... x_k}{1-x_2 x_3 ... x_k}\left[1-\left(1-(x_0 x_1) x_2 x_3 ... x_k\right)^i\right].
\end{aligned}
\tag{61}
$$

The case $m_0 = 0$, $m_1 = 0$ and $x_1 = 1$ has to be excluded. However, with an appropriate choice of the standard form for S-sums (c.f. eq. 28) this case never occurs.

3.4 Algorithm D

Here we consider sums of the form

$$
\begin{aligned}
& -\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} \frac{\Gamma(i+a_1+b_1\varepsilon)}{\Gamma(i+c_1+d_1\varepsilon)} ... \frac{\Gamma(i+a_k+b_k\varepsilon)}{\Gamma(i+c_k+d_k\varepsilon)} \\
& \quad \times S(i+o, m_1, ..., m_l, x_1, ..., x_l) \\
& \quad \times \frac{y^{n-i}}{(n-i+c')^{m'}} \frac{\Gamma(n-i+a_1'+b_1'\varepsilon)}{\Gamma(n-i+c_1'+d_1'\varepsilon)} ... \frac{\Gamma(n-i+a_{k'}'+b_{k'}'\varepsilon)}{\Gamma(n-i+c_{k'}'+d_{k'}'\varepsilon)} \\
& \quad \times S(n-i+o', m_1', ..., m_{l'}', x_1', ..., x_{l'}').
\end{aligned}
\tag{62}
$$

Here, all a_j, a_j', c_j and c_j' are integers, c, c', are nonnegative integers and o, o' are integers. Note that the upper summation limit is $(n-1)$. The upper summation limit should not be infinity. As in the case of sums of type C, we cannot relate these sums to Z-sums with upper summation limit $(n-1)$ alone, but we can reduce them to Z-sums with upper summation limit $(n-1)$ and multiple polylogarithms (which are Z-sums to infinity).

After the expansion of the Gamma functions and the synchronization of the subsums we have sums of the form

$$
-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} S(i, m_1, ...) \frac{y^{n-i}}{(n-i+c')^{m'}} S(n-i, m_1', ...). \tag{63}
$$

Partial fractioning leads to

$$
-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x^i}{(i+c)^m} S(i, m_1, ...) S(n-i, m_1', ...) \tag{64}
$$

with $c \geq 0$. In order to reduce the offset c to zero one rewrites eq. (64) as

$$
\left(-\frac{1}{x}\right) \frac{1}{n+1} (-1) \sum_{i=1}^{n+1-1} \binom{n+1}{i} (-1)^i \frac{x^i}{(i+c-1)^m} i S(i-1, ...) S(n+1-i, m_1', ...). \tag{65}
$$

We arrive at sums of the form

$$-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x^i}{i^m} S(i,m_1,...) S(n-i,m_1',....). \tag{66}$$

If the depth of $S(n-i,m_1',....)$ is zero, we have a sum of type C:

$$\begin{aligned} & -\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x^i}{i^m} S(i,m_1,...) \\ = & \ -\sum_{i=1}^{n} \binom{n}{i} (-1)^i \frac{x^i}{i^m} S(i,m_1,...) + \frac{(-x)^n}{n^m} S(n,m_1,...). \end{aligned} \tag{67}$$

Otherwise, we first reduce m to zero. For $m>0$ we rewrite eq. (66) as

$$\begin{aligned} & \sum_{j=1}^{n} \frac{1}{j} \left[(-1) \sum_{i=1}^{j-1} \binom{j}{i} (-1)^i \frac{x^i}{i^{m-1}} S(i,m_1,...) S(j-i,m_1',....) \right] \\ & + \sum_{j=1}^{n} \frac{1}{j} \left[(-1) \sum_{i=1}^{j-1} \binom{j}{i} (-1)^i \frac{x^i}{i^m} S(i,m_1,...) \frac{{x'_1}^{j-i}}{(j-i)^{m_1'-1}} S(j-i,m_2',....) \right]. \end{aligned} \tag{68}$$

For $m<0$ we rewrite eq. (66) as

$$\begin{aligned} & -nx(-1) \sum_{i=1}^{n-2} \binom{n-1}{i} (-1)^i \frac{x^i}{(i+1)^{m+1}} S(i+1,m_1,...) S(n-1-i,m_1',....) \\ & + nx S(1,m_1,...) S(n-1,m_1',...). \end{aligned} \tag{69}$$

Having reduced m to zero we arrive at sums of the form

$$-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i x^i S(i,m_1,...) S(n-i,m_1',....). \tag{70}$$

We can eliminate x^i by rewriting it as

$$x^i = 1 - \frac{1-x}{x} \sum_{j=1}^{i} x^j = 1 - \frac{1-x}{x} S(i;0;x). \tag{71}$$

The sum $S(i;0;x)$ can be multiplied with the other sum $S(i,m_1,...)$ to yield single sums and we therefore arrive at sums of the form

$$-\sum_{i=1}^{n-1} \binom{n}{i} (-1)^i S(i,m_1,...) S(n-i,m_1',....). \tag{72}$$

After some algebra we obtain for eq. (72)

$$\begin{aligned} & \frac{1}{n}(-1) \sum_{i=1}^{n-1} \binom{n}{i} (-1)^i \frac{x_1^i}{i^{m_1-1}} S(i,m_2,...) S(n-i,m_1',....) \\ & + \frac{1}{n}(-1) \sum_{i=1}^{n-1} \binom{n}{i} (-1)^i S(i,m_1,...) \frac{{x'_1}^{n-i}}{(n-i)^{m_1'-1}} S(n-i,m_2',....) \end{aligned} \tag{73}$$

where the original problem is reduced to one of the same type but with lower weight. The above algorithm yields thus a recursion to treat sums of type D.

4 Applications

The algorithms given in this paper can be used for the expansion of higher transcendental functions around integer values of their indices, where the expansion parameter occurs in the Pochhammer symbols. In this section we give a few examples. Additionally, we illustrate the applicability of the algorithms for nested sums to the calculation of loop integrals, in particular to integrals with several scales. As an example, we discuss the C-topology and show that the integral can be written as a nested sum of the type previously discussed.

4.1 Generalized hypergeometric functions

The generalized hypergeometric functions are defined by [1, 2]

$$ {}_{J+1}F_J(a_1,...,a_{J+1};b_1,...,b_J;x) = \sum_{n=0}^{\infty} \frac{(a_1)_n...(a_{J+1})_n}{(b_1)_n...(b_J)_n} \frac{x^n}{n!}, \tag{74} $$

where $(a)_n = \Gamma(n+a)/\Gamma(a)$ denotes a Pochhammer symbol. These functions can be rewritten as

$$ \begin{aligned} & {}_{J+1}F_J(a_1,...,a_{J+1};b_1,...,b_J;x) \\ = \; & 1 + \frac{\Gamma(b_1)...\Gamma(b_J)}{\Gamma(a_1)...\Gamma(a_{J+1})} \sum_{i=1}^{\infty} x^i \frac{\Gamma(i+a_1)}{\Gamma(i+b_1)} ... \frac{\Gamma(i+a_J)}{\Gamma(i+b_J)} \frac{\Gamma(i+a_{J+1})}{\Gamma(i+1)} \end{aligned} \tag{75} $$

and fall therefore into the category of transcendental sums of type A. We give a few examples obtained using the algorithms given in sec. 3.1:

$$ \begin{aligned} {}_2F_1(a\varepsilon, b\varepsilon; 1-c\varepsilon; x) &= 1 + ab\,\mathrm{Li}_2(x)\varepsilon^2 + ab\,(c\,\mathrm{Li}_3(x) + (a+b+c)\,\mathrm{S}_{1,2}(x))\,\varepsilon^3 + O(\varepsilon^4), \\ {}_2F_1(1, -\varepsilon; 1-\varepsilon; x) &= 1 + \ln(1-x)\varepsilon - \mathrm{Li}_2(x)\varepsilon^2 - \mathrm{Li}_3(x)\varepsilon^3 - \mathrm{Li}_4(x)\varepsilon^4 - \mathrm{Li}_5(x)\varepsilon^5 \\ & \quad - \mathrm{Li}_6(x)\varepsilon^6 - \mathrm{Li}_7(x)\varepsilon^7 + O(\varepsilon^8), \end{aligned} \tag{76} $$

$$ {}_3F_2(-2\varepsilon, -2\varepsilon, 1-\varepsilon; 1-2\varepsilon, 1-2\varepsilon; x) = 1 + 4\,\mathrm{Li}_2(x)\varepsilon^2 + O(\varepsilon^3), \tag{77} $$

which all agree with known results in the literature [41, 42].

4.2 Appell functions

The first Appell function is defined by [43, 2]

$$ F_1(a, b_1, b_2; c; x_1, x_2) = \sum_{m_1=0}^{\infty} \sum_{m_2=0}^{\infty} \frac{(a)_{m_1+m_2} (b_1)_{m_1} (b_2)_{m_2}}{(c)_{m_1+m_2}} \frac{x_1^{m_1}}{m_1!} \frac{x_2^{m_2}}{m_2!}. \tag{78} $$

It can be rewritten as

$$ \begin{aligned} & F_1(a, b_1, b_2; c; x_1, x_2) \\ = \; & 1 + \frac{\Gamma(c)}{\Gamma(a)\Gamma(b_1)} \sum_{i=1}^{\infty} x_1^i \frac{\Gamma(i+a)\Gamma(i+b_1)}{\Gamma(i+c)\Gamma(i+1)} + \frac{\Gamma(c)}{\Gamma(a)\Gamma(b_2)} \sum_{i=1}^{\infty} x_2^i \frac{\Gamma(i+a)\Gamma(i+b_2)}{\Gamma(i+c)\Gamma(i+1)} \\ & + \frac{\Gamma(c)}{\Gamma(a)\Gamma(b_1)\Gamma(b_2)} \sum_{n=1}^{\infty} \frac{\Gamma(n+a)}{\Gamma(n+c)} \sum_{i=1}^{n-1} x_1^i \frac{\Gamma(i+b_1)}{\Gamma(i+1)} x_2^{n-i} \frac{\Gamma(n-i+b_2)}{\Gamma(n-i+1)}. \end{aligned} \tag{79} $$

The inner sum of the last term is of type B. The first Appell function can therefore be expanded with the help of the algorithms A and B.

The second Appell function is defined by [43, 2]

$$F_2(a,b_1,b_2;c_1,c_2;x_1,x_2) = \sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty} \frac{(a)_{m_1+m_2}(b_1)_{m_1}(b_2)_{m_2}}{(c_1)_{m_1}(c_2)_{m_2}} \frac{x_1^{m_1}}{m_1!}\frac{x_2^{m_2}}{m_2!}. \tag{80}$$

It can be rewritten as

$$\begin{aligned}
& F_2(a,b_1,b_2;c_1,c_2;x_1,x_2) \\
&= 1+\frac{\Gamma(c_1)}{\Gamma(a)\Gamma(b_1)}\sum_{i=1}^{\infty} x_1^i \frac{\Gamma(i+a)\Gamma(i+b_1)}{\Gamma(i+c_1)\Gamma(i+1)} + \frac{\Gamma(c_2)}{\Gamma(a)\Gamma(b_2)}\sum_{i=1}^{\infty} x_2^i \frac{\Gamma(i+a)\Gamma(i+b_2)}{\Gamma(i+c_2)\Gamma(i+1)} \\
& \quad -\frac{\Gamma(c_1)\Gamma(c_2)}{\Gamma(a)\Gamma(b_1)\Gamma(b_2)}\sum_{n=1}^{\infty}\frac{\Gamma(n+a)}{\Gamma(n+1)} \\
& \quad \times(-1)\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i(-x_1)^i\frac{\Gamma(i+b_1)}{\Gamma(i+c_1)} x_2^{n-i}\frac{\Gamma(n-i+b_2)}{\Gamma(n-i+c_2)}.
\end{aligned} \tag{81}$$

The inner sum of the last term is of type D. The second Appell function can therefore be expanded with the help of the algorithms A to D. As an example we give

$$F_2(1,1,\varepsilon;1+\varepsilon,1-\varepsilon;x,y) = \frac{1}{1-x}+\frac{1}{1-x}\left(2\ln(1-x)-\ln(1-x-y)\right)\varepsilon+O(\varepsilon^2). \tag{82}$$

After taking into account a typo in eq. (A.47) of ref. [44] this result agrees with the one obtained along the lines of ref. [44].

4.3 Kampé de Fériet function

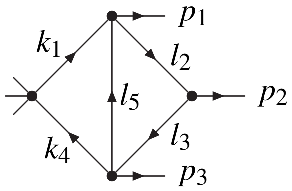
The Kampé de Fériet function is defined by [43]

$$S_1(a_1,a_2,b_1;c,c_1;x_1,x_2) = \sum_{m_1=0}^{\infty}\sum_{m_2=0}^{\infty} \frac{(a_1)_{m_1+m_2}(a_2)_{m_1+m_2}(b_1)_{m_1}}{(c)_{m_1+m_2}(c_1)_{m_1}} \frac{x_1^{m_1}}{m_1!}\frac{x_2^{m_2}}{m_2!}. \tag{83}$$

It can be rewritten as

$$\begin{aligned}
& S_1(a_1,a_2,b_1;c,c_1;x_1,x_2) \\
&= 1+\frac{\Gamma(c)\Gamma(c_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1)}\sum_{i=1}^{\infty} x_1^i \frac{\Gamma(i+a_1)\Gamma(i+a_2)\Gamma(i+b_1)}{\Gamma(i+c)\Gamma(i+c_1)\Gamma(i+1)} \\
& \quad +\frac{\Gamma(c)}{\Gamma(a_1)\Gamma(a_2)}\sum_{i=1}^{\infty} x_2^i \frac{\Gamma(i+a_1)\Gamma(i+a_2)}{\Gamma(i+c)\Gamma(i+1)} \\
& \quad -\frac{\Gamma(c)\Gamma(c_1)}{\Gamma(a_1)\Gamma(a_2)\Gamma(b_1)}\sum_{n=1}^{\infty} x_2^n \frac{\Gamma(n+a_1)\Gamma(n+a_2)}{\Gamma(n+c)\Gamma(n+1)} \\
& \quad \times(-1)\sum_{i=1}^{n-1}\binom{n}{i}(-1)^i\left(-\frac{x_1}{x_2}\right)^i\frac{\Gamma(i+b_1)}{\Gamma(i+c_1)}.
\end{aligned} \tag{84}$$

The inner sum of the last term is of type C. The Kampé de Fériet function can therefore be expanded with the help of the algorithms A and C.



$$= c \int_0^1 da\, a^{\nu_2-1} \bar{a}^{\nu_3-1}$$

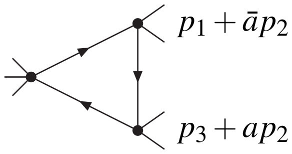


Figure 3: The C-topology reduces to a triangle with three external masses and an additional integration over the Feynman parameter a.

4.4 The C-topology

Here we study the C-topology with one massive external leg and arbitrary powers of the propagators and arbitray dimensions, which can be solved using the algorithms given in this paper. The importance of this result lies in the fact that one avoids having to solve a system of equations obtained from partial integration or Lorentz invariance. Solving such a system becomes quite difficult if one external leg is massive. The result obtained here is thus a useful ingredient for the calculation of the two-loop amplitudes with one massive external leg, such as $e^+e^- \to 3$ jets.
The second C-topology, where the massive leg is attached to the other corner, as well as all simpler topologies, can be obtained along the same lines. The two-loop C-topology with one massive external leg is defined by

$$I = \int \frac{d^D k_1}{i\pi^{D/2}} \int \frac{d^D l_5}{i\pi^{D/2}} \frac{1}{\left(-k_1^2\right)^{\nu_1}} \frac{1}{\left(-l_2^2\right)^{\nu_2}} \frac{1}{\left(-l_3^2\right)^{\nu_3}} \frac{1}{\left(-k_4^2\right)^{\nu_4}} \frac{1}{\left(-l_5^2\right)^{\nu_5}} \tag{85}$$

with

$$\begin{aligned} l_2 &= k_1 + l_5 - p_1, \\ l_3 &= l_2 - p_2, \\ k_4 &= k_1 - p_{123}. \end{aligned} \tag{86}$$

Fig. 3 shows the corresponding Feynman diagram. We first perform the l_5-integration. Combining with Feynman parameters first l_2^2 and l_3^2 and then the resulting propagator with l_5^2 we obtain:

$$\begin{aligned} I &= \frac{\Gamma(\nu_{235} - m + \varepsilon)}{\Gamma(\nu_2)\Gamma(\nu_3)\Gamma(\nu_5)} \frac{\Gamma(-\nu_{23} + m - \varepsilon)\Gamma(-\nu_5 + m - \varepsilon)}{\Gamma(-\nu_{235} + 2m - 2\varepsilon)} \int_0^1 da\, a^{\nu_2-1} \bar{a}^{\nu_3-1} \\ &\times \int \frac{d^D k_1}{i\pi^{D/2}} \frac{1}{\left(-k_1^2\right)^{\nu_1}} \frac{1}{\left(-(k_1 - p_1 - \bar{a} p_2)^2\right)^{\nu_{235}-m+\varepsilon}} \frac{1}{\left(-k_4^2\right)^{\nu_4}}. \end{aligned} \tag{87}$$

As a short hand notation we used $D = 2m - 2\varepsilon$, $\bar{a} = 1 - a$ and $\nu_{235} = \nu_2 + \nu_3 + \nu_5$. The second line is a one-loop triangle with three external masses. The solution for this one-loop integral with arbitrary powers of the propagators and arbitrary dimensions is known [45]. We use the solution given in [44] and perform the remaining integration. We obtain

$$I = \frac{\Gamma(2m - 2\varepsilon - \nu_{1235})\Gamma(1 + \nu_{1235} - 2m + 2\varepsilon)\Gamma(2m - 2\varepsilon - \nu_{2345})\Gamma(1 + \nu_{2345} - 2m + 2\varepsilon)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(\nu_3)\Gamma(\nu_4)\Gamma(\nu_5)\Gamma(3m - 3\varepsilon - \nu_{12345})}$$

$$
\begin{aligned}
&\times \frac{\Gamma(m-\varepsilon-\nu_5)\Gamma(m-\varepsilon-\nu_{23})}{\Gamma(2m-2\varepsilon-\nu_{235})} \left(-s_{123}\right)^{2m-2\varepsilon-\nu_{12345}} \sum\limits_{i_1=0}^{\infty} \sum\limits_{i_2=0}^{\infty} \frac{x_1^{i_1}}{i_1!} \frac{x_2^{i_2}}{i_2!} \\
&\times \left[\frac{\Gamma(i_1+\nu_3)\Gamma(i_2+\nu_2)\Gamma(i_1+i_2-2m+2\varepsilon+\nu_{12345})\Gamma(i_1+i_2-m+\varepsilon+\nu_{235})}{\Gamma(i_1+1-2m+2\varepsilon+\nu_{1235})\Gamma(i_2+1-2m+2\varepsilon+\nu_{2345})\Gamma(i_1+i_2+\nu_{23})} \right. \\
&-x_1^{2m-2\varepsilon-\nu_{1235}} \\
&\times \frac{\Gamma(i_1+2m-2\varepsilon-\nu_{125})\Gamma(i_2+\nu_2)\Gamma(i_1+i_2+\nu_4)\Gamma(i_1+i_2+m-\varepsilon-\nu_1)}{\Gamma(i_1+1+2m-2\varepsilon-\nu_{1235})\Gamma(i_2+1-2m+2\varepsilon+\nu_{2345})\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{15})} \\
&-x_2^{2m-2\varepsilon-\nu_{2345}} \\
&\times \frac{\Gamma(i_1+\nu_3)\Gamma(i_2+2m-2\varepsilon-\nu_{345})\Gamma(i_1+i_2+\nu_1)\Gamma(i_1+i_2+m-\varepsilon-\nu_4)}{\Gamma(i_1+1-2m+2\varepsilon+\nu_{1235})\Gamma(i_2+1+2m-2\varepsilon-\nu_{2345})\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{45})} \\
&+x_1^{2m-2\varepsilon-\nu_{1235}} x_2^{2m-2\varepsilon-\nu_{2345}} \frac{\Gamma(i_1+2m-2\varepsilon-\nu_{125})\Gamma(i_2+2m-2\varepsilon-\nu_{345})}{\Gamma(i_1+1+2m-2\varepsilon-\nu_{1235})\Gamma(i_2+1+2m-2\varepsilon-\nu_{2345})} \\
&\left. \times \frac{\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{235})\Gamma(i_1+i_2+3m-3\varepsilon-\nu_{12345})}{\Gamma(i_1+i_2+4m-4\varepsilon-\nu_{12345}-\nu_5)} \right], \qquad (88)
\end{aligned}
$$

where we set $x_1 = (-s_{12})/(-s_{123})$ and $x_2 = (-s_{23})/(-s_{123})$. Changing the summation indices as in the case of the second Appell function yields a sum of type D. For specific (integer) values of ν_i and m this expression can be expanded in ε with the algorithm given in sec. 3. This is a new and useful result. Up to now this integral has only been known for $m = 2$ and the sets $(1,1,1,1,1)$ and $(1,1,1,1,2)$ for $(\nu_1,\nu_2,\nu_3,\nu_4,\nu_5)$ [8]. It is easy to verify that for these specific two cases the terms proportional to ε^{-3} and ε^{-2} of eq. (88) agree with the result given in [8]. A complete comparison has to wait until the necessary computer programs are finished and will be reported elsewhere.

5 Conclusions

In this paper we studied some algebraic properties of nested sums. Based on these properties we developed a number of algorithms which can be used to expand a certain class of mathematical functions. All presented algorithms are suitable for the implementation on a computer. These algorithms allow the evaluation of integrals occuring in high-energy physics. As an application we have shown how the two-loop C-topology can be evaluated for arbitrary powers of the propagators and arbitrary dimensions. Furthermore we have shown that the nested sums satisfy a Hopf algebra and established the connection with the Hopf algebra of Kreimer.

Acknowledgements

We would like to thank Jos Vermaseren for useful discussions.

A The Hopf algebra of Z-sums

In this section we show that the Z-sums form a Hopf algebra [36, 37]. It is sufficient to demonstrate that the Z-sums form a quasi-shuffle algebra. A general theorem [46] guarantees then, that they also form a Hopf algebra. We also discuss the connection with the Hopf algebra of Kreimer [47].

Before we start, we have to introduce some notation. We call a pair $(m_j;x_j)$ a letter and the set of all letters the alphabet A. We further call m_j the degree of the letter (m_j,x_j). On the alphabet A we define a multiplication

$$\begin{aligned} \cdot \ : \ & A \times A \to A, \\ & (m_1,x_1)\cdot(m_2,x_2) = (m_1+m_2,x_1x_2), \end{aligned} \tag{89}$$

e.g. the x_j's are multiplied and the degrees are added. As a short-hand notation we will in the following denote a letter just by $X_j = (m_j;x_j)$. A word is an ordered sequence of letters, e.g.

$$W = X_1,X_2,...,X_k. \tag{90}$$

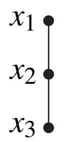
We denote the word of length zero by e. The sums defined in (1) are therefore completely specified by the upper summation limit n and a word W. In particular for any positive n the sum corresponding to the empty word e equals 1. A quasi-shuffle algebra $\mathcal{A}$ on the vectorspace of words is defined by [46]

$$\begin{aligned} e \circ W &= W \circ e = W, \\ (X_1,W_1)\circ(X_2,W_2) &= X_1,(W_1\circ(X_2,W_2)) + X_2,((X_1,W_1)\circ W_2) \\ &\quad +(X_1\cdot X_2),(W_1\circ W_2). \end{aligned} \tag{91}$$

Note that "$\cdot$" denotes multiplication of letters as defined in eq. (89), whereas "$\circ$" denotes the product in the algebra $\mathcal{A}$, recursively defined in eq. (91). We observe that the formula for the multiplication of Z-sums eq. (7) is identical to eq. (91). The Z-sums form therefore a quasi-shuffle algebra.

We now discuss the connection with the Hopf algebra of Kreimer [47]. Kreimer showed that the process of renormalization of UV-divergences occuring in quantum field theories can be formulated in terms of a Hopf algebra structure. We first recall the properties of an algebra and a coalgebra: An algebra has a unit and a multiplication, whereas a coalgebra has a counit and a comultiplication. A Hopf algebra is an algebra and a coalgebra at the same time, such that the two structures are compatible with each other. In addition there is an antipode. We show that the coalgebra structure of Z-sums is identical to the coalgebra structure of the Hopf algebra of Kreimer. To this aim we introduce the explicit definitions of the counit, the coproduct and the antipode. It is convenient to phrase the coalgebra structure in terms of rooted trees. A Z-sums can be represented as rooted trees without any sidebranchings. As a concrete example we write down the pictorial representation of a sum of depth three :

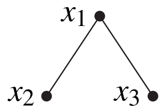
$$Z(n;m_1,m_2,m_3;x_1,x_2,x_3) = \sum_{i_1=1}^{n}\sum_{i_2=1}^{i_1-1}\sum_{i_3=1}^{i_2-1} \frac{x_1^{i_1}}{i_1^{m_1}}\frac{x_2^{i_2}}{i_2^{m_2}}\frac{x_3^{i_3}}{i_3^{m_3}} = \tag{92}$$



The pictorial representation views a Z-sum as a rooted tree without any sidebranchings. The outermost sum corresponds to the root. By convention, the root is always drawn on the top.

Trees with sidebranchings are given by nested sums with more than one subsum, for example:

$$\sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} Z(i-1;m_2,x_2) Z(i-1;m_3;x_3) \quad = \tag{93}$$



Of course, due to the multiplication formula, trees with sidebranchings can always be reduced to trees without any sidebranchings:

$$\begin{aligned}
& \sum_{i=1}^{n} \frac{x_1^i}{i^{m_1}} Z(i-1;m_2,x_2) Z(i-1;m_3;x_3) = \\
& \qquad Z(n;m_1,m_2,m_3;x_1,x_2,x_3) + Z(n;m_1,m_3,m_2;x_1,x_3,x_2) \\
& \qquad + Z(n;m_1,m_2+m_3;x_1,x_2x_3).
\end{aligned} \tag{94}$$

The coalgebra structure is formulated in terms of rooted trees (e.g. there is no need to convert rooted trees to a basis of rooted trees without sidebranchings). We first introduce some notation how to manipulate rooted trees. We adopt the notation of Kreimer and Connes [47, 48]. An elementary cut of a rooted tree is a cut at a single chosen edge. An admissible cut is any assignment of elementary cuts to a rooted tree such that any path from any vertex of the tree to the root has at most one elementary cut. An admissible cut maps a tree t to a monomial in trees $t_1 \circ ... \circ t_{k+1}$. Note that precisely one of these subtrees t_j will contain the root of t. We denote this distinguished tree by $R^C(t)$, and the monomial delivered by the k other factors by $P^C(t)$. The counit $\bar{e}$ is given by

$$\begin{aligned}
\bar{e}(e) &= 1, \\
\bar{e}(t) &= 0, \quad t \neq e.
\end{aligned} \tag{95}$$

The coproduct Δ is defined by the equations

$$\begin{aligned}
\Delta(e) &= e \otimes e, \\
\Delta(t) &= e \otimes t + t \otimes e + \sum_{\text{adm. cuts } C \text{ of } t} P^C(t) \otimes R^C(t), \\
\Delta(t_1 \circ ... \circ t_k) &= \Delta(t_1)(\circ \otimes \circ) ... (\circ \otimes \circ)\Delta(t_k).
\end{aligned} \tag{96}$$

The antipode $\mathcal{S}$ is given by

$$\begin{aligned}
\mathcal{S}(e) &= e, \\
\mathcal{S}(t) &= -t - \sum_{\text{adm. cuts } C \text{ of } t} \mathcal{S}\left(P^C(t)\right) \circ R^C(t), \\
\mathcal{S}(t_1 \circ ... \circ t_k) &= \mathcal{S}(t_1) \circ ... \circ \mathcal{S}(t_k).
\end{aligned} \tag{97}$$

The proof that these definitions yield a Hopf algebra can be found in [46] and is not repeated here. The Hopf algebra of Kreimer and Connes [47, 48], which emerged in the context of renormalization of UV-divergences, has a slightly different algebra structure. There the algebra is generated by rooted trees. In this algebra a product of two rooted trees is not necessarily a rooted tree again. However, the coalgebra structures are identical, which is a remarkable observation.

Let us give some examples for the coproduct and the antipode for Z-sums:

$$\begin{aligned}\Delta Z(n;m_1;x_1) &= e\otimes Z(n;m_1;x_1)+Z(n;m_1;x_1)\otimes e,\\ \Delta Z(n;m_1,m_2;x_1,x_2) &= e\otimes Z(n;m_1,m_2;x_1,x_2)+Z(n;m_1,m_2;x_1,x_2)\otimes e\\ &\quad +Z(n;m_2;x_2)\otimes Z(n;m_1;x_1),\end{aligned} \tag{98}$$

$$\begin{aligned}\mathcal{S}Z(n;m_1;x_1) &= -Z(n;m_1;x_1),\\ \mathcal{S}Z(n;m_1,m_2;x_1,x_2) &= Z(n;m_2,m_1;x_2,x_1)+Z(n;m_1+m_2;x_1x_2).\end{aligned} \tag{99}$$

B Review of Goncharov's multiple polylogarithms

At the end of the day we express our results in terms of Goncharov's multiple polylogarithms. They form therefore an important specialization of nested sums and we review therefore some of their properties. After the introduction by Gonacharov [5] they have been extensively studied by Borwein et al. [6]. They use a different notation which is related to the one of Goncharov by

$$\text{Li}_{m_k,...,m_1}(x_k,...,x_1)=\lambda\left(\begin{array}{c}m_1,...,m_k\\ b_1,...,b_k\end{array}\right),\qquad b_j=\frac{1}{x_1x_2...x_j}. \tag{100}$$

Most of the material reviewed in this section is based on the work of Borwein et al. [6].

B.1 Integral representations

We first define the notation for iterated integrals

$$\int\limits_0^\Lambda \frac{dt}{a_n-t}\circ...\circ\frac{dt}{a_1-t} = \int\limits_0^\Lambda \frac{dt_n}{a_n-t_n}\int\limits_0^{t_n}\frac{dt_{n-1}}{a_{n-1}-t_{n-1}}\times...\times\int\limits_0^{t_2}\frac{dt_1}{a_1-t_1}. \tag{101}$$

We further use the following short hand notation:

$$\int\limits_0^\Lambda\left(\frac{dt}{t}\circ\right)^m\frac{dt}{a-t} = \int\limits_0^\Lambda\underbrace{\frac{dt}{t}\circ...\frac{dt}{t}}_{m\,\text{times}}\circ\frac{dt}{a-t}. \tag{102}$$

The integral representation for $\text{Li}_{m_k,...,m_1}(x_k,...,x_1)$ reads:

$$\begin{aligned}\text{Li}_{m_k,...,m_1}(x_k,...,x_1) &= \int\limits_0^{x_1x_2...x_k}\left(\frac{dt}{t}\circ\right)^{m_1-1}\frac{dt}{x_2x_3...x_k-t}\\ &\quad\circ\left(\frac{dt}{t}\circ\right)^{m_2-1}\frac{dt}{x_3...x_k-t}\circ...\circ\left(\frac{dt}{t}\circ\right)^{m_k-1}\frac{dt}{1-t}.\end{aligned} \tag{103}$$

In the notation of Borwein et al. this representation reads

$$\begin{aligned}\text{Li}_{m_k,...,m_1}(x_k,...,x_1) &= (-1)^k\int\limits_0^1\left(\frac{dt}{t}\circ\right)^{m_1-1}\frac{dt}{t-b_1}\\ &\quad\circ\left(\frac{dt}{t}\circ\right)^{m_2-1}\frac{dt}{t-b_2}\circ...\circ\left(\frac{dt}{t}\circ\right)^{m_k-1}\frac{dt}{t-b_k},\end{aligned} \tag{104}$$

where the b_j's are related to the x_j's as in eq. (100). Changing the integration variables according to $t \to 1-t$ yields the dual integral representation:

$$\begin{aligned}
\mathrm{Li}_{m_k,...,m_1}(x_k,...,x_1) &= (-1)^k \int_0^1 \frac{dt}{1-b_k-t} \circ \left(\frac{dt}{1-t}\circ\right)^{m_k-1} \\
&\quad \frac{dt}{1-b_{k-1}-t} \circ \left(\frac{dt}{1-t}\circ\right)^{m_{k-1}-1} \circ ... \circ \frac{dt}{1-b_1-t} \circ \left(\frac{dt}{1-t}\circ\right)^{m_1-1}.
\end{aligned} \tag{105}$$

In addition to these weight-dimensional integral representations there is also a depth-dimensional integral representation:

$$\begin{aligned}
\mathrm{Li}_{m_k,...,m_1}(x_k,...,x_1) &= \frac{1}{\Gamma(m_1)...\Gamma(m_k)} \int_1^\infty \frac{dt_1}{t_1} \frac{(\ln t_1)^{m_1-1}}{\frac{t_1}{x_1}-1} \\
&\quad \times \int_1^\infty \frac{dt_2}{t_2} \frac{(\ln t_2)^{m_2-1}}{\frac{t_1 t_2}{x_1 x_2}-1} \times ... \times \int_1^\infty \frac{dt_k}{t_k} \frac{(\ln t_k)^{m_k-1}}{\frac{t_1...t_k}{x_1...x_k}-1}.
\end{aligned} \tag{106}$$

B.2 The shuffle algebra

Instead of specifying a multiple polylogarithm by the x_j's and m_j's, we may denote the function by a single string

$$(\alpha_1,\alpha_2,...,\alpha_w) = (0,...,0,b_1,0,...,0,b_2,...,0,...,0,b_k), \tag{107}$$

where (m_j-1) zeros preceed b_j. Defining further

$$\Omega(\alpha_i) = \frac{dt}{t-\alpha_i} \tag{108}$$

allows us to rewrite the integral representation eq. (104) as

$$\mathrm{Li}_{m_k,...,m_1}(x_k,...,x_1) = (-1)^k \int_0^1 \Omega(\alpha_1)\circ ... \circ \Omega(\alpha_w). \tag{109}$$

From the iterated integral representation one deduces a second algebra structure with multiplication given by

$$\begin{aligned}
&\mathrm{Li}_{m_k,...,m_1}(x_k,...,x_1) \times \mathrm{Li}_{m_{k+l},...,m_{k+1}}(x_{k+l},...,x_{k+1}) \\
&= (-1)^{k+l} \int_0^1 \Omega(\alpha_1)\circ ... \circ \Omega(\alpha_{w_k}) \int_0^1 \Omega(\alpha_{w_k+1})\circ ... \circ \Omega(\alpha_{w_k+w_l}) \\
&= (-1)^{k+l} \sum_{shuffle} \int_0^1 \Omega(\alpha_{\sigma(1)})\circ ... \circ \Omega(\alpha_{\sigma(w_k+w_l)}),
\end{aligned} \tag{110}$$

where $w_k = m_1+...+m_k$, $w_l = m_{k+1}+...+m_{k+l}$ and the sum is over all permutations, which preserve the relative order of the strings $\Omega(\alpha_1)...\Omega(\alpha_{w_k})$ and $\Omega(\alpha_{w_k+1})...\Omega(\alpha_{w_k+w_l})$.

B.3 Reduction to simpler functions

The multiple polylogarithms contain a variety of other functions as a subset. We start with depth one. As the notation already suggests, the multiple polylogarithms are in this case identical to the classical polylogarithms, e.g.

$$\mathrm{Li}_0(x) = \frac{x}{1-x}, \qquad \mathrm{Li}_1(x) = -\ln(1-x) \tag{111}$$

and

$$\mathrm{Li}_n(x) = \int_0^x dt \frac{\mathrm{Li}_{n-1}(t)}{t}. \tag{112}$$

Nielsen's generalized polylogarithms [4], defined through

$$S_{n,p}(x) \;=\; \frac{(-1)^{n-1+p}}{(n-1)!p!} \int_0^1 dt \frac{\ln^{n-1}(t)\ln^p(1-tx)}{t} \tag{113}$$

are related to the multiple polylogarithms by

$$S_{n,p}(x) \;=\; \mathrm{Li}_{1,\dots,1,n+1}(\underbrace{1,\dots,1}_{p-1},x), \tag{114}$$

where $(p-1)$ one's occur before $n+1$ and x. The harmonic polylogarithms of Remiddi and Vermaseren [7] are related to the multiple polylogarithms for positive indices as

$$H_{m_1,\dots,m_k}(x) \;=\; \mathrm{Li}_{m_k,\dots,m_1}(\underbrace{1,\dots,1}_{k-1},x). \tag{115}$$

The harmonic polylogarithms are defined recursively through

$$H_0(x) = \ln(x), \qquad H_1(x) = -\ln(1-x), \qquad H_{-1}(x) = \ln(1+x)\;, \tag{116}$$

and

$$\begin{aligned} H_{m_1+1,m_2,\dots,m_k} &= \int_0^x dt f_0(t) H_{m_1,m_2,\dots,m_k}(t), \\ H_{\pm 1,m_2,\dots,m_k} &= \int_0^x dt f_{\pm 1}(t) H_{m_2,\dots,m_k}(t), \end{aligned} \tag{117}$$

where the fractions $f_0(x)$, $f_1(x)$ and $f_{-1}(x)$ are given by

$$f_0(x) = \frac{1}{x}, \qquad f_1(x) = \frac{1}{1-x}, \qquad f_{-1}(x) = \frac{1}{1+x}. \tag{118}$$

Recently Gehrmann and Remiddi [8] extended the harmonic polylogarithms to two-dimensional harmonic polylogarithms (2dHPL) by extending the fractions to

$$f(z,x) = \frac{1}{z+x}, \qquad f(1-z,x) = \frac{1}{1-z-x}. \tag{119}$$

From the integral representation eq. (103) it is clear that the 2dHPL are a subset of Goncharov's multiple polylogarithms. If we identitfy $x = x_1 x_2 \times \ldots \times x_k$ we have

$$\begin{aligned}
\int_0^x dt\, f(z,t) \mathrm{Li}_{m_k,\ldots,m_1}\left(x_k,\ldots,x_2,\frac{t}{x_2\ldots x_k}\right) &= -\mathrm{Li}_{m_k,\ldots,m_1,1}\left(x_k,\ldots,x_2,-\frac{z}{x_2\ldots x_k},-\frac{x}{z}\right), \\
\int_0^x dt\, f(1-z,t) \mathrm{Li}_{m_k,\ldots,m_1}\left(x_k,\ldots,x_2,\frac{t}{x_2\ldots x_k}\right) &= \mathrm{Li}_{m_k,\ldots,m_1,1}\left(x_k,\ldots,x_2,\frac{1-z}{x_2\ldots x_k},\frac{x}{1-z}\right).
\end{aligned} \tag{120}$$

References

[1] A. Erdélyi et al., *Higher Transcendental Functions*, (Vol. I, McGraw Hill, 1953).

[2] L. Slater, *Generalized Hypergeometric Functions*, (Cambridge University Press, 1966).

[3] L. Lewin, *Polylogarithmen and associated functions*, (North Holland, Amsterdam, 1981).

[4] N. Nielsen, Nova Acta Leopoldina (Halle) **90**, 123 (1909).

[5] A. B. Goncharov, Math. Res. Lett. **5**, 497 (1998), available at http://www.math.uiuc.edu/K-theory/0297.

[6] J. M. Borwein, D. M. Bradley, D. J. Broadhurst and P. Lisonek, math.CA/9910045.

[7] E. Remiddi and J. A. M. Vermaseren, Int. J. Mod. Phys. **A15**, 725 (2000), hep-ph/9905237.

[8] T. Gehrmann and E. Remiddi, Nucl. Phys. **B601**, 248 (2001), hep-ph/0008287.

[9] L. Euler, Novi Comm. Acad. Sci. Petropol. **20**, 140 (1775).

[10] D. Zagier, First European Congress of Mathematics, Vol. II, Birkhauser, Boston , 497 (1994).

[11] A. Gonzalez-Arroyo, C. Lopez, and F. J. Yndurain, Nucl. Phys. **B153**, 161 (1979); A. Gonzalez-Arroyo and C. Lopez, Nucl. Phys. **B166**, 429 (1980).

[12] J. A. M. Vermaseren, Int. J. Mod. Phys. **A14**, 2037 (1999), hep-ph/9806280.

[13] J. Blümlein and S. Kurth, Phys. Rev. **D60**, 014018 (1999), hep-ph/9810241.

[14] D. I. Kazakov and A. V. Kotikov, Nucl. Phys. **B307**, 721 (1988); D. I. Kazakov and A. V. Kotikov, Nucl. Phys. **B345**, 299 (1990), Erratum.

[15] S. Moch and J. A. M. Vermaseren, Nucl. Phys. **B573**, 853 (2000), hep-ph/9912355.

[16] J. A. M. Vermaseren and S. Moch, Nucl. Phys. Proc. Suppl. **89**, 131 (2000), hep-ph/0004235.

[17] Z. Bern, L. Dixon, and A. Ghinculov, Phys. Rev. **D63**, 053007 (2001), hep-ph/0010075.

[18] Z. Bern, L. Dixon, and D. A. Kosower, JHEP **01**, 027 (2000), hep-ph/0001001.

[19] C. Anastasiou, E. W. N. Glover, C. Oleari, and M. E. Tejeda-Yeomans, Nucl. Phys. **B601**, 318 (2001), hep-ph/0010212;
C. Anastasiou, E. W. N. Glover, C. Oleari, and M. E. Tejeda-Yeomans, Nucl. Phys. **B601**, 341 (2001), hep-ph/0011094;
C. Anastasiou, E. W. N. Glover, C. Oleari, and M. E. Tejeda-Yeomans, Phys. Lett. **B506**, 59 (2001), hep-ph/0012007;
C. Anastasiou, E. W. N. Glover, C. Oleari, and M. E. Tejeda-Yeomans, Nucl. Phys. **B605**, 486 (2001), hep-ph/0101304.

[20] E. W. N. Glover, C. Oleari, and M. E. Tejeda-Yeomans, Nucl. Phys. **B605**, 467 (2001), hep-ph/0102201.

[21] Z. Bern, A. De Freitas, L. J. Dixon, A. Ghinculov, and H. L. Wong, (2001), hep-ph/0109079.

[22] Z. Bern, A. De Freitas, and L. J. Dixon, (2001), hep-ph/0109078.

[23] V. A. Smirnov, Phys. Lett. **B460**, 397 (1999), hep-ph/9905323;
V. A. Smirnov, Phys. Lett. **B491**, 130 (2000), hep-ph/0007032;
V. A. Smirnov, Phys. Lett. **B500**, 330 (2001), hep-ph/0011056.

[24] J. B. Tausk, Phys. Lett. **B469**, 225 (1999), hep-ph/9909506.

[25] T. Gehrmann and E. Remiddi, Nucl. Phys. **B580**, 485 (2000), hep-ph/9912329;
T. Gehrmann and E. Remiddi, Nucl. Phys. **B601**, 287 (2001), hep-ph/0101124.

[26] T. Binoth and G. Heinrich, Nucl. Phys. **B585**, 741 (2000), hep-ph/0004013.

[27] S. Laporta, Phys. Lett. **B504**, 188 (2001), hep-ph/0102032;
S. Laporta, Int. J. Mod. Phys. **A15**, 5087 (2000), hep-ph/0102033.

[28] L. Phaf and S. Weinzierl, JHEP **04**, 006 (2001), hep-ph/0102207.

[29] A. I. Davydychev, (1993), hep-ph/9307323.

[30] A. I. Davydychev, Phys. Rev. **D61**, 087701 (2000), hep-ph/9910224.

[31] A. I. Davydychev and M. Y. Kalmykov, Nucl. Phys. **B605**, 266 (2001), hep-th/0012189.

[32] J. Fleischer, A. V. Kotikov, and O. L. Veretin, Nucl. Phys. **B547**, 343 (1999), hep-ph/9808242.

[33] J. Fleischer and M. Y. Kalmykov, Phys. Lett. **B470**, 168 (1999), hep-ph/9910223.

[34] M. Y. Kalmykov and O. Veretin, Phys. Lett. **B483**, 315 (2000), hep-th/0004010.

[35] O. V. Tarasov, Nucl. Phys. Proc. Suppl. **89**, 237 (2000), hep-ph/0102271.

[36] H. Hopf, Ann. of Math. **42**, 22 (1941).

[37] J. W. Milnor and J. C. Moore, Ann. of Math. **81**, 210 (1965).

[38] C. Bauer, A. Frink, and R. Kreckel, (2000), cs/0004015.

[39] J. A. M. Vermaseren, (2000), math-ph/0010025.

[40] S. Weinzierl and R. Marani, (2001), http://www.fis.unipr.it/~stefanw/gtybalt.html.

[41] D. A. Kosower and P. Uwer, Nucl. Phys. **B563**, 477 (1999), hep-ph/9903515.

[42] C. Anastasiou, E. W. N. Glover, and C. Oleari, Nucl. Phys. **B565**, 445 (2000), hep-ph/9907523.

[43] P. Appell and J. K. de Fériet, *Fonctions Hypergéométriques et Hypersphériques, Polynomes D'Hermite*, (Gauthiers-Villars, Paris, 1926).

[44] C. Anastasiou, E. W. N. Glover, and C. Oleari, Nucl. Phys. **B572**, 307 (2000), hep-ph/9907494.

[45] E. E. Boos and A. I. Davydychev, Theor. Math. Phys. **89**, 1052 (1991).

[46] M. E. Hoffman, J. Algebraic Combin. **11**, 49 (2000), math.QA/9907173.

[47] D. Kreimer, Adv. Theor. Math. Phys. **2**, 303 (1998), q-alg/9707029.

[48] A. Connes and D. Kreimer, Commun. Math. Phys. **199**, 203 (1998), hep-th/9808042.