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Kurzfassung

Diese Arbeit behandelt spezielle verschachtelte Objekte, die in massiven Störungsberechnungen höherer Ordnung renormierbarer Quantenfeldtheorien auftreten. Einerseits bearbeiten wir verschachtelte Summen, wie harmonische Summen und deren Verallgemeinerungen (S-Summen, cyclotomische harmonische Summen, cyclotomische S-Summen) und andererseits arbeiten wir mit iterierten Integralen nach Poincaré und Chen, wie harmonischen Polylogarithmen und deren Verallgemeinerungen (multiple Polylogarithmen, cyclotomische harmonische Polylogarithmen). Die iterierten Integrale sind über die Mellin-Transformation (und Erweiterungen der Mellin-Transformation) mit den verschachtelten Summen verknüpft und wir zeigen wie diese Transformation berechnet werden kann. Wir leiten algebraische und strukturelle Relationen zwischen den verschachtelten Summen und zusätzlich zwischen den Werten der Summen bei Unendlich und den damit verbundenen Werten der iterierten Integrale ausgewertet bei speziellen Konstanten her. Darüber hinaus präsentieren wir Algorithmen zur Berechnung der asymptotischen Entwicklung dieser Objekte und wir beschreiben einen Algorithmus der bestimmte verschachtelte Summen in Ausdrücke bestehend aus cyclotomische S-Summen umwandelt. Des Weiteren fassen wir die wichtigsten Funktionen des Computeralgebra Pakets `HarmonicSums` zusammen, in welchem alle diese Algorithmen und Transformationen implementiert sind. Ferner präsentieren wir Anwendungen des multivariaten Almkvist-Zeilberger Algorithmuses und Erweiterungen dieses Algorithmuses auf spezielle Typen von Feynman-Integralen und wir stellen das dazugehörige Computeralgebra Paket `MultiIntegrate` vor.

Abstract

This work deals with special nested objects arising in massive higher order perturbative calculations in renormalizable quantum field theories. On the one hand we work with nested sums such as harmonic sums and their generalizations (S-sums, cyclotomic harmonic sums, cyclotomic S-sums) and on the other hand we treat iterated integrals of the Poincaré and Chen-type, such as harmonic polylogarithms and their generalizations (multiple polylogarithms, cyclotomic harmonic polylogarithms). The iterated integrals are connected to the nested sums via (generalizations of) the Mellin-transformation and we show how this transformation can be computed. We derive algebraic and structural relations between the nested sums as well as relations between the values of the sums at infinity and connected to it the values of the iterated integrals evaluated at special constants. In addition we state algorithms to compute asymptotic expansions of these nested objects and we state an algorithm which rewrites certain types of nested sums into expressions in terms of cyclotomic S-sums. Moreover we summarize the main functionality of the computer algebra package `HarmonicSums` in which all these algorithms and transformations are implemented. Furthermore, we present application of and enhancements of the multivariate Almkvist-Zeilberger algorithm to certain types of Feynman integrals and the corresponding computer algebra package `MultiIntegrate`.

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Notations

\mathbb{N}	$\mathbb{N} = \{1, 2, \dots\}$, natural numbers
\mathbb{N}_0	$\mathbb{N}_0 = \{0, 1, 2, \dots\}$
\mathbb{Z}	integers
\mathbb{Z}^*	$\mathbb{Z} \setminus \{0\}$
\mathbb{Q}	rational numbers
\mathbb{R}	real numbers
\mathbb{R}^*	$\mathbb{R} \setminus \{0\}$
$S_{a_1, a_2, \dots}(n)$	harmonic sum; see page 6
$S_a(\mathbf{b}; n)$	S-sum; see page 53
$S_{(a_1, b_1, c_1), \dots}(n)$	cyclotomic harmonic sum; see page 119
$S_{(a_1, b_1, c_1), \dots}(\mathbf{b}; n)$	cyclotomic S-sum; see page 169
$\mathcal{S}(n)$	the set of polynomials in the harmonic sums; see page 25
$\mathcal{C}(n)$	the set of polynomials in the cyclotomic harmonic sums; see page 142
$\mathcal{CS}(n)$	the set of polynomials in the cyclotomic S-sums; see page 170
$H_{m_1, m_2, \dots}(x)$	harmonic/multiple polylogarithm; see pages 9 and 54
$H_{(m_1, n_1), (m_2, n_2), \dots}(x)$	cyclotomic harmonic polylogarithm; see page 125
\sqcup	the shuffle product; see page 10
sign	sign(a) gives the sign of the number a
$ $	$ \mathbf{w} $ gives the degree of a word \mathbf{w} ; $ a $ is the absolute value of the number a
\wedge	$a \wedge b = \text{sign}(a) \text{sign}(b) (a + b)$; see page
$\mu(n)$	the Möbius function; see page 27
ζ_n	ζ_n is the value of the Riemann zeta-function at n
$M(f(x), n)$	the Mellin transform of $f(x)$; see pages 19, 70 and 136
$M^+(f(x), n)$	the extended Mellin transform of $f(x)$; see page 19
$\mathbf{0}_k$	$(\underbrace{0, 0, \dots, 0}_{k \times})$

Chapter 1

Introduction

Harmonic sums and harmonic polylogarithms associated to them by a Mellin transform [85, 27], emerge in perturbative calculations of massless or massive single scale problems in quantum field theory [45, 44, 59, 22]. In order to facilitate these computations, many properties and methods have been worked out for these special functions. In particular, that the harmonic polylogarithms form a shuffle algebra [73], while the harmonic sums form a quasi shuffle algebra [47, 49, 48, 72, 19, 85, 1]. Various relations between harmonic sums, i.e., algebraic and structural relations have already been considered [19, 20, 21, 22], and the asymptotic behavior and the analytic continuation of these sums was worked out up to certain weights [18, 21, 22]. Moreover, algorithms to compute the Mellin transform of harmonic polylogarithms and the inverse Mellin transform [73] as well as algorithms to compute the asymptotic expansion of harmonic sums (with positive indices) are known [60]. In addition, argument transforms and power series expansions of harmonic polylogarithms were worked out [73, 1]. Note that harmonic sums at infinity and harmonic polylogarithms at one are closely related to the multiple zeta values [73]; relations between them and basis representation of them are considered, e.g., in [23, 85, 32, 33, 50]. For the exploration of related objects, like Euler sums, and their applications with algorithms see, e.g., [30, 31, 41, 83].

In recent calculations generalizations of harmonic sums and harmonic polylogarithms, i.e., S-sums (see e.g., [62, 7, 5, 2]) and cyclotomic harmonic sums (see e.g., [8, 4]) on the one hand and multiple polylogarithms and cyclotomic polylogarithms (see e.g., [8, 4]) on the other hand emerge. Both generalizations of the harmonic sums, i.e., cyclotomic harmonic sums and S-sums can be viewed as subsets of the more general class of cyclotomic S-sums $S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n)$ defined as

$$S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n) = \sum_{i_1 \geq i_2, \dots, i_k \geq 1} \frac{x_1^{i_1}}{(a_1 i_1 + b_1)^{c_1}} \frac{x_2^{i_2}}{(a_2 i_2 + b_2)^{c_2}} \cdots \frac{x_k^{i_k}}{(a_k i_k + b_k)^{c_k}},$$

which form a quasi-shuffle algebra. In addition, the corresponding generalizations of the harmonic polylogarithms to multiple polylogarithms and cyclotomic polylogarithms fall into the class of Poincaré iterated integrals (see [71, 55]).

We conclude that so far only some basic properties of S-sums [62] are known and these generalized objects need further investigations for, e.g., ongoing calculations.

One of the main goals of this theses is to extend known properties of harmonic sums and harmonic polylogarithms to their generalizations and to provide algorithms to deal with these quantities, in particular, to find relations between them, to compute series expansions, to compute Mellin transforms, etc.

Due to the complexity of higher order calculations the knowledge of as many as possible relations between the finite harmonic sums, S-sums and cyclotomic harmonic sums is of importance to simplify the calculations and to obtain as compact as possible analytic results. Therefore we derive not only algebraic but also structural relations originating from differentiation and multiplication of the upper summation limit. Concerning harmonic sums these relations have already been considered in [1, 21, 22] and for the sake of completeness we briefly summarize these results here and extend them to S-sums and cyclotomic harmonic sums.

In physical applications (see e.g., [27, 18, 19, 63, 64, 65, 28, 20, 4, 7, 6, 2]) an analytic continuation of these nested sums is required (which is already required in order to establish differentiation) and eventually one has to derive the complex analysis for these nested sums. Hence we look at integral representations of them which leads to Mellin type transformations of harmonic polylogarithms, multiple polylogarithms and cyclotomic polylogarithms.

Starting from the integral representation of the nested sums we derive algorithms to determine the asymptotic behavior of harmonic sums, S-sums and cyclotomic harmonic sums, i.e., we are able to compute asymptotic expansions up to arbitrary order of these sums.

In the context of Mellin transforms and asymptotic expansions the values of the nested sums at infinity and connected to them the values of harmonic polylogarithms, multiple polylogarithms and cyclotomic polylogarithms at certain constants are of importance. For harmonic sums this leads to multiple zeta values and for example in [23] relations between these constants have been investigated. Here we extend these consideration to S-sums and cyclotomic harmonic sums (compare [8]).

Besides several argument transformations of harmonic polylogarithms, multiple polylogarithms and cyclotomic polylogarithms we derive algorithms to compute power series expansions about zero as well as algorithms to determine the asymptotic behavior of these iterated integrals.

The various relations between the nested sums together with the values at infinity on the one hand and the nested integrals together with the values at special constants on the other hand are summarized by Figure 1.1.

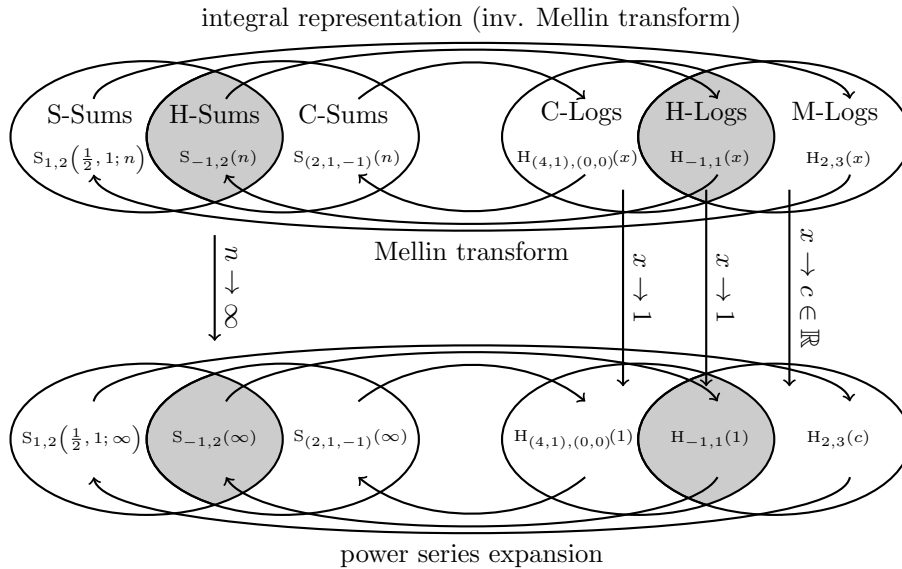


Figure 1.1: Connection between harmonic sums (H-Sums), S-sums (S-Sums) and cyclotomic harmonic sums (C-Sums), their values at infinity and harmonic polylogarithms (H-Logs), multiple polylogarithms (M-Logs) and cyclotomic harmonic polylogarithms (C-Logs) and their values at special constants.

All the algorithms for the harmonic sums, S-sums, cyclotomic harmonic sums, cyclotomic S-sums, harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms which are presented in this theses are implemented in the Mathematica package `HarmonicSums` which was developed in [1] originally for harmonic sums and which was extended and generalized in the frame of this thesis.

In the last chapter we extend the multivariate Almkvist-Zeilberger algorithm [14] in several directions using ideas and algorithms from [26] in order to apply it to special Feynman integrals emerging in renormalizable Quantum field Theories (see [26]). We will look on integrals of the form

$$\mathcal{I}(\varepsilon, N) = \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d; \varepsilon) dx_1 \dots dx_d,$$

with $d, N \in \mathbb{N}$, $F(n; x_1, \dots, x_d; \varepsilon)$ a hyperexponential term (for details see [14] or Theorem 7.1.1), $\varepsilon > 0$ a real parameter and $u_i, o_i \in \mathbb{R} \cup \{-\infty, \infty\}$. As indicated by several examples, the solution of these integrals may lead to harmonic sums, cyclotomic harmonic sums and S-sums.

Our Mathematica package `MultiIntegrate`, which was developed in the frame of this theses, can be considered as an enhanced implementation of the multivariate Almkvist Zeilberger algorithm to compute recurrences for the integrands and integrals. Together with the summation package `Sigma` [77, 78, 79, 80, 81, 82] our package provides methods

to compute representations of $\mathcal{I}(\varepsilon, N)$ in terms of harmonic sums, cyclotomic harmonic sums and S-sums and to compute Laurent series expansions of $\mathcal{I}(\varepsilon, N)$ in the form

$$\mathcal{I}(\varepsilon, N) = I_t(N)\varepsilon^t + I_{t+1}(N)\varepsilon^{t+1} + I_{t+2}(N)\varepsilon^{t+2} + \dots$$

where $t \in \mathbb{Z}$ and the I_k are expressed in terms of harmonic sums, cyclotomic harmonic sums and S-sums, and even more generally in terms of indefinite nested sums and products [82].

The remainder of the thesis is structured as follows: In Chapter 2 harmonic sums and harmonic polylogarithms are introduced. We seek power series expansions and the asymptotic behavior of harmonic polylogarithms and harmonic sums. We look for integral representations of harmonic sums and Mellin-transforms of harmonic polylogarithms. In addition we consider algebraic and structural relations between harmonic sums and we consider values of harmonic sums at infinity and values of harmonic polylogarithms at one. In Chapter 3 S-sums and multiple polylogarithms are introduced and we generalize the theorems and algorithms from Chapter 2 to S-sums and multiple polylogarithms, while in Chapter 4 cyclotomic harmonic sums and cyclotomic harmonic polylogarithms are defined and we seek to generalize the theorems and algorithms from Chapter 2 to these structures. Chapter 5 introduces cyclotomic S-sums and provides mainly an algorithms that transforms indefinite nested sums and products to cyclotomic S-sums whenever this is possible. In Chapter 6 we briefly summarize the main features of the packages `HarmonicSums` in which the algorithms and procedures presented in the foregoing chapters are implemented. Finally, Chapter 7 deals with the application of (extensions of) the multivariate Almkvist-Zeilberger to certain types of Feynman integrals and the corresponding package `MultiIntegrate`.

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Chapter 2

Harmonic Sums

One of the main goals of this chapter is to present a new algorithm which computes the asymptotic expansions of harmonic sums (see, e.g., [18, 21, 22, 85]). Asymptotic expansions of harmonic sums with positive indices have already been considered in [60], but here we will derive an algorithm which is suitable for harmonic sums in general (so negative indices are allowed as well). Our approach is inspired by [21, 22] and uses an integral representation of harmonic sums and in addition makes use of several properties of harmonic sums. Therefore we will state first several known and needed facts about harmonic sums.

Note that the major part of this chapter up to Section 2.8 can already be found in [1], however there are some differences and some complementary facts are added.

The integral representation which is used in the algorithm is based on the Mellin transformation of harmonic polylogarithms defined in [73]; note that the Mellin transformation defined here slightly differs. We will show how the Mellin transformation of harmonic polylogarithms can be computed using a new approach different from [73].

The Mellin transformation also leads to harmonic polylogarithms at one and connected to them to harmonic sums at infinity. Since this relation is of importance for further considerations, we repeat how these quantities are related (see [73]). Since the algorithm utilizes algebraic properties of harmonic sums, we will shortly comment on the structure of harmonic sums (for details see, e.g., [49]) and we will look at algebraic and structural relations (compare [1, 19, 20, 21, 22]). In addition we derive new formulas that count the number of basis sums at a specified weight.

We state some of the argument transformations of harmonic polylogarithms from [73], which will for example allow us to determine the asymptotic behavior of harmonic polylogarithms. One of these argument transformations will be used in the algorithm which computes asymptotic expansions of harmonic sums. But since harmonic polylogarithms are not closed under this transformation, we will extend harmonic polylogarithms by adding a new letter to the index set. This new letter is added in a way such that the extended harmonic polylogarithms are closed under the required transformation.

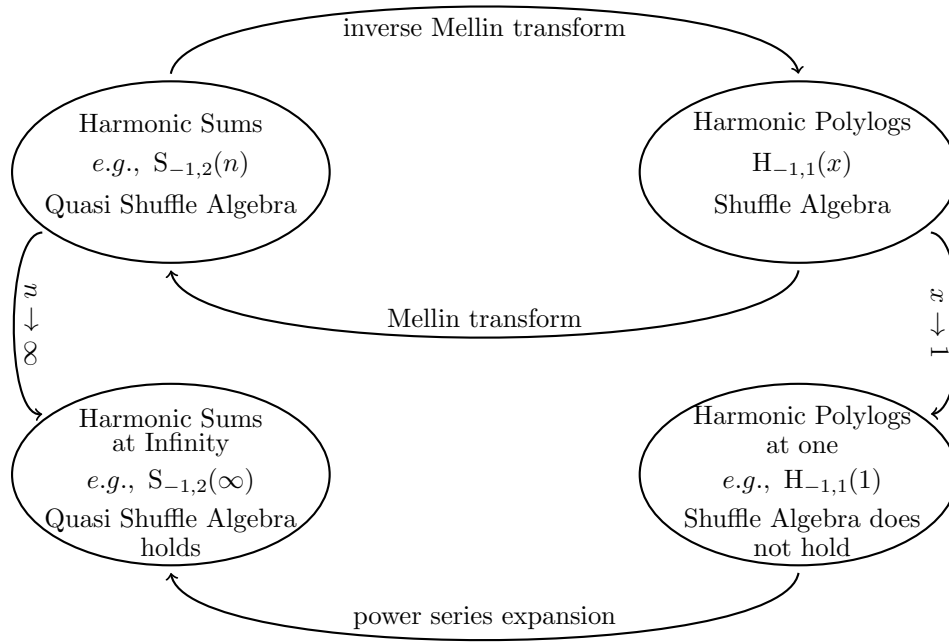


Figure 2.1: Connection between harmonic sums and harmonic polylogarithms (compare [1]).

The stated material will finally allow us to compute asymptotic expansion of the harmonic sums.

The connection between harmonic sums, their values at infinity, harmonic polylogarithms and their values at one are summarized in Figure 2.1. Note that this chapter can be viewed as a model for Chapter 3 and Chapter 4, since there we will extend the properties of harmonic sums and harmonic polylogarithms, which will lead to asymptotic expansion of generalizations of harmonic sums.

2.1 Definition and Structure of Harmonic Sums

We start by defining multiple harmonic sums; see, e.g., [19, 85].

Definition 2.1.1 (Harmonic Sums). *For $k \in \mathbb{N}$, $n \in \mathbb{N}_0$ and $a_i \in \mathbb{Z}^*$ with $1 \leq i \leq k$ we define*

$$S_{a_1, \dots, a_k}(n) = \sum_{n \geq i_1 \geq i_2 \geq \dots \geq i_k \geq 1} \frac{\text{sign}(a_1)^{i_1}}{i_1^{|a_1|}} \dots \frac{\text{sign}(a_k)^{i_k}}{i_k^{|a_k|}}.$$

k is called the depth and $w = \sum_{i=1}^k |a_i|$ is called the weight of the harmonic sum $S_{a_1, \dots, a_k}(n)$.

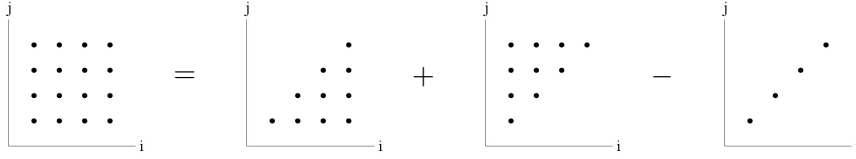


Figure 2.2: Sketch of the proof of the multiplication of harmonic sums (compare [62]).

One of the properties of harmonic sums is the following identity: for $n \in \mathbb{N}$,

$$\begin{aligned}
S_{a_1, \dots, a_k}(n) S_{b_1, \dots, b_l}(n) &= \sum_{i=1}^n \frac{\text{sign}(a_1)^i}{i^{|a_1|}} S_{a_2, \dots, a_k}(i) S_{b_1, \dots, b_l}(i) \\
&+ \sum_{i=1}^n \frac{\text{sign}(b_1)^i}{i^{|b_1|}} S_{a_1, \dots, a_k}(i) S_{b_2, \dots, b_l}(i) \\
&- \sum_{i=1}^n \frac{\text{sign}(a_1 * b_1)^i}{i^{|a_1|+|b_1|}} S_{a_2, \dots, a_k}(i) S_{b_2, \dots, b_l}(i). \quad (2.1)
\end{aligned}$$

The proof of equation (2.1) follows immediately from

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} = \sum_{i=1}^n \sum_{j=1}^i a_{ij} + \sum_{j=1}^n \sum_{i=1}^j a_{ij} - \sum_{i=1}^n a_{ii};$$

for a graphical illustration of the proof see Figure 2.2. As a consequence, any product of harmonic sums with the same upper summation limit can be written as a linear combination of harmonic sums by iterative application of (2.1). Together with this product, harmonic sums form a quasi shuffle algebra (for further details see Section 2.6.1 and, e.g., [47, 48, 49]).

Example 2.1.2.

$$\begin{aligned}
S_{2,3}(n) S_{2,2}(n) &= S_{4,5}(n) - 2S_{2,2,5}(n) - S_{2,4,3}(n) - S_{2,5,2}(n) - S_{4,2,3}(n) - \\
&S_{4,3,2}(n) + 3S_{2,2,2,3}(n) + 2S_{2,2,3,2}(n) + S_{2,3,2,2}(n).
\end{aligned}$$

Definition 2.1.3. We say that a harmonic sum $S_{a_1, a_2, \dots, a_k}(n)$ has trailing ones if there is an $i \in \{1, 2, \dots, k\}$ such that for all $j \in \mathbb{N}$ with $i \leq j \leq k$, $a_j = 1$.

Likewise, we say that a harmonic sum $S_{a_1, a_2, \dots, a_k}(n)$ has leading ones if there is an $i \in \{1, 2, \dots, k\}$ such that for all $j \in \mathbb{N}$ with $1 \leq j \leq i$, $a_j = 1$.

Choosing one of the harmonic sums in (2.1) with depth one we get

$$\begin{aligned}
S_a(n) S_{b_1, \dots, b_l}(n) &= S_{a, b_1, \dots, b_l}(n) + S_{b_1, a, b_2, \dots, b_l}(n) + \dots + S_{b_1, b_2, \dots, b_l, a}(n) \\
&- S_{a \wedge b_1, b_2, \dots, b_l}(n) - \dots - S_{b_1, b_2, \dots, a \wedge b_m}(n). \quad (2.2)
\end{aligned}$$

Here the symbol \wedge is defined as

$$a \wedge b = \text{sign}(a) \text{sign}(b) (|a| + |b|).$$

We can use (2.2) now to single out terms of $S_1(n)$ from harmonic sums whose indices have leading ones. Taking $a = 1$ in (2.2), we get:

$$\begin{aligned} S_1(n) S_{b_1, \dots, b_l}(n) &= S_{1, b_1, \dots, b_l}(n) + S_{b_1, 1, b_2, \dots, b_l}(n) + \dots + S_{b_1, b_2, \dots, b_l, 1}(n) \\ &\quad - S_{1 \wedge b_1, b_2, \dots, b_l}(n) - \dots - S_{b_1, b_2, \dots, 1 \wedge b_m}(n), \end{aligned}$$

or equivalently:

$$\begin{aligned} S_{1, b_1, \dots, b_l}(n) &= S_1(n) S_{b_1, \dots, b_l}(n) - S_{b_1, 1, b_2, \dots, b_l}(n) - \dots - S_{b_1, b_2, \dots, b_l, 1}(n) \\ &\quad + S_{1 \wedge b_1, b_2, \dots, b_l}(n) + \dots + S_{b_1, b_2, \dots, 1 \wedge b_m}(n). \end{aligned}$$

If b_1 is 1 as well, we can move $S_{b_1, 1, b_2, \dots, b_l}(n)$ to the left and can divide by two. This leads to

$$\begin{aligned} S_{1, b_1, \dots, b_l}(n) &= \frac{1}{2} (S_1(n) S_{b_1, \dots, b_l}(n) - S_{b_1, b_2, 1, \dots, b_l}(n) - \dots - S_{b_1, b_2, \dots, b_l, 1}(n) \\ &\quad + S_{1 \wedge b_1, b_2, \dots, b_l}(n) + \dots + S_{b_1, b_2, \dots, 1 \wedge b_m}(n)). \end{aligned}$$

Now we can use (2.2) for all the other terms, and we get an identity which extracts two leading ones. We can repeat this strategy as often as needed in order to extract all the powers of $S_1(n)$ from a harmonic sum.

Example 2.1.4. For $x \in \mathbb{N}$,

$$\begin{aligned} S_{1,1,2,3}(n) &= \frac{1}{2} S_{2,3}(n) S_1(n)^2 + (S_{2,4}(n) + S_{3,3}(n) - S_{2,1,3}(n) - S_{2,3,1}(n)) S_1(n) \\ &\quad + \frac{1}{2} S_{2,5}(n) + S_{3,4}(n) + \frac{1}{2} S_{4,3}(n) - S_{2,1,4}(n) - \frac{1}{2} S_{2,3,2}(n) - S_{2,4,1}(n) \\ &\quad - S_{3,1,3}(n) - S_{3,3,1}(n) + S_{2,1,1,3}(n) + S_{2,1,3,1}(n) + S_{2,3,1,1}(n). \end{aligned}$$

Remark 2.1.5. We can decompose a harmonic sum $S_{b_1, \dots, b_l}(n)$ in a univariate polynomial in $S_1(n)$ with coefficients in the harmonic sums without leading ones. If the harmonic sum has exactly r leading ones, the highest power of $S_1(n)$, which will appear, is r .

Note, that in a similar way it is possible to extract trailing ones. Hence we can also decompose a harmonic sum $S_{b_1, \dots, b_l}(n)$ in a univariate polynomial in $S_1(n)$ with coefficients in the harmonic sums without trailing ones.

2.2 Definition and Structure of Harmonic Polylogarithms

In this section we define harmonic polylogarithms as introduced in [73]. In addition we will state some basic properties, which can already be found in [73]. We start with defining the auxiliary functions f_a for $a \in \{-1, 0, 1\}$ as follows:

$$f_a : (0, 1) \mapsto \mathbb{R}$$

$$f_a(x) = \begin{cases} \frac{1}{x}, & \text{if } a = 0 \\ \frac{1}{|a| - \text{sign}(a)x}, & \text{otherwise.} \end{cases}$$

Definition 2.2.1 (Harmonic Polylogarithms). *For $m_i \in \{-1, 0, 1\}$, we define harmonic polylogarithms for $x \in (0, 1)$:*

$$\begin{aligned} \mathbf{H}(x) &= 1, \\ \mathbf{H}_{m_1, m_2, \dots, m_w}(x) &= \begin{cases} \frac{1}{w!} (\log x)^w, & \text{if } (m_1, \dots, m_w) = (0, \dots, 0) \\ \int_0^x f_{m_1}(y) \mathbf{H}_{m_2, \dots, m_w}(y) dy, & \text{otherwise.} \end{cases} \end{aligned}$$

The length w of the vector $\mathbf{m} = (m_1, \dots, m_w)$ is called the weight of the harmonic polylogarithm $\mathbf{H}_{\mathbf{m}}(x)$.

Example 2.2.2. For $x \in (0, 1)$,

$$\begin{aligned} \mathbf{H}_1(x) &= \int_0^x \frac{dy}{1-y} = -\log(1-x), \\ \mathbf{H}_{-1}(x) &= \int_0^x \frac{dy}{1+y} = \log(1+x), \\ \mathbf{H}_{-1,1}(x) &= \int_0^x \frac{\mathbf{H}_1(y)}{1+y} dy = \int_0^x \frac{\log(1-y)}{1+y} dy. \end{aligned}$$

A harmonic polylogarithm $\mathbf{H}_{\mathbf{m}}(x) = \mathbf{H}_{m_1, \dots, m_w}(x)$ is an analytic functions for $x \in (0, 1)$. For the limits $x \rightarrow 0$ and $x \rightarrow 1$ we have the following facts (compare [73]):

- It follows from the definition that if $\mathbf{m} \neq \mathbf{0}_w$, $\mathbf{H}_{\mathbf{m}}(0) = 0$.
- If $m_1 \neq 1$ or if $m_1 = 1$ and $m_v = 0$ for all v with $1 < v \leq w$ then $\mathbf{H}_{\mathbf{m}}(1)$ is finite.
- If $m_1 = 1$ and $m_v \neq 0$ for some v with $1 < v \leq w$, $\lim_{x \rightarrow 1^-} \mathbf{H}_{\mathbf{m}}(x)$ behaves as a combination of powers of $\log(1-x)$ as we will see later in more detail.

We define $\mathbf{H}_{\mathbf{m}}(0) := \lim_{x \rightarrow 0^+} \mathbf{H}_{\mathbf{m}}(x)$ and $\mathbf{H}_{\mathbf{m}}(1) := \lim_{x \rightarrow 1^-} \mathbf{H}_{\mathbf{m}}(x)$ if the limits exist.

Remark 2.2.3. For the derivatives we have for all $x \in (0, 1)$ that

$$\frac{d}{dx} \mathbf{H}_{\mathbf{m}}(x) = f_{m_1}(x) \mathbf{H}_{m_2, m_3, \dots, m_w}(x).$$

The product of two harmonic polylogarithms of the same argument can be expressed using the formula

$$\mathbf{H}_p(x) \mathbf{H}_q(x) = \sum_{r=p \sqcup q} \mathbf{H}_r(x) \quad (2.3)$$

in which $p \sqcup q$ represent all merges of p and q in which the relative orders of the elements of p and q are preserved. For details see [73, 1]. The following remarks are in place.

Remark 2.2.4. *The product of two harmonic polylogarithms of weights w_1 and w_2 can be expressed as a linear combination of $(w_1 + w_2)!/(w_1!w_2!)$ harmonic polylogarithms of weight $w = w_1 + w_2$.*

Definition 2.2.5. *We say that a harmonic polylogarithm $\mathbf{H}_{m_1, m_2, \dots, m_w}(x)$ has trailing zeros if there is an $i \in \{1, 2, \dots, w\}$ such that for all $j \in \mathbb{N}$ with $i \leq j \leq w$, $m_j = 0$. Likewise, we say that a harmonic polylogarithm $\mathbf{H}_{m_1, m_2, \dots, m_w}(x)$ has leading ones if there is an $i \in \{1, 2, \dots, w\}$ such that for all $j \in \mathbb{N}$ with $1 \leq j \leq i$, $a_j = 1$.*

Analogously to harmonic sums, we proceed as follows; compare [73]. Choosing one of the harmonic polylogarithms is in (2.3) with weight one yields:

$$\begin{aligned} \mathbf{H}_a(x) \mathbf{H}_{m_1, \dots, m_w}(x) &= \mathbf{H}_{a, m_1, m_2, \dots, m_w}(x) \\ &+ \mathbf{H}_{m_1, a, m_2, \dots, m_w}(x) \\ &+ \mathbf{H}_{m_1, m_2, a, m_3, \dots, m_w}(x) \\ &+ \cdots + \\ &+ \mathbf{H}_{m_1, m_2, \dots, m_w, a}(x). \end{aligned} \quad (2.4)$$

We can use (2.4) now to single out terms of $\log x = \mathbf{H}_0(x)$ from harmonic polylogarithms whose indices have trailing zeros. Let $a = 0$ in (2.4); then after using the definition of harmonic polylogarithms we get:

$$\begin{aligned} \mathbf{H}_0(x) \mathbf{H}_{m_1, \dots, m_w}(x) &= \mathbf{H}_{0, m_1, \dots, m_w}(x) + \mathbf{H}_{m_1, 0, m_2, \dots, m_w}(x) \\ &+ \mathbf{H}_{m_1, m_2, 0, m_3, \dots, m_w}(x) + \cdots + \mathbf{H}_{m_1, \dots, m_w, 0}(x), \end{aligned}$$

or equivalently:

$$\begin{aligned} \mathbf{H}_{m_1, \dots, m_w, 0}(x) &= \mathbf{H}_0(x) \mathbf{H}_{m_1, \dots, m_w}(x) - \mathbf{H}_{0, m_1, \dots, m_w}(x) \\ &- \mathbf{H}_{m_1, 0, m_2, \dots, m_w}(x) - \cdots - \mathbf{H}_{m_1, \dots, 0, m_w}(x). \end{aligned}$$

If m_w is 0 as well, we can move the last term to the left and can divide by two. This leads to

$$\begin{aligned} \mathbf{H}_{m_1, \dots, 0, 0}(x) &= \frac{1}{2} \left(\mathbf{H}_0(x) \mathbf{H}_{m_1, \dots, m_{w-1}, 0}(x) - \mathbf{H}_{0, m_1, \dots, m_{w-1}, 0}(x) \right. \\ &\left. - \mathbf{H}_{m_1, 0, m_2, \dots, m_{w-1}, 0}(x) - \cdots - \mathbf{H}_{m_1, \dots, 0, m_{w-1}}(x) \right). \end{aligned}$$

Now we can use (2.4) for all the other terms, and we get an identity which extracts the logarithmic singularities due to two trailing zeros. We can repeat this strategy as often as needed in order to extract all the powers of $\log(x)$ or equivalently $H_0(x)$ from a harmonic polylogarithm.

Example 2.2.6. For $x \in (0, 1)$,

$$\begin{aligned} H_{1,-1,0,0}(x) &= \frac{1}{2}H_0(x)^2 H_{1,-1}(x) - H_0(x) H_{0,1,-1}(x) \\ &\quad - H_0(x) H_{1,0,-1}(x) + H_{0,0,1,-1}(x) + H_{0,1,0,-1}(x) \\ &\quad + H_{1,0,0,-1}(x) \\ &= \frac{1}{2}H_0(x)^2 H_{1,-1}(x) - H_0(x) H_{0,1,-1}(x) \\ &\quad - H_0(x) H_{1,0,-1}(x) + H_{0,0,1,-1}(x) + H_{0,1,0,-1}(x) \\ &\quad + H_{1,0,0,-1}(x). \end{aligned}$$

Remark 2.2.7. We can decompose a harmonic polylogarithm $H_{m_1, m_2, \dots, m_w}(x)$ in a univariate polynomial in $H_0(x)$ with coefficients in the harmonic polylogarithms without trailing zeros. If the harmonic polylogarithm has exactly r trailing zeros, the highest power of $H_0(x)$, which will appear, is r .

Similarly, we can use (2.4) to extract powers of $\log(1-x)$, or equivalently $-H_1(x)$ from harmonic polylogarithms whose indices have leading ones and hence are singular around $x = 1$.

Example 2.2.8. For $x \in (0, 1)$,

$$\begin{aligned} H_{1,1,0,-1}(x) &= -H_{0,-1}(x) H_{1,1}(x) - H_1(x) H_{0,-1,1}(x) \\ &\quad - H_1(x) H_{0,1,-1}(x) + H_{0,-1,1,1}(x) \\ &\quad + H_{0,1,-1,1}(x) + H_{0,1,1,-1}(x) \\ &= -\frac{1}{2}H_{0,-1}(x) H_1(x)^2 - H_1(x) H_{0,-1,1}(x) \\ &\quad - H_1(x) H_{0,1,-1}(x) + H_{0,-1,1,1}(x) \\ &\quad + H_{0,1,-1,1}(x) + H_{0,1,1,-1}(x). \end{aligned}$$

Remark 2.2.9. We can decompose a harmonic polylogarithm $H_{m_1, m_2, \dots, m_w}(x)$ in a univariate polynomial in $H_1(x)$ with coefficients in the harmonic polylogarithms without leading ones. If the harmonic polylogarithm has exactly r leading ones, the highest power of $H_1(x)$, which will appear, is r . So all divergences of harmonic polylogarithms for $x \rightarrow 1$ can be traced back to the basic divergence of $H_1(x) = -\log(1-x)$ for $x \rightarrow 1$.

Remark 2.2.10. We can combine these two strategies to extract both, leading ones and trialling zeros. Hence, it is always possible to express a harmonic polylogarithm in a bivariate polynomial in $H_0(x) = \log(x)$ and $H_1(x) = -\log(1-x)$ with coefficients in the

harmonic polylogarithms without leading ones or trailing zeros, which are continuous on $[0, 1]$ and finite at $x = 0$ and $x = 1$.

Example 2.2.11. For $x \in (0, 1)$,

$$\begin{aligned} \mathbb{H}_{1,-1,0}(x) &= -\mathbb{H}_0(x) \mathbb{H}_{-1,1}(x) + \mathbb{H}_1(x) (\mathbb{H}_{-1}(x) \mathbb{H}_0(x) \\ &\quad - \mathbb{H}_{0,-1}(x)) + \mathbb{H}_{0,-1,1}(x) \\ &= -\log(x) \mathbb{H}_{-1,1}(x) + \log(1-x) (\mathbb{H}_{-1}(x) \log(x) \\ &\quad - \mathbb{H}_{0,-1}(x)) + \mathbb{H}_{0,-1,1}(x). \end{aligned}$$

2.3 Identities between Harmonic Polylogarithms of Related Arguments

In this section we look at special transforms of the argument of harmonic polylogarithms. Again they can be already found in [73].

2.3.1 $1-x \rightarrow x$

For the transformation $1-x \rightarrow x$ we restrict to harmonic polylogarithms with index sets that do not contain -1 (we will include the index -1 later in Section 2.8.1). We proceed recursively on the weight w of the harmonic polylogarithm, For the base cases we have for $x \in (0, 1)$

$$\mathbb{H}_0(1-x) = -\mathbb{H}_1(x) \tag{2.5}$$

$$\mathbb{H}_1(1-x) = -\mathbb{H}_0(x). \tag{2.6}$$

Now let us look at higher weights $w > 1$. We consider $\mathbb{H}_{m_1, m_2, \dots, m_w}(1-x)$ with $m_i \in \{0, 1\}$ and suppose that we can already apply the transformation for harmonic polylogarithms of weight $< w$. If $m_1 = 1$, we can remove leading ones and end up with harmonic polylogarithms without leading ones and powers of $\mathbb{H}_1(1-x)$. For the powers of $\mathbb{H}_1(1-x)$ we can use (2.6); therefore, only the cases in which the first index $m_1 \neq 1$ are to be considered. If $m_i = 0$ for all $1 < i \leq w$, we are in fact dealing with a power of $\mathbb{H}_0(1-x)$ and hence we can use (2.5); if $m_1 = 0$ and there exists an i such that $m_i \neq 0$ we get for $x \in (0, 1)$ (see [73]):

$$\begin{aligned} \mathbb{H}_{0, m_2, \dots, m_w}(1-x) &= \int_0^{1-x} \frac{\mathbb{H}_{m_2, \dots, m_w}(y)}{y} dy \\ &= \int_0^1 \frac{\mathbb{H}_{m_2, \dots, m_w}(y)}{y} dy - \int_{1-x}^1 \frac{\mathbb{H}_{m_2, \dots, m_w}(y)}{y} dy \end{aligned}$$

$$= \mathbb{H}_{0,m_2,\dots,m_w}(1) - \int_0^x \frac{\mathbb{H}_{m_2,\dots,m_w}(1-t)}{1-t} dt, \quad (2.7)$$

where the constant $\mathbb{H}_{0,m_2,\dots,m_w}(1)$ is finite. Since we know the transform for weights $< w$ we can apply it to $\mathbb{H}_{m_2,\dots,m_w}(1-t)$ and finally we obtain the required weight w identity.

2.3.2 $\frac{1-x}{1+x} \rightarrow x$

Proceeding recursively on the weight w of the harmonic polylogarithm, the base case is for $x \in (0, 1)$

$$\mathbb{H}_{-1}\left(\frac{1-x}{1+x}\right) = \mathbb{H}_{-1}(1) - \mathbb{H}_{-1}(x) \quad (2.8)$$

$$\mathbb{H}_0\left(\frac{1-x}{1+x}\right) = -\mathbb{H}_1(x) + \mathbb{H}_{-1}(x) \quad (2.9)$$

$$\mathbb{H}_1\left(\frac{1-x}{1+x}\right) = -\mathbb{H}_{-1}(1) - \mathbb{H}_0(x) + \mathbb{H}_{-1}(x). \quad (2.10)$$

Now let us look at higher weights $w > 1$. We consider $\mathbb{H}_{m_1,m_2,\dots,m_w}\left(\frac{1-x}{1+x}\right)$ with $m_i \in \{-1, 0, 1\}$ and we suppose that we can already apply the transformation for harmonic polylogarithms of weight $< w$. If $m_1 = 1$, we can remove leading ones and end up with harmonic polylogarithms without leading ones and powers of $\mathbb{H}_1\left(\frac{1-x}{1+x}\right)$. For the powers of $\mathbb{H}_1\left(\frac{1-x}{1+x}\right)$ we can use (2.10); therefore, only the cases in which the first index $m_1 \neq 1$ are to be considered. For $m_1 \neq 1$ we get for $x \in (0, 1)$ (see [73]):

$$\begin{aligned} \mathbb{H}_{-1,m_2,\dots,m_w}\left(\frac{1-x}{1+x}\right) &= \mathbb{H}_{-1,m_2,\dots,m_w}(1) - \int_0^x \frac{1}{1+t} \mathbb{H}_{m_2,\dots,m_w}\left(\frac{1-t}{1+t}\right) dt \\ \mathbb{H}_{0,m_2,\dots,m_w}\left(\frac{1-x}{1+x}\right) &= \mathbb{H}_{0,m_2,\dots,m_w}(1) - \int_0^x \frac{1}{1-t} \mathbb{H}_{m_2,\dots,m_w}\left(\frac{1-t}{1+t}\right) dt \\ &\quad - \int_0^x \frac{1}{1-t} \mathbb{H}_{m_2,\dots,m_w}\left(\frac{1+t}{1+t}\right) dt. \end{aligned}$$

Again we have to consider the case for $\mathbb{H}_{0,\dots,0}\left(\frac{1-x}{1+x}\right)$ separately, however we can handle this case since we can handle $\mathbb{H}_0\left(\frac{1-x}{1+x}\right)$. Since we know the transform for weights $< w$, we can apply it to $\mathbb{H}_{m_2,\dots,m_w}\left(\frac{1+t}{1+t}\right)$, and finally we obtain the required weight w identity by using the definition of the extended harmonic polylogarithms.

2.3.3 $\frac{1}{x} \rightarrow x$

We first restrict this transformation to harmonic polylogarithms with index sets that do not contain 1. Proceeding recursively on the weight w of the harmonic polylogarithm we use the base case for $x \in (0, 1)$:

$$\begin{aligned} \mathbf{H}_{-1}\left(\frac{1}{x}\right) &= \mathbf{H}_{-1}(x) - \mathbf{H}_0(x) \\ \mathbf{H}_0\left(\frac{1}{x}\right) &= -\mathbf{H}_0(x). \end{aligned}$$

Now let us look at higher weights $w > 1$. We consider $\mathbf{H}_{m_1, m_2, \dots, m_w}\left(\frac{1}{x}\right)$ with $m_i \in \{-1, 0\}$ and suppose that we can already apply the transformation for harmonic polylogarithms of weight $< w$. For $m_1 \neq 1$ we get for $x \in (0, 1)$ (compare [73]):

$$\begin{aligned} \mathbf{H}_{-1, m_2, \dots, m_w}\left(\frac{1}{x}\right) &= \mathbf{H}_{-1, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t^2(1+1/t)} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ &= \mathbf{H}_{-1, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ &\quad - \int_x^1 \frac{1}{1+t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ \mathbf{H}_{0, m_2, \dots, m_w}\left(\frac{1}{x}\right) &= \mathbf{H}_{0, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t^2(1/t)} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ &= \mathbf{H}_{0, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt. \end{aligned}$$

Again we have to consider the case for $\mathbf{H}_{0, \dots, 0}\left(\frac{1}{x}\right)$ separately, however we can handle this case since we can handle $\mathbf{H}_0\left(\frac{1}{x}\right)$. Since we know the transformation for weights $< w$ we can apply it to $\mathbf{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right)$ and finally we obtain the required weight w identity by using the definition of the harmonic polylogarithms.

The index 1 in the index set leads to a branch point at 1 and a branch cut discontinuity in the complex plane for $x \in (1, \infty)$. This corresponds to the branch point at $x = 1$ and the branch cut discontinuity in the complex plane for $x \in (1, \infty)$ of $-\log(1-x) = \mathbf{H}_1(x)$. However the analytic properties of the logarithm are well known and we can set for $0 < x < 1$ for instance

$$\mathbf{H}_1\left(\frac{1}{x}\right) = \mathbf{H}_1(x) + \mathbf{H}_0(x) - i\pi, \quad (2.11)$$

by approaching the argument $\frac{1}{x}$ from the lower half complex plane. The strategy now is as follows. If a harmonic polylogarithm has leading ones, we remove them and end up with harmonic polylogarithms without leading ones and powers of $\mathbf{H}_1\left(\frac{1}{x}\right)$. We know how to deal with the harmonic polylogarithms without leading ones due to the previous part of this section and for the powers of $\mathbf{H}_1\left(\frac{1}{x}\right)$ we can use (2.11).

2.4 Power Series Expansion of Harmonic Polylogarithms

Due to trailing zeros in the index, harmonic polylogarithms in general do not have regular Taylor series expansions. To be more precise, the expansion is separated into two parts, one in x and one in $\log(x)$; see also Remark 2.2.10. E.g., it can be seen easily that trailing zeros are responsible for powers of $\log(x)$ in the expansion; see [73]. Subsequently, we only consider the case without trailing zeros in more detail. For weight one we get the following well known expansions.

Lemma 2.4.1. *For $x \in [0, 1)$,*

$$\begin{aligned} H_1(x) &= -\log(1-x) = \sum_{i=1}^{\infty} \frac{x^i}{i}, \\ H_{-1}(x) &= \log(1+x) = \sum_{i=1}^{\infty} -\frac{(-x)^i}{i}. \end{aligned}$$

For higher weights we proceed inductively (see [73]). If we assume that m has no trailing zeros and that for $x \in [0, 1]$ we have

$$H_m(x) = \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^a} S_n(i),$$

then for $x \in [0, 1)$ the following theorem holds.

Theorem 2.4.2. *For $x \in [0, 1)$,*

$$\begin{aligned} H_{0,m}(x) &= \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^{a+1}} S_n(i), \\ H_{1,m}(x) &= \sum_{i=1}^{\infty} \frac{x^i}{i} S_{\sigma a, n}(i-1) = \sum_{i=1}^{\infty} \frac{x^i}{i} S_{\sigma a, n}(i) - \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^{a+1}} S_n(i), \\ H_{-1,m}(x) &= -\sum_{i=1}^{\infty} \frac{(-1)^i x^i}{i} S_{-\sigma a, n}(i-1) = -\sum_{i=1}^{\infty} \frac{(-1)^i x^i}{i} S_{-\sigma a, n}(i) + \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^{a+1}} S_n(i). \end{aligned}$$

Example 2.4.3. *For $x \in [0, 1]$,*

$$H_{-1,1}(x) = \sum_{i=1}^{\infty} \frac{x^i}{i^2} - \sum_{i=1}^{\infty} \frac{(-x)^i}{i} S_{-1}(i).$$

Note that even the reverse direction is possible, i.e., given a sum of the form

$$\sum_i (\pm x)^i \frac{S_n(i)}{i^k}$$

with $k \in \mathbb{N}_0$, we can find a linear combination of (possibly weighted) harmonic polylogarithms $h(x)$ such that for $x \in (0, 1)$:

$$h(x) = \sum_i x^i \frac{S_n(i)}{i^k}.$$

Example 2.4.4. For $x \in (0, 1)$ we have

$$\sum_i x^i \frac{S_{1,-2}(i)}{i} = -H_{0,0,0,-1}(x) - H_{0,1,0,-1}(x) - H_{1,0,0,-1}(x) - H_{1,1,0,-1}(x).$$

2.4.1 Asymptotic Behavior of Harmonic Polylogarithms

Combining Section 2.3.3 together with the power series expansion of harmonic polylogarithms we can determine the asymptotic behavior of harmonic polylogarithms. Let us look at the harmonic polylogarithm $H_m(x)$ and define $y := \frac{1}{x}$. Using Section 2.3.3 on $H_m\left(\frac{1}{y}\right) = H_m(x)$ we can rewrite $H_m(x)$ in terms of harmonic polylogarithms at argument y together with some constants. Now we can get the power series expansion of the harmonic polylogarithms at argument y about 0 easily using the previous part of this section. Since sending x to infinity corresponds to sending y to zero, we get the asymptotic behavior of $H_m(x)$.

Example 2.4.5. For $x \in (0, \infty)$ we have

$$\begin{aligned} H_{-1,0}(x) &= 2H_{-1,0}(1) - H_{-1,0}\left(\frac{1}{x}\right) - H_{0,0}(1) + H_{0,0}\left(\frac{1}{x}\right) \\ &= \frac{1}{2} H_0(x)^2 - H_0(x) \left(\sum_{i=1}^{\infty} \frac{\left(-\frac{1}{x}\right)^i}{i} \right) - \sum_{i=1}^{\infty} \frac{\left(-\frac{1}{x}\right)^i}{i^2} \\ &\quad + 2H_{-1,0}(1). \end{aligned}$$

2.4.2 Values of Harmonic Polylogarithms at 1 Expressed by Harmonic Sums at Infinity

As worked out earlier, the expansion of the harmonic polylogarithms without trailing zeros is a combination of sums of the form:

$$\sum_{i=1}^{\infty} x^i \frac{\sigma^i S_n(i)}{i^a}, \quad \sigma \in \{-1, 1\}, \quad a \in \mathbb{N}.$$

For $x \rightarrow 1$ these sums turn into harmonic sums at infinity if $\sigma a \neq 1$:

$$\sum_{i=1}^{\infty} x^i \frac{\sigma^i S_n(i)}{i^a} \rightarrow S_{\sigma a, n}(\infty).$$

Example 2.4.6.

$$H_{-1,1,0}(1) = -2S_3(\infty) + S_{-1,-2}(\infty) + S_{-2,-1}(\infty).$$

If $\sigma a = 1$, these sums turn into

$$\sum_{i=1}^{\infty} x^i \frac{S_n(i)}{i},$$

and sending x to one gives:

$$\lim_{x \rightarrow 1} \sum_{i=1}^{\infty} x^i \frac{S_n(i)}{i} = \infty.$$

We see that these limits do not exist: this corresponds to the infiniteness of the harmonic sums with leading ones: $\lim_{k \rightarrow \infty} S_{1,n}(k) = \infty$. Hence the values of harmonic polylogarithms at one are related to the values of the multiple harmonic sums at infinity (see [73]). For further details see Section 2.7.

2.5 Integral Representation of Harmonic Sums

In this section we want to derive an integral representation of harmonic sums. First we will find a multidimensional integral which can afterwards be rewritten as a sum of one-dimensional integrals in terms of harmonic polylogarithms using integration by parts. We start with the base case of a harmonic sum of depth one.

Lemma 2.5.1. *Let $m \in \mathbb{N}$, and $n \in \mathbb{N}$ then*

$$\begin{aligned} S_1(n) &= \int_0^1 \frac{x_1^n - 1}{x_1 - 1} dx_1 \\ S_{-1}(n) &= \int_0^1 \frac{(-x_1)^n - 1}{x_1 + 1} dx_1 \\ S_m(n) &= \int_0^1 \frac{1}{x_m} \int_0^{x_m} \frac{1}{x_{m-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^n - 1}{x_1 - 1} dx_1 dx_2 \cdots dx_{m-1} dx_m \\ S_{-m}(n) &= \int_0^1 \frac{1}{x_m} \int_0^{x_m} \frac{1}{x_{m-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{(-x_1)^n - 1}{x_1 + 1} dx_1 dx_2 \cdots dx_{m-1} dx_m. \end{aligned}$$

Proof. We proceed by induction on the weight m . For $m = 1$ we get:

$$\int_0^1 \frac{x_1^n - 1}{x_1 - 1} dx_1 = \int_0^1 \sum_{i=0}^{n-1} x_1^i dx_1 = \sum_{i=0}^{n-1} \int_0^1 x_1^i dx_1 = \sum_{i=0}^{n-1} \frac{1}{i+1} = \sum_{i=1}^n \frac{1}{i} = S_1(n)$$

and

$$\begin{aligned} \int_0^1 \frac{(-x_1)^n - 1}{x_1 + 1} dx_1 &= - \int_0^1 \sum_{i=0}^{n-1} (-x_1)^i dx_1 = - \sum_{i=0}^{n-1} \int_0^1 (-x_1)^i dx_1 = - \sum_{i=0}^{n-1} \frac{(-1)^i}{i+1} \\ &= \sum_{i=1}^n \frac{(-1)^i}{i} = S_{-1}(n). \end{aligned}$$

Now suppose the theorem holds for weight $m - 1$. We get

$$\begin{aligned} \int_0^1 \frac{1}{x_m} \int_0^{x_m} \frac{1}{x_{m-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^n - 1}{x_1 - 1} dx_1 dx_2 \cdots dx_{m-1} dx_m &= \\ \int_0^1 \frac{S_{m-1}(x_m; n)}{x_m} dx_m &= \int_0^1 \sum_{i=1}^n \frac{x_m^{i-1}}{i^{m-1}} dx_m = \sum_{i=1}^n \int_0^1 \frac{x_m^{i-1}}{i^{m-1}} dx_m = \\ \sum_{i=1}^n \frac{1}{i} \frac{1}{i^{m-1}} &= S_m(n). \end{aligned}$$

For $-m$ the theorem follows similarly. □

Now we can look at the general cases:

Theorem 2.5.2. For $m_i \in \mathbb{N}$, $b_i \in \{-1, 1\}$ and $n \in \mathbb{N}$, then

$$\begin{aligned} S_{b_1 m_1, b_2 m_2, \dots, b_k m_k}(n) &= \\ \int_0^{b_1 \cdots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \int_0^{x_k^{m_k}} \frac{dx_k^{m_k-1}}{x_k^{m_k-1}} \cdots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_1 \cdots b_{k-1}} & \\ \int_{b_1 \cdots b_{k-1}}^{x_k^1} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \int_0^{x_{k-1}^{m_{k-1}}} \frac{dx_{k-1}^{m_{k-1}-1}}{x_{k-1}^{m_{k-1}-1}} \cdots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_1 \cdots b_{k-2}} & \\ \int_{b_1 \cdots b_{k-2}}^{x_{k-1}^1} \frac{dx_{k-2}^{m_{k-2}}}{x_{k-2}^{m_{k-2}}} \int_0^{x_{k-2}^{m_{k-2}}} \frac{dx_{k-2}^{m_{k-2}-1}}{x_{k-2}^{m_{k-2}-1}} \cdots \int_0^{x_{k-2}^3} \frac{dx_{k-2}^2}{x_{k-2}^2} \int_0^{x_{k-2}^2} \frac{dx_{k-2}^1}{x_{k-2}^1 - b_1 \cdots b_{k-3}} & \\ \vdots & \\ \int_{b_1 b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \int_0^{x_3^{m_3}} \frac{dx_3^{m_3-1}}{x_3^{m_3-1}} \cdots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_1 b_2} & \\ \int_{b_1 b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \int_0^{x_2^{m_2}} \frac{dx_2^{m_2-1}}{x_2^{m_2-1}} \cdots \int_0^{x_2^3} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{dx_2^1}{x_2^1 - b_1} & \\ \int_{b_1}^{x_2^1} \frac{dx_1^{m_1}}{x_1^{m_1}} \int_0^{x_1^{m_1}} \frac{dx_1^{m_1-1}}{x_1^{m_1-1}} \cdots \int_0^{x_1^3} \frac{dx_1^2}{x_1^2} \int_0^{x_1^2} \frac{(x_1^1)^n - 1}{x_1^1 - 1} dx_1^1. & \end{aligned}$$

We will not give a proof of this theorem at this point, since it is a special case of Theorem 3.4.3, which is proven in Chapter 3. Applying integration by parts to this integral representation it is possible to arrive at one-dimensional integral representations containing harmonic polylogarithms; for details we again refer to Chapter 3. A different way to arrive at a one-dimensional integral representation in terms of harmonic polylogarithms of harmonic sums is shown in the following subsection.

2.5.1 Mellin Transformation of Harmonic Polylogarithms

In this section we look at the so called Mellin-transform of harmonic polylogarithms; compare [69].

Definition 2.5.3 (Mellin-Transform). *Let $f(x)$ be a locally integrable function on $(0, 1)$ and $n \in \mathbb{N}$. Then the Mellin transform is defined by:*

$$M(f(x), n) = \int_0^1 x^n f(x) dx, \text{ when the integral converges.}$$

Remark 2.5.4. *A locally integrable function on $(0, 1)$ is one that is absolutely integrable on all closed subintervals of $(0, 1)$.*

For $f(x) = 1/(1-x)$ the Mellin transform is not defined since the integral $\int_0^1 \frac{x^n}{1-x}$ does not converge. We modify the definition of the Mellin transform to include functions like $1/(1-x)$ as follows (compare [27]).

Definition 2.5.5. *Let $h(x)$ be a harmonic polylogarithm or $h(x) = 1$ for $x \in [0, 1]$. Then we define the extended and modified Mellin-transform as follows:*

$$\begin{aligned} M^+(h(x), n) &= M(h(x), n) = \int_0^1 x^n h(x) dx, \\ M^+\left(\frac{h(x)}{1+x}, n\right) &= M\left(\frac{h(x)}{1+x}, n\right) = \int_0^1 \frac{x^n h(x)}{1+x} dx, \\ M^+\left(\frac{h(x)}{1-x}, n\right) &= \int_0^1 \frac{(x^n - 1)h(x)}{1-x} dx. \end{aligned}$$

Remark 2.5.6. *Note that in [1] and [73] the Mellin-transform is defined slightly differently.*

Remark 2.5.7. *It is possible that for a harmonic polylogarithm the original Mellin transform $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{1-x}, n\right)$ exists, but also in this case we modified the definition. Namely, we get*

$$M\left(\frac{H_{\mathbf{m}}(x)}{1-x}, n\right) = M^+\left(\frac{H_{\mathbf{m}}(x)}{1-x}, n\right) + H_{1, \mathbf{m}}(1).$$

Since $M^+\left(\frac{H_{\mathbf{m}}(x)}{1-x}, n\right)$ converges as well, $H_{1, \mathbf{m}}(1)$ has to be finite. But this is only the case if $H_{1, \mathbf{m}}(x) = H_{1, 0, \dots, 0}(x)$. Hence we modified the definition only for functions of the form $\frac{H_{0, 0, \dots, 0}(x)}{1-x}$ all the other cases are extensions.

Remark 2.5.8. *From now on we will call the extended and modified Mellin transform M^+ just Mellin transform and we will write M instead of M^+ .*

In the rest of this section we want to study how we can actually calculate the Mellin transform of harmonic polylogarithms weighted by $1/(1+x)$ or $1/(1-x)$, i.e., we want to represent the Mellin transforms in terms of harmonic sums at n , harmonic sums at infinity and harmonic polylogarithms at one. This will be possible due to the following lemmas. We will proceed recursively on the depth of the harmonic polylogarithms.

Lemma 2.5.9. *For $n \in \mathbb{N}$ and $\mathbf{m} \in \{0, -1, 1\}^k$,*

$$\begin{aligned} M\left(\frac{H_{\mathbf{m}}(x)}{1-x}, n\right) &= -n \cdot M(H_{1, \mathbf{m}}(x), n-1), \\ M\left(\frac{H_{\mathbf{m}}(x)}{1+x}, n\right) &= -n \cdot M(H_{-1, \mathbf{m}}(x), n-1) + H_{-1, \mathbf{m}}(1). \end{aligned}$$

Proof. We have

$$\begin{aligned} \int_0^1 x^n H_{1, \mathbf{m}}(x) dx &= \frac{1}{n+1} \lim_{\epsilon \rightarrow 1^-} \left(\epsilon^{n+1} H_{1, \mathbf{m}}(\epsilon) - \int_0^\epsilon \frac{x^{n+1} - 1}{1-x} H_{\mathbf{m}}(x) dx - H_{1, \mathbf{m}}(\epsilon) \right) \\ &= -\frac{1}{n+1} \int_0^1 \frac{x^{n+1} - 1}{1-x} H_{\mathbf{m}}(x) dx \\ &= -\frac{1}{n+1} M\left(\frac{H_{1, \mathbf{m}}(x)}{1-x}, n+1\right) \end{aligned}$$

and

$$\begin{aligned} \int_0^1 x^n H_{-1, \mathbf{m}}(x) dx &= \frac{H_{-1, \mathbf{m}}(1)}{n+1} - \frac{1}{n+1} \int_0^1 \frac{x^{n+1}}{(1+x)} H_{\mathbf{m}}(x) dx \\ &= \frac{H_{-1, \mathbf{m}}(1)}{n+1} - \frac{1}{n+1} M\left(\frac{H_{\mathbf{m}}(x)}{1+x}, n+1\right). \end{aligned}$$

Hence we get

$$\begin{aligned} M\left(\frac{H_m(x)}{1-x}, n+1\right) &= -(n+1)M(H_{1,m}(x), n), \\ M\left(\frac{H_m(x)}{1+x}, n+1\right) &= -(n+1)M(H_{-1,m}(x), n) + H_{-1,m}(1). \end{aligned}$$

This is equivalent to the lemma. \square

Due to Lemma 2.5.9 we are able to reduce the calculation of the Mellin transform of harmonic polylogarithms weighted by $1/(1+x)$ or $1/(1-x)$ to the calculation of the Mellin transform which are not weighted, i.e., to the calculation of expressions of the form $M(H_m(x), n)$. To calculate $M(H_m(x), n)$ we proceed by recursion. First let us state the base cases i.e., the Mellin transforms of extended harmonic polylogarithms with weight one [73]; see also [1].

Lemma 2.5.10. *For $n \in \mathbb{N}$ we have*

$$\begin{aligned} M(H_0(x), n) &= -\frac{1}{(n+1)^2}, \\ M(H_1(x), n) &= \frac{S_1(n+1)}{n+1}, \\ M(H_{-1}(x), n) &= (-1)^n \frac{S_{-1}(n+1)}{n+1} + \frac{H_{-1}(1)}{n+1} (1 + (-1)^n). \end{aligned}$$

The higher depth results can now be obtained by recursion.

Lemma 2.5.11. *For $n \in \mathbb{N}$ and $m \in \{0, -1, 1\}^k$,*

$$\begin{aligned} M(H_{0,m}(x), n) &= \frac{H_{0,m}(1)}{n+1} - \frac{1}{n+1} M(H_m(x), n), \\ M(H_{1,m}(x), n) &= \frac{1}{n+1} \sum_{i=0}^n M(H_m(x), i), \\ M(H_{-1,m}(x), n) &= \frac{1 + (-1)^n}{n+1} H_{-1,m}(1) - \frac{(-1)^n}{n+1} \sum_{i=0}^n (-1)^i M(H_m(x), i). \end{aligned}$$

Proof. We get the following results by integration by parts:

$$\begin{aligned} \int_0^1 x^n H_{0,m}(x) dx &= \frac{x^{n+1}}{n+1} H_{0,m}(x) \Big|_0^1 - \int_0^1 \frac{x^n}{n+1} H_m(x) dx \\ &= \frac{H_{0,m}(1)}{n+1} - \frac{1}{n+1} M(H_m(x), n), \end{aligned}$$

$$\begin{aligned}
\int_0^1 x^n H_{1,m}(x) dx &= \lim_{\epsilon \rightarrow 1^-} \int_0^\epsilon x^n H_{1,m}(x) dx \\
&= \lim_{\epsilon \rightarrow 1^-} \left(\frac{x^{n+1}}{n+1} H_{1,m}(x) \Big|_0^\epsilon - \int_0^\epsilon \frac{x^{n+1}}{(n+1)(1-x)} H_m(x) dx \right) \\
&= \frac{1}{n+1} \lim_{\epsilon \rightarrow 1^-} \left(\epsilon^{n+1} H_{1,m}(\epsilon) - \int_0^\epsilon \frac{x^{n+1}-1}{1-x} H_m(x) dx - H_{1,m}(\epsilon) \right) \\
&= \frac{1}{n+1} \left(\lim_{\epsilon \rightarrow 1^-} (\epsilon^{n+1} - 1) H_{1,m}(\epsilon) + \lim_{\epsilon \rightarrow 1^-} \int_0^\epsilon \sum_{i=0}^n x^i H_m(x) dx \right) \\
&= \frac{1}{n+1} \left(0 + \int_0^1 \sum_{i=0}^n x^i H_m(x) dx \right) \\
&= \frac{1}{n+1} \sum_{i=0}^n M(H_m(x), n), \\
\int_0^1 x^n H_{-1,m}(x) dx &= \frac{x^{n+1}}{n+1} H_{-1,m}(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1}}{(n+1)(1+x)} H_m(x) dx \\
&= \frac{H_{-1,m}(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} + (-1)^n}{1+x} H_m(x) dx \right. \\
&\quad \left. - (-1)^n \int_0^1 \frac{H_m(x)}{1+x} dx \right) = \frac{H_{-1,m}(1) + (-1)^n H_{-1,m}(1)}{n+1} \\
&\quad - \frac{(-1)^n}{n+1} \int_0^1 \sum_{i=0}^n (-1)^i x^i H_m(x) dx \\
&= \frac{1 + (-1)^n}{n+1} H_{-1,m}(1) - \frac{(-1)^n}{n+1} \sum_{i=0}^n (-1)^i M(H_m(x), n).
\end{aligned}$$

□

Remark 2.5.12. Combining the Lemmas 2.5.9, 2.5.10 and 2.5.11 we can represent the Mellin transforms of Definition 2.5.5 in terms of harmonic sums at n , harmonic sums at infinity and harmonic polylogarithms at one.

Remark 2.5.13. As already mentioned (see Remark 2.5.7), our definition of the Mellin transform slightly differs from the definitions in [1] and [73], however we can easily connect these different definitions. In fact the difference of the results is just a constant; this constant can be computed and we can use the strategy presented here as well to compute the Mellin-transform as defined in [1] and [73].

2.5.2 The Inverse Mellin Transform

In this subsection we want to summarize briefly how the inverse Mellin transform of harmonic sums can be computed. For details we refer to [1, 73]. First we define as in [1] an order on harmonic sums.

Definition 2.5.14 (Order on harmonic sums). *Let $S_{m_1}(n)$ and $S_{m_2}(n)$ be harmonic sums with weights w_1, w_2 and depths d_1 and d_2 , respectively. Then*

$$S_{m_1}(n) \prec S_{m_2}(n), \text{ if } w_1 < w_2, \text{ or } (w_1 = w_2 \text{ and } d_1 < d_2).$$

We say that a harmonic sum s_1 is more complicated than a harmonic sum s_2 if $s_2 \prec s_1$. For a set of harmonic sums we call a harmonic sum most complicated if it is a largest function with respect to \prec .

From [73] (worked out in detail in [1]) we know that there is only one *most complicated* harmonic sum in the the Mellin transform of a harmonic polylogarithm and this single *most complicated* harmonic sum can be calculated using, e.g., Algorithm 2 of [1]. But even the reverse direction is possible: given a harmonic sum, we can find a harmonic polylogarithm weighted by $1/(1-x)$ or $1/(1+x)$ such that the harmonic sum is the *most complicated* harmonic sum in the Mellin transform of this weighted harmonic polylogarithm. We will call this weighted harmonic polylogarithm the *most complicated* weighted harmonic polylogarithm in the inverse Mellin transform of the harmonic sum. Equipped with these facts the computation of the inverse Mellin transform is relatively easy. As stated in [73] we can proceed as follows:

- Locate the most complicated harmonic sum.
- Construct the corresponding most complicated harmonic polylogarithm.
- Add it and subtract it.
- Perform the Mellin transform to the subtracted version. This will cancel the original harmonic sum.
- Repeat the above steps until there are no more harmonic sums.
- Let c be the remaining constant term, replace it by $M^{-1}(c)$, or equivalently, multiply c by $\delta(1-x)$.

Here δ is the Dirac- δ -distribution [89].

Remark 2.5.15. *A second way to compute the inverse Mellin transform of a harmonic sum uses the integral representation of Theorem 2.5. After repeated suitable integration by parts we can find the inverse Mellin transform.*

Example 2.5.16.

$$S_{-2}(n) = \int_0^1 \frac{1}{y} \int_0^y \frac{(-x)^n - 1}{x+1} dy dx$$

$$\begin{aligned}
&= -\mathrm{H}_{0,1}(1) + \mathrm{H}_0(y) \int_0^y \frac{(-x)^n}{x+1} dx \Big|_0^y - \int_0^1 \frac{(-x)^n \mathrm{H}_0(x)}{1+x} dx \\
&= -\mathrm{H}_{0,1}(1) - (-1)^n \mathrm{M}\left(\frac{\mathrm{H}_0(x)}{1+x}, n\right).
\end{aligned}$$

2.5.3 Differentiation of Harmonic Sums

Due to the previous section we are able to calculate the inverse Mellin transform of harmonic sums. It turned out that they are usually linear combinations of harmonic polylogarithms weighted by the factors $1/(1 \pm x)$ and they can be distribution-valued (compare [1]). By computing the Mellin transform of a harmonic sum we find in fact an analytic continuation of the sum to $n \in \mathbb{R}$. For explicitly given analytic continuations see [27, 18, 19, 28, 20]. The differentiation of harmonic sums in the physic literature has been considered the first time in [27]. Worked out in [20, 21, 22] this allows us to consider differentiation with respect to n , since we can differentiate the analytic continuation. Afterwards we may transform back to harmonic sums with the help of the Mellin transform. Differentiation turns out to be relatively easy if we represent the harmonic sum using its inverse Mellin transform as the following example suggests (see [69, p.81] and [1]):

Example 2.5.17. For $n \in \mathbb{R}$ we have

$$\frac{d}{dn} \int_0^1 x^n \mathrm{H}_{-1}(x) dx = \int_0^1 x^n \log(x) \mathrm{H}_{-1}(x) dx = \int_0^1 x^n \mathrm{H}_{-1,0}(x) dx + \int_0^1 x^n \mathrm{H}_{0,-1}(x) dx.$$

Based on this example, if we want to differentiate $S_a(n)$ with respect to n , we can proceed as follows:

- Calculate the inverse Mellin transform of $S_a(n)$.
- Set the constants to zero and multiply the terms of the inverse Mellin transform where x^n is present by $\mathrm{H}_0(x)$. This is in fact differentiation with respect to n .
- Use the Mellin transform to transform back the multiplied inverse Mellin transform of $S_a(n)$ to harmonic sums.

Example 2.5.18. Let us differentiate $S_{2,1}(n)$. We have:

$$S_{2,1}(n) = \int_0^1 \frac{(x^n - 1) \mathrm{H}_{1,0}(x)}{1-x} dx.$$

Differentiating the right hand side with respect to n yields:

$$\frac{d}{dn} \int_0^1 \frac{(x^n - 1) \mathrm{H}_{1,0}(x)}{1-x} dx = \int_0^1 \frac{x^n \mathrm{H}_0(x) \mathrm{H}_{1,0}(x)}{1-x} dx$$

$$\begin{aligned}
&= \int_0^1 \frac{(x^n - 1)H_0(x) H_{1,0}(x)}{1 - x} dx + \int_0^1 \frac{H_0(x) H_{1,0}(x)}{1 - x} dx \\
&= M\left(\frac{H_{0,1,0}(x)}{1 - x}, n\right) + 2M\left(\frac{H_{1,0,0}(x)}{1 - x}, n\right) - H_{0,1,1,0}(1) \\
&= -S_{2,2}(n) - 2S_{1,3}(n) + 2H_{0,0,1}(1)S_1(n) - H_{0,1,1,0}(1).
\end{aligned}$$

To evaluate $\int_0^1 \frac{H_0(x)H_{1,d}(x)}{1-x} dx$ we use the following lemma:

Lemma 2.5.19. *For a harmonic polylogarithm $H_m(x)$ the integral*

$$\int_0^1 \frac{H_0(x) H_m(x)}{1 - x} dx$$

exists and equals $-H_{0,1,m}(1)$.

Proof. Using integration by parts we get

$$\begin{aligned}
\int_0^1 \frac{H_0(x) H_m(x)}{1 - x} dx &= \lim_{b \rightarrow 1^-} \lim_{a \rightarrow 0^+} \int_a^b \frac{H_0(x) H_m(x)}{1 - x} dx \\
&= \lim_{b \rightarrow 1^-} \lim_{a \rightarrow 0^+} \left(H_0(x) H_{1,m}(x) \Big|_a^b - \int_a^b \frac{H_{1,m}(x)}{x} dx \right) \\
&= \lim_{b \rightarrow 1^-} \left(H_0(b) H_{1,m}(b) - \lim_{a \rightarrow 0^+} H_0(a) H_{1,m}(a) - H_{0,1,m}(b) \right) \\
&= \lim_{b \rightarrow 1^-} (H_0(b) H_{1,m}(b)) - H_{0,1,m}(1) = -H_{0,1,m}(1).
\end{aligned}$$

□

2.6 Relations between Harmonic Sums

In this section we look for the sake of completeness at various relations between harmonic sums as already done in [1, 19, 20, 21, 22].

2.6.1 Algebraic Relations

We already mentioned in Section 2.1 that harmonic sums form a quasi shuffle algebra. We will now take a closer look at the quasi shuffle algebra property (for details see for example [49] or [1]). Subsequently, we define the following sets:

$$\begin{aligned}
\mathcal{S}(n) &= \{q(s_1, \dots, s_r) \mid r \in \mathbb{N}; s_i \text{ a harmonic sum at } n; q \in \mathbb{R}[x_1, \dots, x_r]\} \\
\mathcal{S}_p(n) &= \{q(s_1, \dots, s_r) \mid r \in \mathbb{N}; s_i \text{ a harmonic sum with positive indices at } n; \\
&\quad q \in \mathbb{R}[x_1, \dots, x_r]\}.
\end{aligned}$$

From Section 2.1 we know that we can always expand a product of harmonic sums with the same upper summation limit into a linear combination of harmonic sums. Let $L(s_1, s_2)$ denote the expansion of $s_1 s_2$ into a linear combination of harmonic sums. Now we can define the ideals \mathcal{I} and \mathcal{I}_p on $\mathcal{S}(n)$ respectively $\mathcal{S}_p(n)$:

$$\begin{aligned}\mathcal{I}(n) &= \{s_1 s_2 - L(s_1, s_2) \mid s_i \text{ a harmonic sum at } n\} \\ \mathcal{I}_p(n) &= \{s_1 s_2 - L(s_1, s_2) \mid s_i \text{ a harmonic sum at } n \text{ with positive indices}\}.\end{aligned}$$

By construction $\mathcal{S}(n)/\mathcal{I}$ and $\mathcal{S}_p(n)/\mathcal{I}_p$ are quasi shuffle algebras (for further details we again refer to [1]). We remark that it has been shown in [60] that

$$\mathcal{S}_p(n)/\mathcal{I}_p \cong \mathcal{S}_p(n)/\sim$$

where $a(n) \sim b(n) \Leftrightarrow \forall k \in \mathbb{N} a(k) = b(k)$, i.e., the quasi-shuffle algebra is equivalent to the harmonic sums considered as sequences. To our knowledge it has not been shown so far that

$$\mathcal{S}(n)/\mathcal{I} \cong \mathcal{S}(n)/\sim$$

where $a(n) \sim b(n) \Leftrightarrow \forall k \in \mathbb{N} a(k) = b(k)$. Nevertheless, we strongly believe in this fact; see also Remark 2.6.3.

For further considerations let A be a totally ordered, graded set. The degree of $a \in A$ is denoted by $|a|$. Let A^* denote the free monoid over A , i.e.,

$$A^* = \{a_1 \cdots a_n \mid a_i \in A, n \geq 1\} \cup \{\epsilon\},$$

where ϵ is the empty word. We extend the degree function to A^* by $|a_1 a_2 \cdots a_n| = |a_1| + |a_2| + \cdots + |a_n|$ for $a_i \in A$ and $|\epsilon| = 0$. Suppose now that the set A of letters is totally ordered by $<$. We extend this order to words with the following lexicographic order:

$$\begin{cases} \mathbf{u} < \mathbf{w} \text{ for } v \in A^+ \text{ and } \mathbf{u} \in A^*, \\ \mathbf{w}_1 a_1 \mathbf{w}_2 < \mathbf{w}_1 a_2 \mathbf{w}_3, \text{ if } a_1 < a_2 \text{ for } a_1, a_2 \in A \text{ and } \mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3 \in A^*. \end{cases}$$

Definition 2.6.1. We refer to elements of A as letters and to elements of A^* as words. For a word $\mathbf{w} = pxs$ with $p, x, s \in A^*$, p is called a prefix of w if $p \neq \epsilon$ and any s is called a suffix of \mathbf{w} if $s \neq \epsilon$. A word \mathbf{w} is called a Lyndon word if it is smaller than any of its suffixes. The set of all Lyndon words on A is denoted by $\text{Lyndon}(A)$.

Inspired by [49] it has been shown in [1] directly that the quasi shuffle algebras $\mathcal{S}(n)/\mathcal{I}$ and $\mathcal{S}_p(n)/\mathcal{I}_p$ are the free polynomial algebras on the Lyndon words with alphabet $A = \mathbb{Z}^*$ and $A = \mathbb{N}$ respectively, where we define the degree of a letter $|\pm n| = n$ for all $n \in \mathbb{N}$ and we order the letters by $-n \prec n$ and $n \prec m$ for all $n, m \in \mathbb{N}$ with $n < m$, and extend this order lexicographically (see [49, 1]). Hence the number of algebraic

independent sums in $\mathcal{S}_p(n)/\mathcal{I}$, respectively $\mathcal{S}(n)/\mathcal{I}$ which we also call basis sums is connected to the number of *Lyndon* words. In order to count the number of *Lyndon* words belonging to a specific index set we use the second Witt formula [87, 88, 74]:

$$l_n(n_1, \dots, n_q) = \frac{1}{n} \sum_{d|n} \mu(d) \frac{\binom{n}{d}!}{\binom{n_1}{d}! \dots \binom{n_q}{d}!}, \quad n = \sum_{k=1}^q n_k; \quad (2.12)$$

here n_i denotes the multiplicity of the indices that appear in the index set and

$$\mu(n) = \begin{cases} 1 & \text{if } n = 1 \\ 0 & \text{if } n \text{ is divided by the square of a prime} \\ (-1)^s & \text{if } n \text{ is the product of } s \text{ different primes} \end{cases}$$

is the Möbius function. The number of *Lyndon* words of length n over an alphabet of length q is given by the first Witt formula [87, 88, 74]:

$$l_n(q) = \frac{1}{n} \sum_{d|n} \mu(d) q^{n/d}. \quad (2.13)$$

In order to use this formula to count the number of algebraic basis sums at a specific weight, we introduce a modified notation of harmonic sums compare [85] and [19]. Of course we can identify a harmonic sum at n by its index set viewed as a word:

$$S_{a_1, a_2, \dots, a_k}(n) \rightarrow a_1 a_2 \dots a_k.$$

In addition, we can represent each such word using the alphabet $\{-1, 0, 1\}$ where a letter zero which is followed by an letter that is nonzero indicates that one should be added to the absolute value of the nonzero letter.

$$\begin{aligned} S_{a_1, a_2, \dots, a_k}(n) &\rightarrow a_1 a_2 \dots a_k \rightarrow \underbrace{0 \dots 0}_{|a_1|-1 \times} \text{sign}(a_1) \underbrace{0 \dots 0}_{|a_2|-1 \times} \text{sign}(a_2) \dots \underbrace{0 \dots 0}_{|a_k|-1 \times} \text{sign}(a_k) \\ 0100-11 &\rightarrow S_{2, -3, 1}(n). \end{aligned}$$

Note that the last letter is either -1 or 1 , The advantage of this notation is that a harmonic sum of weight w is expressed by a word of length w in the alphabet $\{-1, 0, 1\}$ and hence we can use (2.13) to count the number of basis harmonic sums at specified weight $w \geq 2$:

$$\frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d. \quad (2.14)$$

For $w = 3$ this formula gives 8 and hence there are 8 algebraic basis harmonic sums spanning the quasi shuffle algebra at weight 3.

A method to find the basis sums together with the relations for the dependent sums was presented in [19]. Efficient implementations and further variations are developed in [1]. Here we want to give an example for harmonic sums at weight $w = 3$.

Example 2.6.2. *At weight $w = 3$ we have for instance the 8 basis sums:*

$$S_{-3}(n), S_3(n), S_{-2,-1}(n), S_{-2,1}(n), S_{2,-1}(n), S_{2,1}(n), S_{-1,1,-1}(n), S_{-1,1,1}(n)$$

together with the relations for remaining sums:

$$\begin{aligned} S_{1,-2}(n) &= S_{-3}(n) + S_{-2}(n) S_1(n) - S_{-2,1}(n) \\ S_{1,2}(n) &= S_1(n) S_2(n) + S_3(n) - S_{2,1}(n) \\ S_{1,-1,-1}(n) &= \frac{1}{2} S_{-2}(n) S_{-1}(n) - \frac{1}{2} S_{-1,1}(n) S_{-1}(n) + \frac{1}{2} S_3(n) + \frac{1}{2} S_{-2,-1}(n) \\ &\quad + S_1(n) S_{-1,-1}(n) - \frac{1}{2} S_{2,1}(n) - \frac{1}{2} S_{-1,1,-1}(n) \\ S_{1,-1,1}(n) &= S_{-3}(n) + S_{-1}(n) S_2(n) + S_{-2,1}(n) + S_1(n) S_{-1,1}(n) - S_{2,-1}(n) \\ &\quad - 2S_{-1,1,1}(n) \\ S_{1,1,-1}(n) &= \frac{1}{2} S_{-2}(n) S_1(n) - \frac{1}{2} S_{-1,1}(n) S_1(n) + \frac{1}{2} S_{1,-1}(n) S_1(n) \\ &\quad - \frac{1}{2} S_{-1}(n) S_2(n) - S_{-2,1}(n) + S_{2,-1}(n) + S_{-1,1,1}(n) \\ S_{1,1,1}(n) &= \frac{1}{3} S_1(n) S_2(n) + \frac{1}{3} S_3(n) + \frac{1}{3} S_1(n) S_{1,1}(n) \\ S_{-1,-2}(n) &= S_{-2}(n) S_{-1}(n) + S_3(n) - S_{-2,-1}(n) \\ S_{-1,2}(n) &= S_{-3}(n) + S_{-1}(n) S_2(n) - S_{2,-1}(n) \\ S_{-1,-1,-1}(n) &= \frac{1}{3} S_{-3}(n) + \frac{1}{3} S_{-1}(n) S_2(n) + \frac{1}{3} S_{-1}(n) S_{-1,-1}(n) \\ S_{-1,-1,1}(n) &= \frac{1}{2} S_{-2}(n) S_{-1}(n) + \frac{1}{2} S_{-1,1}(n) S_{-1}(n) + \frac{1}{2} S_3(n) - \frac{1}{2} S_{-2,-1}(n) \\ &\quad + \frac{1}{2} S_{2,1}(n) - \frac{1}{2} S_{-1,1,-1}(n). \end{aligned}$$

Hence we can use the 8 basis sums together with sums of lower weight to express all sums of weight $w = 3$. Note that the sums of lower weight in this example are not yet reduced to a basis.

Remark 2.6.3 (compare [1]). *In the difference field setting of $\Pi\Sigma$ -fields one can verify algebraic independence of sums algorithmically for a particular given finite set of sums; see [81]. We could verify up to weight 8 that the figures \mathbf{N}_A in Table 2.1 are correct, interpreting the objects in $\mathcal{S}(n)/\sim$, i.e., as sequences (see [9]). Nevertheless, unless we do not have a rigorous proof for $\mathcal{S}(n)/\mathcal{I} \cong \mathcal{S}(n)/\sim$, we can only assume that the figures in Table 2.1 give an upper bound.*

Using the difference field setting of $\Pi\Sigma$ -fields it is possible to verify the algebraic independence of a special set of harmonic sums. As an example we could prove that for $m \in \mathbb{N}$ the harmonic sums $\{S_{i,m}(n) \mid i \geq 1\}$ are algebraically independent over $\mathbb{Q}(n)$ (for details we refer to [10]).

2.6.2 Differential Relations

In Section 2.5.3 we described the differentiation of harmonic sums with respect to the upper summation limit. The differentiation leads to new relation, for instance we find

$$\frac{\partial}{\partial n} S_{2,1}(n) = \frac{7\zeta_2^2}{10} + \zeta_2 S_2(n) - S_{2,2}(n) - 2S_{3,1}(n).$$

Example 2.6.4 (Example 2.6.2 continued). *From differentiation we get the additional relations*

$$\begin{aligned} S_{-3}(n) &= S_{-3}(\infty) - \frac{1}{2} \frac{\partial}{\partial n} S_{-2}(n) \\ S_3(n) &= S_3(\infty) - \frac{1}{2} \frac{\partial}{\partial n} S_2(n) \\ S_{-2,1}(n) &= \frac{1}{2} \frac{\partial}{\partial n} S_{-2}(n) - \frac{\partial}{\partial n} S_{-1,1}(n) + S_{-1}(n) S_2(\infty) - S_{-1}(n) S_2(n) \\ &\quad + S_{2,-1}(n) - S_{-3}(\infty) - S_3(\infty) + S_{-2,-1}(\infty). \end{aligned}$$

Hence we could reduce the number of basis sums at weight $w = 3$ to 5 by introducing differentiation. The basis sums are:

$$S_{-2,-1}(n), S_{2,-1}(n), S_{2,1}(n), S_{-1,1,-1}(n), S_{-1,1,1}(n).$$

Note that we collect the derivatives in

$$S_{a_1, \dots, a_k}(n)^{(D)} = \left\{ \frac{\partial^N}{\partial n^N} S_{a_1, \dots, a_k}(n); N \in \mathbb{N} \right\},$$

and identify an appearance of a derivative of a harmonic sum with the harmonic sum itself. This makes sense, since a given finite harmonic sum $S_{a_1, \dots, a_k}(n)$ is determined for $n \in \mathbb{C}$ by its asymptotic representation (see Section 2.8) and the corresponding recursion from $n \rightarrow (n - 1)$ and both, the asymptotic representation and the recursion can be easily differentiated analytically. Hence the differentiation of a harmonic sum with respect to n is closely related to the original sum.

2.6.3 Duplication Relations

Considering harmonic sums up to n together with harmonic sums up to $2 \cdot n$ we find new relations, which are summarized in the following theorem.

Theorem 2.6.5. (see [85, 1]) Let $n, m \in \mathbb{N}$ and $a_i \in \mathbb{N}$ for $i \in \mathbb{N}$. Then we have the following relation:

$$\sum S_{\pm a_m, \pm a_{m-1}, \dots, \pm a_1}(2 \cdot n) = \frac{1}{2^{\sum_{i=1}^m a_i - m}} S_{a_m, a_{m-1}, \dots, a_1}(n) \quad (2.15)$$

where we sum on the left hand side over the 2^m possible combinations concerning \pm .

As for differentiation, when we are counting basis elements, we identify an appearance of a harmonic sum $S_a(2 \cdot n)$ with the harmonic sum $S_a(n)$. We can continue Example 2.6.4:

Example 2.6.6 (Example 2.6.4 continued).

$$\begin{aligned} S_{-2,-1}(n) &= -\frac{1}{2} \frac{\partial}{\partial n} S_{-2}(n) + \frac{\partial}{\partial n} S_{-1,1}(n) + \frac{1}{2} S_{2,1}\left(\frac{n}{2}\right) - S_{-1}(n) S_2(\infty) - 2 S_{2,-1}(n) \\ &\quad + S_{-1}(n) S_2(n) - S_{2,1}(n) + S_{-3}(\infty) + S_3(\infty) - S_{-2,-1}(\infty). \end{aligned}$$

Hence we could reduce the number of basis sums at weight $w = 3$ to 4 by introducing duplication. The basis sums are:

$$S_{2,-1}(n), S_{2,1}(n), S_{-1,1,-1}(n), S_{-1,1,1}(n).$$

2.6.4 Number of Basis Elements

We know that the number of harmonic sums $N_S(w)$ at a specified weight $w \geq 1$ is given by

$$N_S(w) = 2 \cdot 3^{w-1}.$$

This can be seen using the representation of harmonic sums as words in the alphabet $\{-1, 0, 1\}$ as explained on page 27: the last letter is either -1 or 1 , the other $w - 1$ are chosen out of $\{-1, 0, 1\}$. Of course we have $N_S(0) = 0$.

On page 27 we have already seen that the number of algebraic basis harmonic sums for weight $w \geq 2$ is given by

$$N_A(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d.$$

Again we have $N_A(0) = 0$ and $N_A(1) = 2$. This means we can express all the sums of weight w by algebraic relations using $N_A(w)$ harmonic sums of weight w (of course we can not choose them randomly, but there is at least one choice) and sums of lower weight.

Using other types of relations (i.e., those emerging from differentiation, or duplication relations) we can also count the numbers concerning these relations. Of course we can also combine the different types of relations and hence get a different number of basis harmonic sums (as we did in the previous sections for harmonic sums at weight 3). Here we want to present all the different formulas which arise using algebraic, differential and duplication relations.

We start with the formulas which arise if we do not mix the different relations. We already stated the number of algebraic basis harmonic sums, so it remains to give respective numbers concerning differential ($\mathbf{N}_D(w)$) and duplication ($\mathbf{N}_H(w)$) relations:

Proposition 2.6.7.

$$\mathbf{N}_D(w) = \begin{cases} 4 \cdot 3^{w-2}, & w \geq 2 \\ 2, & w = 1 \end{cases} \quad (2.16)$$

$$\mathbf{N}_H(w) = 2 \cdot 3^{w-1} - 2^{w-1}, \quad w \geq 1 \quad (2.17)$$

Proof. Let us start to prove (2.17). From Theorem 2.6.5 we know that there are as many duplication relations at weight w as there are harmonic sums with only positive indices at weight w . The harmonic sums of weight w with positive indices can be viewed as the words of length w out of an alphabet with two letters i.e., $\{0, 1\}$ (compare page 27). Hence there are 2^{w-1} such relations. Since each sum of weight w appears in exactly one of these relations, we can express 2^{w-1} of the $\mathbf{N}_S(w)$ sums by using the remaining sums. Thus $\mathbf{N}_H(w) \leq 2 \cdot 3^{w-1} - 2^{w-1}$ and since we used all possible relations we have $\mathbf{N}_H(w) = 2 \cdot 3^{w-1} - 2^{w-1}$.

In order to prove (2.16), we first take a look at the action of the differential operator $\frac{\partial}{\partial n}$ on a harmonic sum of weight $w - 1$:

$$\begin{aligned} \frac{\partial}{\partial n}(\mathbf{S}_{a_1, a_2, \dots, a_k}(n)) &= -|a_1| \mathbf{S}_{a_1 \wedge 1, a_2, \dots, a_k}(n) - |a_2| \mathbf{S}_{a_1, a_2 \wedge 1, \dots, a_k}(n) \\ &\quad - \dots - |a_k| \mathbf{S}_{a_1, a_2, \dots, a_k \wedge 1}(n) + R(n) \\ &= - \sum_{i=1}^k |a_i| \mathbf{S}_{a_1, \dots, a_{i-1}, a_i \wedge 1, a_{i+1}, \dots, a_k}(n) + R(n); \end{aligned}$$

the harmonic sums popping up in $R(n)$ are of weight less than w and

$$a \wedge b = \text{sign}(a) \text{sign}(b) (|a| + |b|).$$

Note that differentiation increases the weight by 1. Hence only the differentiation of the $\mathbf{N}_S(w - 1)$ sums of weight $w - 1$ leads to relations including harmonic sums of weight w . Let $\mathbf{S}_{a_1, a_2, \dots, a_k}(n)$ be a sum of weight $w - 1$. We use the differentiation of this sum to express, e.g., the sum $\mathbf{S}_{\text{sign}(a_1)(|a_1|+1), a_2, \dots, a_k}(n)$ of weight w . In this way we can

express $N_S(w-1)$ sums (note that we cannot express more sums because the number of relations equals $N_S(w-1)$), hence

$$N_D(w) = N_S(w) - N_S(w-1) = \begin{cases} 2 \cdot 3^{w-1} - 2 \cdot 3^{w-2} = 4 \cdot 3^{w-2}, & w \geq 2 \\ 2 - 0 = 2, & w = 1. \end{cases}$$

□

Note that we have of course $N_D(0) = 0$ and $N_H(0) = 0$. Let us consider the formulas which arise if we mix two different types of relations. There are three different ways to combine 2 types of relations. We give the numbers using algebraic and differential ($N_{AD}(w)$), using algebraic and duplication ($N_{AH}(w)$) and using differential and duplication ($N_{DH}(w)$) relations:

Proposition 2.6.8.

$$N_{AD}(w) = \begin{cases} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) 3^d, & w \geq 2 \\ 2, & w = 1 \end{cases} \quad (2.18)$$

$$N_{AH}(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) [3^d - 2^d] \quad (2.19)$$

$$N_{DH}(w) = \begin{cases} 4 \cdot 3^{w-2} - 2^{w-2}, & w \geq 2 \\ 1, & w = 1. \end{cases} \quad (2.20)$$

Proof. In order to prove (2.18), we first use the algebraic relations to get a basis out of $N_A(w)$ harmonic sums for the sums at weight w . From the differentiation of the harmonic sums of weight $w-1$ we get $N_S(w-1)$ new relations (indeed these relations are different and independent from the algebraic ones since in each relation there is a new symbol; the differential operator applied to a sum of weight $w-1$, i.e., $\frac{\partial}{\partial n} S_{a_1, \dots, a_k}(n)$). However not all of these new relations are independent since the sums of weight $w-1$ fulfill algebraic relations and so do the new symbols. Since there are $N_A(w-1)$ algebraic basis sums of weight $w-1$, we get the same number of independent relations. We can use these $N_A(w-1)$ relations (these are all relations we can use). This reduces the number of algebraic harmonic sums and we get

$$\begin{aligned} N_{AD}(w) &= N_A(w) - N_A(w-1) \\ &= \begin{cases} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) 3^d, & w \geq 2 \\ 2 - 0 = 2, & w = 1. \end{cases} \end{aligned}$$

In order to prove (2.19), we first use the algebraic relations to get a basis out of $N_A(w)$ harmonic sums for the sums at weight w . From the duplication relations of the harmonic sums we get $N_H(w)$ new relations (indeed these relations are different and independent from the algebraic ones since in each relation there is a new symbol; the operator H

applied to a sum of weight w with positive indices, i.e., $H(S_{a_1, \dots, a_k}(n))$). However not all of these new relations are independent since the sums with positive indices of weight w fulfill algebraic relations and so do the new symbols. The harmonic sums of weight w with positive indices can be viewed as the words of length w out of an alphabet with two letters i.e., $\{0, 1\}$ (compare page 27), hence there are $\frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 2^d$ algebraic basis sums for harmonic sums with positive indices (compare this to the explanation for $N_A(w)$). Therefore we get $\frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 2^d$ new independent relations. We can use these $\frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 2^d$ relations (but not more) and reduce the number of algebraic harmonic sums and we get

$$N_{AH}(w) = N_A(w) - \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 2^d = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) [3^d - 2^d].$$

In order to prove (2.20) we first use the duplication relations to get a basis out of $N_H(w)$ harmonic sums for the sums at weight w . From the differentiation of the harmonic sums of weight $w-1$ we get $N_S(w-1)$ new relations (as earlier these relations are different and independent from the duplication relations since in each relation there is a new symbol; the differential operator applied to a sum of weight $w-1$, i.e., $\frac{\partial}{\partial n} S_{a_1, \dots, a_k}(n)$). However not all of these new relations are independent since the sums of weight $w-1$ fulfill duplication relations and so do the new symbols. Since there are $N_H(w-1)$ duplication basis sums of weight $w-1$ we get the same number of independent relations. We can use these $N_H(w-1)$ relations (but not more). This reduces the number of basis duplication harmonic sums further and we get

$$\begin{aligned} N_{DH}(w) &= N_H(w) - N_H(w-1) \\ &= \begin{cases} (2 \cdot 3^{w-1} - 2^{w-1}) - (2 \cdot 3^{w-2} - 2^{w-2}) = 4 \cdot 3^{w-2} - 2^{w-2}, & w \geq 2 \\ 1 - 0 = 1, & w = 1. \end{cases} \end{aligned}$$

□

Note, obviously we have $N_{AD}(0) = 0$, $N_{AH}(0) = 0$ and $N_{DH}(0) = 0$. Let us now consider consider all three types of relations together:

Proposition 2.6.9.

$$N_{ADH}(w) = \begin{cases} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) [3^d - 2^d] - \frac{1}{w-1} \sum_{d|w-1} \mu\left(\frac{w-1}{d}\right) [3^d - 2^d], & w \geq 2 \\ 1, & w = 1. \end{cases}$$

Proof. In order to prove this formula, we first use the algebraic and the duplication relations to get a basis out of $N_{AH}(w)$ harmonic sums for the sums at weight w . From the differentiation of the harmonic sums of weight $w-1$ we get $N_S(w-1)$ new relations (indeed these relations are different and independent from the algebraic together with

the duplication relations since in each relation there is a new symbol; the differential operator applied to a sum of weight $w - 1$, i.e., $\frac{\partial}{\partial n} S_{a_1, \dots, a_k}(n)$. However not all of these new relations are independent since the sums of weight $w - 1$ fulfill algebraic and duplication relations and so do the new symbols. Since there are $N_{\text{AH}}(w - 1)$ algebraic-duplication basis sums of weight $w - 1$, we get the same number of independent relations. We can use these $N_{\text{AH}}(w - 1)$ relations (but not more). This reduces the number of algebraic-duplication basis harmonic sums further and we get

$$\begin{aligned} N_{\text{ADH}}(w) &= N_{\text{AH}}(w) - N_{\text{AH}}(w - 1) \\ &= \begin{cases} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) [3^d - 2^d] - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) [3^d - 2^d], & w \geq 2 \\ 1 - 0 = 1, & w = 1. \end{cases} \end{aligned}$$

□

Let us finally summarize all these formulas:

$$\begin{aligned} N_{\text{S}}(w) &= 2 \cdot 3^{w-1} \\ N_{\text{A}}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d \\ N_{\text{D}}(w) &= 4 \cdot 3^{w-2} \\ N_{\text{H}}(w) &= 2 \cdot 3^{w-1} - 2^{w-1} \\ N_{\text{AD}}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) 3^d \\ N_{\text{AH}}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) [3^d - 2^d] \\ N_{\text{DH}}(w) &= 4 \cdot 3^{w-2} - 2^{w-2} \\ N_{\text{ADH}}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) [3^d - 2^d] - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) [3^d - 2^d]. \end{aligned}$$

Concrete values up to weight 8 are given in Table 2.1; note that the corresponding relations that lead to this amount of basis sums have been explicitly computed using the package `HarmonicSums` and are now available within it.

2.7 Harmonic Sums at Infinity

Not all harmonic sums are finite at infinity, since for example $\lim_{n \rightarrow \infty} S_1(n)$ does not exist. In fact, we have the following lemma, compare [60]:

Lemma 2.7.1. *Let $a_1, a_2, \dots, a_p \in \mathbb{Z}^*$ for $p \in \mathbb{N}$. The harmonic sum $S_{a_1, a_2, \dots, a_p}(n)$ is convergent, when $n \rightarrow \infty$, if and only if $a_1 \neq 1$.*

Weight	Number of							
	N _S	N _A	N _D	N _H	N _{AD}	N _{AH}	N _{DH}	N _{ADH}
1	2	2	2	1	2	1	1	1
2	6	3	4	4	1	2	3	1
3	18	8	12	14	5	6	10	4
4	54	18	36	46	10	15	32	9
5	162	48	108	146	30	42	100	27
6	486	116	324	454	68	107	308	65
7	1458	312	972	1394	196	294	940	187
8	4374	810	2916	4246	498	780	2852	486

Table 2.1: Number of basis sums concerning different relations up to weight 8.

Note that a refined (and generalized) version of this lemma is given in Theorem 3.7.1. As already mentioned in Section 2.1 we are always able to express a harmonic sum as an expression consisting only of sums without leading ones and sums of the type $S_{\mathbf{I}_w}(n)$ with $w \in \mathbb{N}$. Since sums without leading ones are convergent, they do not produce any problems. For sums of the type $S_{\mathbf{I}_w}(n)$ we have the following proposition which is a direct consequence of Corollary 3 of [37] and Proposition 2.1 of [52].

Proposition 2.7.2. *For $w \geq 1$ and $n \in \mathbb{N}$, we have*

$$S_{\mathbf{I}_w}(n) = \sum_{i=1}^n (-1)^{i-1} \binom{n}{i} \frac{1}{i^w} = -\frac{1}{w} Y_w(\dots, (j-1)! S_j(n), \dots),$$

where $Y_w(\dots, x_i, \dots)$ are the Bell polynomials.

Note that the explicit formulas were found empirically in [27]; for a determinant evaluation formula we refer to [27, 36, 15]. Using this proposition we can express each sum of the type $S_{\mathbf{I}_w}(n)$ by sums of the form $S_i(n)$, where $i \in \mathbb{Z}$. Hence we can decompose each harmonic sum $S_{a_1, a_2, \dots, a_p}(n)$ in a univariate polynomial in $S_1(n)$ with coefficients in the convergent harmonic sums. So all divergences can be traced back to the basic divergence of $S_1(n)$ when $n \rightarrow \infty$.

Notation 2.7.3. *We will define the symbol $S_1(\infty) := \lim_{n \rightarrow \infty} S_1(n)$, and every time it is present, we are in fact dealing with limit processes. For $k \in \mathbb{N}$ with $k > 1$ the harmonic sums $S_k(\infty)$ turn into zeta-values and we will sometimes write ζ_k for $S_k(\infty)$.*

Example 2.7.4.

$$\begin{aligned} \lim_{n \rightarrow \infty} S_{1,1,2}(n) &= \lim_{n \rightarrow \infty} \left\{ \frac{1}{2} S_1(n)^2 S_2(n) + S_1(n) (S_3(n) - S_{2,1}(n)) \right. \\ &\quad \left. - S_{3,1}(n) + \frac{1}{2} S_4(n) + S_{2,1,1}(n) \right\} \\ &= S_1(\infty)^2 \frac{\zeta_2}{2} - S_1(\infty) \zeta_3 + \frac{9\zeta_2^2}{10}. \end{aligned}$$

For the computation of the actual values of the harmonic sums at infinity see [85].

2.7.1 Relations between Harmonic Sums at Infinity

In this section we just want to give several types of relations between the values of harmonic sums at infinity which are of importance in the following chapters. Note that harmonic sums at infinity are closely related to the multiple zeta values; for details we refer to [23, 85, 32, 33, 50, 90].

- The first type of relations originate from the algebraic relations of harmonic sums, see Section 2.6.1. These relations remain valid when we consider them at infinity. We will refer to this relations as the stuffle relations.
- The duplication relations from Section 2.6.3 remain valid if we consider sums which are finite at infinity (i.e., do not have leading ones), since it makes no difference whether the argument is ∞ or $\frac{\infty}{2}$.
- In [85] the following relation for not both $m_1 = 1$ and $k_1 = 1$ can be found:

$$S_{m_1, \dots, m_p}(\infty) S_{k_1, \dots, k_q}(\infty) = \lim_{n \rightarrow \infty} \sum_{i=1}^n \frac{\text{sign}(k_1)^i S_{m_1, \dots, m_p}(n-i) S_{k_2, \dots, k_q}(i)}{i^{|k_1|}}.$$

Using

$$\begin{aligned} \sum_{i=1}^n \frac{\text{sign}(k_1)^i S_{m_1, \dots, m_p}(n-i) S_{k_2, \dots, k_q}(i)}{i^{|k_1|}} &= \sum_{a=1}^k \binom{|k_1| + |m_1| - 1 - a}{|m_1| - 1} \sum_{i=1}^n \frac{\text{sign}(m_1)^i}{i^{|m_1| + |k_1| - a}} \\ &\quad \sum_{j=1}^i \frac{\text{sign}\left(\frac{k_1}{m_1}\right)^j S_{m_2, \dots, m_p}(i-j) S_{k_2, \dots, k_q}(j)}{j^a} \\ &+ \sum_{a=1}^{m_1} \binom{|k_1| + |m_1| - 1 - a}{|m_1| - 1} \sum_{i=1}^n \frac{\text{sign}(m_1)^i}{i^{|m_1| + |k_1| - a}} \\ &\quad \sum_{j=1}^i \frac{\text{sign}\left(\frac{k_1}{m_1}\right)^j S_{m_2, \dots, m_p}(j) S_{k_2, \dots, k_q}(i-j)}{j^a}, \end{aligned}$$

we can rewrite the right hand side in terms of harmonic sums. We will refer to these relations as the shuffle relations since one could also obtain them from the shuffle algebra of harmonic polylogarithms.

- In [23] in addition so called generalized doubling relations are considered.

All these relations enable us to express harmonic sums at infinity up to weight 8 using the following 19 constants:

$$\{S_{-1}(\infty), S_2(\infty), S_3(\infty), S_5(\infty), S_7(\infty), S_{-1,1,1,1}(\infty), S_{-1,1,1,1,1}(\infty), \\ S_{-1,1,1,1,1,1}(\infty), S_{-5,-1}(\infty), S_{-1,1,1,1,1,1,1}(\infty), S_{-5,1,1}(\infty), S_{5,-1,-1}(\infty), \\ S_{-1,1,1,1,1,1,1,1}(\infty), S_{5,3}(\infty), S_{-7,-1}(\infty), S_{-5,-1,-1,-1}(\infty), S_{-5,-1,1,1}(\infty)\}.$$

The way we chose these constants is not unique, one could look for other basis constants. Note, that the corresponding relations, that enables one to rewrite an expression with infinite harmonic sums up to weight 8 to an expression with these basis sums, are available within the `HarmonicSums` package.

2.8 Asymptotic Expansion of Harmonic Sums

In [60] an algorithm to compute asymptotic expansions of harmonic sums with positive indices was introduced, while in [12] a different approach was used to compute asymptotic expansions of harmonic sums including negative indices. In this section we will use a new approach and provide an efficient algorithm to compute asymptotic expansions of harmonic sums (including negative indices); this approach is inspired by [21, 22].

In general we say that the function $f : \mathbb{R} \rightarrow \mathbb{R}$ is expanded in an asymptotic series

$$f(x) \sim \sum_{n=1}^{\infty} \frac{a_n}{x^n}, \quad x \rightarrow \infty,$$

where a_n are constants from \mathbb{R} , if for all $N \geq 0$

$$R_N(x) = f(x) - \sum_{n=0}^N \frac{a_n}{x^n} \in o\left(\frac{1}{x^N}\right), \quad x \rightarrow \infty;$$

note, here a function $g(x) \in o(G(x)) \Leftrightarrow \lim_{x \rightarrow \infty} \left| \frac{g(x)}{G(x)} \right| = 0$.

In order to compute asymptotic series for harmonic sums, we will use their representations as Mellin transforms of harmonic polylogarithms. But first we have to state several details.

2.8.1 Extending Harmonic Polylogarithms

In the following we look again at the change of the variable $1 - x \rightarrow x$ for harmonic polylogarithms (compare Section 2.3.1). This transformation can as well be found in [73], however we will generalize it to index sets including -1 . In order to accomplish this extension, we will first introduce an extension for the harmonic polylogarithms. We introduce 2 as a member of the index set as follows.

Definition 2.8.1. *Let $m_i \in \{-1, 0, 1, 2\}$; for $x \in (0, 1)$ we extend the harmonic polylogarithms from Definition 2.2.1 by introducing in addition*

$$H_2(x) = \int_0^x \frac{1}{2-y} dy$$

and

$$H_{2,m_2,\dots,m_w}(x) = \int_0^x \frac{H_{m_2,\dots,m_w}(x)}{2-y} dy.$$

Remark 2.8.2. *The extended harmonic polylogarithms are still analytic functions for $x \in (0, 1)$ and the differentiation extends as follows:*

$$\frac{d}{dx} H_{2,m_2,\dots,m_w}(x) = \frac{H_{m_2,\dots,m_w}(x)}{2-x}.$$

The product of these extended harmonic polylogarithms is still the shuffle product and still only harmonic polylogarithms with leading 1 and not followed only by zeroes are not finite at 1.

Example 2.8.3.

$$\begin{aligned} H_{1,2}(x) H_{0,2,-1}(x) &= H_{0,1,2,-1,2}(x) + 2 H_{0,1,2,2,-1}(x) + H_{0,2,-1,1,2}(x) + H_{0,2,1,-1,2}(x) \\ &\quad + H_{0,2,1,2,-1}(x) + H_{1,0,2,-1,2}(x) + 2 H_{1,0,2,2,-1}(x) + H_{1,2,0,2,-1}(x). \end{aligned}$$

Remark 2.8.4. *For further extensions of the index set, we refer to the later chapters.*

Extension of the $1 - x \rightarrow x$ Transform

Let us again look at the transformation $1 - x \rightarrow x$ (compare Section 2.3.1). Proceeding recursively on the weight w of the harmonic polylogarithm we have for $x \in (0, 1)$

$$H_0(1-x) = -H_1(x) \tag{2.21}$$

$$H_1(1-x) = -H_0(x) \tag{2.22}$$

$$H_{-1}(1-x) = H_{-1}(1) - H_2(x) \tag{2.23}$$

$$H_2(1-x) = H_2(1) - H_{-1}(x). \tag{2.24}$$

Now let us look at higher weights $w > 1$. We consider $H_{m_1, m_2, \dots, m_w}(1-x)$ and suppose that we can already apply the transform for harmonic polylogarithms of weight $< w$. If $m_1 = 1$ we can remove leading ones and end up with harmonic polylogarithms without leading ones and powers of $H_1(1-x)$. For the powers of $H_1(1-x)$ we can use (2.22); therefore, only the cases in which the first index $m_1 \neq 1$ are to be considered. For $m_1 = 0$ we get (see [73]):

$$\begin{aligned} H_{0, m_2, \dots, m_w}(1-x) &= \int_0^{1-x} \frac{H_{m_2, \dots, m_w}(y)}{y} dy \\ &= \int_0^1 \frac{H_{m_2, \dots, m_w}(y)}{y} dy - \int_{1-x}^1 \frac{H_{m_2, \dots, m_w}(y)}{y} dy \\ &= H_{0, m_2, \dots, m_w}(1) - \int_0^x \frac{H_{m_2, \dots, m_w}(1-t)}{1-t} dt, \end{aligned} \quad (2.25)$$

where the constant $H_{0, m_2, \dots, m_w}(1)$ is finite. For $m_1 = -1$ we get:

$$\begin{aligned} H_{-1, m_2, \dots, m_w}(1-x) &= \int_0^{1-x} \frac{H_{m_2, \dots, m_w}(y)}{1+y} dy \\ &= \int_0^1 \frac{H_{m_2, \dots, m_w}(y)}{1+y} dy - \int_{1-x}^1 \frac{H_{m_2, \dots, m_w}(y)}{1+y} dy \\ &= H_{-1, m_2, \dots, m_w}(1) - \int_0^x \frac{H_{m_2, \dots, m_w}(1-t)}{2-t} dt, \end{aligned} \quad (2.26)$$

where the constant $H_{-1, m_2, \dots, m_w}(1)$ is finite. Finally for $m_1 = 2$ we get:

$$\begin{aligned} H_{2, m_2, \dots, m_w}(1-x) &= \int_0^{1-x} \frac{H_{m_2, \dots, m_w}(y)}{2-y} dy \\ &= \int_0^1 \frac{H_{m_2, \dots, m_w}(y)}{2-y} dy - \int_{1-x}^1 \frac{H_{m_2, \dots, m_w}(y)}{2-y} dy \\ &= H_{2, m_2, \dots, m_w}(1) - \int_0^x \frac{H_{m_2, \dots, m_w}(1-t)}{1+t} dt, \end{aligned} \quad (2.27)$$

where the constant $H_{2, m_2, \dots, m_w}(1)$ is finite. Since we know the transform for weights $< w$, we can apply it to $H_{m_2, \dots, m_w}(1-t)$ and finally we obtain the required weight w identity by using the definition of the extended harmonic polylogarithms.

Example 2.8.5. For $x \in (0, 1)$

$$\begin{aligned} H_{-1,1}(1-x) &= H_{-1,1}(1) + H_{2,0}(x) \\ H_{1,-1,2}(1-x) &= -H_0(x) H_{-1,2}(1) + H_2(1) H_{0,2}(x) - H_{-1,1,2}(1) \\ &\quad - H_{-1,2,1}(1) - H_{0,2,-1}(x). \end{aligned}$$

Remark 2.8.6. If we apply the transform $1-x \rightarrow x$ to the harmonic polylogarithm $H_{m_1, m_2, \dots, m_w}(1-x)$ and if we afterwards expand all the products of polylogarithms at x it is easy to see, that there will be just one harmonic polylogarithm $H_{n_1, n_2, \dots, n_w}(x)$ at x with weight w . The index set of this harmonic polylogarithm changed as follows:

- if $m_i = 1$ then $n_i = 0$
- if $m_i = 0$ then $n_i = 1$
- if $m_i = -1$ then $n_i = 2$
- if $m_i = 2$ then $n_i = -1$.

If we want to apply the transform $x \rightarrow 1 - x$ to the harmonic polylogarithm $H_{n_1, n_2, \dots, n_w}(x)$, we have two possibilities:

1. Set $x = 1 - y$; apply the transform $1 - y \rightarrow y$; replace y by $1 - x$.
2. By Remark 2.8.6 we construct $H_{m_1, m_2, \dots, m_w}(1 - x)$; we apply the transform to $H_{m_1, m_2, \dots, m_w}(1 - x)$; in the result we find $H_{n_1, n_2, \dots, n_w}(x)$. Note that there might still be other harmonic polylogarithms at x but their weight is smaller than w ; for all these harmonic polylogarithms we can apply the same strategy.

The advantage of the second strategy is that if we apply first the transform $1 - x \rightarrow x$ to $H_{m_1, m_2, \dots, m_w}(1 - x)$ and then $x \rightarrow 1 - x$ to the result, we get back $H_{m_1, m_2, \dots, m_w}(1 - x)$ immediately. Using the first strategy we might have to know various relations to get back to $H_{m_1, m_2, \dots, m_w}(1 - x)$. We will illustrate this with an example:

Example 2.8.7. *Transforming $H_{1,0,1}(1 - x)$ we get $H_0(x)H_{0,1}(1) - H_{0,1,0}(x) - 2H_{0,1,1}(1)$. If we transform back using the first strategy, we end up with $-H_{0,1,0}(1) - 2H_{0,1,1}(1) + H_{1,0,1}(1 - x)$; note that we introduced $-H_{0,1,0}(1) - 2H_{0,1,1}(1)$ which turns out to be zero. But using the second strategy we do not need this additional knowledge to remove possibly introduced zeros.*

Lemma 2.8.8. *Let $x \in (0, 1)$. If we perform the the transformation $1 - x \rightarrow x$ to the harmonic polylogarithm $H_{m_1, m_2, \dots, m_w}(1 - x)$, where $m_i \neq -1$ and express it by harmonic polylogarithms with argument x , then the index 2 does not appear in the resulting harmonic polylogarithms with argument x . It is however possible that 2 appears in the resulting harmonic polylogarithms at 1.*

Proof. For $w = 1$ we have:

$$\begin{aligned}
 H_0(1 - x) &= -H_1(x) \\
 H_1(1 - x) &= -H_0(x) \\
 H_2(1 - x) &= H_2(1) - H_{-1}(x).
 \end{aligned} \tag{2.28}$$

Assume the lemma holds for weights $< w$. We have:

$$\mathbb{H}_{2,m_2,\dots,m_w}(1-x) = \mathbb{H}_{2,m_2,\dots,m_w}(1) - \int_0^x \frac{\mathbb{H}_{m_2,\dots,m_w}(1-t)}{1+t} dt \quad (2.29)$$

$$\mathbb{H}_{0,m_2,\dots,m_w}(1-x) = \mathbb{H}_{0,m_2,\dots,m_w}(1) - \int_0^x \frac{\mathbb{H}_{m_2,\dots,m_w}(1-t)}{1-t} dt. \quad (2.30)$$

Since the lemma holds for weights $< w$, it holds for $\mathbb{H}_{m_2,\dots,m_w}(1-t)$, thus it can be written in the right format. If $m_1 = 1$ then we extract the leading ones (this does not generate the index -1) and afterwards we can use (2.28), (2.29) and (2.30) to obtain the desired format. \square

Lemma 2.8.9. *If we perform the the transformation $x \rightarrow 1-x$ (no matter which strategy of the two we use) to the harmonic polylogarithm $\mathbb{H}_{m_1,m_2,\dots,m_w}(x)$, where $m_i \neq 2$, and express it by harmonic polylogarithms with argument $1-x$, then the index -1 does not appear in the resulting harmonic polylogarithms with argument $1-x$. It is however possible that -1 appears in the resulting harmonic polylogarithms at 1.*

Proof. We just give a proof for the second strategy. For $w = 1$ we have:

$$\begin{aligned} \mathbb{H}_0(x) &= -\mathbb{H}_1(1-x) \\ \mathbb{H}_1(x) &= -\mathbb{H}_0(1-x) \\ \mathbb{H}_{-1}(x) &= \mathbb{H}_2(1) - \mathbb{H}_2(1-x). \end{aligned} \quad (2.31)$$

Assume the lemma holds for weights $< w$. $\mathbb{H}_{m_1,\dots,m_w}(x)$ arises from $\mathbb{H}_{n_1,\dots,n_w}(1-x)$ where $n_i = 2, 0, 1$ if $m_i = -1, 1, 0$, so $n_i \neq -1$. Hence, according to the previous lemma in the transform of $\mathbb{H}_{n_1,\dots,n_w}(1-x)$ there is no index 2 in the harmonic polylogarithms at x . All the the harmonic polylogarithms in the transform at x (except $\mathbb{H}_{m_1,\dots,m_w}(x)$ itself) have weight less than w and therefore the index -1 does not appear in their transform (except in harmonic sums at 1). \square

Remark 2.8.10. *If we want to remove the index 2 from $\mathbb{H}_{m_1,\dots,m_w}(1)$, we can use the transform $x \rightarrow 1-x$ for $\mathbb{H}_{m_1,\dots,m_w}(x)$ and afterwards we replace x by 1 in the result. All the indices 2 are removed.*

2.8.2 Asymptotic Representations of Factorial Series

We can use the Mellin transform of harmonic polylogarithms to represent harmonic sums. Hence any partial result to derive asymptotic expansions of integrals of the form

$$\int_0^1 \frac{x^n \mathbb{H}_m(x)}{1+x} dx \quad \text{and} \quad \int_0^1 \frac{(x^n - 1) \mathbb{H}_m(x)}{1-x} dx$$

will support us to obtain asymptotic expansions of the harmonic sums. For the following we refer to [21, 67, 53]. Let us look at the Mellin transform

$$M(\varphi(x), n) = \int_0^1 x^n \varphi(x) dx$$

where $\varphi(x)$ is analytic at $x = 1$ and has the following Taylor series expansion about $x = 1$,

$$\varphi(1-x) = \sum_{k=0}^{\infty} a_k x^k.$$

For $\operatorname{Re}(x) > 0$, $M(\varphi(x), n)$ is given by the factorial series

$$M(\varphi(x), n) = \sum_{k=0}^{\infty} \frac{a_k k!}{(n+1)(n+2)\dots(n+k+1)}.$$

$M(\varphi(x), n)$ has poles at the negative integers and one may continue $M(\varphi(x), n)$ analytically to values of $n \in \mathbb{C}$ as a meromorphic function. The asymptotic representation is

$$M(\varphi(x), n) \sim \sum_{k=0}^{\infty} \frac{b_k}{n^{k+1}}, \quad n \rightarrow \infty, \quad (2.32)$$

where

$$\begin{aligned} b_0 &= a_0 \\ b_k &= \sum_{l=0}^{k-1} (-1)^{l+1} S_{k-l}^k a_{k-l} (k-l)! \end{aligned}$$

and S_l^k are the Stirling numbers of 2nd kind.

Example 2.8.11 (Asymptotic expansion of $S_{-1}(n)$). *First we express $S_{-1}(n)$ using the Mellin transformation:*

$$S_{-1}(n) = \int_0^1 x^n \overbrace{\frac{1}{1+x}}^{\varphi(x)} dx + \log(2) = M(\varphi(x), n) + \log(2).$$

The Taylor series expansion of $\varphi(1-x)$ yields:

$$\varphi(1-x) = \frac{1}{2-x} = \sum_{k=0}^{\infty} \frac{1}{2^{k+1}} x^k.$$

Hence the factorial series of $M(\varphi(x), n)$ is given by

$$M(\varphi(x), n) = \frac{1}{2(1+n)} + \frac{1}{4(1+n)(1+n)} + \frac{2}{8n(1+n)(2+n)(3+n)}$$

$$+ \frac{6}{16n(1+n)(2+n)(3+n)(4+n)} + \dots,$$

which leads to the following asymptotic representation of $M(\varphi(x), n)$:

$$M(\varphi(x), n) = \frac{1}{2n} - \frac{1}{4n^2} + \frac{1}{8n^4} + o\left(\frac{1}{n^6}\right).$$

Combining the results yields

$$S_{-1}(n) = \log(2) + \frac{1}{2n} - \frac{1}{4n^2} + \frac{1}{8n^4} + o\left(\frac{1}{n^6}\right).$$

If we are interested in accuracy of this expansion, the following considerations may help. From repeated integration by parts we get:

$$M(\varphi(x), n) = \sum_{s=0}^k \frac{a_s s!}{(n+1)(n+2)\dots(n+k+1)} + \frac{(-1)^{k+1} R_{k+1}(n)}{(n+1)(n+2)\dots(n+k+1)}$$

with

$$R_{k+1}(n) = \int_0^1 x^{n+k} \varphi^{(k)}(x) dx,$$

or similarly

$$M(\varphi(x), n) = \sum_{s=0}^k \frac{b_s}{n^{s+1}} + \underbrace{\frac{(-1)^{k+1}}{n^{k+1}} \int_0^1 x^{n-1} (D_x)^k (x \varphi(x)) dx}_{\bar{R}_{k+1}(n):=}$$

with

$$D_x(f(x)) := x f'(x);$$

for the estimate \bar{R}_{k+1} we can use in addition

$$(D_x)^k (x f(x)) = \sum_{i=0}^k g(i+1, k) x^{i+1} f^{(i)}(x), \quad \text{with } g(i, k) := \sum_{j=1}^i (-1)^j \frac{j^{k+1}}{(i-j)! j!}.$$

Example 2.8.12 (Asymptotic expansion of $S_{-1}(n)$ continued). *We get*

$$\begin{aligned} \int_0^1 \frac{x^n}{1+x} dx &= \int_0^1 x^{n-1} \frac{x}{1+x} dx = \frac{x^n}{n} \frac{x}{1+x} \Big|_0^1 - \int_0^1 \frac{x^n}{n} \frac{1}{(1+x)^2} dx \\ &= \frac{1}{2n} - \int_0^1 x^{n-1} \frac{x}{n(1+x)^2} dx \\ &= \frac{1}{2n} - \frac{x^n}{n} \frac{x}{n(1+x)^2} \Big|_0^1 + \int_0^1 \frac{x^n}{n} \frac{(1-x)}{n(1+x)^3} dx \\ &= \frac{1}{2n} - \frac{1}{4n^2} + \int_0^1 x^{n-1} \frac{x(1-x)}{n^2(1+x)^3} dx \end{aligned}$$

$$= \dots = \frac{1}{2n} - \frac{1}{4n^2} + \frac{1}{8n^4} - \frac{1}{4n^6} + \frac{1}{n^6} \bar{R}_6(n)$$

with $|\bar{R}_6(n)| \leq 2$. Hence

$$\left| \int_0^1 \frac{x^{20}}{1+x} dx - \frac{6240199}{256000000} \right| \leq \frac{1}{32000000}.$$

As the previous example suggests, we can use repeated integration by parts to get the b_k of equation (2.32) directly. Unfortunately not all integrals of the form

$$\int_0^1 \frac{x^n \mathbf{H}_{m_1, m_2, \dots, m_{k-1}, m_k}(x)}{1 \pm x} dx$$

can be expanded in that way up to arbitrary order, since $\frac{\mathbf{H}_{m_1, m_2, \dots, m_{k-1}, m_k}(x)}{1 \pm x}$ does not have to be analytic at $x = 1$. In the following we will explore certain functions (see Lemma 2.8.14 and Lemma 2.8.15), which are analytic at 1 (and hence infinitely times differentiable). We will try afterwards to transform all the integrals $\int_0^1 \frac{x^n \mathbf{H}_{m_1, m_2, \dots, m_{k-1}, m_k}(x)}{1 \pm x} dx$ as far as possible into a form given in terms of these analytic functions at 1 and therefore we can use the method mentioned above to find an asymptotic representation. In the following lemma we will summarize some properties of the n -th derivatives of functions that we will come across.

Lemma 2.8.13. *Let $f : D \rightarrow \mathbb{R}$ be an analytic function on D with $D \subset \mathbb{R}$. For $x \in D$ and $n \in \mathbb{N}$ we have,*

$$\begin{aligned} \left(\frac{f(x)}{1-x} \right)^{(n)} &= \frac{1}{(1-x)^{n+1}} \sum_{k=0}^n \frac{n!}{k!} f^{(k)}(x) (1-x)^k \\ \left(\frac{f(x)}{1+x} \right)^{(n)} &= \frac{(-1)^n}{(1+x)^{n+1}} \sum_{k=0}^n (-1)^k \frac{n!}{k!} f^{(k)}(x) (1+x)^k \\ \left(\frac{f(x)}{x} \right)^{(n)} &= \frac{(-1)^n}{x^{n+1}} \sum_{k=0}^n (-1)^k \frac{n!}{k!} f^{(k)}(x) x^k. \end{aligned}$$

Proof. All three identities follow from the Leibniz rule; for instance:

$$\begin{aligned} \left(\frac{f(x)}{1-x} \right)^{(n)} &= \sum_{k=0}^n \binom{n}{k} f^{(k)}(x) \left(\frac{1}{1-x} \right)^{(n-k)} = \sum_{k=0}^n \binom{n}{k} f^{(k)}(x) \frac{(n-k)!}{(1-x)^{n-k+1}} \\ &= \frac{1}{(1-x)^{n+1}} \sum_{k=0}^n \frac{n!}{k!} f^{(k)}(x) (1-x)^k. \end{aligned}$$

□

Lemma 2.8.14. *Let $H_{m_1, m_2, \dots, m_k}(x)$ be a harmonic polylogarithm with $m_i \in \{0, -1\}$ for $1 \leq i \leq k$. Then*

$$H_{m_1, m_2, \dots, m_k}(x), \frac{H_{m_1, m_2, \dots, m_k}(x)}{1+x}$$

and

$$\frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{1-x}$$

are analytic for $x \in (0, \infty)$.

Proof. We know that $H_0(x)$ and $H_{-1}(x)$ are analytic $\in (0, \infty)$. Now we suppose the harmonic polylogarithms with indices $\in \{0, -1\}$ of depth $k-1$ are analytic and consider the the n -th derivative of $H_{m_1, m_2, \dots, m_k}(x)$: If $m_1 = -1$, we get

$$\begin{aligned} H_{-1, m_2, \dots, m_k}(x)^{(n)} &= \left(\frac{H_{m_2, \dots, m_k}(x)}{1+x} \right)^{(n-1)} \\ &= \frac{(-1)^{n-1}}{(1+x)^n} \sum_{k=0}^{n-1} (-1)^k \frac{(n-1)!}{k!} H_{m_2, \dots, m_k}(x)^{(k)} (1+x)^k \end{aligned}$$

using Lemma 2.8.13. Similarly, if $m_1 = 0$, we get

$$H_{-1, m_2, \dots, m_k}(x)^{(n)} = \frac{(-1)^{n-1}}{x^n} \sum_{k=0}^{n-1} (-1)^k \frac{(n-1)!}{k!} H_{m_2, \dots, m_k}(x)^{(k)} x^k.$$

In both cases $H_{m_1, m_2, \dots, m_k}(x)$ is analytic for $x \in (0, \infty)$ since $H_{m_2, \dots, m_k}(x)$ is analytic for $x \in (0, \infty)$. Moreover, $\frac{H_{m_1, m_2, \dots, m_k}(x)}{1+x}$ is analytic since $H_{m_1, m_2, \dots, m_k}(x)$ and $\frac{1}{1+x}$ are analytic. Finally we look at

$$\frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{1-x};$$

for $x \in (0, 1) \cup (1, \infty)$ the analyticity can be seen as in the previous case. In the following we will use the abbreviation $f(x) := H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)$. For $x = 1$ we get using Lemma 2.8.13 and by using de l'Hospital's rule $n+1$ times (note that $\frac{\partial^{n+1}}{\partial x^{n+1}}(1-x)^{n+1} = (-1)^{n+1}(n+1)!$):

$$\begin{aligned} \lim_{x \rightarrow 1} \left(\frac{f(x)}{1-x} \right)^{(n)} &= \lim_{x \rightarrow 1} \frac{1}{(1-x)^{n+1}} \sum_{k=0}^n \frac{n!}{k!} f(x)^{(k)} (1-x)^k \\ &= \lim_{x \rightarrow 1} \frac{(-1)^{n+1}}{(n+1)!} \sum_{k=0}^n \frac{n!}{k!} \left(f(x)^{(k)} (1-x)^k \right)^{(n+1)} \\ &= \lim_{x \rightarrow 1} \frac{(-1)^{n+1}}{n+1} \sum_{k=0}^n \frac{1}{k!} \sum_{i=0}^{n+1} \binom{n+1}{i} f(x)^{(k+i)} ((1-x)^k)^{(n+1-i)} \\ &= \lim_{x \rightarrow 1} \frac{(-1)^{n+1}}{n+1} \sum_{k=0}^n \frac{1}{k!} \sum_{i=n-k+1}^{n+1} \binom{n+1}{i} f(x)^{(k+i)} \end{aligned}$$

$$\begin{aligned} & \times \frac{k!(-1)^{n+1-i}}{(k-n-1+i)!} (1-x)^{k-n-1+i} \\ & = \frac{1}{n+1} \sum_{k=0}^n \binom{n+1}{n-k+1} f(1)^{(n+1)} (-1)^{n-k+1} = -\frac{f(1)^{(n+1)}}{n+1}. \end{aligned}$$

Hence $\frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{1-x}$ is analytic for $x \in (0, \infty)$. \square

Using similar arguments as in the proof of the previous lemma we get the following lemma.

Lemma 2.8.15. *Let $H_{m_1, m_2, \dots, m_k}(x)$ be a harmonic polylogarithm with $m_i \in \{1, 0, -1, 2\}$ for $1 \leq i \leq k$, and $m_k \neq 0$. Then*

$$\frac{H_{m_1, m_2, \dots, m_k}(1-x)}{1+x}$$

and

$$\frac{H_{m_1, m_2, \dots, m_k}(1-x)}{1-x}$$

are analytic for $x \in (0, 2)$.

Lemma 2.8.16. *Let $H_m(x) = H_{m_1, m_2, \dots, m_k}(x)$ and $H_b(x) = H_{b_1, b_2, \dots, b_l}(x)$ be harmonic polylogarithms with $m_i, b_i \in \{1, 0, -1, 2\}$, $m_1 \neq 1$ and $b_l \neq 0$. Then we have*

$$M\left(\frac{H_m(x)}{1-x}, n\right) = \int_0^1 \frac{x^n (H_m(x) - H_m(1))}{1-x} dx - \int_0^1 \frac{H_m(x) - H_m(1)}{1-x} dx - S_1(n) H_m(1),$$

and

$$M\left(\frac{H_b(1-x)}{1-x}, n\right) = \int_0^1 \frac{x^n H_b(1-x)}{1-x} dx - H_{0, b}(1)$$

where

$$\int_0^1 \frac{H_m(x) - H_m(1)}{1-x} dx, \quad H_m(1) \quad \text{and} \quad H_{0, b}(1)$$

are finite constants.

Proof. By integration by parts we get

$$\begin{aligned} & \int_0^1 \frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{1-x} dx \\ & = \lim_{\epsilon \rightarrow 1^-} \int_0^\epsilon \frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{1-x} dx \\ & = \lim_{\epsilon \rightarrow 1^-} \left((H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)) H_1(x) \Big|_0^\epsilon \right. \\ & \quad \left. - \int_0^\epsilon \frac{H_{m_2, m_3, \dots, m_k}(x) H_1(x)}{x - m_1} dx \right) \\ & = 0 - \lim_{\epsilon \rightarrow 1^-} \int_0^\epsilon \frac{H_{1, m_2, \dots, m_k}(x) + H_{m_2, 1, m_3, \dots, m_k}(x) + \dots + H_{m_2, \dots, m_k, 1}(x)}{x - m_1} dx \end{aligned}$$

$$\begin{aligned}
&= - \lim_{\epsilon \rightarrow 1^-} (\mathbf{H}_{m_1,1,m_2,\dots,m_k}(\epsilon) + \mathbf{H}_{m_1,m_2,1,m_3,\dots,m_k}(\epsilon) + \dots + \mathbf{H}_{m_1,m_2,\dots,m_k,1}(\epsilon)) \\
&= -\mathbf{H}_{m_1,1,m_2,\dots,m_k}(1) - \mathbf{H}_{m_1,m_2,1,m_3,\dots,m_k}(1) - \dots - \mathbf{H}_{m_1,m_2,\dots,m_k,1}(1).
\end{aligned}$$

Since $m_1 \neq 1$ all these harmonic polylogarithms are finite. The same is true for $\mathbf{H}_m(1)$ and $\mathbf{H}_{0,b}(1)$. Now we get

$$\begin{aligned}
\mathbf{M}\left(\frac{\mathbf{H}_m(x)}{1-x}, n\right) &= \int_0^1 \frac{(x^n - 1)\mathbf{H}_m(x)}{1-x} dx \\
&= \int_0^1 \frac{x^n \mathbf{H}_m(x) - \mathbf{H}_m(x) - x^n \mathbf{H}_m(1) + x^n \mathbf{H}_m(1) - \mathbf{H}_m(1) + \mathbf{H}_m(1)}{1-x} dx \\
&= \int_0^1 \frac{x^n (\mathbf{H}_m(x) - \mathbf{H}_m(1))}{1-x} dx - \int_0^1 \frac{\mathbf{H}_m(x) - \mathbf{H}_m(1)}{1-x} dx + \mathbf{H}_m(1) \int_0^1 \frac{x^n - 1}{1-x} dx \\
&= \int_0^1 \frac{x^n (\mathbf{H}_m(x) - \mathbf{H}_m(1))}{1-x} dx - \int_0^1 \frac{\mathbf{H}_m(x) - \mathbf{H}_m(1)}{1-x} dx - \mathbf{S}_1(n) \mathbf{H}_m(1)
\end{aligned}$$

and

$$\begin{aligned}
\mathbf{M}\left(\frac{\mathbf{H}_b(1-x)}{1-x}, n\right) &= \int_0^1 \frac{(x^n - 1)\mathbf{H}_b(1-x)}{1-x} dx \\
&= \int_0^1 \frac{x^n \mathbf{H}_b(1-x)}{1-x} dx - \int_0^1 \frac{\mathbf{H}_b(1-x)}{1-x} dx \\
&= \int_0^1 \frac{x^n \mathbf{H}_b(1-x)}{1-x} dx - \mathbf{H}_{0,b}(1).
\end{aligned}$$

□

Remark 2.8.17. Combining Lemma 2.8.14, Lemma 2.8.15 and 2.8.16 we are able to compute the asymptotic expansion of Mellin transforms of the form

$$\mathbf{M}\left(\frac{\mathbf{H}_{m_1,m_2,\dots,m_k}(x)}{1 \pm x}, n\right) \quad \text{and} \quad \mathbf{M}\left(\frac{\mathbf{H}_{b_1,b_2,\dots,b_k}(1-x)}{1 \pm x}, n\right)$$

where $m_i \in \{-1, 0\}$, $b_i \in \{-1, 0, 1, 2\}$ and $b_l \neq 0$ using the method presented in the beginning of this section, or using repeated integration by parts.

2.8.3 Computation of Asymptotic Expansions of Harmonic Sums

The following observation is crucial.

Lemma 2.8.18. 1. If a harmonic sum $\mathbf{S}_{a_1,a_2,\dots,a_k}(n)$ has no trailing ones, i.e., $a_k \neq 1$ then the most complicated harmonic polylogarithm in the inverse Mellin transform of $\mathbf{S}_{a_1,a_2,\dots,a_k}(n)$ has no trailing ones.

2. If a harmonic polylogarithm $\mathbf{H}_{m_1,m_2,\dots,m_k}(x)$ has no trailing ones, i.e., $m_k \neq 1$ then the most complicated harmonic sum in the Mellin transform of $\mathbf{H}_{m_1,m_2,\dots,m_k}(x)$ has no trailing ones.

Proof. Due to [1, Remark 3.5.18.] 1. and 2. are equivalent. The proof of 2. follows by using Algorithm 2 of [1] for each of the possible values of m_k . \square

According to the previous lemma we know that if $H_{m_1, m_2, \dots, m_k}(x)$ is the most complicated harmonic polylogarithm in the inverse Mellin transform of a harmonic sum without trailing ones then $m_k \neq 1$. Due to Remark 2.8.17 we can expand the resulting integrals (either we can handle it directly, or we have to transform the argument of the harmonic polylogarithm).

Moreover, a harmonic sum with trailing ones might lead to a harmonic polylogarithm with trailing ones. But $\frac{H_{m_1, m_2, \dots, m_{k-1}, 1}(x)}{1 \pm x}$ is not analytic at 1 and hence we cannot use the strategy mentioned in Section 2.8.2 to find an asymptotic representation of such integrals. Fortunately we can always extract trailing ones such that we end up in a univariate polynomial in $S_1(n)$ with coefficients in the harmonic sums without trailing ones (see Section 2.1). Hence we only need to deal with powers of $S_1(n)$ and harmonic sums without trailing ones.

First we consider $S_1(n)$. Since $\frac{1}{1-x}$ is not analytic at 1, we cannot use the strategy mentioned in Section 2.8.2 to find an asymptotic representation of $\int_0^1 \frac{x^n - 1}{1 \pm x} dx = S_1(n)$, however we have the following well known lemma.

Lemma 2.8.19. *The asymptotic representation of $S_1(n)$ is given by*

$$\gamma + \log(n) + \frac{1}{2n} - \sum_{k=1}^{\infty} \frac{B_{2k}}{2k n^{2k}}$$

where γ is the Euler-Mascheroni constant and B_{2k} are Bernoulli numbers.

Remark 2.8.20. *To compute the asymptotic representation of $S_1(n)$, we can as well proceed in the following way: we compute the expansion of $-\int_0^1 \frac{x^n H_d(x)}{1-x} dx$; integrate the result and add the constant γ . This is possible since $S_1(n) = \int_0^1 \frac{x^n - 1}{1-x} dx$ and $\frac{d}{dn} \int_0^1 \frac{x^n - 1}{1-x} dx = -\int_0^1 \frac{x^n H_d(x)}{1-x} dx$.*

Now we are ready to state an algorithm to compute asymptotic expansions of harmonic sums. If we want to find the asymptotic expansions of a harmonic sum $S_{a_1, a_2, \dots, a_k}(n)$ we can proceed as follows:

- If $S_{a_1, a_2, \dots, a_k}(n)$ has trailing ones, i.e., $a_k = 1$, we first extract them such that we end up in a univariate polynomial in $S_1(n)$ with coefficients in the harmonic sums without trailing ones; apply the following items to each of the harmonic sums without trailing ones.

- Suppose now $S_{a_1, a_2, \dots, a_k}(n)$ has no trailing ones, i.e., $a_k \neq 1$; let $\frac{H_{m_1, m_2, \dots, m_l}(x)}{1+sx}$ be the most complicated weighted harmonic polylogarithm in the inverse Mellin transform of $S_{a_1, a_2, \dots, a_k}(n)$; express $S_{a_1, a_2, \dots, a_k}(n)$ as

$$S_{a_1, a_2, \dots, a_k}(n) = M\left(\frac{H_{m_1, m_2, \dots, m_l}(x)}{1+sx}, n\right) + T. \quad (2.33)$$

Note that T is an expression in harmonic sums (which are less complicated than $S_{a_1, a_2, \dots, a_k}(n)$) and constants.

- We proceed by expanding $M\left(\frac{H_{m_1, m_2, \dots, m_l}(x)}{1+sx}, n\right)$:

all $m_i \neq 1$: expand $M\left(\frac{H_{m_1, m_2, \dots, m_l}(x)}{1+sx}, n\right)$ directly see Remark 2.8.17

not all $m_i \neq 1$:

– transform $x \rightarrow 1-x$ in $H_m(x)$; expand all products; now we can rewrite

$$M\left(\frac{H_m(x)}{1+sx}, n\right) = \sum_{i=1}^p c_i M\left(\frac{H_{b_i}(1-x)}{1+sx}, n\right) + c \quad \text{with } c, c_i \in \mathbb{R} \quad (2.34)$$

– for each Mellin transform $M\left(\frac{H_{b_1, \dots, b_j}(1-x)}{1+sx}, n\right)$ do

$b_j \neq 0$: expand $\int_0^1 \frac{x^n H_b(1-x)}{1+sx} dx$ see Remark 2.8.17

$b_j = 0$: transform back $1-x \rightarrow x$ in $H_b(1-x)$; expand all products by shuffling; write

$$M\left(\frac{H_b(1-x)}{1+sx}, n\right) = \sum_{i=1}^p d_i M\left(\frac{H_{g_i}(x)}{1+sx}, n\right) + d \quad (2.35)$$

with $d, d_i \in \mathbb{R}$ and perform the Mellin transforms $M\left(\frac{H_{g_i}(x)}{1-x}, n\right)$.

- Replace $M\left(\frac{H_{m_1, m_2, \dots, m_l}(x)}{1+sx}, n\right)$ in equation (2.33) by the result of this process.
- Expand the powers of $S_1(n)$ using Lemma 2.8.19 and perform the Cauchy product to the expansions.
- For all harmonic sums that remain in equation (2.33) apply the above points; since these harmonic sums are less complicated this process will terminate.

Some remarks are in place: Since $a_k \neq 1$ in equation (2.33), we know due to Lemma 2.8.18 that $m_l \neq 0$ in equation (2.33). If not all $m_i \neq 1$ in equation (2.33), we have to transform $x \rightarrow 1 - x$ in $H_{m_1, m_2, \dots, m_l}(x)$. From Remark 2.8.6 we know that the s harmonic polylogarithm at argument x with weight l which will pop up will not have trailing zeroes since $m_l \neq 1$. Therefore the harmonic sums which will appear in equation (2.35) are less complicated (i.e., smaller in the sense of Definition 2.5.14) than $S_{a_1, a_2, \dots, a_k}(n)$ of (2.33) and hence this algorithm will eventually terminate.

Example 2.8.21. *Let us now consider the asymptotic expansion of $S_{2,1}(n)$. First we remove the trailing ones:*

$$S_{2,1}(n) = S_1(n) S_2(n) + S_3(n) - S_{1,2}(n).$$

We can expand $S_1(n)$ using Lemma 2.8.19. For $S_2(n)$ we get:

$$S_2(n) = M\left(\frac{H_0(x)}{1-x}, n\right) = \int_0^1 \frac{x^n(H_0(x) - H_0(1))}{1-x} dx - \int_0^1 \frac{H_0(x) - H_0(1)}{1-x} dx.$$

The second integral is a constant. Expanding the first integral leads to

$$S_2(n) \sim -H_{1,0}(1) - \frac{1}{n} + \frac{1}{2n^2} - \frac{1}{6n^3} + \frac{1}{30n^5}.$$

Analogously for $S_3(n)$ we get:

$$\begin{aligned} S_3(n) &= -M\left(\frac{H_{0,0}(x)}{1-x}, n\right) \\ &= -\int_0^1 \frac{x^n(H_{0,0}(x) - H_{0,0}(1))}{1-x} dx + \int_0^1 \frac{H_{0,0}(x) - H_{0,0}(1)}{1-x} dx, \end{aligned}$$

and hence:

$$S_3(n) \sim H_{1,0,0}(1) - \frac{1}{2n} + \frac{1}{2n^3} - \frac{1}{4n^4}.$$

Finally for $S_{1,2}(n)$ we have

$$\begin{aligned} S_{1,2}(n) = M\left(\frac{H_{1,0}(x)}{1-x}, n\right) &= \int_0^1 \frac{x^n(H_{1,0}(x) - H_{1,0}(1))}{1-x} dx \\ &\quad - \int_0^1 \frac{H_{1,0}(x) - H_{1,0}(1)}{1-x} dx - S_1(n) H_{1,0}(1), \end{aligned}$$

and consequently:

$$S_{1,2}(n) \sim -H_{1,0,0}(1) + \frac{1}{n} - \frac{3}{4n^2} + \frac{17}{36n^3} - \frac{5}{24n^4} + \frac{7}{450n^5} - H_{1,0}(1) S_1(n).$$

Combining these results we find the asymptotic expansion of $S_{2,1}(n)$:

$$S_{2,1}(n) \sim 2H_{1,0,0}(1) - \frac{1}{n} - \frac{1}{4n^2} + \frac{13}{36n^3} - \frac{1}{6n^4} - \frac{1}{100n^5}$$

$$+(\log(n) + \gamma) \left(-\frac{1}{n} + \frac{1}{2n^2} - \frac{1}{6n^3} + \frac{1}{30n^5} \right).$$

Chapter 3

S-Sums

The main goal of this chapter is to extend the ideas from Chapter 2 to a generalization of harmonic sums (see Definition 2.1.1), i.e., we generalize the harmonic sums to the S-sums of [62].

3.1 Definition and Structure of S-Sums and Multiple Polylogarithms

Definition 3.1.1 (S-Sums). For $a_i \in \mathbb{N}$ and $x_i \in \mathbb{R}^*$ we define

$$S_{a_1, \dots, a_k}(x_1, \dots, x_k; n) = \sum_{n \geq i_1 \geq i_2 \geq \dots \geq i_k \geq 1} \frac{x_1^{i_1}}{i_1^{a_1}} \dots \frac{x_k^{i_k}}{i_k^{a_k}}. \quad (3.1)$$

k is called the depth and $w = \sum_{i=0}^k a_i$ is called the weight of the S-sum $S_{a_1, \dots, a_k}(x_1, \dots, x_k; n)$.

As for harmonic sums a product of two S-sums with the same upper summation limit can be written in terms of single S-sums (see [62]): for $n \in \mathbb{N}$,

$$\begin{aligned} S_{a_1, \dots, a_k}(x_1, \dots, x_k; n) S_{b_1, \dots, b_l}(y_1, \dots, y_l; n) = & \\ & \sum_{i=1}^n \frac{a_1^i}{i^{a_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) S_{b_1, \dots, b_l}(y_1, \dots, y_l; i) \\ & + \sum_{i=1}^n \frac{b_1^i}{i^{|b_1|}} S_{a_1, \dots, a_k}(x_1, \dots, x_k; i) S_{b_2, \dots, b_l}(y_2, \dots, y_l; i) \\ & - \sum_{i=1}^n \frac{(a_1 \cdot b_1)^i}{i^{a_1+b_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) S_{b_2, \dots, b_l}(y_2, \dots, y_l; i). \quad (3.2) \end{aligned}$$

Recursive application of (3.2) leads to a linear combination of single S-sums. Together with this product S-sums form a quasi shuffle algebra.

The quasi shuffle algebra property will allow us again to look for algebraic relations, however we are as well interested in structural relations and asymptotic expansions of S-sums. Therefore we will again use an integral representation of these sums, which leads to an extension of the harmonic polylogarithms. In Section 2.8.1 we already extended harmonic polylogarithms which were originally defined on the alphabet $\{-1, 0, 1\}$ (see Definition 2.2.1) to the alphabet $\{-1, 0, 1, 2\}$. In this section we will extend harmonic polylogarithms even further (for an equivalent definition see [43]).

Definition 3.1.2 (Multiple Polylogarithms). *Let $a \in \mathbb{R}$ and*

$$q = \begin{cases} a, & \text{if } a > 0 \\ \infty, & \text{otherwise.} \end{cases}$$

We define the auxiliary function as follows:

$$f_a : (0, q) \mapsto \mathbb{R}$$

$$f_a(x) = \begin{cases} \frac{1}{x}, & \text{if } a = 0 \\ \frac{1}{|a| - \text{sign}(a)x}, & \text{otherwise.} \end{cases}$$

Now we can define the multiple polylogarithms \mathbf{H} . Let $m_i \in \mathbb{R}$ and let $q = \min_{m_i > 0} m_i$; we define for $x \in (0, q)$:

$$\mathbf{H}(x) = 1,$$

$$\mathbf{H}_{m_1, m_2, \dots, m_w}(x) = \begin{cases} \frac{1}{w!} (\log x)^w, & \text{if } (m_1, \dots, m_k) = (0, \dots, 0) \\ \int_0^x f_{m_1}(y) \mathbf{H}_{m_2, \dots, m_k}(y) dy, & \text{otherwise.} \end{cases}$$

The length w of the vector \mathbf{m} is called the weight of the shifted multiple polylogarithm $\mathbf{H}_{\mathbf{m}}(x)$.

Example 3.1.3.

$$\mathbf{H}_1(x) = \int_0^x \frac{1}{1-x_1} dx_1 = -\log(1-x)$$

$$\mathbf{H}_{-2}(x) = \int_0^x \frac{1}{2+x_1} dx_1 = \log(2+x) - \log(2)$$

$$\mathbf{H}_{2,0,-\frac{1}{2}}(x) = \int_0^x \frac{1}{2-x_1} \int_0^{x_1} \frac{1}{x_2} \int_0^{x_2} \frac{1}{\frac{1}{2}+x_3} dx_3 dx_2 dx_1.$$

A multiple polylogarithm $\mathbf{H}_{\mathbf{m}}(x) = \mathbf{H}_{m_1, \dots, m_w}(x)$ with $q := \min_{m_i > 0} m_i$ is an analytic functions for $x \in (0, q)$. For the limits $x \rightarrow 0$ and $x \rightarrow q$ we have:

- It follows from the definition that if $\mathbf{m} \neq \mathbf{0}_w$, $\mathbf{H}_{\mathbf{m}}(0) = 0$.

- If $m_1 \neq q$ or if $m_1 = 1$ and $m_v = 0$ for all v with $1 < v \leq w$ then $H_m(q)$ is finite.

We define $H_m(0) := \lim_{x \rightarrow 0^+} H_m(x)$ and $H_m(1) := \lim_{x \rightarrow 1^-} H_m(x)$ if the limits exist.

Note that for multiple polylogarithms of the form

$$H_{m_1, \dots, m_k, 1, 0, \dots, 0}(x)$$

with $c := \min_{m_i > 0} m_i$ we can extend the definition range from $x \in (0, 1)$ to $x \in (0, c)$. These multiple polylogarithms are analytic functions for $x \in (0, c)$. The limit $x \rightarrow q$ exists if and only if $m_1 \neq c$.

Remark 3.1.4. *In the following we will always assume that the arguments of the considered multiple polylogarithms are chosen in a way such that multiple polylogarithms are defined and finite.*

Remark 3.1.5. *For the derivatives we have for all $x \in (0, \min_{m_i > 0} m_i)$ that*

$$\frac{d}{dx} H_m(x) = f_{m_1}(x) H_{m_2, m_3, \dots, m_w}(x).$$

Remark 3.1.6. *Again the product of two multiple polylogarithms of the same argument can be expressed using the formula (compare (2.3))*

$$H_p(x) H_q(x) = \sum_{r=p \sqcup q} H_r(x) \quad (3.3)$$

in which $p \sqcup q$ represent all merges of p and q in which the relative orders of the elements of p and q are preserved.

Note that we can use the shuffle algebra property to extract trailing zeroes using the ideas of Section 2.2. There is one situation we have to take care of: given a multiple polylogarithm in the form

$$H_{m_1, \dots, m_k, 1, 0, \dots, 0}(x)$$

with $1 < q := \min_{m_i > 0} m_i$ then we cannot use the strategy to extract trailing zeroes if $x \geq 1$ since this would lead to infinities. The shuffle algebra would suggest to rewrite $H_{2,1,0}(x)$ as

$$H_0(x) H_{2,1}(x) - H_{0,2,1}(x) - H_{2,0,1}(x),$$

however for $x > 1$ for instance $H_{2,0,1}(x)$ is not defined. Thus, if we consider the extraction of trailing zeroes in the following then trailing zeroes of multiple polylogarithm in the form $H_{m_1, \dots, m_k, 1, 0, \dots, 0}(x)$ will not be extracted and these multiple polylogarithms will remain untouched if $x \geq 1$.

Along with the integral representation multiple polylogarithms at special constants and connected to them S-sums at infinity will pop up. Hence we will take a closer look at

relations between these quantities. This will lead to power series expansions of multiple polylogarithms and identities between multiple polylogarithms of related arguments.

3.2 Identities between Multiple Polylogarithms of Related Arguments

In the following we want to look at several special transforms of the argument of multiple polylogarithms which will be useful in later considerations.

3.2.1 $x + b \rightarrow x$

Lemma 3.2.1. *Let $m_i \in \mathbb{R} \setminus (0, 1)$ and $x > 0$ such that the multiple polylogarithm $\mathbf{H}_{m_1, \dots, m_l}(x + 1)$ is defined. If $(m_1, \dots, m_l) \neq (1, 0, \dots, 0)$,*

$$\begin{aligned} \mathbf{H}_{m_1, \dots, m_l}(x + 1) &= \\ &\mathbf{H}_{m_1, \dots, m_l}(1) + \mathbf{H}_{m_1-1}(x) \mathbf{H}_{m_2, \dots, m_l}(1) + \mathbf{H}_{m_1-1, m_2-1}(x) \mathbf{H}_{m_3, \dots, m_l}(1) \\ &+ \dots + \mathbf{H}_{m_1-1, \dots, m_{l-1}-1}(x) \mathbf{H}_{m_l}(1) + \mathbf{H}_{m_1-1, \dots, m_l-1}(x). \end{aligned}$$

If $(m_1, \dots, m_l) = (1, 0, \dots, 0)$,

$$\mathbf{H}_{1, 0, \dots, 0}(x + 1) = \mathbf{H}_{1, 0, \dots, 0}(1) - \mathbf{H}_{0, -1, \dots, -1}(x).$$

Proof. We proceed by induction on l . For $l = 1$ and $m_1 > 1$ we have:

$$\begin{aligned} \mathbf{H}_{m_1}(x + 1) &= \int_0^{x+1} \frac{1}{m_1 - u} du = \mathbf{H}_{m_1}(1) + \int_1^{x+1} \frac{1}{m_1 - u} du \\ &= \mathbf{H}_{m_1}(1) + \int_0^x \frac{1}{m_1 - (u + 1)} du = \mathbf{H}_{m_1}(1) + \mathbf{H}_{m_1-1}(x). \end{aligned}$$

For $l = 1$ and $m_1 < 0$ we have:

$$\begin{aligned} \mathbf{H}_{m_1}(x + 1) &= \int_0^{x+1} \frac{1}{|m_1| + u} du = \mathbf{H}_{m_1}(1) + \int_1^{x+1} \frac{1}{|m_1| + u} du \\ &= \mathbf{H}_{m_1}(1) + \int_0^x \frac{1}{|m_1| + (u + 1)} du = \mathbf{H}_{m_1}(1) + \mathbf{H}_{m_1-1}(x). \end{aligned}$$

For $l = 1$ and $m_1 = 0$ we have:

$$\mathbf{H}_0(x + 1) = \mathbf{H}_0(1) + \int_1^{x+1} \frac{1}{u} du = \int_0^x \frac{1}{1 + u} du = \mathbf{H}_0(1) + \mathbf{H}_{-1}(x).$$

Suppose the theorem holds for $l - 1$. If $m_1 \neq 0$ we get

$$\begin{aligned}
\mathbb{H}_{m_1, \dots, m_l}(x+1) &= \mathbb{H}_{m_1, \dots, m_l}(1) + \int_1^{x+1} \frac{\mathbb{H}_{m_2, \dots, m_l}(u)}{|m_1| - \text{sign}(m_1)u} du \\
&= \mathbb{H}_{m_1, \dots, m_l}(1) + \int_0^x \frac{\mathbb{H}_{m_2, \dots, m_l}(u+1)}{|m_1| - \text{sign}(m_1)(u+1)} du \\
&= \mathbb{H}_{m_1, \dots, m_l}(1) + \int_0^x \frac{1}{|m_1| - \text{sign}(m_1)(u+1)} \left(\mathbb{H}_{m_2, \dots, m_l}(1) \right. \\
&\quad \left. + \mathbb{H}_{m_2-1}(x) \mathbb{H}_{m_3, \dots, m_l}(1) + \mathbb{H}_{m_2-1, m_3-1}(x) \mathbb{H}_{m_4, \dots, m_l}(1) + \dots \right. \\
&\quad \left. + \mathbb{H}_{m_2-1, \dots, m_{l-1}-1}(x) \mathbb{H}_{m_l}(1) + \mathbb{H}_{m_2-1, \dots, m_{l-1}}(x) \right) du \\
&= \mathbb{H}_{m_1, \dots, m_l}(1) + \mathbb{H}_{m_1-1}(x) \mathbb{H}_{m_2, \dots, m_l}(1) \\
&\quad + \mathbb{H}_{m_1-1, m_2-1}(x) \mathbb{H}_{m_3, \dots, m_l}(1) + \dots + \\
&\quad + \mathbb{H}_{m_1-1, \dots, m_{l-1}-1}(x) \mathbb{H}_{m_l}(1) + \mathbb{H}_{m_1-1, \dots, m_{l-1}}(x).
\end{aligned}$$

If $m_1 = 0$ we get

$$\begin{aligned}
\mathbb{H}_{0, m_2, \dots, m_l}(x+1) &= \mathbb{H}_{0, m_2, \dots, m_l}(1) + \int_1^{x+1} \frac{\mathbb{H}_{m_2, \dots, m_l}(u)}{u} du \\
&= \mathbb{H}_{0, m_2, \dots, m_l}(1) + \int_0^x \frac{\mathbb{H}_{m_2, \dots, m_l}(u+1)}{(1+u)} du \\
&= \mathbb{H}_{0, m_2, \dots, m_l}(1) + \int_0^x \frac{1}{1+u} \left(\mathbb{H}_{m_2, \dots, m_l}(1) + \right. \\
&\quad \left. + \mathbb{H}_{m_2-1}(x) \mathbb{H}_{m_3, \dots, m_l}(1) + \mathbb{H}_{m_2-1, m_3-1}(x) \mathbb{H}_{m_4, \dots, m_l}(1) + \right. \\
&\quad \left. + \dots + \mathbb{H}_{m_2-1, \dots, m_{l-1}-1}(x) \mathbb{H}_{m_l}(1) + \mathbb{H}_{m_2-1, \dots, m_{l-1}}(x) \right) du \\
&= \mathbb{H}_{0, m_2, \dots, m_l}(1) + \mathbb{H}_{-1}(x) \mathbb{H}_{m_2, \dots, m_l}(1) \\
&\quad + \mathbb{H}_{-1, m_2-1}(x) \mathbb{H}_{m_3, \dots, m_l}(1) + \dots + \\
&\quad + \mathbb{H}_{-1, \dots, m_{l-1}-1}(x) \mathbb{H}_{m_l}(1) + \mathbb{H}_{-1, \dots, m_{l-1}}(x).
\end{aligned}$$

□

The proofs of the following three lemmas are similar to the proof of the previous one, hence we will omit them here.

Lemma 3.2.2. *Let $b > 0$, $m_1 \in \mathbb{R} \setminus (0, b]$, $m_i \in \mathbb{R} \setminus (0, b)$ for $i \in \{2, 3, \dots, l\}$ such that $(m_j, \dots, m_l) \neq (1, 0, \dots, 0)$ for all $j \in \{1, \dots, l\}$. For $x > 0$ we have*

$$\begin{aligned}
\mathbb{H}_{m_1, \dots, m_l}(x+b) &= \mathbb{H}_{m_1, m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b}(x) \mathbb{H}_{m_2, \dots, m_l}(b) \\
&\quad + \mathbb{H}_{m_1-b, m_2-b}(x) \mathbb{H}_{m_3, \dots, m_l}(b) + \dots + \\
&\quad + \mathbb{H}_{m_1-b, \dots, m_{l-1}-b}(x) \mathbb{H}_{m_l}(b) + \mathbb{H}_{m_1-b, \dots, m_{l-1}}(x).
\end{aligned}$$

Lemma 3.2.3. *Let $(m_1, \dots, m_l) = (1, 0, \dots, 0)$. For $1 > b > 0$ and $1 - b > x > 0$ we have*

$$\begin{aligned} \mathbb{H}_{m_1, \dots, m_l}(x + b) &= \\ &\mathbb{H}_{m_1, m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b}(x) \mathbb{H}_{m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b, m_2-b}(x) \mathbb{H}_{m_3, \dots, m_l}(b) \\ &+ \cdots + \mathbb{H}_{m_1-b, \dots, m_{l-1}-b}(x) \mathbb{H}_{m_l}(b) + \mathbb{H}_{m_1-b, \dots, m_l-b}(x). \end{aligned}$$

For $x > 0$ and $b \geq 1$ we have

$$\begin{aligned} \mathbb{H}_{m_1, \dots, m_l}(x + b) &= \\ &\mathbb{H}_{m_1, m_2, \dots, m_l}(b) - \mathbb{H}_{m_1-b}(x) \mathbb{H}_{m_2, \dots, m_l}(b) - \mathbb{H}_{m_1-b, m_2-b}(x) \mathbb{H}_{m_3, \dots, m_l}(b) \\ &- \cdots - \mathbb{H}_{m_1-b, \dots, m_{l-1}-b}(x) \mathbb{H}_{m_l}(b) - \mathbb{H}_{m_1-b, \dots, m_l-b}(x). \end{aligned}$$

Lemma 3.2.4. *Let $b > 0$, $m_1 \in \mathbb{R} \setminus (0, b]$, $m_i \in \mathbb{R} \setminus (0, b)$ for $i \in \{2, 3, \dots, k\}$ and $(m_{k+1}, \dots, m_l) = (1, 0, \dots, 0)$. For $1 - b > x > 0$ and $1 > b > 0$ we have*

$$\begin{aligned} \mathbb{H}_{m_1, \dots, m_l}(x + b) &= \\ &\mathbb{H}_{m_1, m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b}(x) \mathbb{H}_{m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b, m_2-b}(x) \mathbb{H}_{m_3, \dots, m_l}(b) \\ &+ \cdots + \mathbb{H}_{m_1-b, \dots, m_k-b}(x) \mathbb{H}_{m_{k+1}, \dots, m_l}(b) + \mathbb{H}_{m_1-b, \dots, m_{k+1}-b}(x) \mathbb{H}_{m_{k+2}, \dots, m_l}(b) \\ &+ \cdots + \mathbb{H}_{m_1-b, \dots, m_{l-1}-b}(x) \mathbb{H}_{m_l}(b) + \mathbb{H}_{m_1-b, \dots, m_l-b}(x). \end{aligned}$$

For $x > 0$ and $b \geq 1$ we have

$$\begin{aligned} \mathbb{H}_{m_1, \dots, m_l}(x + b) &= \\ &\mathbb{H}_{m_1, m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b}(x) \mathbb{H}_{m_2, \dots, m_l}(b) + \mathbb{H}_{m_1-b, m_2-b}(x) \mathbb{H}_{m_3, \dots, m_l}(b) \\ &+ \cdots + \mathbb{H}_{m_1-b, \dots, m_k-b}(x) \mathbb{H}_{m_{k+1}, \dots, m_l}(b) - \mathbb{H}_{m_1-b, \dots, m_{k+1}-b}(x) \mathbb{H}_{m_{k+2}, \dots, m_l}(b) \\ &- \cdots - \mathbb{H}_{m_1-b, \dots, m_{l-1}-b}(x) \mathbb{H}_{m_l}(b) - \mathbb{H}_{m_1-b, \dots, m_l-b}(x). \end{aligned}$$

3.2.2 $b - x \rightarrow x$

In this subsection we assume that $b > 0$ and we consider indices $m_i \in \mathbb{R} \setminus (0, b)$. Proceeding recursively on the weight w of the multiple polylogarithm we have for $m_1 \neq b$:

$$\mathbb{H}_{m_1}(b - x) = \mathbb{H}_{m_1}(b) - \mathbb{H}_{b-m_1}(x) \quad (3.4)$$

$$\mathbb{H}_b(b - x) = \mathbb{H}_0(x) - \mathbb{H}_0(b). \quad (3.5)$$

Now let us look at higher weights $w > 1$. We consider $H_{m_1, m_2, \dots, m_w}(b-x)$ with $m_i \in \mathbb{R} \setminus (0, b)$ and suppose that we can already apply the transformation for multiple polylogarithms of weight $< w$. If $m_1 = b$, we can remove leading b 's (similar to the extraction of leading ones) and end up with multiple polylogarithms without leading b 's and powers of $H_b(b-x)$. For the powers of $H_b(b-x)$ we can use (3.5); therefore, only the cases in which the first index $m_1 \neq 1$ are to be considered. For $b \neq 0$:

$$H_{m_1, m_2, \dots, m_w}(b-x) = H_{m_1, m_2, \dots, m_w}(b) - \int_0^x \frac{H_{m_2, \dots, m_w}(b-t)}{|-m_1 + b| - \text{sign}(-m_1 + b)t} dt.$$

Since we know the transform for weights $< w$, we can apply it to $H_{m_2, \dots, m_w}(b-t)$ and finally we obtain the required weight w identity by using the definition of the multiple polylogarithms.

3.2.3 $\frac{1-x}{1+x} \rightarrow x$

In this subsection we restrict the indices again. We consider indices that are greater equal 1 or less equal 0. Proceeding recursively on the weight w of the multiple polylogarithm we have for $0 < \frac{1-x}{1+x} < 1$, $y_1 < -1$, $-1 < y_2 < 0$ and $y_3 > 1$:

$$H_{y_1}\left(\frac{1-x}{1+x}\right) = -H_0(-y_1) - H_{-1}(x) + H_0(1-y_1) + H_{\frac{1-y_1}{1+y_1}}(x) \quad (3.6)$$

$$H_{-1}\left(\frac{1-x}{1+x}\right) = H_{-1}(1) - H_{-1}(x) \quad (3.7)$$

$$H_{y_2}\left(\frac{1-x}{1+x}\right) = -H_0(-y_2) - H_{-1}(x) + H_0(1-y_2) - H_{\frac{1-y_2}{1+y_2}}(x) \quad (3.8)$$

$$H_0\left(\frac{1-x}{1+x}\right) = -H_1(x) + H_{-1}(x) \quad (3.9)$$

$$H_1\left(\frac{1-x}{1+x}\right) = -H_{-1}(1) - H_0(x) + H_{-1}(x) \quad (3.10)$$

$$H_{y_3}\left(\frac{1-x}{1+x}\right) = H_0(y_3) + H_{-1}(x) - H_0(y_3-1) - H_{\frac{1-y_3}{1+y_3}}(x). \quad (3.11)$$

Now let us look at higher weights $w > 1$. We consider $H_{m_1, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right)$ with $m_i \in \mathbb{R} \setminus (0, 1)$ and suppose that we can already apply the transformation for multiple polylogarithms of weight $< w$. If $m_1 = 1$, we can remove leading ones and end up with multiple polylogarithms without leading ones and powers of $H_1\left(\frac{1-x}{1+x}\right)$. For the powers of $H_1\left(\frac{1-x}{1+x}\right)$ we can use (3.10); therefore, only the cases in which the first index $m_1 \neq 1$ are to be considered. For $y_1 < 0$, $y_1 \neq -1$ and $y_3 > 1$ we get (compare Section 2.3.2):

$$H_{y_1, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) = H_{y_2, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt$$

$$\begin{aligned}
& + \int_0^x \frac{1}{\frac{1-y_1}{1+y_1} + t} \mathbf{H}_{m_2, \dots, m_w} \left(\frac{1-t}{1+t} \right) dt \\
\mathbf{H}_{-1, m_2, \dots, m_w} \left(\frac{1-x}{1+x} \right) &= \mathbf{H}_{-1, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t} \mathbf{H}_{m_2, \dots, m_w} \left(\frac{1-t}{1+t} \right) dt \\
\mathbf{H}_{0, m_2, \dots, m_w} \left(\frac{1-x}{1+x} \right) &= \mathbf{H}_{0, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1-t} \mathbf{H}_{m_2, \dots, m_w} \left(\frac{1-t}{1+t} \right) dt \\
& - \int_0^x \frac{1}{1-t} \mathbf{H}_{m_2, \dots, m_w} \left(\frac{1+t}{1+t} \right) dt \\
\mathbf{H}_{y_2, m_2, \dots, m_w} \left(\frac{1-x}{1+x} \right) &= \mathbf{H}_{y_2, m_2, \dots, m_w}(1) + \int_0^x \frac{1}{1+t} \mathbf{H}_{m_2, \dots, m_w} \left(\frac{1-t}{1+t} \right) dt \\
& - \int_0^x \frac{1}{\frac{1-y_2}{1+y_2} + t} \mathbf{H}_{m_2, \dots, m_w} \left(\frac{1-t}{1+t} \right) dt.
\end{aligned}$$

We have to consider the case for $\mathbf{H}_{0, \dots, 0} \left(\frac{1-x}{1+x} \right)$ separately, however we can deal with this case since it reduces by Definition 3.1.2 to $\mathbf{H}_0 \left(\frac{1-x}{1+x} \right)$, which we handled in (3.9). Since we know the transform for weights $< w$, we can apply it to $\mathbf{H}_{m_2, \dots, m_w} \left(\frac{1+t}{1+t} \right)$ and finally we obtain the required weight w identity by using the definition of the multiple polylogarithms.

3.2.4 $kx \rightarrow x$

Lemma 3.2.5. *If $m_i \in \mathbb{R}, m_l \neq 0, x \in \mathbb{R}^+$ and $k \in \mathbb{R}^+$ such that the multiple polylogarithm $\mathbf{H}_{m_1, \dots, m_l}(k \cdot x)$ is defined then we have*

$$\mathbf{H}_{m_1, \dots, m_l}(k \cdot x) = \mathbf{H}_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x). \quad (3.12)$$

Proof. We proceed by induction on l . For $l = 1$ we have:

$$\mathbf{H}_{m_1}(k \cdot x) = \int_0^{kx} \frac{1}{|m_1| - \text{sign}(m_1) u} du = \int_0^x \frac{k}{|m_1| - \text{sign}(m_1) ku} du = \mathbf{H}_{\frac{m_1}{k}}(x).$$

Suppose the lemma holds for l . For $m_1 \neq 0$ we get

$$\begin{aligned}
\mathbf{H}_{m_1, \dots, m_{l+1}}(k \cdot x) &= \int_0^{kx} \frac{\mathbf{H}_{m_2, \dots, m_{l+1}}(u)}{|m_1| - \text{sign}(m_1) u} du = \int_0^x \frac{\mathbf{H}_{m_2, \dots, m_{l+1}}(ku)}{|m_1| - \text{sign}(m_1) ku} k du \\
&= \int_0^x \frac{\mathbf{H}_{\frac{m_2}{k}, \dots, \frac{m_{l+1}}{k}}(u)}{\frac{|m_1|}{k} - \text{sign}(m_1) u} du = \mathbf{H}_{\frac{m_1}{k}, \dots, \frac{m_{l+1}}{k}}(x).
\end{aligned}$$

For $m_1 = 0$ we get

$$\mathbf{H}_{0, m_2, \dots, m_{l+1}}(k \cdot x) = \int_0^{kx} \frac{\mathbf{H}_{m_2, \dots, m_{l+1}}(u)}{u} du = \int_0^x \frac{\mathbf{H}_{m_2, \dots, m_{l+1}}(ku)}{ku} k du$$

$$= \int_0^x \frac{\mathbb{H}_{\frac{m_2}{k}, \dots, \frac{m_{l+1}}{k}}(u)}{u} du = \mathbb{H}_{\frac{0}{k}, \frac{m_2}{k}, \dots, \frac{m_{l+1}}{k}}(x).$$

□

3.2.5 $-x \rightarrow x$

The proof of the following lemma is straightforward (compare [73], where it is stated for harmonic polylogarithms).

Lemma 3.2.6. *If $m_i \in \mathbb{R}, m_l \neq 0$ and $x \in \mathbb{R}^-$ such that the multiple polylogarithm $\mathbb{H}_{m_1, \dots, m_l}(-x)$ is defined then we have*

$$\mathbb{H}_{m_1, \dots, m_l}(-x) = (-1)^{l-k} \mathbb{H}_{-m_1, \dots, -m_l}(x), \quad (3.13)$$

here k denotes the number of m_i which equal zero.

3.2.6 $\frac{1}{x} \rightarrow x$

In this subsection we restrict the indices again. We consider negative indices together with the index 0. Proceeding recursively on the weight w of the multiple polylogarithm we have for $0 < x < 1$ and $y < 0$:

$$\begin{aligned} \mathbb{H}_y\left(\frac{1}{x}\right) &= \mathbb{H}_{\frac{1}{y}}(x) - \mathbb{H}_0(x) - \mathbb{H}_0(-y) \\ \mathbb{H}_0\left(\frac{1}{x}\right) &= -\mathbb{H}_0(x). \end{aligned}$$

Now let us look at higher weights $w > 1$. We consider $\mathbb{H}_{m_1, m_2, \dots, m_w}\left(\frac{1}{x}\right)$ with $m_i \leq 0$ and suppose that we can already apply the transformation for multiple polylogarithms of weight $< w$. For $m_1 < 0$ we get (compare [73] and Section 2.3.3):

$$\begin{aligned} \mathbb{H}_{m_1, m_2, \dots, m_w}\left(\frac{1}{x}\right) &= \mathbb{H}_{m_1, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t^2(-m_1 + 1/t)} \mathbb{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ &= \mathbb{H}_{m_1, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t} \mathbb{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ &\quad - \int_x^1 \frac{1}{-\frac{1}{m_1} + t} \mathbb{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ \mathbb{H}_{0, m_2, \dots, m_w}\left(\frac{1}{x}\right) &= \mathbb{H}_{0, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t^2(1/t)} \mathbb{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt \\ &= \mathbb{H}_{0, m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t} \mathbb{H}_{m_2, \dots, m_w}\left(\frac{1}{t}\right) dt. \end{aligned}$$

Since we know the transform for weights $< w$, we can apply it to $H_{m_2, \dots, m_w}(\frac{1}{t})$ and finally we obtain the required weight w identity by using the definition of the multiple polylogarithms.

An index $m > 0$ in the index set leads to a branch point at m and a branch cut discontinuity in the complex plane for $x \in (m, \infty)$. This corresponds to the branch point at $x = m$ and the branch cut discontinuity in the complex plane for $x \in (m, \infty)$ of $\log(m - x) = \log(m) - H_m(x)$. However, the analytic properties of the logarithm are well known and we can set for $0 < x < 1$ for instance

$$H_m\left(\frac{1}{x}\right) = H_{\frac{1}{m}}(x) + H_0(m) + H_0(x) - i\pi, \quad (3.14)$$

by approaching the argument $\frac{1}{x}$ from the lower half complex plane. We can now consider an alphabet with at most one letter $m \geq 1$ (note that we could as well assume $m > 0$ however for simplicity we restrict to $m \geq 1$). For such an alphabet the strategy is as follows: if a multiple polylogarithm has leading m 's, we remove them and end up with multiple polylogarithms without leading m 's and powers of $H_m(\frac{1}{x})$. To deal with the multiple polylogarithms without leading m , we can slightly modify the previous part of this section and for the powers of $H_m(\frac{1}{x})$ we can use (3.14).

3.3 Power Series Expansion of Multiple Polylogarithms

As stated in Section 2.4 in general, the harmonic polylogarithms $H_m(x)$ do not have a regular Taylor series expansion. This is due to the effect that trailing zeroes in the index field may cause powers of $\log(x)$. Hence the proper expansion is one in terms of both x and $\log x$. The same is true for multiple polylogarithms with indices in \mathbb{R} . In this case we have for $j \in \mathbb{R}$ and $x \in (0, |j|)$:

$$H_j(x) = \begin{cases} -\sum_{i=1}^{\infty} \frac{j^{-i}(-x)^i}{i}, & \text{if } j < 0 \\ \sum_{i=1}^{\infty} \frac{j^{-i}x^i}{i}, & \text{if } j > 0. \end{cases}$$

Set $\mathbf{m} = (m_1, \dots, m_l)$ and $q = \min_{m_i \neq 0} |m_i|$. Assuming that for $x \in (0, q)$

$$H_{\mathbf{m}}(x) = \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^a} S_n(\mathbf{b}; i)$$

one can write the relations for $j > 0$ and $x \in (0, \min(j, q))$

$$H_{0, \mathbf{m}}(x) = \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^{a+1}} S_n(\mathbf{b}; i)$$

$$\begin{aligned}
H_{j,m}(x) &= \sum_{i=1}^{\infty} \frac{x^i}{ij^i} S_{a,n}(\sigma j, \mathbf{b}; i-1) \\
&= \sum_{i=1}^{\infty} \frac{x^i}{ij^i} S_{a,n}(\sigma j, \mathbf{b}; i) - \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^{a+1}} S_n(\mathbf{b}; i) \\
H_{-j,m}(x) &= -\sum_{i=1}^{\infty} \frac{x^i}{i(-j)^i} S_{a,n}(-\sigma j, \mathbf{b}; i-1) \\
&= -\sum_{i=1}^{\infty} \frac{x^i}{i(-j)^i} S_{a,n}(-\sigma j, \mathbf{b}; i) + \sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^{a+1}} S_n(\mathbf{b}; i).
\end{aligned}$$

Proof. We just prove the case that $j > 0$. The other cases follow analogously.

$$\begin{aligned}
H_{j,m}(x) &= \int_0^x \frac{1}{j-y} \sum_{i=1}^{\infty} \frac{\sigma^i y^i}{i^a} S_n(\mathbf{b}; i) dy \\
&= \int_0^x \frac{1}{j} \sum_{k=0}^{\infty} \left(\frac{y}{j}\right)^k \sum_{i=1}^{\infty} \frac{\sigma^i y^i}{i^a} S_n(\mathbf{b}; i) dy \\
&= \frac{1}{j} \int_0^x \sum_{k=0}^{\infty} \left(\frac{y}{j}\right)^k \sum_{i=0}^{\infty} \frac{\sigma^{i+1} y^{i+1}}{(i+1)^a} S_n(\mathbf{b}; i+1) dy \\
&= \frac{1}{j} \int_0^x \sum_{i=0}^{\infty} \sum_{k=0}^i \left(\frac{y}{j}\right)^{i-k} \frac{\sigma^{k+1} y^{k+1}}{(k+1)^a} S_n(\mathbf{b}; k+1) dy \\
&= \int_0^x \sum_{i=0}^{\infty} \frac{y^{i+1}}{j^{i+2}} S_{a,n}(\sigma j, \mathbf{b}; i+1) dy \\
&= \sum_{i=1}^{\infty} \frac{x^{i+1}}{j^{i+1}(i+1)} S_{a,n}(\sigma j, \mathbf{b}; i) \\
&= \sum_{i=1}^{\infty} \frac{x^i}{ij^i} S_{a,n}(\sigma j, \mathbf{b}; i-1).
\end{aligned}$$

□

Note that again the reverse direction is possible, i.e., given a sum of the form

$$\sum_i (cx)^i \frac{S_n(\mathbf{b}; i)}{i^k}$$

with $k \in \mathbb{N}_0$ and $c \in \mathbb{R}^*$, we can find an linear combination of (possibly weighted) multiple polylogarithms $h(x)$ such that for $x \in (0, j)$ with $j > 0$ small enough

$$\sum_i (cx)^i \frac{S_n(\mathbf{b}; i)}{i^k} = h(x).$$

Example 3.3.1. For $x \in (0, \frac{1}{2})$ we have

$$\sum_i^{\infty} \frac{2^i x^i S_{1,1} \left(3, \frac{1}{2}; i\right)}{i} = H_{0,0,\frac{1}{3}}(x) + H_{0,\frac{1}{6},\frac{1}{3}}(x) + H_{\frac{1}{2},0,\frac{1}{3}}(x) + H_{\frac{1}{2},\frac{1}{6},\frac{1}{3}}(x).$$

3.3.1 Asymptotic Behavior of Multiple Polylogarithms

Similar to Section 2.4.1 we can combine Section 3.2.6 together with the power series expansion of multiple polylogarithms to determine the asymptotic behavior of multiple polylogarithms. Let us look at the multiple polylogarithm $H_m(x)$ and define $y := \frac{1}{x}$. Using Section 3.2.6 on $H_m\left(\frac{1}{y}\right) = H_m(x)$ we can rewrite $H_m(x)$ in terms of multiple polylogarithms at argument y together with some constants. Now we can get the power series expansion of the multiple polylogarithms at argument y around 0 easily using the previous part of this Section. Since sending x to infinity corresponds to sending y to zero, we get the asymptotic behavior of $H_m(x)$.

Example 3.3.2.

$$\begin{aligned} H_{-2,0}(x) &= H_{-2,0}(1) + H_{-\frac{1}{2},0}(1) - H_{-\frac{1}{2},0}\left(\frac{1}{x}\right) - H_{0,0}(1) + H_{0,0}\left(\frac{1}{x}\right) \\ &= \frac{1}{2} H_0(x)^2 - H_0(x) \left(\sum_{i=1}^{\infty} \frac{\left(-\frac{2}{x}\right)^i}{i} \right) - \sum_{i=1}^{\infty} \frac{\left(-\frac{2}{x}\right)^i}{i^2} \\ &\quad + H_{-2,0}(1) + H_{-\frac{1}{2},0}(1) - H_{0,0}(1). \end{aligned}$$

3.3.2 Values of Multiple Polylogarithms Expressed by S-Sums at Infinity

For $x = c, c \in (0, 1]$ we have that

$$\sum_{i=1}^{\infty} \frac{\sigma^i x^i}{i^a} S_n(\mathbf{b}; i) \rightarrow S_{a,n}(c\sigma, \mathbf{b}; \infty)$$

and hence (due to the previous part of this section) the values of the multiple polylogarithms in $x = c$ are related to the values of the generalized multiple harmonic sums at infinity. In this section we look at the problem to rewrite a multiple polylogarithm $H_m(c)$ (c such that $H_m(c)$ is finite) in terms of finite S-sums at infinity.

If $c < 0$, we use Lemma 3.2.6 to transform $H_m(c)$ to an expression out of multiple polylogarithms at argument $-c$. Hence we can assume $c > 0$. If the multiple polylogarithm $H_m(c)$ has trailing zeroes we first extract them. If $0 < c \leq 1$, we end up in an expression of multiple polylogarithms without trailing zeroes and powers of $H_0(c)$, while there can

also contribute multiple polylogarithms of the form $H_{a_1, a_2, \dots, a_k, 1, 0, \dots, 0}(c)$ if $c > 1$ (see Section 3.1).

To rewrite multiple polylogarithms of the form $H_{a_1, a_2, \dots, a_k}(c)$ where $a_k \neq 0$ and $\min_{a_i \neq 0} |a_i| > c$ we use the power series expansion of $H_{a_1, a_2, \dots, a_k}(x)$ and finally sending $x \rightarrow c$.

We can use the following lemma to rewrite powers of $H_0(c)$.

Lemma 3.3.3. *Let $c > 0$. We have*

$$\begin{aligned} 0 < c < 1 : & \quad H_0(c) = -S_1(1 - c; \infty) \\ c = 1 : & \quad H_0(c) = 0 \\ 1 < c \leq 2 : & \quad H_0(c) = -S_1(1 - c; \infty) \\ 2 < c : & \quad H_0(c) = H_0(2) - H_0\left(\frac{c}{2}\right). \end{aligned}$$

To rewrite $H_{a_1, a_2, \dots, a_k}(c)$ with $(a_1, a_2, \dots, a_k) = (1, 0, \dots, 0)$ and $c > 1$ we use the following lemma.

Lemma 3.3.4. *For $c > 0$ and $(a_1, a_2, \dots, a_k) = (1, 0, \dots, 0)$ we have*

$$H_{a_1, a_2, \dots, a_k}(c) = H_{a_1, a_2, \dots, a_k}(1) - H_{0, a_1 - 1, \dots, a_k - 1}(c - 1).$$

To rewrite multiple polylogarithms of the form $H_{a_1, a_2, \dots, a_k}(c)$ where $a_1 \in \mathbb{R} \setminus (0, c]$, $a_k \neq 0$, $\min_{a_i > 0} |a_i| \geq c$ and $s := \max_{a_i < 0} a_i > -c$ we use Lemma 3.2.2 to rewrite $H_{a_1, a_2, \dots, a_k}(x - s)$ and afterwards send $x \rightarrow c + s$. Now there are two cases: Either we can already handle the arising polylogarithms since we arrive in a previous case or we have to apply the same strategy once more.

Finally, to rewrite multiple polylogarithms of the form $H_{a_1, a_2, \dots, a_k, 1, 0, \dots, 0}(c)$ where $c > 1$ we can proceed similar to the previous case: we use Lemma 3.2.4 to rewrite $H_{a_1, a_2, \dots, a_k}(x + 1)$ and afterwards send $x \rightarrow c - 1$. Now we arrive at multiple polylogarithms at values we can already handle.

Summarizing, we can rewrite all finite multiple polylogarithms $H_{a_1, a_2, \dots, a_k}(c)$ in terms of S-sums at infinity.

Example 3.3.5.

$$\begin{aligned} H_{4,1,0}(3) = & \quad -S_{-3}(\infty) + 2S_3(\infty) + S_{-2}(\infty) S_1\left(\frac{1}{2}; \infty\right) - S_2(\infty) S_1\left(\frac{2}{3}; \infty\right) \\ & \quad - S_3\left(-\frac{1}{2}; \infty\right) + S_{-1}(\infty) \left(S_{-2}(\infty) - S_{1,1}\left(\frac{1}{2}, -2; \infty\right) \right) \end{aligned}$$

$$\begin{aligned}
& -S_{1,2}\left(\frac{1}{4}, 4; \infty\right) + S_{1,2}\left(\frac{1}{3}, -3; \infty\right) + S_{1,2}\left(\frac{1}{2}, -1; \infty\right) \\
& + S_{2,1}\left(-1, \frac{1}{2}; \infty\right) - S_{2,1}\left(\frac{1}{4}, 4; \infty\right) - S_{1,1,1}\left(\frac{1}{2}, -2, \frac{1}{2}; \infty\right).
\end{aligned}$$

Note that this process can be reversed. In particular, using Algorithm 1 also the other direction is possible; given a finite S-sum at infinity we can rewrite it in terms of multiple polylogarithms at one.

Example 3.3.6.

$$\begin{aligned}
S_{2,3,1}\left(-\frac{1}{2}, \frac{1}{3}, 2; \infty\right) &= -H_{0,-2,0,0,-6,-3}(1) + H_{0,-2,0,0,0,-3}(1) + H_{0,0,0,0,-6,-3}(1) \\
&\quad - H_{0,0,0,0,0,-3}(1).
\end{aligned}$$

Algorithm 1

input: a finite S-sum $S_{a_1, \dots, a_k}(b_1, \dots, b_k; \infty)$, with $a_i \in \mathbb{N}$ and $b_i \in \mathbb{R}^*$
output: expression in terms of multiple polylogarithms evaluating to finite constants
procedure SINFTOH($S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$)
 $c_1 = \frac{1}{b_1}$
for $i = 2$ **to** k **do**
 $c_i = \frac{b_{i-1}}{b_i}$
end for
 $l =$ number of entries < 0 in (c_1, \dots, c_k)
 $\bar{k} = \sum_{i=1}^k a_i$
 $j = 1$
for $i = 1$ **to** k **do**
while $a_i > 1$ **do**
 $a_i = a_i - 1$
 $d_j = 0$
 $j = j + 1$
end while
 $d_j = c_i$
 $j = j + 1$
end for
 $h = (-1)^l \cdot H_{d_1, d_2, \dots, d_{\bar{k}}}(1)$
rewrite h in terms of S-sums $\rightarrow \bar{h}$
return $h + \text{SINFTOH}(S_{a_1, \dots, a_k}(b_1, \dots, b_k; n) - \bar{h})$
end procedure

3.4 Integral Representation of S-Sums

In this section we want to derive an integral representation for S-sums. First we will find a multidimensional integral which can afterwards be rewritten as a sum of one-

dimensional integrals over multiple polylogarithms using integration by parts. We start with the base case of a S-sum of depth one and then give a detailed example.

Lemma 3.4.1 (Compare Lemma 2.5.1). *Let $m \in \mathbb{N}$, $b \in \mathbb{R}^*$ and $n \in \mathbb{N}$, then*

$$\begin{aligned} S_1(b; n) &= \int_0^b \frac{x_1^n - 1}{x_1 - 1} dx_1 \\ S_2(b; n) &= \int_0^b \frac{1}{x_2} \int_0^{x_2} \frac{x_1^n - 1}{x_1 - 1} dx_1 dx_2 \\ S_m(b; n) &= \int_0^b \frac{1}{x_m} \int_0^{x_m} \frac{1}{x_{m-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^n - 1}{x_1 - 1} dx_1 dx_2 \cdots dx_{m-1} dx_m. \end{aligned}$$

Proof. We proceed by induction on the weight m . For $m = 1$ we get:

$$\int_0^b \frac{x_1^n - 1}{x_1 - 1} dx_1 = \int_0^b \sum_{i=0}^{n-1} x_1^i dx_1 = \sum_{i=0}^{n-1} \int_0^b x_1^i dx_1 = \sum_{i=0}^{n-1} \frac{b^{i+1}}{i+1} = \sum_{i=1}^n \frac{b^i}{i} = S_1(b; n).$$

Now suppose the theorem holds for weight $m - 1$, we get

$$\begin{aligned} &\int_0^b \frac{1}{x_m} \int_0^{x_m} \frac{1}{x_{m-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^n - 1}{x_1 - 1} dx_1 dx_2 \cdots dx_{m-1} dx_m = \\ &\int_0^b \frac{S_{m-1}(x_m; n)}{x_m} dx_m = \int_0^b \sum_{i=1}^n \frac{x_m^{i-1}}{i^{m-1}} dx_m = \sum_{i=1}^n \int_0^b \frac{x_m^{i-1}}{i^{m-1}} dx_m = \\ &\sum_{i=1}^n \frac{b^i}{i} \frac{1}{i^{m-1}} = S_m(b; n). \end{aligned}$$

□

Example 3.4.2. *We consider the sum $S_{1,2,1}(a, b, c; n)$ with $a, b, c \in \mathbb{R}^*$. Due to the definition and Lemma 3.4.1 we have*

$$\begin{aligned} S_{1,2,1}(a, b, c; n) &= \sum_{k=1}^n \frac{a^k}{k} S_{2,1}(b, c; k) = \sum_{k=1}^n \frac{a^k}{k} \sum_{j=1}^k \frac{b^j}{j^2} S_1(c; j) \\ &= \sum_{k=1}^n \frac{a^k}{k} \sum_{j=1}^k \frac{b^j}{j^2} \int_0^c \frac{x^j - 1}{x - 1} dx \\ &= \sum_{k=1}^n \frac{a^k}{k} \int_0^c \frac{1}{x - 1} \sum_{j=1}^k \frac{b^j}{j^2} (x^j - 1) dx \\ &= \sum_{k=1}^n \frac{a^k}{k} \int_0^c \frac{1}{x - 1} (S_2(bx; k) - S_2(b; k)) dx \\ &= \sum_{k=1}^n \frac{a^k}{k} \int_0^c \frac{1}{x - 1} \int_b^{bx} \frac{1}{y} \int_0^y \frac{z^k - 1}{z - 1} dz dy dx \end{aligned}$$

$$\begin{aligned}
&= \sum_{k=1}^n \frac{a^k}{k} \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^y \frac{z^k - 1}{z-1} dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^y \frac{1}{z-1} \sum_{k=1}^n \frac{a^k (z^k - 1)}{k} dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^y \frac{a}{z-1} \int_1^z \sum_{k=1}^n (aw)^{k-1} dw dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^y \frac{a}{z-1} \int_1^z \frac{(aw)^n - 1}{aw-1} dw dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^y \frac{1}{z-1} \int_a^{za} \frac{w^n - 1}{w-1} dw dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^{ya} \frac{1}{\frac{z}{a}-1} \frac{1}{a} \int_a^z \frac{w^n - 1}{w-1} dw dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_b^x \frac{1}{y} \int_0^{ya} \frac{1}{z-a} \int_a^z \frac{w^n - 1}{w-1} dw dz dy dx \\
&= \int_0^{bc} \frac{1}{x-b} \int_{ba}^{xa} \frac{1}{y} \int_0^y \frac{1}{z-a} \int_a^z \frac{w^n - 1}{w-1} dw dz dy dx \\
&= \int_0^{abc} \frac{1}{x-ab} \int_{ab}^x \frac{1}{y} \int_0^y \frac{1}{z-a} \int_a^z \frac{w^n - 1}{w-1} dw dz dy dx.
\end{aligned}$$

Inspired by the previous example we arrive at the following theorem.

Theorem 3.4.3 (Compare Theorem 2.5.2). *Let $m_i \in \mathbb{N}$, $b_i \in \mathbb{R}^*$ and $n \in \mathbb{N}$, then*

$$\begin{aligned}
S_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; n) &= \\
&\int_0^{b_1 \dots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \int_0^{x_k^{m_k}} \frac{dx_k^{m_k-1}}{x_k^{m_k-1}} \dots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_1 \dots b_{k-1}} \\
&\int_{b_1 \dots b_{k-1}}^{x_k^1} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \int_0^{x_{k-1}^{m_{k-1}}} \frac{dx_{k-1}^{m_{k-1}-1}}{x_{k-1}^{m_{k-1}-1}} \dots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_1 \dots b_{k-2}} \\
&\int_{b_1 \dots b_{k-2}}^{x_{k-1}^1} \frac{dx_{k-2}^{m_{k-2}}}{x_{k-2}^{m_{k-2}}} \int_0^{x_{k-2}^{m_{k-2}}} \frac{dx_{k-2}^{m_{k-2}-1}}{x_{k-2}^{m_{k-2}-1}} \dots \int_0^{x_{k-2}^3} \frac{dx_{k-2}^2}{x_{k-2}^2} \int_0^{x_{k-2}^2} \frac{dx_{k-2}^1}{x_{k-2}^1 - b_1 \dots b_{k-3}} \\
&\vdots \\
&\int_{b_1 b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \int_0^{x_3^{m_3}} \frac{dx_3^{m_3-1}}{x_3^{m_3-1}} \dots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_1 b_2} \\
&\int_{b_1 b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \int_0^{x_2^{m_2}} \frac{dx_2^{m_2-1}}{x_2^{m_2-1}} \dots \int_0^{x_2^3} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{dx_2^1}{x_2^1 - b_1} \\
&\int_{b_1}^{x_2^1} \frac{dx_1^{m_1}}{x_1^{m_1}} \int_0^{x_1^{m_1}} \frac{dx_1^{m_1-1}}{x_1^{m_1-1}} \dots \int_0^{x_1^3} \frac{dx_1^2}{x_1^2} \int_0^{x_1^2} \frac{(x_1^1)^n - 1}{x_1^1 - 1} dx_1^1.
\end{aligned}$$

Proof. We proceed by induction on depth k . For $k = 1$ see Lemma 3.4.1. Now let $k > 1$. Due to the induction hypothesis we get

$$\begin{aligned}
S_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; n) &= \sum_{i=1}^n \frac{b_1^i}{i^{m_1}} S_{m_2, \dots, m_k}(b_2, \dots, b_k; i) \\
&= \sum_{i=1}^n \frac{b_1^i}{i^{m_1}} \int_0^{b_2 \cdots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \cdots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_2 \cdots b_{k-1}} \\
&\quad \int_{b_2 \cdots b_{k-1}}^{x_{k-1}} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \cdots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_2 \cdots b_{k-2}} \\
&\quad \vdots \\
&\quad \int_{b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \cdots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_2} \\
&\quad \int_{b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \cdots \int_{x_2^3}^{x_2^1} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{(x_2^1)^i - 1}{x_2^1 - 1} dx_2^1 \\
&= \int_0^{b_2 \cdots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \cdots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_2 \cdots b_{k-1}} \\
&\quad \int_{b_2 \cdots b_{k-1}}^{x_{k-1}} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \cdots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_2 \cdots b_{k-2}} \\
&\quad \vdots \\
&\quad \int_{b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \cdots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_2} \\
&\quad \int_{b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \cdots \int_{x_2^3}^{x_2^1} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{dx_2^1}{x_2^1 - 1} \sum_{i=1}^n \frac{b_1^i \left((x_2^1)^i - 1 \right)}{i^{m_1}} \\
&= \int_0^{b_2 \cdots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \cdots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_2 \cdots b_{k-1}} \\
&\quad \int_{b_2 \cdots b_{k-1}}^{x_{k-1}} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \cdots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_2 \cdots b_{k-2}} \\
&\quad \vdots \\
&\quad \int_{b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \cdots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_2} \\
&\quad \int_{b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \cdots \int_{x_2^3}^{x_2^1} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{dx_2^1}{x_2^1 - 1} (S_{m_1}(b_1 x_2^1; i) - S_{m_1}(b_1; i)) \\
&= \int_0^{b_2 \cdots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \cdots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_2 \cdots b_{k-1}} \\
&\quad \int_{b_2 \cdots b_{k-1}}^{x_{k-1}} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \cdots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_2 \cdots b_{k-2}} \\
&\quad \vdots \\
&\quad \int_{b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \cdots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_2} \\
&\quad \int_{b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \cdots \int_0^{x_2^3} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{dx_2^1}{x_2^1 - 1}
\end{aligned}$$

$$\begin{aligned}
& \int_{b_1}^{b_1 x_2^1} \frac{dx_1^{m_1}}{x_1^{m_1}} \cdots \int_0^{x_{13}} \frac{1}{x_1^2} \int_0^{x_1^1} \frac{(x_1^1)^n - 1}{x_1^1 - 1} \\
&= \int_0^{b_1 b_2 \cdots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \cdots \int_0^{x_k^3} \frac{dx_k^2}{x_k^2} \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_1 b_2 \cdots b_{k-1}} \\
& \int_{b_1 b_2 \cdots b_{k-1}}^{x_{k1}} \frac{dx_{k-1}^{m_{k-1}}}{x_{k-1}^{m_{k-1}}} \cdots \int_0^{x_{k-1}^3} \frac{dx_{k-1}^2}{x_{k-1}^2} \int_0^{x_{k-1}^2} \frac{dx_{k-1}^1}{x_{k-1}^1 - b_1 b_2 \cdots b_{k-2}} \\
& \quad \vdots \\
& \int_{b_1 b_2 b_3}^{x_4^1} \frac{dx_3^{m_3}}{x_3^{m_3}} \cdots \int_0^{x_3^3} \frac{dx_3^2}{x_3^2} \int_0^{x_3^2} \frac{dx_3^1}{x_3^1 - b_1 b_2} \\
& \int_{b_1 b_2}^{x_3^1} \frac{dx_2^{m_2}}{x_2^{m_2}} \cdots \int_0^{x_2^3} \frac{dx_2^2}{x_2^2} \int_0^{x_2^2} \frac{dx_2^1}{x_2^1 - b_1} \\
& \int_{b_1}^{x_2^1} \frac{dx_1^{m_1}}{x_1^{m_1}} \cdots \int_0^{x_{13}} \frac{1}{x_1^2} \int_0^{x_1^1} \frac{(x_1^1)^n - 1}{x_1^1 - 1}.
\end{aligned}$$

□

3.4.1 Mellin Transformation of Multiple Polylogarithms with Indices in $\mathbb{R} \setminus (0, 1)$

In this section we look at the Mellin-transform of multiple polylogarithms with indices in $\mathbb{R} \setminus (0, 1)$. It will turn out that these transforms can be expressed using a subclass of the S-sums together with certain constants.

For $f(x) = 1/(a - x)$ with $a \in (0, 1)$, the Mellin transform is not defined since the integral $\int_0^1 \frac{x^n}{a-x}$ does not converge. We modify the definition of the Mellin transform Definition 2.5.5 to include these functions, like $1/(a - x)$, as follows (note that all the arising integrals are well defined).

Definition 3.4.4 (Compare Definition 2.5.5). *Let $h(x)$ be a multiple polylogarithm with indices in $\mathbb{R} \setminus (0, 1)$ or $h(x) = 1$ for $x \in [0, 1]$; let $a \in (0, \infty)$, $a_1 \in (1, \infty)$, $a_2 \in (0, 1]$. Then we define the extended and modified Mellin-transform as follows:*

$$M^+(h(x), n) = M(h(x), n) = \int_0^1 x^n h(x) dx, \quad (3.15)$$

$$M^+\left(\frac{h(x)}{a+x}, n\right) = M\left(\frac{h(x)}{a+x}, n\right) = \int_0^1 \frac{x^n h(x)}{a+x} dx, \quad (3.16)$$

$$M^+\left(\frac{h(x)}{a_1-x}, n\right) = M\left(\frac{h(x)}{a_1-x}, n\right) = \int_0^1 \frac{x^n h(x)}{a_1-x} dx, \quad (3.17)$$

$$M^+\left(\frac{h(x)}{a_2-x}, n\right) = \int_0^{\frac{1}{a_2}} \frac{(x^n - 1)h(a_2 x)}{1-x} dx = \int_0^1 \frac{\left(\frac{x}{a_2}\right)^n - 1}{a_2 - x} h(x) dx. \quad (3.18)$$

Remark 3.4.5. The definitions (3.15), (3.16), (3.17) are just the original Mellin transform (see (2.12)). Only in (3.18) we extended the original Mellin transform; besides that an additional difference was already mentioned in Remark 2.5.7.

Remark 3.4.6. In (3.18) both extensions $\int_0^{\frac{1}{a_2}} \frac{x^{n-1}}{1-x} dx$ and $\int_0^1 \frac{((\frac{x}{a_2})^n - 1)h(x)}{a_2 - x} dx$ are equivalent, which can be seen using a simple substitution. Since from an algorithmic point of view it is easier to handle the second integral, we prefer this representation.

Remark 3.4.7. From now on we will call the extended and modified Mellin transform M^+ just Mellin transform and we will write M instead of M^+ .

Subsequently, we want to study how we can actually calculate the Mellin transform of multiple polylogarithms with indices in $\mathbb{R} \setminus (0, 1)$ weighted by $1/(a+x)$ or $1/(a-x)$ for $a \in \mathbb{R}$. This will be possible due to the following lemma which is an extension of Lemma 2.5.9.

Lemma 3.4.8 (Compare Lemma 2.5.9). For $n \in \mathbb{N}$, $\mathbf{m} = (m_1, \bar{\mathbf{m}}) = (m_1, m_2, \dots, m_k)$ with $m_i \in \mathbb{R} \setminus (0, 1)$ and $a \in (0, \infty)$, $a_1 \in (1, \infty)$, $a_2 \in (0, 1)$, we have

$$\begin{aligned} M\left(\frac{1}{a+x}, n\right) &= \begin{cases} (-a)^n (S_1(-\frac{1}{a}; n) + H_{-a}(1)), & \text{if } 0 < a < 1 \\ (-a)^n (S_1(-\frac{1}{a}; n) - S_1(-\frac{1}{a}; \infty)), & \text{if } 1 \geq a \end{cases} \\ M\left(\frac{1}{a-x}, n\right) &= \begin{cases} -S_1(\frac{1}{a}; n), & \text{if } 0 < a \leq 1 \\ a^n (-S_1(\frac{1}{a}; n) + S_1(\frac{1}{a}; \infty)), & \text{if } 1 < a \end{cases} \\ M\left(\frac{H_{\mathbf{m}}(x)}{a+x}, n\right) &= -n M(H_{-a, \mathbf{m}}(x), n-1) + H_{-a, \mathbf{m}}(1), \\ M\left(\frac{H_{\mathbf{m}}(x)}{1-x}, n\right) &= -n M(H_{1, \mathbf{m}}(x), n-1), \\ M\left(\frac{H_{\mathbf{m}}(x)}{a_1-x}, n\right) &= -n M(H_{a_1, \mathbf{m}}(x), n-1) + H_{a_1, \mathbf{m}}(1), \\ M\left(\frac{H_{m_1, \bar{\mathbf{m}}}(x)}{a_2-x}, n\right) &= \begin{cases} -H_{m_1, \bar{\mathbf{m}}}(1) S_1(\frac{1}{a_2}; n) - \sum_{i=1}^n \frac{(\frac{1}{a_2})^i M(\frac{H_{\bar{\mathbf{m}}}(x)}{|m_1|+x}, i)}{i}, & \text{if } m_1 < 0 \\ -H_{0, \bar{\mathbf{m}}}(1) S_1(\frac{1}{a_2}; n) + \sum_{i=1}^n \frac{(\frac{1}{a_2})^i M(\frac{H_{\bar{\mathbf{m}}}(x)}{x}, i)}{i}, & \text{if } m_1 = 0 \\ \sum_{i=1}^n \frac{(\frac{1}{a_2})^i M(\frac{H_{\bar{\mathbf{m}}}(x)}{1-x}, i)}{i}, & \text{if } m_1 = 1, \\ -H_{m_1, \bar{\mathbf{m}}}(1) S_1(\frac{1}{a_2}; n) + \sum_{i=1}^n \frac{(\frac{1}{a_2})^i M(\frac{H_{\bar{\mathbf{m}}}(x)}{m_1-x}, i)}{i}, & \text{if } m_1 > 1, \end{cases} \end{aligned}$$

where the arising constants on the right hand side are finite.

Proof. For $a > 0$ we get

$$\begin{aligned} M\left(\frac{1}{a+x}, n\right) &= \int_0^1 \frac{x^n}{a+x} dx = \int_0^1 \frac{x^n - (-a)^n}{a+x} dx + \int_0^1 \frac{(-a)^n}{a+x} dx \\ &= \int_0^1 (-a)^{n-1} \sum_{i=0}^{n-1} \frac{x^i}{(-a)^i} dx + (-a)^n H_{-a}(1) \end{aligned}$$

$$\begin{aligned}
&= (-a)^{n-1} \sum_{i=0}^{n-1} \frac{1}{(-a)^i(i+1)} + (-a)^n \mathbf{H}_{-a}(1) \\
&= (-a)^n \mathbf{S}_1\left(-\frac{1}{a}; n\right) + (-a)^n \mathbf{H}_{-a}(1).
\end{aligned}$$

If $a \geq 1$ this is equal to $(-a)^n \mathbf{S}_1(-\frac{1}{a}; n) - \mathbf{S}_1(-\frac{1}{a}; \infty)$.

For $0 < a \leq 1$ we get

$$\begin{aligned}
\mathbf{M}\left(\frac{1}{a-x}, n\right) &= \frac{1}{a^n} \int_0^1 \frac{x^n - a^n}{a-x} dx = -\frac{1}{a^n} \int_0^1 a^{n-1} \sum_{i=0}^{n-1} \left(\frac{x}{a}\right)^i dx \\
&= -\frac{1}{a} \sum_{i=0}^{n-1} \frac{1}{a^i} \int_0^1 x^i dx = -\frac{1}{a} \sum_{i=0}^{n-1} \frac{1}{a^i(1+i)} \\
&= -\mathbf{S}_1\left(\frac{1}{a}; n\right).
\end{aligned}$$

For $a > 1$ we get

$$\begin{aligned}
\mathbf{M}\left(\frac{1}{a-x}, n\right) &= \int_0^1 \frac{x^n}{a-x} dx = \int_0^1 \frac{x^n - a^n}{a-x} dx + a^n \int_0^1 \frac{1}{a-x} dx \\
&= -a^n \mathbf{S}_1\left(\frac{1}{a}; n\right) + a^n \mathbf{H}_a(1) = -a^n \mathbf{S}_1\left(\frac{1}{a}; n\right) + a^n \mathbf{S}_1\left(\frac{1}{a}; \infty\right).
\end{aligned}$$

For $a > 0$ we get

$$\begin{aligned}
\int_0^1 x^n \mathbf{H}_{-a,m}(x) dx &= \frac{\mathbf{H}_{-a,m}(1)}{n+1} - \frac{1}{n+1} \int_0^1 \frac{x^{n+1}}{(a+x)} \mathbf{H}_m(x) dx \\
&= \frac{\mathbf{H}_{-a,m}(1)}{n+1} - \frac{1}{n+1} \mathbf{M}\left(\frac{\mathbf{H}_m(x)}{a+x}, n+1\right).
\end{aligned}$$

Hence we get

$$\mathbf{M}\left(\frac{\mathbf{H}_m(x)}{a+x}, n+1\right) = -(n+1) \mathbf{M}(\mathbf{H}_{-a,m}(x), n) + \mathbf{H}_{-a,m}(1).$$

Similarly we get

$$\begin{aligned}
\int_0^1 x^n \mathbf{H}_{1,m}(x) dx &= \frac{1}{n+1} \lim_{\epsilon \rightarrow 1} \left(\epsilon^{n+1} \mathbf{H}_{1,m}(\epsilon) - \int_0^\epsilon \frac{x^{n+1} - 1}{1-x} \mathbf{H}_m(x) dx + \mathbf{H}_{1,m}(\epsilon) \right) \\
&= \frac{1}{n+1} \int_0^1 \frac{x^{n+1} - 1}{1-x} \mathbf{H}_m(x) dx \\
&= \frac{1}{n+1} \mathbf{M}\left(\frac{\mathbf{H}_{1,m}(x)}{1-x}, n+1\right).
\end{aligned}$$

And hence

$$\mathbf{M}\left(\frac{\mathbf{H}_m(x)}{1-x}, n+1\right) = -(n+1) \mathbf{M}(\mathbf{H}_{1,m}(x), n). \quad (3.19)$$

For $a_1 \in (1, \infty)$ we get

$$\begin{aligned} \int_0^1 x^n H_{a_1, m}(x) dx &= \frac{H_{a_1, m}(1)}{n+1} - \frac{1}{n+1} \int_0^1 \frac{x^{n+1}}{(a_1 - x)} H_m(x) dx \\ &= \frac{H_{a_1, m}(1)}{n+1} - \frac{1}{n+1} M\left(\frac{H_m(x)}{a_1 - x}, n+1\right). \end{aligned}$$

Hence we get

$$M\left(\frac{H_m(x)}{a_1 - x}, n+1\right) = -(n+1)M(H_{a_1, m}(x), n) + H_{a_1, m}(1).$$

For $a_2 \in (0, 1)$ and $m_1 < 0$ we get

$$\begin{aligned} M\left(\frac{H_{m_1, m}(x)}{a_2 - x}, n\right) &= \frac{1}{a_2^n} \int_0^1 \frac{(x^n - a_2^n) H_{m_1, m}(x)}{a_2 - x} dx \\ &= -H_{m_1, m}(x) \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} \Bigg|_0^1 + \int_0^1 \frac{H_m(x)}{|m_1| + x} \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} dx \\ &= -H_{m_1, m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^1 \frac{x^i H_m(x)}{|m_1| + x} dx \\ &= -H_{m_1, m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} M\left(\frac{H_m(x)}{|m_1| + x}, i\right), \end{aligned}$$

$$\begin{aligned} M\left(\frac{H_{0, m}(x)}{a_2 - x}, n\right) &= \frac{1}{a_2^n} \int_0^1 \frac{(x^n - a_2^n) H_{0, m}(x)}{a_2 - x} dx \\ &= -H_{0, m}(x) \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} \Bigg|_0^1 + \int_0^1 \frac{H_m(x)}{x} \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} dx \\ &= -H_{0, m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^1 \frac{x^i H_m(x)}{x} dx \\ &= -H_{0, m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} M\left(\frac{H_m(x)}{x}, i\right), \end{aligned}$$

and

$$\begin{aligned} M\left(\frac{H_{1, m}(x)}{a_2 - x}, n\right) &= \frac{1}{a_2^n} \lim_{\epsilon \rightarrow 1} \int_0^\epsilon \frac{(x^n - a_2^n) H_{m_1, m}(x)}{a_2 - x} dx \\ &= \lim_{\epsilon \rightarrow 1} \left(-H_{1, m}(x) \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} \Bigg|_0^\epsilon + \int_0^\epsilon \frac{H_m(x)}{1-x} \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} dx \right) \end{aligned}$$

$$\begin{aligned}
&= \lim_{\epsilon \rightarrow 1} \left(-\mathbf{H}_{1,\mathbf{m}}(\epsilon) \mathbf{S}_1\left(\frac{\epsilon}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^\epsilon \frac{x^i \mathbf{H}_{\mathbf{m}}(x)}{1-x} dx \right) \\
&= \lim_{\epsilon \rightarrow 1} \left(-\mathbf{H}_{1,\mathbf{m}}(\epsilon) \mathbf{S}_1\left(\frac{\epsilon}{a_2}; n\right) + \mathbf{S}_1\left(\frac{1}{a_2}; n\right) \mathbf{H}_{1,\mathbf{m}}(\epsilon) \right. \\
&\quad \left. + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^\epsilon \frac{(x^i - 1) \mathbf{H}_{\mathbf{m}}(x)}{1-x} dx \right) \\
&= \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \mathbf{M}\left(\frac{\mathbf{H}_{\mathbf{m}}(x)}{1-x}, i\right).
\end{aligned}$$

For $a_2 \in (0, 1)$ and $m_1 > 0$ we get

$$\begin{aligned}
\mathbf{M}\left(\frac{\mathbf{H}_{m_1, \mathbf{m}}(x)}{a_2 - x}, n\right) &= \frac{1}{a_2^n} \int_0^1 \frac{(x^n - a_2^n) \mathbf{H}_{m_1, \mathbf{m}}(x)}{a_2 - x} dx \\
&= -\mathbf{H}_{m_1, \mathbf{m}}(x) \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} \Big|_0^1 + \int_0^1 \frac{\mathbf{H}_{\mathbf{m}}(x)}{m_1 - x} \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} dx \\
&= -\mathbf{H}_{m_1, \mathbf{m}}(1) \mathbf{S}_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^1 \frac{x^i \mathbf{H}_{\mathbf{m}}(x)}{m_1 - x} dx \\
&= -\mathbf{H}_{m_1, \mathbf{m}}(1) \mathbf{S}_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \mathbf{M}\left(\frac{\mathbf{H}_{\mathbf{m}}(x)}{m_1 - x}, i\right).
\end{aligned}$$

□

Due to Lemma 3.4.8 we are able to reduce the calculation of the Mellin transform of multiple polylogarithms with indices in $\mathbb{R} \setminus (0, 1)$ weighted by $1/(a+x)$ or $1/(a-x)$ to the calculation of the Mellin transform of multiple polylogarithms with indices in $\mathbb{R} \setminus (0, 1)$ which are not weighted, i.e., to the calculation of expressions of the form $\mathbf{M}(\mathbf{H}_{\mathbf{m}}(x), n)$. To calculate $\mathbf{M}(\mathbf{H}_{\mathbf{m}}(x), n)$ we proceed by recursion. First let us state the base cases, i.e., the Mellin transforms of multiple polylogarithms with depth 1.

Lemma 3.4.9 (Compare Lemma 2.5.10). *For $n \in \mathbb{N}$, $a \in \mathbb{R} \setminus (0, 1)$ we have*

$$M(H_a(x), n) = \begin{cases} \frac{-1}{(n+1)^2} \left((1 + a^{n+1}(n+1)S_1\left(\frac{1}{a}; n\right) \right. \\ \quad \left. - (a^{n+1} - 1)(n+1)S_1\left(\frac{1}{a}; \infty\right) \right), & \text{if } a \leq -1 \\ \frac{-1}{(n+1)^2} \left((1 + a^{n+1}(n+1)S_1\left(\frac{1}{a}; n\right) \right. \\ \quad \left. + (a^{n+1} - 1)(n+1)H_a(1) \right), & \text{if } -1 < a < 0 \\ \frac{-1}{(n+1)^2}, & \text{if } a = 0 \\ \frac{1}{(n+1)^2} (1 + (n+1)S_1(n)), & \text{if } a = 1 \\ \frac{1}{(n+1)^2} \left((1 + a^{n+1}(n+1)S_1\left(\frac{1}{a}; n\right) \right. \\ \quad \left. - (a^{n+1} - 1)(n+1)S_1\left(\frac{1}{a}; \infty\right) \right), & \text{if } a > 1 \end{cases}$$

where the arising constants are finite.

Proof. First let $a \leq -1$. By integration by parts we get:

$$\begin{aligned} M(H_a(x), n) &= \int_0^1 x^n H_a(x) dx = \frac{x^{n+1}}{n+1} H_a(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1}}{n+1} \frac{1}{|a|+x} dx \\ &= \frac{H_a(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} - a^{n+1}}{|a|+x} dx + a^{n+1} \int_0^1 \frac{1}{|a|+x} dx \right) \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{1}{n+1} \int_0^1 a^n \sum_{i=0}^n \frac{x^i}{a^i} dx \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{a^n}{n+1} \sum_{i=0}^n \frac{1}{a^i (i+1)} \\ &= \frac{-S_1\left(\frac{1}{a}; \infty\right)}{n+1} (1 - a^{n+1}) - \frac{a^{n+1}}{n+1} S_1\left(\frac{1}{a}; n+1\right) \\ &= \frac{-1}{n+1} \left(\frac{1}{n+1} + a^{n+1} S_1\left(\frac{1}{a}; n\right) - (a^{n+1} - 1) S_1\left(\frac{1}{a}; \infty\right) \right). \end{aligned}$$

For $-1 < a < 0$ we obtain:

$$\begin{aligned} M(H_a(x), n) &= \int_0^1 x^n H_a(x) dx = \frac{x^{n+1}}{n+1} H_a(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1}}{n+1} \frac{1}{|a|+x} dx \\ &= \frac{H_a(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} - a^{n+1}}{|a|+x} dx + a^{n+1} \int_0^1 \frac{1}{|a|+x} dx \right) \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{1}{n+1} \int_0^1 a^n \sum_{i=0}^n \frac{x^i}{a^i} dx \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{a^n}{n+1} \sum_{i=0}^n \frac{1}{a^i (i+1)} \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{a^{n+1}}{n+1} S_1\left(\frac{1}{a}; n+1\right) \end{aligned}$$

$$= \frac{-1}{(n+1)^2} \left(1 + a^{n+1}(n+1)S_1\left(\frac{1}{a}; n\right) + (a^{n+1} - 1)(n+1)H_a(1) \right).$$

For $a = 0$ it follows that

$$\begin{aligned} M(H_0(x), n) &= \int_0^1 x^n H_0(x) dx = \frac{x^{n+1}}{n+1} H_0(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1}}{n+1} \frac{1}{x} dx \\ &= - \int_0^1 \frac{x^n}{n+1} dx = - \frac{x^{n+1}}{(n+1)^2} \Big|_0^1 = - \frac{1}{(n+1)^2}. \end{aligned}$$

For $a = 1$ we get:

$$\begin{aligned} \int_0^1 x^n H_1(x) dx &= \lim_{\epsilon \rightarrow 1} \int_0^\epsilon x^n H_1(x) dx \\ &= \lim_{\epsilon \rightarrow 1} \left(\frac{x^{n+1}}{n+1} H_1(x) \Big|_0^\epsilon - \int_0^\epsilon \frac{x^{n+1}}{(n+1)(1-x)} dx \right) \\ &= \frac{1}{n+1} \lim_{\epsilon \rightarrow 1} \left(\epsilon^{n+1} H_1(\epsilon) - \int_0^\epsilon \frac{x^{n+1} - 1}{1-x} x dx - H_1(\epsilon) \right) \\ &= \frac{1}{n+1} \left(\lim_{\epsilon \rightarrow 1} (\epsilon^{n+1} - 1) H_1(\epsilon) + \lim_{\epsilon \rightarrow 1} \int_0^\epsilon \sum_{i=0}^n x^i dx \right) \\ &= \frac{1}{n+1} \left(0 + \int_0^1 \sum_{i=0}^n x^i dx \right) \\ &= \frac{1}{n+1} \sum_{i=0}^n \frac{1}{i+1} = \frac{1}{(n+1)^2} (1 + (n+1)S_1(n)). \end{aligned}$$

Finally for $a > 1$ we conclude that

$$\begin{aligned} M(H_a(x), n) &= \int_0^1 x^n H_a(x) dx = \frac{x^{n+1}}{n+1} H_a(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1}}{n+1} \frac{1}{a-x} dx \\ &= \frac{H_a(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} - a^{n+1}}{a-x} dx + a^{n+1} \int_0^1 \frac{1}{a-x} dx \right) \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) + \frac{1}{n+1} \int_0^1 a^n \sum_{i=0}^n \frac{x^i}{a^i} dx \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) + \frac{a^n}{n+1} \sum_{i=0}^n \frac{1}{a^i (i+1)} \\ &= \frac{S_1\left(\frac{1}{a}; \infty\right)}{n+1} (1 - a^{n+1}) + \frac{a^{n+1}}{n+1} S_1\left(\frac{1}{a}; n+1\right) \\ &= \frac{1}{n+1} \left(\frac{1}{n+1} + a^{n+1} S_1\left(\frac{1}{a}; n\right) - (a^{n+1} - 1) S_1\left(\frac{1}{a}; \infty\right) \right). \end{aligned}$$

□

The higher depth results for $M(H_m(x), n)$ can now be obtained by recursion:

Lemma 3.4.10 (Compare Lemma 2.5.11). For $n \in \mathbb{N}$, $a \in \mathbb{R} \setminus (0, 1)$ and $\mathbf{m} \in (\mathbb{R} \setminus (0, 1))^k$,

$$M(H_{a,\mathbf{m}}(x), n) = \begin{cases} \frac{(1-a^{n+1})H_{a,\mathbf{m}}(1)}{n+1} - \frac{a^n}{n+1} \sum_{i=0}^n \frac{M(H_{\mathbf{m}}(x), i)}{a^i}, & \text{if } a < 0 \\ \frac{H_{0,\mathbf{m}}(1)}{n+1} - \frac{1}{n+1} M(H_{\mathbf{m}}(x), n), & \text{if } a = 0 \\ \frac{1}{n+1} \sum_{i=0}^n M(H_{\mathbf{m}}(x), i), & \text{if } a = 1 \\ \frac{(1-a^{n+1})H_{a,\mathbf{m}}(1)}{n+1} + \frac{a^n}{n+1} \sum_{i=0}^n \frac{M(H_{\mathbf{m}}(x), i)}{a^i}, & \text{if } a > 1 \end{cases}$$

where the arising constants are finite.

Proof. We get the following results by integration by parts. For $a < 0$ we get:

$$\begin{aligned} M(H_{a,\mathbf{m}}(x), n) &= \int_0^1 x^n H_{a,\mathbf{m}}(x) dx = \frac{x^{n+1}}{n+1} H_{a,\mathbf{m}}(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1} H_{\mathbf{m}}(x)}{n+1} \frac{1}{|a|+x} dx \\ &= \frac{H_{a,\mathbf{m}}(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} - a^{n+1}}{|a|+x} H_{\mathbf{m}}(x) dx + a^{n+1} \int_0^1 \frac{H_{\mathbf{m}}(x)}{|a|+x} dx \right) \\ &= \frac{H_{a,\mathbf{m}}(1)}{n+1} (1 - a^{n+1}) - \frac{1}{n+1} \int_0^1 a^n \sum_{i=0}^n \frac{x^i H_{\mathbf{m}}(x)}{a^i} dx \\ &= \frac{H_{a,\mathbf{m}}(1)}{n+1} (1 - a^{n+1}) - \frac{a^n}{n+1} \sum_{i=0}^n \frac{1}{a^i} M(H_{\mathbf{m}}(x), i). \end{aligned}$$

For $a = 0$ we get:

$$\begin{aligned} \int_0^1 x^n H_{0,\mathbf{m}}(x) dx &= \frac{x^{n+1}}{n+1} H_{0,\mathbf{m}}(x) \Big|_0^1 - \int_0^1 \frac{x^n}{n+1} H_{\mathbf{m}}(x) dx \\ &= \frac{H_{0,\mathbf{m}}(1)}{n+1} - \frac{1}{n+1} M(H_{\mathbf{m}}(x), n). \end{aligned}$$

For $a = 1$ we it follows that

$$\begin{aligned} \int_0^1 x^n H_{1,\mathbf{m}}(x) dx &= \lim_{\epsilon \rightarrow 1} \int_0^\epsilon x^n H_{1,\mathbf{m}}(x) dx \\ &= \lim_{\epsilon \rightarrow 1} \left(\frac{x^{n+1}}{n+1} H_{1,\mathbf{m}}(x) \Big|_0^\epsilon - \int_0^\epsilon \frac{x^{n+1}}{(n+1)(1-x)} H_{\mathbf{m}}(x) dx \right) \\ &= \frac{1}{n+1} \lim_{\epsilon \rightarrow 1} \left(\epsilon^{n+1} H_{1,\mathbf{m}}(\epsilon) - \int_0^\epsilon \frac{x^{n+1} - 1}{1-x} H_{\mathbf{m}}(x) dx - H_{1,\mathbf{m}}(\epsilon) \right) \\ &= \frac{1}{n+1} \left(\lim_{\epsilon \rightarrow 1} (\epsilon^{n+1} - 1) H_{1,\mathbf{m}}(\epsilon) + \lim_{\epsilon \rightarrow 1} \int_0^\epsilon \sum_{i=0}^n x^i H_{\mathbf{m}}(x) dx \right) \\ &= \frac{1}{n+1} \left(0 + \int_0^1 \sum_{i=0}^n x^i H_{\mathbf{m}}(x) dx \right) \\ &= \frac{1}{n+1} \sum_{i=0}^n M(H_{\mathbf{m}}(x), i). \end{aligned}$$

For $a > 1$ we conclude that

$$\begin{aligned}
M(H_{a,m}(x), n) &= \int_0^1 x^n H_{a,m}(x) dx = \frac{x^{n+1}}{n+1} H_{a,m}(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1} H_m(x)}{n+1} \frac{1}{a-x} dx \\
&= \frac{H_{a,m}(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} - a^{n+1}}{a-x} H_m(x) dx + a^{n+1} \int_0^1 \frac{H_m(x)}{a-x} dx \right) \\
&= \frac{H_{a,m}(1)}{n+1} (1 - a^{n+1}) + \frac{1}{n+1} \int_0^1 a^n \sum_{i=0}^n \frac{x^i H_m(x)}{a^i} dx \\
&= \frac{H_{a,m}(1)}{n+1} (1 - a^{n+1}) + \frac{a^n}{n+1} \sum_{i=0}^n \frac{1}{a^i} M(H_m(x), i).
\end{aligned}$$

□

Using Lemma 3.4.8 together with Lemma 3.4.9 and Lemma 3.4.10 we are able to calculate the Mellin transform of multiple polylogarithms with indices in $\mathbb{R} \setminus (0, 1)$. In addition, the polylogarithms can be weighted by $1/(a+x)$ or $1/(a-x)$ for $a \in \mathbb{R}$. These Mellin transforms can be expressed using S-sums. If we restrict the indices of the multiple polylogarithms to $\mathbb{R} \setminus ((-1, 0) \cup (0, 1))$, it turns out that these Mellin transforms can be expressed using a subset of the S-sums. This subset consists of S-sums $S_{a_1, a_2, \dots, a_l}(b_1, b_2, \dots, b_k; n)$ with $(a_1, \dots, a_k) \in \mathbb{Z}^k$, $(b_2, \dots, b_k) \in ([-1, 1] \setminus \{0\})^{k-1}$ and $b_1 \in \mathbb{R} \setminus \{0\}$. We will call these sums \bar{S} -sums, see the following definition.

Definition 3.4.11 (\bar{S} -sums and \bar{H} -multiple polylogarithms). *We define the set*

$$\bar{S} := \left\{ S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n) \mid \begin{array}{l} a_i \in \mathbb{Z}^* \text{ for } 1 \leq i \leq k; b_1 \in \mathbb{R}^*; \\ b_i \in [-1, 1] \setminus \{0\} \text{ for } 2 \leq i \leq k \end{array} \right\}$$

and call the elements \bar{S} -sums and the set

$$\bar{H} := \{ H_{m_1, m_2, \dots, m_k}(x) \mid m_i \in \mathbb{R} \setminus ((-1, 0) \cup (0, 1)) \text{ for } 1 \leq i \leq k \}$$

and call the elements \bar{H} -multiple polylogarithms.

Remark 3.4.12. *Restricting to this class, we are able to construct the inverse Mellin transform.*

3.4.2 The Inverse Mellin Transform of \bar{S} -sums

As in the cases of harmonic sums, we can define an order on S-sums.

Definition 3.4.13 (Order on S-sums). *Let $S_{m_1}(\mathbf{b}_1; n)$ and $S_{m_2}(\mathbf{b}_2; n)$ be S-sums with weights w_1, w_2 and depths d_1 and d_2 , respectively. Then*

$$S_{m_1}(\mathbf{b}_1; n) \prec S_{m_2}(\mathbf{b}_2; n), \text{ if } w_1 < w_2, \text{ or } (w_1 = w_2 \text{ and } d_1 < d_2).$$

We say that an S-sum s_1 is more complicated than an S-sum s_2 if $s_2 \prec s_1$. For a set of S-sums we call an S-sum most complicated if it is a largest element with respect to \prec .

The following proposition guarantees that there is only one *most complicated* S-sum in the the Mellin transform of an \bar{H} -multiple polylogarithm.

Proposition 3.4.14 (Compare [1]). *In the Mellin transform of a multiple polylogarithm $H_m(x) \in \bar{H}$ weighted by $1/(c-x)$ or $1/(c+x)$ ($c \in \mathbb{R}^*$) there is only one most complicated S-sum $S_a(\mathbf{b}; n) \in \bar{S}$, i.e.,*

$$M\left(\frac{H_m(x)}{c \pm x}, n\right) = p \cdot S_a(\mathbf{b}; n) + t \quad (3.20)$$

where $p \in \mathbb{R}^$ and all S-sums in t occur linearly and are smaller than $S_a(\mathbf{b}; n)$.*

The *most complicated* S-sum in the Mellin transform of a \bar{H} -multiple polylogarithm can be calculated using Algorithm 2. Since all S-sums that occur in the Mellin transform are \bar{S} -sums, it is in fact a \bar{S} -sum. But even the reverse direction is possible: given an \bar{S} -sum, we can find an \bar{H} -multiple polylogarithm weighted by $1/(c-x)$ or $1/(c+x)$ such that the \bar{S} -sum is the *most complicated* S-sum in the Mellin transform of this weighted multiple polylogarithm. We will call this weighted multiple polylogarithm the *most complicated* weighted multiple polylogarithm in the inverse Mellin transform of the \bar{S} -sum. We can use Algorithm 3 to compute the most-complicated multiple polylogarithm in the inverse Mellin transform of a \bar{S} -sum. The proof of Proposition 3.4.14, in particular the correctness of Algorithms 2 and 3 are similar to the proof given in [1] and is thus skipped here.

The computation of the inverse Mellin transform of a \bar{S} -sum $S_{a_1, a_2, \dots, a_l}(b_1, b_2, \dots, b_l; n)$ now is straightforward just as in Section 2.5.2 (compare[1, 73]):

- Locate the most complicated \bar{S} -sum.
- Construct the corresponding most complicated multiple polylogarithm.
- Add it and subtract it.
- Perform the Mellin transform to the subtracted version. This will cancel the original \bar{S} -sum.

- Repeat the above steps until there are no more \bar{S} -sums.
- Let c be the remaining constant term; replace it by $M^{-1}(c)$, or equivalently, multiply c by $\delta(1-x)$.

Algorithm 2 The Most-Complicated S-Sum

input: $\frac{H_{m_1, \dots, m_k}(x)}{d+s*x}$, with $d \in \mathbb{R}^+$, $s \in \{-1, 1\}$ and $H_{m_1, \dots, m_k}(x) \in \bar{H}(x)$

output: $p \cdot S_a(\mathbf{b}; n)$ as in (3.20)

procedure MOSTCOMPS($\frac{H_{m_1, \dots, m_k}(x)}{d+s*x}$)

$(a_1, \dots, a_k, a_{k+1}) = (\text{sign}(m_1), \dots, \text{sign}(m_k), 1)$

for $i = k$ to 1 **do**

if $a_i \neq 0$ **then**

$j = i - 1$

while $j > 0$ and $a_j = 0$ **do**

$j = j - 1$

end while

if $j > 0$ and $a_j < 0$ **then**

$a_i = -a_i$

end if

if $j = 0$ and $s = 1$ **then**

$a_i = -a_i$

end if

end if

end for

 delete the zeros in $(|m_1|, \dots, |m_k|, 1)$; let $(b_1, \dots, b_{\bar{k}})$ be the result

for $i = \bar{k}$ to 2 **do**

$b_i = \frac{b_i}{b_{i-1}}$

end for

$b_1 = \frac{b_1}{d}$

$l = \text{number of entries } \leq 0 \text{ in } (m_1, \dots, m_k)$

 let $S_{\bar{a}_1, \dots, \bar{a}_{\bar{k}}}(n)$ be the sum that is denoted by the word $a_1 \cdots a_k$ (see Section 2.6.1)

$(b_1, \dots, b_{\bar{k}}) = (\text{sign}(\bar{a}_1) b_1, \dots, \text{sign}(\bar{a}_{\bar{k}}) b_{\bar{k}})$

$(\bar{a}_1, \dots, \bar{a}_{\bar{k}}) = (|\bar{a}_1|, \dots, |\bar{a}_{\bar{k}}|)$

return $s \cdot (-1)^l \cdot S_{\bar{a}_1, \dots, \bar{a}_{\bar{k}}}(b_1, \dots, b_{\bar{k}}; n)$

end procedure

Remark 3.4.15. *Again there is a second way to compute the inverse Mellin transform of an \bar{S} -sum: We can use the integral representation of Theorem 3.4.3. After repeated suitable integration by parts we can find the inverse Mellin transform.*

3.5 Differentiation of S-Sums

We present two strategies to compute the differentiation of S-sums. The first approach follows the ideas carried out in Section 2.5.3 for harmonic sums. Since we rely here

Algorithm 3 The Most-Complicated Harmonic Polylogarithm

input: $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$, with $a_i \in \mathbb{Z}$ and $b_i \in \mathbb{R}^*$

output: the most-complicated multiple polylogarithm in the inverse Mellin transform of $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ together with a possibly arising factor $(-1)^n$

procedure MOSTCOMPH($S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$)

$(a_1, \dots, a_k) = (\text{sign}(b_1) a_1, \dots, \text{sign}(b_k) a_k)$

$l =$ number of entries < 0 in (a_1, \dots, a_k)

$v = ((-1)^l)^n$

$s = -(-1)^l$

 let $m_1 \cdots m_{\bar{k}}$ be the notation in the alphabet $\{-1, 0, 1\}$ of $S_{a_1, \dots, a_k}(n)$ (see Section 2.6.1)

$j = 1$

if $s = 1$ and $\bar{k} \neq 1$ **then**

while $m_j = 0$ and $j < \bar{k} - 1$ **do**

$j = j + 1$

end while

$m_j = -m_j$

end if

if $\bar{k} \neq 1$ **then**

$d = \text{sign}(m_j)$

end if

for $i = j + 1$ to $\bar{k} - 1$ **do**

if $m_i \neq 0$ **then**

if $d = -1$ **then**

$m_i = -m_i$

end if

$d = \text{sign}(m_i)$

end if

end for

$l =$ number of entries ≤ 0 in $(m_1, \dots, m_{\bar{k}-1})$

$v = v \cdot s \cdot (-1)^l$

$b_k = \frac{1}{b_k}$

for $i = k - 1$ to 1 **do**

$b_i = \frac{b_{i+1}}{b_i}$

end for

$d = b_1$

$j = 1$

for $i = 1$ to $\bar{k} - 1$ **do**

if $m_i \neq 0$ **then**

$m_i = b_j m_i$

$j = j + 1$

end if

$b_i = \frac{b_{i+1}}{b_i}$

end for

if $(d > 1$ and $\bar{k} \neq 1)$ or $s \neq -1$ **then**

$v = \frac{v}{d^n}$

end if

return $v \cdot \frac{H_{m_1, \dots, m_{\bar{k}-1}}(x)}{d+sx}$

end procedure

on the inverse Mellin transform, this method is restricted to \bar{S} -sums using our current technologies. Finally, we will develop a second approach that will work for S-sums in general.

3.5.1 First Approach: Differentiation of \bar{S} -sums

We are able to calculate the inverse Mellin transform of \bar{S} -sums $S_{a_1, \dots, a_l}(b_1, \dots, b_l; n)$. It turned out that they are linear combinations of multiple polylogarithms weighted by the factors $1/(a \pm x)$. By computing the Mellin transform of a \bar{S} -sum we find in fact an analytic continuation of the sum to $n \in \mathbb{C}$ up to countable many isolated points. As for harmonic sums (see Section 2.5.3) this allows us to consider differentiation with respect to n , since we can differentiate the analytic continuation. Afterwards we may transform back to \bar{S} -sums applying the Mellin transformation.

Again differentiation turns out to be relatively easy if we represent the \bar{S} -sums using its inverse Mellin transform. If we want to differentiate $S_a(\mathbf{b}; n)$ with respect to n we can proceed as follows:

- Calculate the inverse Mellin transform of $S_a(\mathbf{b}; n)$.
- Set the constants to zero and multiply the remaining terms of the inverse Mellin transform by $H_0(x)$. This is in fact differentiation with respect to n .
- Calculate the Mellin transform of the multiplied inverse Mellin transform of $S_a(\mathbf{b}; n)$

Looking in detail at this procedure, we see that first we express the \bar{S} -sum as a linear combination of expressions of the form $M\left(\frac{H_m(x)}{k \pm x}, n\right)$ with $H_m(x) \in \bar{H}(x)$. Next we have to differentiate these summands. For “+” and $k \in \mathbb{R}^+$ this leads to:

$$\begin{aligned} \frac{d}{dn} M\left(\frac{H_m(x)}{k+x}, n\right) &= \frac{d}{dn} \int_0^1 \frac{x^n H_m(x)}{k+x} dx = \int_0^1 \frac{x^n H_0(x) H_m(x)}{k+x} dx \\ &= \int_0^1 \frac{x^n (H_{0, m_1, \dots, m_l}(x) + H_{m_1, 0, m_2, \dots, m_l}(x) + \dots + H_{m_1, \dots, m_l, 0}(x))}{k+x} dx \\ &= M\left(\frac{H_{0, m_1, \dots, m_l}(x)}{k+x}, n\right) + \dots + M\left(\frac{H_{m_1, \dots, m_l, 0}(x)}{k+x}, n\right). \end{aligned}$$

For “−” and $k \in (1, \infty)$ this leads to:

$$\begin{aligned} \frac{d}{dn} M\left(\frac{H_m(x)}{k-x}, n\right) &= \frac{d}{dn} \int_0^1 \frac{x^n H_m(x)}{k-x} dx = \int_0^1 \frac{x^n H_0(x) H_m(x)}{k-x} dx \\ &= \int_0^1 \frac{x^n (H_{0, m_1, \dots, m_l}(x) + H_{m_1, 0, m_2, \dots, m_l}(x) + \dots + H_{m_1, \dots, m_l, 0}(x))}{k-x} dx \end{aligned}$$

$$= M\left(\frac{H_{0,m_1,\dots,m_l}(x)}{k-x}, n\right) + \dots + M\left(\frac{H_{m_1,\dots,m_l,0}(x)}{k-x}, n\right).$$

For “–” and $k \in (0, 1]$ this leads to:

$$\begin{aligned} \frac{d}{dn} M\left(\frac{H_{\mathbf{m}}(x)}{k-x}, n\right) &= \frac{d}{dn} \int_0^1 \frac{\left(\frac{x^n}{k^n} - 1\right) H_{\mathbf{m}}(x)}{k-x} dx = \int_0^1 \frac{\frac{x^n}{k^n} (H_0(x) - H_0(k)) H_{\mathbf{m}}(x)}{k-x} dx \\ &= \int_0^1 \frac{\left(\frac{x^n}{k^n} - 1\right) H_0(x) H_{\mathbf{m}}(x)}{k-x} dx - H_0(k) \int_0^1 \frac{\left(\frac{x^n}{k^n} - 1\right) H_{\mathbf{m}}(x)}{k-x} dx \\ &\quad + \int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_{\mathbf{m}}(x)}{k-x} dx. \end{aligned} \quad (3.21)$$

In the following lemmas we will see that $\int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_{\mathbf{m}}(x)}{k-x} dx$ is finite and in other words, the last integral in (3.21) is well defined. We will see how we can evaluate this constant in terms of multiple polylogarithms. Hence in all three cases we eventually arrive at Mellin transforms of multiple polylogarithms.

Lemma 3.5.1. *For a multiple polylogarithm $H_{\mathbf{m}}(x)$ with $\mathbf{m} = (m_1, m_2, \dots, m_l)$, $m_i \in \mathbb{R} \setminus (0, 1]$ and $i \in \mathbb{N}$ the integral*

$$\int_0^1 \frac{H_0(x)^i H_{\mathbf{m}}(x)}{1-x} dx$$

exists and can be expressed in terms of multiple polylogarithms.

Proof. Using integration by parts we get

$$\begin{aligned} \int_0^1 \frac{H_0(x)^i H_{\mathbf{m}}(x)}{1-x} dx &:= \lim_{b \rightarrow 1^-} \lim_{a \rightarrow 0^+} \int_a^b \frac{H_0(x)^i H_{\mathbf{m}}(x)}{1-x} dx \\ &= \lim_{b \rightarrow 1^-} \lim_{a \rightarrow 0^+} \left(H_0(x)^i H_{1,\mathbf{m}}(x) \Big|_a^b - i \int_a^b \frac{H_0(x)^{i-1} H_{1,\mathbf{m}}(x)}{x} dx \right) \\ &= -i \int_0^1 \frac{H_0(x)^{i-1} H_{1,\mathbf{m}}(x)}{x} dx. \end{aligned}$$

After expanding the product $H_0(x)^{i-1} H_{1,\mathbf{m}}(x)$ and applying the integral we end up in multiple polylogarithms at one with leading zero. Hence the integral is finite. \square

Lemma 3.5.2. *For $k \in (0, 1)$ and $\mathbf{a} = (a_1, a_2, \dots, a_l)$, $m_i \in \mathbb{R} \setminus (0, 1]$ we have that*

$$\int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_{\mathbf{a}}(x)}{k-x} dx$$

is finite and can be expressed in terms of multiple polylogarithms.

Proof. If $H_a(x)$ has trailing zeroes, i.e., $a_l = 0$, we first extract them and get a linear combination of expressions of the form

$$\int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_0(x)^w H_m(x)}{k-x} dx$$

with $w \in \mathbb{N}$. Now let us look at such an expression:

$$\begin{aligned} \int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_0(x)^w H_m(x)}{k-x} dx &= \int_0^{\frac{1}{k}} \frac{H_0(x) H_0(kx)^w H_m(kx)}{k-kx} k dx \\ &= \int_0^{\frac{1}{k}} \frac{H_0(x) (H_0(x) + H_0(k))^w H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x)}{1-x} dx \\ &= \int_0^{\frac{1}{k}} \frac{H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x) \sum_{i=0}^w \binom{w}{i} H_0(x)^{i+1} H_0(k)^{w-i}}{1-x} dx \\ &= \sum_{i=0}^w \binom{w}{i} H_0(k)^{w-i} \underbrace{\int_0^{\frac{1}{k}} \frac{H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x) H_0(x)^{i+1}}{1-x} dx}_A \end{aligned}$$

$$\begin{aligned} A &= \int_0^1 \frac{H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x) H_0(x)^{i+1}}{1-x} dx + \int_1^{\frac{1}{k}} \frac{H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x) H_0(x)^{i+1}}{1-x} dx \\ &= \underbrace{\int_0^1 \frac{H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x) H_0(x)^{i+1}}{x} dx}_B - \underbrace{\int_0^{\frac{1}{k}-1} \frac{H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x+1) H_0(x+1)^{i+1}}{x} dx}_C. \end{aligned}$$

The integral B is finite and expressible in terms of multiple polylogarithms due to the previous lemma. After expanding the product $H_{\frac{m_1}{k}, \dots, \frac{m_l}{k}}(x+1) H_0(x+1)^{i+1}$, applying Lemma 3.2.1 and applying the integral we end up in multiple polylogarithms at one and at $\frac{1}{k} - 1$ which are all finite. Hence C is finite. Summarizing

$$\int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_a(x)}{k-x} dx$$

is finite, since we can write it as a sum of finite integrals. \square

Example 3.5.3. Let us differentiate $S_2(2; n)$. We have:

$$S_2(2; n) = M\left(\frac{H_0(x)}{\frac{1}{2}-x}, n\right) = \int_0^1 \frac{(2^n x^n - 1) H_0(x)}{\frac{1}{2}-x} dx.$$

Differentiating with respect to n yields:

$$\begin{aligned} \frac{d}{dn} \int_0^1 \frac{(2^n x^n - 1) H_0(x)}{\frac{1}{2}-x} dx &= \int_0^1 \frac{2^n x^n (H_0(x) + H_0(2)) H_0(x)}{\frac{1}{2}-x} dx \\ &= 2 \int_0^1 \frac{(2^n x^n - 1) H_{0,0}(x)}{\frac{1}{2}-x} dx + H_0(2) \int_0^1 \frac{(2^n x^n - 1) H_0(x)}{\frac{1}{2}-x} dx \end{aligned}$$

$$\begin{aligned}
& + \int_0^1 \frac{H_0(2x) H_0(x)}{\frac{1}{2} - x} dx \\
& = 2M\left(\frac{H_{0,0}(x)}{\frac{1}{2} - x}, n\right) + H_0(2) M\left(\frac{H_0(x)}{\frac{1}{2} - x}, n\right) + \int_0^1 \frac{H_0(2x) H_0(x)}{\frac{1}{2} - x} dx \\
& = -2S_3(2; n) + H_0(2) S_2(2; n) + H_{0,0,-1}(1) + 2H_{0,0,1}(1) + H_{0,1,-1}(1).
\end{aligned}$$

3.5.2 Second Approach: Differentiation of S-sums

Using the first approach we were able to compute the derivative for \bar{S} -sums. However we are also interested in the derivative of S-sums which are not in this subset. For those sums we failed in the first approach since we were not able to compute their inverse Mellin transform. Therefore we look at a different approach, which we will first illustrate using the following detailed example.

Example 3.5.4 (Differentiation of $S_{1,2,1}(\frac{1}{2}, 2, \frac{1}{3}; n)$). *Using Theorem 3.4.3 leads to*

$$\begin{aligned}
S_{1,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_1^x \frac{1}{y} \int_0^y \frac{1}{z-\frac{1}{2}} \int_{\frac{1}{2}}^z \frac{w^n-1}{w-1} dw dz dy dx \\
&= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^1 -\frac{1}{y} \int_0^y \frac{1}{\frac{1}{2}-z} \int_{\frac{1}{2}}^z \frac{w^n-1}{w-1} dw dz dy dx.
\end{aligned}$$

Differentiation of the integral representation with respect to n yields

$$\int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^1 -\frac{1}{y} \int_0^y \frac{1}{\frac{1}{2}-z} \int_{\frac{1}{2}}^z \frac{w^n H_0(w)}{w-1} dw dz dy dx =: A.$$

We want to rewrite A in terms of S-sums at n and finite S-sums at ∞ (or finite multiple polylogarithms). Therefore we first rewrite A in the following form:

$$\begin{aligned}
A &= \underbrace{\int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^1 -\frac{1}{y} \int_0^y \frac{1}{\frac{1}{2}-z} \int_{\frac{1}{2}}^z \frac{w^n-1}{w-1} H_0(w) dw dz dy dx}_{B:=} + \\
&\quad \underbrace{\int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^1 -\frac{1}{y} \int_0^y \frac{1}{\frac{1}{2}-z} \int_{\frac{1}{2}}^z \frac{H_0(w)}{w-1} dw dz dy dx}_{C:=}.
\end{aligned}$$

Let us first consider B : we split the integral at the zeroes of the denominators and get:

$$\begin{aligned}
B &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{1}{y} \int_0^y \frac{1}{z-\frac{1}{2}} \int_z^{\frac{1}{2}} -\frac{w^n-1}{w-1} H_0(w) dw dz dy dx + \\
&\quad \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_{\frac{1}{2}}^1 -\frac{1}{y} \int_0^{\frac{1}{2}} \frac{1}{z-\frac{1}{2}} \int_z^{\frac{1}{2}} -\frac{w^n-1}{w-1} H_0(w) dw dz dy dx + \\
&\quad \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_{\frac{1}{2}}^1 -\frac{1}{y} \int_{\frac{1}{2}}^y \frac{1}{z-\frac{1}{2}} \int_{\frac{1}{2}}^z \frac{w^n-1}{w-1} H_0(w) dw dz dy dx \\
&= B_1 + B_2 + B_3.
\end{aligned}$$

Starting from the inner integral and integrating integral by integral leads to

$$\begin{aligned}
B_1 &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{1}{y} \int_0^y \frac{1}{z-\frac{1}{2}} \left(H_0\left(\frac{1}{2}\right) S_1\left(\frac{1}{2}; n\right) - H_0(z) S_1(z; n) \right. \\
&\quad \left. + S_2\left(\frac{1}{2}; n\right) - S_2(z; n) \right) dz dy dx \\
&= \dots = \\
&= -H_3(1)H_{0,1,0}(1)S_1\left(\frac{1}{2}; n\right) + H_0(2)H_{3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - H_0(3)H_{3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) \\
&\quad - H_{0,3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - 2H_{3,0,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - H_0(2)H_3(1)S_{1,2}\left(\frac{1}{2}, 1; n\right) \\
&\quad + H_0(3)H_3(1)S_{1,2}\left(\frac{1}{2}, 2; n\right) + H_{0,3}(1)S_{1,2}\left(\frac{1}{2}, 2; n\right) - 2H_3(1)S_{1,3}\left(\frac{1}{2}, 1; n\right) \\
&\quad + 2H_3(1)S_{1,3}\left(\frac{1}{2}, 2; n\right) - H_3(1)S_{2,2}\left(\frac{1}{2}, 1; n\right) + H_3(1)S_{2,2}\left(\frac{1}{2}, 2; n\right) \\
&\quad - H_0(3)S_{1,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) - S_{1,2,2}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) - 2S_{1,3,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) \\
&\quad - S_{2,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right).
\end{aligned}$$

Applying the same strategy to B_2 and B_3 leads to

$$\begin{aligned}
B &= -H_3(1)H_{0,1,0}(2)S_1\left(\frac{1}{2}; n\right) + H_0(2)H_{3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - H_0(3)H_{3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) \\
&\quad - H_{0,3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - 2H_{3,0,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) + H_0(3)H_3(1)S_{1,2}\left(\frac{1}{2}, 2; n\right) \\
&\quad + H_{0,3}(1)S_{1,2}\left(\frac{1}{2}, 2; n\right) - H_0(3)S_{1,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) - S_{1,2,2}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) \\
&\quad - 2S_{1,3,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) - S_{2,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right).
\end{aligned}$$

Let us now consider C : again we split the integral at the zeroes of the denominators and get:

$$\begin{aligned}
C &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{1}{y} \int_0^y \frac{1}{z-\frac{1}{2}} \int_z^{\frac{1}{2}} -\frac{H_0(w)}{w-1} dw dz dy dx + \\
&\quad \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_{\frac{1}{2}}^1 -\frac{1}{y} \int_0^{\frac{1}{2}} \frac{1}{z-\frac{1}{2}} \int_z^{\frac{1}{2}} -\frac{H_0(w)}{w-1} dw dz dy dx + \\
&\quad \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_{\frac{1}{2}}^1 -\frac{1}{y} \int_{\frac{1}{2}}^y \frac{1}{z-\frac{1}{2}} \int_{\frac{1}{2}}^z \frac{H_0(w)}{w-1} dw dz dy dx \\
&= C_1 + C_2 + C_3.
\end{aligned}$$

Starting from the inner integral and integrating integral by integral leads to

$$\begin{aligned}
C_1 &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{1}{y} \int_0^y \frac{H_{1,0}\left(\frac{1}{2}\right) - H_{1,0}(z)}{z-\frac{1}{2}} dz dy dx \\
&= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{H_{\frac{1}{2}}(y) H_{1,0}\left(\frac{1}{2}\right) + H_{\frac{1}{2},1,0}(y)}{y} dy dx \\
&= \int_0^{\frac{1}{3}} \frac{H_{1,0}\left(\frac{1}{2}\right) \left(H_{0,\frac{1}{2}}\left(\frac{1}{2}\right) - H_{0,\frac{1}{2}}(x) \right) - H_{0,\frac{1}{2},1,0}\left(\frac{1}{2}\right) + H_{0,\frac{1}{2},1,0}(x)}{x-1} dx
\end{aligned}$$

$$\begin{aligned}
&= H_0(2)H_2(1)H_3(1)H_{0,1}(1) + H_3(1)H_{0,2}(1)H_{0,1}(1) - H_0(2)H_3(1)H_{0,1,2}(1) \\
&\quad - H_0(2)H_2(1)H_{3,0,\frac{3}{2}}(1) - H_{0,2}(1)H_{3,0,\frac{3}{2}}(1) - 2H_3(1)H_{0,0,1,2}(1) - H_3(1)H_{0,1,0,2}(1) \\
&\quad + H_0(3)H_{3,0,\frac{3}{2},3}(1) + H_{0,3,0,\frac{3}{2},3}(1) + 2H_{3,0,0,\frac{3}{2},3}(1) + H_{3,0,\frac{3}{2},0,3}(1).
\end{aligned}$$

Applying the same strategy to C_2 and C_3 leads to

$$\begin{aligned}
C &= H_3(1)H_0(2)^2H_{0,-1}(1) + H_2(1)H_3(1)H_0(2)H_{0,1}(1) + H_3(1)H_0(2)H_{-1,0,1}(1) \\
&\quad + H_3(1)H_0(2)H_{0,-1,1}(1) - H_3(1)H_0(2)H_{0,1,2}(1) - H_2(1)H_0(2)H_{3,0,\frac{3}{2}}(1) \\
&\quad + H_3(1)H_{0,1}(1)H_{0,2}(1) - H_{0,2}(1)H_{3,0,\frac{3}{2}}(1) - H_3(1)H_{-1,0,1,-1}(1) - 2H_3(1)H_{0,0,1,2}(1) \\
&\quad - H_3(1)H_{0,1,0,2}(1) + H_0(3)H_{3,0,\frac{3}{2},3}(1) + H_{0,3,0,\frac{3}{2},3}(1) + 2H_{3,0,0,\frac{3}{2},3}(1) + H_{3,0,\frac{3}{2},0,3}(1).
\end{aligned}$$

Adding B and C leads to the final result:

$$\begin{aligned}
&\frac{\partial S_{1,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right)}{\partial n} = \\
&H_0(2)H_{3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - H_3(1)H_{0,1,0,2}S_1\left(\frac{1}{2}; n\right) - H_0(3)H_{3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) \\
&- H_{0,3,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) - 2H_{3,0,0,\frac{3}{2}}(1)S_1\left(\frac{1}{2}; n\right) + H_0(3)H_3(1)S_{1,2}\left(\frac{1}{2}, 2; n\right) \\
&+ H_0(3)S_{1,2}\left(\frac{1}{2}, 2; n\right) - H_0(3)S_{1,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) - S_{1,2,2}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) \\
&- 2S_{1,3,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) - S_{2,2,1}\left(\frac{1}{2}, 2, \frac{1}{3}; n\right) + H_3(1)H_0(2)^2H_{0,-1}(1) \\
&+ H_2(1)H_3(1)H_0(2)H_{0,1}(1) + H_3(1)H_0(2)H_{-1,0,1}(1) + H_3(1)H_0(2)H_{0,-1,1}(1) \\
&- H_3(1)H_0(2)H_{0,1,2}(1) - H_2(1)H_0(2)H_{3,0,\frac{3}{2}}(1) + H_3(1)H_{0,1}(1)H_{0,2}(1) - H_0(2)H_{3,0,\frac{3}{2}}(1) \\
&- H_3(1)H_{-1,0,1,-1}(1) - 2H_3(1)H_{0,0,1,2}(1) - H_3(1)H_{0,1,0,2}(1) \\
&+ H_0(3)H_{3,0,\frac{3}{2},3}(1) + H_{0,3,0,\frac{3}{2},3}(1) + 2H_{3,0,0,\frac{3}{2},3}(1) + H_{3,0,\frac{3}{2},0,3}(1).
\end{aligned}$$

Details of the Method

Let us now look in detail at this method to compute the differentiation of a S-sum $S_m(\mathbf{b}; n) = S_{m_1, \dots, m_k}(b_1, \dots, b_l; n)$. We start with the integral representation of $S_m(\mathbf{b}; n)$ given in Theorem 3.4.3. We split the integral at 0 and 1 and at all zeroes of the denominators, i.e., at $0, 1, b_1, b_1b_2, \dots, b_1b_2 \cdots b_{l-1}$ such that $0, 1, b_1, b_1b_2, \dots, b_1b_2 \cdots b_{k-1}$ are always at the borders of the integration domains and never inside the integration domains. We end up with a sum of integrals of the form

$$\begin{aligned}
&\pm \int_a^b \frac{dx_k}{x_k - c_k} \int_{u_k}^{o_k} \frac{dx_{k-1}}{x_{k-1} - c_{k-1}} \int_{u_{k-1}}^{o_{k-1}} \frac{dx_{k-2}}{x_{k-2} - c_{k-2}} \cdots \int_{u_3}^{o_3} \frac{dx_2}{x_2 - c_2} \int_{u_2}^{o_2} \frac{dx_1}{x_1 - c_1} \\
&\times \int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \int_{s_{r-1}}^{t_{r-1}} \frac{dy_{r-2}}{y_{r-2} - g_{r-2}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{y_1^n - 1}{y_1 - 1} dy_1
\end{aligned}$$

where $(u_i, o_i) = (a, x_i) \vee (u_i, o_i) = (x_i, b) \vee (u_i, o_i) = (a, b)$; $b > a \geq 0 \vee 0 \geq b > a$; $c_i \in \mathbb{R} \setminus (a, b)$; $a \neq c_1 \neq b$ and $(s_i, t_i) = (e, y_i) \vee (s_i, t_i) = (y_i, f)$; $f > e \geq 1 \vee 1 \geq$

$f > e \geq 0 \vee 0 \geq f > e$; $g_i \in \mathbb{R} \setminus (e, f)$.

Note that due to the structure of the integral representation we have in addition:

$$\begin{aligned} \text{if } c_i = a &\longrightarrow u_i = a \\ \text{if } c_i = b &\longrightarrow o_i = b \\ \text{if } g_i = e &\longrightarrow s_i = e \\ \text{if } g_i = f &\longrightarrow t_i = f. \end{aligned}$$

In the case that $0 \geq b > a$ we apply the transform $x_i \rightarrow -x_i$ to the integral and get

$$\pm \int_{\bar{a}}^{\bar{b}} \frac{dx_k}{x_k - \bar{c}_k} \int_{\bar{u}_k}^{\bar{o}_k} \frac{dx_{k-1}}{x_{k-1} - \bar{c}_{k-1}} \int_{\bar{u}_{k-1}}^{\bar{o}_{k-1}} \frac{dx_{k-2}}{x_{k-2} - \bar{c}_{k-2}} \cdots \int_{\bar{u}_3}^{\bar{o}_3} \frac{dx_2}{x_2 - \bar{c}_2} \int_{\bar{u}_2}^{\bar{o}_2} \frac{dx_1}{x_1 - \bar{c}_1}$$

with $\bar{a} = -b$; $\bar{b} = -a$ and $\bar{c}_i = -c_i$; where $(\bar{u}_i, \bar{o}_i) = (\bar{a}, x_i) \vee (\bar{u}_i, \bar{o}_i) = (x_i, \bar{b}) \vee (\bar{u}_i, \bar{o}_i) = (\bar{a}, \bar{b})$; $\bar{b} > \bar{a} \geq 0$; $\bar{c}_i \in \mathbb{R} \setminus (\bar{a}, \bar{b})$; $\bar{a} \neq \bar{c}_1 \neq \bar{b}$ and

$$\begin{aligned} \text{if } \bar{c}_i = \bar{a} &\longrightarrow \bar{u}_i = \bar{a} \\ \text{if } \bar{c}_i = \bar{b} &\longrightarrow \bar{o}_i = \bar{b}. \end{aligned}$$

Hence we can always assume $b > a \geq 0$.

In the case that $0 \geq f > e$ we apply the transform $y_i \rightarrow -y_i$ to the integral and get

$$\pm \int_{\bar{e}}^{\bar{f}} \frac{dy_r}{y_r - \bar{g}_r} \int_{\bar{s}_r}^{\bar{t}_r} \frac{dy_{r-1}}{y_{r-1} - \bar{g}_{r-1}} \int_{\bar{s}_{r-1}}^{\bar{t}_{r-1}} \frac{dx_{r-2}}{y_{r-2} - \bar{g}_{r-2}} \cdots \int_{\bar{s}_3}^{\bar{t}_3} \frac{dx_2}{x_2 - \bar{g}_2} \int_{\bar{s}_2}^{\bar{t}_2} \frac{(-y_1)^n - 1}{y_1 + 1} dy_1$$

with $\bar{e} = -f$; $\bar{f} = -e$ and $\bar{g}_i = -g_i$; where $(\bar{s}_i, \bar{t}_i) = (\bar{e}, y_i) \vee (\bar{s}_i, \bar{t}_i) = (y_i, \bar{f})$; $\bar{f} > \bar{e} \geq 0$; $\bar{g}_i \in \mathbb{R} \setminus (\bar{e}, \bar{f})$ and

$$\begin{aligned} \text{if } \bar{g}_i = \bar{e} &\longrightarrow \bar{s}_i = \bar{e} \\ \text{if } \bar{g}_i = \bar{f} &\longrightarrow \bar{t}_i = \bar{f}. \end{aligned}$$

Hence we can rewrite the integral representation of Theorem 3.4.3 as a sum of integrals of the form

$$\begin{aligned} &\pm \int_a^b \frac{dx_k}{x_k - c_k} \int_{u_k}^{o_k} \frac{dx_{k-1}}{x_{k-1} - c_{k-1}} \cdots \int_{u_3}^{o_3} \frac{dx_2}{x_2 - c_2} \int_{u_2}^{o_2} \frac{dx_1}{x_1 - c_1} \\ &\times \int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{(\pm y_1)^n - 1}{y_1 \mp 1} dy_1 \quad (3.22) \end{aligned}$$

where $(u_i, o_i) = (a, x_i) \vee (u_i, o_i) = (x_i, b)$; $b > a \geq 0$; $c_i \in \mathbb{R} \setminus (a, b)$; $a \neq c_1 \neq b$ and $(s_i, t_i) = (e, y_i) \vee (s_i, t_i) = (y_i, f)$; $f > e \geq 1 \vee 1 \geq f > e \geq 0$; $g_i \in \mathbb{R} \setminus (e, f)$ and

$$\begin{aligned} \text{if } c_i = a &\longrightarrow u_i = a \\ \text{if } c_i = b &\longrightarrow o_i = b \end{aligned}$$

$$\begin{aligned} \text{if } g_i = e &\longrightarrow s_i = e \\ \text{if } g_i = f &\longrightarrow t_i = f. \end{aligned}$$

Differentiating of an integral of the form (3.22) with respect to n leads to (note that we did not differentiate the factor $(-1)^n$):

$$\begin{aligned} &\pm \int_a^b \frac{dx_k}{x_k - c_k} \int_{u_k}^{o_k} \frac{dx_{k-1}}{x_{k-1} - c_{k-1}} \cdots \int_{u_3}^{o_3} \frac{dx_2}{x_2 - c_2} \int_{u_2}^{o_2} \frac{dx_1}{x_1 - c_1} \\ &\times \int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{(\pm y_1)^n \mathbb{H}_0(y_1)}{y_1 \mp 1} dy_1 \\ &= \pm \int_a^b \frac{dx_k}{x_k - c_k} \int_{u_k}^{o_k} \frac{dx_{k-1}}{x_{k-1} - c_{k-1}} \cdots \int_{u_3}^{o_3} \frac{dx_2}{x_2 - c_2} \int_{u_2}^{o_2} \frac{dx_1}{x_1 - c_1} \\ &\times \int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{(\pm y_1)^n - 1}{y_1 \mp 1} \mathbb{H}_0(y_1) dy_1 \\ &\pm \int_a^b \frac{dx_k}{x_k - c_k} \int_{u_k}^{o_k} \frac{dx_{k-1}}{x_{k-1} - c_{k-1}} \cdots \int_{u_3}^{o_3} \frac{dx_2}{x_2 - c_2} \int_{u_2}^{o_2} \frac{dx_1}{x_1 - c_1} \\ &\times \int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{\mathbb{H}_0(y_1)}{y_1 \mp 1} dy_1. \end{aligned}$$

Now we want to transform these integrals back to S-sums and constants related to S-sums, i.e., S-sums at infinity or multiple polylogarithms evaluated at constants. For this task we have to consider the following 5 different classes of integrals

- (a) $\int_a^b \frac{dx_k}{x_k - c_k} \int_{u_k}^{o_k} \frac{dx_{k-1}}{x_{k-1} - c_{k-1}} \cdots \int_{u_3}^{o_3} \frac{dx_2}{x_2 - c_2} \int_{u_2}^{o_2} \frac{dx_1}{x_1 - c_1}$
- (b) $\int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{\mathbb{H}(y_1)}{y_1 - 1} dy_1$
- (c) $\int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{\mathbb{H}(y_1)}{y_1 + 1} dy_1$
- (d) $\int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{y_1^{n-1}}{y_1 - 1} \mathbb{H}_0(y_1) dy_1$
- (e) $\int_e^f \frac{dy_r}{y_r - g_r} \int_{s_r}^{t_r} \frac{dy_{r-1}}{y_{r-1} - g_{r-1}} \cdots \int_{s_3}^{t_3} \frac{dy_2}{y_2 - g_2} \int_{s_2}^{t_2} \frac{(-y_1)^{n-1}}{y_1 + 1} \mathbb{H}_0(y_1) dy_1$

with $b > a \geq 0$ $f > e \geq 1$ or $1 \geq f > e \geq 0$ $(u_i, o_i) = (a, x_i) \vee (u_i, o_i) = (x_i, b)$; $b > a \geq 0$; $c_i \in \mathbb{R} \setminus (a, b)$; $a \neq c_1 \neq b$ and $(s_i, t_i) = (e, y_i) \vee (s_i, t_i) = (y_i, f)$; $f > e \geq 1 \vee 1 \geq f > e \geq 0$; $g_i \in \mathbb{R} \setminus (e, f)$ and

$$\begin{aligned} \text{if } c_i = a &\longrightarrow u_i = a \\ \text{if } c_i = b &\longrightarrow o_i = b \\ \text{if } g_i = e &\longrightarrow s_i = e \\ \text{if } g_i = f &\longrightarrow t_i = f. \end{aligned}$$

In the following we will use the abbreviations

$$\begin{aligned} \mathbf{H}_m(x|y) &:= \mathbf{H}_m(x) - \mathbf{H}_m(y) \\ S_{m_1, \dots, m_k}(b_1, \dots, b_{k-1}, b_k | b_{k+1}; n) &:= S_{m_1, \dots, m_k}(b_1, \dots, b_{k-1}, b_k; n) \\ &\quad - S_{m_1, \dots, m_k}(b_1, \dots, b_{k-1}, b_{k+1}; n). \end{aligned}$$

We start with integrals of type **(a)**. We will show that we can represent it in the form

$$\sum_{\iota=1}^p z_\iota \mathbf{H}_{m_\iota}(b, a) + \sum_{\iota=1}^q v_\iota \mathbf{H}_{n_\iota}(b_i - c_j | a - c_j) \quad (3.23)$$

with z_ι, v_ι products of multiple polylogarithms evaluated at constants and $j \in \{1, 2, \dots, k\}$. If $k = 1$, we get

$$\int_a^b \frac{dx_1}{x_1 - c_1} = \begin{cases} -\text{sign}(c_1) \mathbf{H}_{c_1}(a|b), & \text{if } c_1 > b \vee 0 \geq c_1 \\ \mathbf{H}_0(a - c_1 | b - c_1), & \text{if } a > c_1 > 0. \end{cases}$$

Let now $1 < i \leq k$. We will see that we can express the first $i - 1$ integrals in the form

$$\sum_{\iota=1}^p z_\iota \mathbf{H}_{m_\iota}(o_i | u_i) + \sum_{\iota=1}^q v_\iota \mathbf{H}_{n_\iota}(o_i - c_j | u_i - c_j)$$

with z_ι, v_ι products of multiple polylogarithms evaluated at constants and $j \in \{1, 2, \dots, i - 1\}$. For $i = 2$ this is obvious. We will now perform the induction step $i \rightarrow i + 1$, therefore we will look at the integrals

$$A := \int_{u_{i+1}}^{o_{i+1}} \frac{\mathbf{H}_m(o_i | u_i)}{x_i - c_i} dx_i \quad \text{and} \quad B := \int_{u_{i+1}}^{o_{i+1}} \frac{\mathbf{H}_m(o_i - c_j | u_i - c_j)}{x_i - c_i} dx_i$$

where $u_{k+1} := a, o_{k+1} := b$ and distinguish several cases:

- $(u_i, o_i) = (a, x_i); c_i > b \vee 0 > c_i :$

$$\begin{aligned} A &= \int_{u_{i+1}}^{o_{i+1}} \frac{\mathbf{H}_m(x_i | a)}{x_i - c_i} dx_i = -\text{sign}(c_i) \mathbf{H}_{c_i, m}(o_{i+1} | u_{i+1}) \\ &\quad + \text{sign}(c_i) \mathbf{H}_{c_i}(o_{i+1} | u_{i+1}) \mathbf{H}_m(a) \\ B &= \int_{u_{i+1}}^{o_{i+1}} \frac{\mathbf{H}_m(x_i - c_j | a - c_j)}{x_i - c_i} dx_i = \int_{u_{i+1} - c_j}^{o_{i+1} - c_j} \frac{\mathbf{H}_m(x_i | a - c_j)}{x_i + c_j - c_i} dx_i \\ &= -\text{sign}(c_i - c_j) \mathbf{H}_{c_i - c_j, m}(o_{i+1} - c_j | u_{i+1} - c_j) \\ &\quad + \text{sign}(c_i - c_j) \mathbf{H}_{c_i - c_j}(o_{i+1} - c_j | u_{i+1} - c_j) \mathbf{H}_m(a - c_j). \end{aligned}$$

Hence in all of the three possible cases, i.e., (u_{i+1}, o_{i+1}) equals (a, x_{i+1}) , (x_{i+1}, b) or (a, b) we arrive at the desired results.

- $(u_i, o_i) = (x_i, b); c_i > b \vee 0 > c_i :$

$$\begin{aligned}
A &= \int_{u_{i+1}}^{o_{i+1}} \frac{\mathbf{H}_m(b|x_i)}{x_i - c_i} dx_i = \text{sign}(c_i) \mathbf{H}_{c_i, m}(o_{i+1}|u_{i+1}) \\
&\quad - \text{sign}(c_i) \mathbf{H}_{c_i}(o_{i+1}|u_{i+1}) \mathbf{H}_m(a) \\
B &= \int_{u_{i+1}}^{o_{i+1}} \frac{\mathbf{H}_m(b - c_j|x_i - c_j)}{x_i - c_i} dx_i = \int_{u_{i+1}-c_j}^{o_{i+1}-c_j} \frac{\mathbf{H}_m(b - c_j|x_i)}{x_i + c_j - c_i} dx_i \\
&= \text{sign}(c_i - c_j) \mathbf{H}_{c_i - c_j, m}(o_{i+1} - c_j|u_{i+1} - c_j) \\
&\quad - \text{sign}(c_i - c_j) \mathbf{H}_{c_i - c_j}(o_{i+1} - c_j|u_{i+1} - c_j) \mathbf{H}_m(b - c_j).
\end{aligned}$$

Hence in all of the three possible cases, i.e., (u_{i+1}, o_{i+1}) equals (a, x_{i+1}) , (x_{i+1}, b) or (a, b) we arrive at the desired results.

- $(u_i, o_i) = (a, x_i); a > c_i \geq 0 :$

$$\begin{aligned}
A &= \int_{u_{i+1}-c_i}^{o_{i+1}-c_i} \frac{\mathbf{H}_m(x_i + c_i) - \mathbf{H}_m(a)}{x_i} dx_i \\
B &= \int_{u_{i+1}-c_i}^{o_{i+1}-c_i} \frac{\mathbf{H}_m(x_i + c_i - c_j) - \mathbf{H}_m(a)}{x_i} dx_i.
\end{aligned}$$

Applying transforms discussed in Section 3.2 to $\mathbf{H}_m(x_i + c_i)$ and to $\mathbf{H}_m(x_i + c_i - c_j)$ leads to

$$\begin{aligned}
A &= \sum_{\rho} \int_{u_{i+1}-c_i}^{o_{i+1}-c_i} \xi_{\rho} \frac{\mathbf{H}_{m_{\rho}}(x_i)}{x_i} - \mathbf{H}_0(o_{i+1} - c_i|u_{i+1} - c_i) \mathbf{H}_m(a) \\
&= \sum_{\rho} \xi_{\rho} \mathbf{H}_{m_{\rho}}(o_{i+1} - c_i|u_{i+1} - c_i) - \mathbf{H}_0(o_{i+1} - c_i|u_{i+1} - c_i) \mathbf{H}_m(a) \\
B &= \sum_{\rho} \int_{u_{i+1}-c_i}^{o_{i+1}-c_i} \xi_{\rho} \frac{\mathbf{H}_{m_{\rho}}(x_i)}{x_i} - \mathbf{H}_0(o_{i+1} - c_i|u_{i+1} - c_i) \mathbf{H}_m(a) \\
&= \sum_{\rho} \mu_{\rho} \mathbf{H}_{m_{\rho}}(o_{i+1} - c_i|u_{i+1} - c_i) - \mathbf{H}_0(o_{i+1} - c_i|u_{i+1} - c_i) \mathbf{H}_m(a),
\end{aligned}$$

where ξ_{ρ} and μ_{ρ} are multiple polylogarithms evaluated at constants. Hence in all of the three possible cases, i.e., (u_{i+1}, o_{i+1}) equals (a, x_{i+1}) , (x_{i+1}, b) or (a, b) we get the desired results.

- $(u_i, o_i) = (x_i, b); a > c_i \geq 0 :$

This case can be basically handled like the previous one.

- $(u_i, o_i) = (x_i, b); c_i = b :$

$$\begin{aligned}
A &= \int_{u_{i+1}-b}^{o_{i+1}-b} \frac{\mathbf{H}_m(x_i + b) - \mathbf{H}_m(a)}{x_i} dx_i \\
B &= \int_{u_{i+1}-b}^{o_{i+1}-b} \frac{\mathbf{H}_m(x_i + b - c_j) - \mathbf{H}_m(a)}{x_i} dx_i.
\end{aligned}$$

Applying transforms discussed in Section 3.2 to $H_m(x_i + c_i)$ and to $H_m(x_i + c_i - c_j)$ leads to

$$\begin{aligned} A &= \sum_{\rho} \int_{u_{i+1}-b}^{o_{i+1}-b} \xi_{\rho} \frac{H_{m_{\rho}}(x_i)}{x_i} = \sum_{\rho} \xi_{\rho} H_{m_{\rho}}(o_{i+1} - b | u_{i+1} - b) \\ B &= \sum_{\rho} \int_{u_{i+1}-b}^{o_{i+1}-b} \xi_{\rho} \frac{H_{m_{\rho}}(x_i)}{x_i} = \sum_{\rho} \mu_{\rho} H_{m_{\rho}}(o_{i+1} - b | u_{i+1} - b), \end{aligned}$$

where ξ_{ρ} and μ_{ρ} are multiple polylogarithms evaluated at constants and none of the leading indices of $H_{m_{\rho}}(x_i)$ equals $o_{i+1} - b$. Hence in all of the three possible cases, i.e., (u_{i+1}, o_{i+1}) equals (a, x_{i+1}) , (x_{i+1}, b) or (a, b) we obtain the desired results.

- $(u_i, o_i) = (a, x_i); c_i = a$:

This case can be handled similarly to the previous one.

Combining all these cases we see that we can always express an integral of type **(a)** in the form:

$$\sum_{\iota=1}^p z_{\iota} H_{m_{\iota}}(b|a) + \sum_{\iota=1}^q v_{\iota} H_{n_{\iota}}(b_i - c_j | a - c_j).$$

Let us now look at the inner integrals of **(b)** and **(c)**. Since we have

$$\int_{s_2}^{t_2} \frac{H_0(y_1)}{y_1 - 1} dy_1 = -H_{1,0}(t_2 | s_2) \quad \text{and} \quad \int_{s_2}^{t_2} \frac{H_0(y_1)}{y_1 + 1} dy_1 = H_{-1,0}(t_2 | s_2)$$

we can use basically the same arguments for integrals of type **(b)** and **(c)** as we used for integrals of type **(a)** to see that we can express them in the same form, i.e., in the form (3.23).

In the following we will show that we can represent integrals of type **(d)** in the form

$$\begin{aligned} &\sum_{\iota=1}^{p_1} z_{\iota} \left(H_0\left(\frac{f}{\alpha_{\iota}}\right) S_{m_{\iota}}\left(\mathbf{b}_{\iota} \middle| \frac{f}{\alpha_{\iota}}; n\right) - H_0\left(\frac{e}{\alpha_{\iota}}\right) S_{m_{\iota}}\left(\mathbf{b}_{\iota} \middle| \frac{e}{\alpha_{\iota}}; n\right) \right) \\ &+ \sum_{\iota=1}^{p_2} \bar{z}_{\iota} \left(S_{w_{\iota}}\left(\mathbf{v}_{\iota} \middle| \frac{f}{\beta_{\iota}}; n\right) - S_{w_{\iota}}\left(\mathbf{v}_{\iota} \middle| \frac{e}{\beta_{\iota}}; n\right) \right) + \sum_{\iota=1}^{p_3} \hat{z}_{\iota} S_h\left(\mathbf{q}_{\iota} \middle| \frac{g_j}{\gamma_{\iota}}; n\right) \end{aligned} \quad (3.24)$$

with $z_{\iota}, \bar{z}_{\iota}, \hat{z}_{\iota}$ products of multiple polylogarithms evaluated at constants and $\alpha_{\iota}, \beta_{\iota}, \gamma_{\iota} \in \mathbb{R}^*$. If $k = 1$, we get

$$\int_e^f \frac{y_1^n - 1}{y_1 - 1} dy_1 = H_0(f) S_1(f; n) - H_0(e) S_1(e; n) - S_2(f; n) + S_2(e; n). \quad (3.25)$$

Let now $1 < i \leq k$. We will see that we can express the first $i - 1$ integrals in the form

$$\begin{aligned} & \sum_{\iota=1}^{p_1} z_{\iota} \left(H_0 \left(\frac{t_i}{\alpha_{\iota}} \right) S_{m_{\iota}} \left(\mathbf{b}_{\iota} \middle| \frac{t_i}{\alpha_{\iota}}; n \right) - H_0 \left(\frac{s_i}{\alpha_{\iota}} \right) S_{m_{\iota}} \left(\mathbf{b}_{\iota} \middle| \frac{s_i}{\alpha_{\iota}}; n \right) \right) \\ & + \sum_{\iota=1}^{p_2} v_{\iota} \left(S_{w_{\iota}} \left(\mathbf{v}_{\iota} \middle| \frac{t_i}{\beta_{\iota}}; n \right) - S_{w_{\iota}} \left(\mathbf{v}_{\iota} \middle| \frac{s_i}{\beta_{\iota}}; n \right) \right) \\ & + \sum_{\iota=1}^{p_3} \hat{z}_{\iota} H_{1,0} \left(\frac{t_i}{g_{i-1}} \middle| \frac{s_i}{g_{i-1}} \right) + \sum_{\iota=1}^{p_4} \tilde{z}_{\iota} H_0(t_i - g_{i-1} | s_i - g_{i-1}) \end{aligned}$$

with $z_{\iota}, \bar{z}_{\iota}, \hat{z}_{\iota}, \tilde{z}_{\iota}$ products of multiple polylogarithms evaluated at constants and S-sums not dependent on a integration variable. For $i = 2$ this is obvious (compare 3.25). We will now perform the induction step $i \rightarrow i + 1$. Therefore we will look at the integrals

$$\begin{aligned} A & := \int_{s_{i+1}}^{t_{i+1}} \frac{H_0 \left(\frac{t_i}{\alpha} \right) S_m \left(\mathbf{b} \middle| \frac{t_i}{\alpha}; n \right) - H_0 \left(\frac{s_i}{\alpha} \right) S_m \left(\mathbf{b} \middle| \frac{s_i}{\alpha}; n \right)}{y_i - g_i} dy_i \\ B & := \int_{s_{i+1}}^{t_{i+1}} \frac{S_w \left(\mathbf{v} \middle| \frac{t_i}{\beta}; n \right) - S_w \left(\mathbf{v} \middle| \frac{s_i}{\beta}; n \right)}{y_i - g_i} dy_i \\ C & := \int_{s_{i+1}}^{t_{i+1}} \frac{H_{1,0} \left(\frac{t_i}{g_{i-1}} \middle| \frac{s_i}{g_{i-1}} \right)}{y_i - g_i} dy_i \\ D & := \int_{s_{i+1}}^{t_{i+1}} \frac{H_0(t_i - g_{i-1} | s_i - g_{i-1})}{y_i - g_i} dy_i \end{aligned}$$

where $s_{k+1} := e, t_{k+1} := f$. Using the method as described for integrals of type (a) we can handle D and using simple integral transforms we can handle C in the same way. For A and B we distinguish several cases:

- $(s_i, t_i) = (e, y_i); g_i > f \vee 0 > g_i :$

$$\begin{aligned} A & = \int_{s_{i+1}}^{t_{i+1}} \frac{H_0 \left(\frac{y_i}{\alpha} \right) S_m \left(\mathbf{b} \middle| \frac{y_i}{\alpha}; n \right) - H_0 \left(\frac{e}{\alpha} \right) S_m \left(\mathbf{b} \middle| \frac{e}{\alpha}; n \right)}{y_i - g_i} dy_i \\ & = H_0(|t_{i+1} - g_i| | |s_{i+1} - g_i|) \left(H_0 \left(\frac{g_i}{\alpha} \right) S_m \left(\mathbf{b} \middle| \frac{g_i}{\alpha}; n \right) - H_0 \left(\frac{e}{\alpha} \right) S_m \left(\mathbf{b} \middle| \frac{e}{\alpha}; n \right) \right) \\ & \quad - H_{1,0} \left(\frac{t_{i+1}}{g_i} \middle| \frac{s_{i+1}}{g_i} \right) S_m \left(\mathbf{b} \middle| \frac{g_i}{\alpha}; n \right) \\ & \quad + H_0 \left(\frac{g_i}{\alpha} \right) \left(S_{m,1} \left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{t_{i+1}}{g_i}; n \right) - S_{m,1} \left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{s_{i+1}}{g_i}; n \right) \right) \\ & \quad + \left(H_0 \left(\frac{t_{i+1}}{g_i} \right) S_{m,1} \left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{t_{i+1}}{g_i}; n \right) - H_0 \left(\frac{s_{i+1}}{g_i} \right) S_{m,1} \left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{s_{i+1}}{g_i}; n \right) \right) \\ & \quad - \left(S_{m,2} \left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{t_{i+1}}{g_i}; n \right) - S_{m,2} \left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{s_{i+1}}{g_i}; n \right) \right) \\ B & = \int_{s_{i+1}}^{t_{i+1}} \frac{S_w \left(\mathbf{v} \middle| \frac{y_i}{\beta}; n \right) - S_w \left(\mathbf{v} \middle| \frac{e}{\beta}; n \right)}{y_i - g_i} dy_i \end{aligned}$$

$$\begin{aligned}
&= S_{w,1}\left(\mathbf{v}, \frac{g_i}{\beta} \middle| \frac{t_{i+1}}{g_i}; n\right) - S_{w,1}\left(\mathbf{v}, \frac{g_i}{\beta} \middle| \frac{s_{i+1}}{g_i}; n\right) \\
&\quad + H_0(|t_{i+1} - g_i| \mid |s_{i+1} - g_i|) \left(S_w\left(\mathbf{v} \middle| \frac{g_i}{\beta}; n\right) - S_w\left(\mathbf{v} \middle| \frac{e}{\beta}; n\right) \right).
\end{aligned}$$

Hence in all of the three possible cases, i.e., (s_{i+1}, t_{i+1}) equals (e, y_{i+1}) , (y_{i+1}, f) or (e, f) , we arrive at the desired results.

- $(s_i, t_i) = (y_i, f); g_i > f \vee 0 > g_i$: This case can be handled similarly to the previous one.
- $(s_i, t_i) = (e, y_i); e > g_i \geq 0$:

$$\begin{aligned}
A &= \int_{s_{i+1}}^{t_{i+1}} \frac{H_0\left(\frac{y_i}{\alpha}\right) S_m\left(\mathbf{b} \middle| \frac{y_i}{\alpha}; n\right) - H_0\left(\frac{e}{\alpha}\right) S_m\left(\mathbf{b} \middle| \frac{e}{\alpha}; n\right)}{y_i - g_i} dy_i \\
&= H_0(t_{i+1} - g_i \mid |s_{i+1} - g_i|) \left(H_0\left(\frac{g_i}{\alpha}\right) S_m\left(\mathbf{b} \middle| \frac{g_i}{\alpha}; n\right) - H_0\left(\frac{e}{\alpha}\right) S_m\left(\mathbf{b} \middle| \frac{e}{\alpha}; n\right) \right) \\
&\quad - H_{1,0}\left(\frac{t_{i+1}}{g_i} \middle| \frac{s_{i+1}}{g_i}\right) S_m\left(\mathbf{b} \middle| \frac{g_i}{\alpha}; n\right) \\
&\quad + H_0\left(\frac{g_i}{\alpha}\right) \left(S_{m,1}\left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{t_{i+1}}{g_i}; n\right) - S_{m,1}\left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{s_{i+1}}{g_i}; n\right) \right) \\
&\quad + \left(H_0\left(\frac{t_{i+1}}{g_i}\right) S_{m,1}\left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{t_{i+1}}{g_i}; n\right) - H_0\left(\frac{s_{i+1}}{g_i}\right) S_{m,1}\left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{s_{i+1}}{g_i}; n\right) \right) \\
&\quad - \left(S_{m,2}\left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{t_{i+1}}{g_i}; n\right) - S_{m,2}\left(\mathbf{b}, \frac{g_i}{\alpha} \middle| \frac{s_{i+1}}{g_i}; n\right) \right) \\
B &= \int_{s_{i+1}}^{t_{i+1}} \frac{S_w\left(\mathbf{v} \middle| \frac{y_i}{\beta}; n\right) - S_w\left(\mathbf{v} \middle| \frac{e}{\beta}; n\right)}{y_i - g_i} dy_i \\
&= S_{w,1}\left(\mathbf{v}, \frac{g_i}{\beta} \middle| \frac{t_{i+1}}{g_i}; n\right) - S_{w,1}\left(\mathbf{v}, \frac{g_i}{\beta} \middle| \frac{s_{i+1}}{g_i}; n\right) \\
&\quad + H_0(t_{i+1} - g_i \mid |s_{i+1} - g_i|) \left(S_w\left(\mathbf{v} \middle| \frac{g_i}{\beta}; n\right) - S_w\left(\mathbf{v} \middle| \frac{e}{\beta}; n\right) \right).
\end{aligned}$$

Hence in all of the three possible cases, i.e., (s_{i+1}, t_{i+1}) equals (e, y_{i+1}) , (y_{i+1}, f) or (e, f) , we arrive at the desired results.

- $(s_i, t_i) = (y_i, f); e > g_i \geq 0$:
This case can be basically handled like the previous one.
- $(s_i, t_i) = (y_i, f); g_i = f$:

$$\begin{aligned}
A &= \int_{s_{i+1}}^{t_{i+1}} \frac{H_0\left(\frac{f}{\alpha}\right) S_m\left(\mathbf{b} \middle| \frac{f}{\alpha}; n\right) - H_0\left(\frac{y_i}{\alpha}\right) S_m\left(\mathbf{b} \middle| \frac{y_i}{\alpha}; n\right)}{y_i - f} dy_i \\
&= H_{1,0}\left(\frac{t_{i+1}}{f} \middle| \frac{s_{i+1}}{f}\right) S_m\left(\mathbf{b} \middle| \frac{f}{\alpha}; n\right)
\end{aligned}$$

$$\begin{aligned}
& -\mathrm{H}_0\left(\frac{f}{\alpha}\right)\left(\mathrm{S}_{m,1}\left(\mathbf{b}, \frac{f}{\alpha}\middle|\frac{t_{i+1}}{f}; n\right) - \mathrm{S}_{m,1}\left(\mathbf{b}, \frac{f}{\alpha}\middle|\frac{s_{i+1}}{f}; n\right)\right) \\
& -\left(\mathrm{H}_0\left(\frac{t_{i+1}}{f}\right)\mathrm{S}_{m,1}\left(\mathbf{b}, \frac{f}{\alpha}\middle|\frac{t_{i+1}}{f}; n\right) - \mathrm{H}_0\left(\frac{s_{i+1}}{f}\right)\mathrm{S}_{m,1}\left(\mathbf{b}, \frac{f}{\alpha}\middle|\frac{s_{i+1}}{f}; n\right)\right) \\
& +\left(\mathrm{S}_{m,2}\left(\mathbf{b}, \frac{f}{\alpha}\middle|\frac{t_{i+1}}{f}; n\right) - \mathrm{S}_{m,2}\left(\mathbf{b}, \frac{f}{\alpha}\middle|\frac{s_{i+1}}{f}; n\right)\right) \\
B & = \int_{s_{i+1}}^{t_{i+1}} \frac{\mathrm{S}_w\left(\mathbf{v}\middle|\frac{f}{\beta}; n\right) - \mathrm{S}_w\left(\mathbf{v}\middle|\frac{y_i}{\beta}; n\right)}{y_i - f} dy_i \\
& = -\mathrm{S}_{w,1}\left(\mathbf{v}, \frac{f}{\beta}\middle|\frac{t_{i+1}}{\beta}; n\right) + \mathrm{S}_{w,1}\left(\mathbf{v}, \frac{f}{\beta}\middle|\frac{s_{i+1}}{\beta}; n\right).
\end{aligned}$$

Hence in all of the three possible cases, i.e., (s_{i+1}, t_{i+1}) equals (e, y_{i+1}) , (y_{i+1}, f) or (e, f) , we arrive at the desired results.

- $(s_i, t_i) = (e, y_i); g_i = e$:

This case can be handled similarly to the previous one.

Combining all these cases we see that we can always express an integral of type (d) in the form given in (3.24). Let us now look at the inner integral of (e). Since we have

$$\int_{s_2}^{t_2} \frac{(-y_1)^n - 1}{y_1 + 1} dy_1 = \mathrm{H}_0(t_2) \mathrm{S}_1(-t_2; n) - \mathrm{H}_0(s_2) \mathrm{S}_1(-s_2; n) - \mathrm{S}_2(-t_2; n) + \mathrm{S}_2(-s_2; n)$$

we can use basically the same arguments for integrals of type (e) as we used for integrals of type (d) to see that we can express them in the same form, i.e., in the form (3.24). Since we are able to express all the integrals in the desired forms, we are able to transform the differentiated integral representation of an S-sum $\mathrm{S}_m(\mathbf{b}; n)$ back to expressions involving S-sums at n and S-sums at infinity (or equivalently multiple polylogarithms at constants) and hence we can differentiate arbitrary S-sums with respect to the upper summation limit.

3.6 Relations between S-Sums

3.6.1 Algebraic Relations

We already mentioned in the beginning of this chapter that S-sums form a quasi shuffle algebra. As showed in [62], ideas from Section 2.6.1 can be carried over to S-sums if we consider an alphabet A , where pairs (m, x) with $m \in \mathbb{N}$ and $x \in \mathbb{R}^*$ form the letters, i.e., we identify a S-sum

$$\mathrm{S}_{m_1, m_2, \dots, m_k}(x_1, x_2, \dots, x_k; n)$$

with the word $(m_1, x_1)(m_2, x_2) \dots (m_k, x_k)$. We define the degree of a letter $(m, x) \in A$ as $|(m, x)| = m$ and we order the letters for $m_1, m_2 \in \mathbb{N}$ and $x_1, x_2 \in \mathbb{R}^*$ by

$$\begin{aligned} (m_1, x_1) &< (m_2, x_2) && \text{if } m_1 < m_2 \\ (m_1, x_1) &< (m_1, x_2) && \text{if } |x_1| < |x_2| \\ (m_1, -x_1) &< (m_1, x_1) && \text{if } x_1 > 0. \end{aligned}$$

We extend this order lexicographically to words. Using this order, it can be showed analogously as in [1] (compare [49]) that the S-sums form a quasi shuffle algebra which is the free polynomial algebra on the *Lyndon* words with alphabet A . Hence the number of algebraic independent sums in this algebra can be counted by counting the number of *Lyndon* words. If we consider for example an alphabet with n letters and we look for the number of basis sums with depth d , we can use the first Witt formula (2.13):

$$N_A(d) = \frac{1}{d} \sum_{q|d} \mu\left(\frac{d}{q}\right) n^q.$$

In the subsequent example we look at S-sums of depth 2 on alphabets of 4 letters. Hence we obtain

$$\frac{1}{2} \sum_{q|2} \mu\left(\frac{2}{q}\right) 4^q = 6$$

basis sums.

We can use an analogous method of the method presented in [19, 1] for harmonic sums to find the basis S-sums together with the relations for the dependent S-sums.

Example 3.6.1. *We consider the letters $(1, \frac{1}{2}), (1, -\frac{1}{2}), (3, \frac{1}{2}), (3, -\frac{1}{2})$. At depth $d = 2$ we obtain 16 sums with these letters. Using the relations*

$$\begin{aligned} S_{1,3}\left(\frac{1}{2}, \frac{1}{2}; n\right) &= -S_{3,1}\left(\frac{1}{2}, \frac{1}{2}; n\right) + S_1\left(\frac{1}{2}; n\right) S_3\left(\frac{1}{2}; n\right) + S_4\left(\frac{1}{4}; n\right) \\ S_{1,3}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) &= -S_{3,1}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) + S_1\left(-\frac{1}{2}; n\right) S_3\left(-\frac{1}{2}; n\right) + S_4\left(\frac{1}{4}; n\right) \\ S_{1,3}\left(\frac{1}{2}, -\frac{1}{2}; n\right) &= -S_{3,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right) + S_1\left(\frac{1}{2}; n\right) S_3\left(-\frac{1}{2}; n\right) + S_4\left(-\frac{1}{4}; n\right) \\ S_{1,3}\left(-\frac{1}{2}, \frac{1}{2}; n\right) &= -S_{3,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right) + S_1\left(-\frac{1}{2}; n\right) S_3\left(\frac{1}{2}; n\right) + S_4\left(-\frac{1}{4}; n\right) \\ S_{1,1}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) &= \frac{1}{2} S_1\left(-\frac{1}{2}; n\right)^2 + \frac{1}{2} S_2\left(\frac{1}{4}; n\right) \\ S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; n\right) &= \frac{1}{2} S_1\left(\frac{1}{2}; n\right)^2 + \frac{1}{2} S_2\left(\frac{1}{4}; n\right) \\ S_{1,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right) &= -S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right) + S_1\left(-\frac{1}{2}; n\right) S_1\left(\frac{1}{2}; n\right) + S_2\left(-\frac{1}{4}; n\right) \\ S_{3,3}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) &= \frac{1}{2} S_3\left(-\frac{1}{2}; n\right)^2 + \frac{1}{2} S_6\left(\frac{1}{4}; n\right) \\ S_{3,3}\left(\frac{1}{2}, \frac{1}{2}; n\right) &= \frac{1}{2} S_3\left(\frac{1}{2}; n\right)^2 + \frac{1}{2} S_6\left(\frac{1}{4}; n\right) \end{aligned}$$

$$S_{3,3}\left(\frac{1}{2}, -\frac{1}{2}; n\right) = -S_{3,3}\left(-\frac{1}{2}, \frac{1}{2}; n\right) + S_3\left(-\frac{1}{2}; n\right) S_3\left(\frac{1}{2}; n\right) + S_6\left(-\frac{1}{4}; n\right)$$

we find the 6 basis sums

$$\begin{aligned} & S_{3,1}\left(\frac{1}{2}, \frac{1}{2}; n\right), S_{3,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right), S_{3,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right), S_{3,1}\left(-\frac{1}{2}, -\frac{1}{2}; n\right), \\ & S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right), S_{3,3}\left(-\frac{1}{2}, \frac{1}{2}; n\right), \end{aligned}$$

in which all the other 10 sums of depth 2 can be expressed.

3.6.2 Differential Relations

In Section 3.5 we described the differentiation of S-sums with respect to the upper summation limit. The differentiation leads to new relations for instance we find

$$\frac{d}{dn} S_2(2; n) = -S_3(2; n) + H_0(2) S_2(2; n) + H_{0,0,-1}(1) + 2H_{0,0,1}(1) + H_{0,1,-1}(1).$$

As for harmonic sums we collect the derivatives with respect to n :

$$S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)^{(D)} = \left\{ \frac{\partial^N}{\partial n^N} S_{a_1, \dots, a_k}(b_1, \dots, b_k; n); N \in \mathbb{N} \right\}. \quad (3.26)$$

Continuing the Example 3.6.1 we get

Example 3.6.2 (Example 3.6.1 continued). *From differentiation we get the additional relations:*

$$\begin{aligned} S_{3,1}\left(\frac{1}{2}, \frac{1}{2}; n\right) &= \frac{1}{12} \frac{\partial}{\partial n} S_3\left(\frac{1}{4}; n\right) - \frac{1}{2} \frac{\partial}{\partial n} S_{2,1}\left(\frac{1}{2}, \frac{1}{2}; n\right) - \frac{1}{2} H_{1,0}\left(\frac{1}{2}\right) S_2\left(\frac{1}{2}; n\right) \\ &\quad + H_0\left(\frac{1}{2}\right) S_{2,1}\left(\frac{1}{2}, \frac{1}{2}; n\right) - \frac{1}{2} H_{\frac{1}{2}}\left(\frac{1}{4}\right) H_{0,1,0}\left(\frac{1}{2}\right) + \frac{1}{12} H_{0,0,1,0}\left(\frac{1}{4}\right) \\ &\quad + \frac{1}{2} H_{\frac{1}{2},0,1,0}\left(\frac{1}{4}\right) - \frac{1}{12} H_0\left(\frac{1}{4}\right) S_3\left(\frac{1}{4}; n\right) - \frac{1}{4} S_2\left(\frac{1}{2}; n\right)^2 \\ S_{3,1}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) &= \frac{1}{12} \frac{\partial}{\partial n} S_3\left(\frac{1}{4}; n\right) - \frac{1}{2} \frac{\partial}{\partial n} S_{2,1}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) + \frac{1}{2} H_{-\frac{1}{2},0}\left(\frac{1}{4}\right) S_2\left(-\frac{1}{2}; n\right) \\ &\quad + \frac{1}{2} H_0\left(\frac{1}{4}\right) S_{2,1}\left(-\frac{1}{2}, -\frac{1}{2}; n\right) - \frac{1}{2} H_{-\frac{1}{2}}\left(\frac{1}{4}\right) H_{0,-1,0}\left(\frac{1}{2}\right) \\ &\quad - \frac{1}{2} H_{-\frac{1}{2},0,1,0}\left(\frac{1}{4}\right) + \frac{1}{12} H_{0,0,1,0}\left(\frac{1}{4}\right) - \frac{1}{2} H_{-\frac{1}{2}}\left(\frac{1}{4}\right) H_0\left(\frac{1}{2}\right) S_2\left(-\frac{1}{2}; n\right) \\ &\quad - \frac{1}{12} H_0\left(\frac{1}{4}\right) S_3\left(\frac{1}{4}; n\right) - \frac{1}{4} S_2\left(-\frac{1}{2}; n\right)^2 \\ S_{3,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right) &= \frac{1}{6} \frac{\partial}{\partial n} S_3\left(-\frac{1}{4}; n\right) - \frac{1}{2} \frac{\partial}{\partial n} S_{2,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right) - \frac{1}{2} \frac{\partial}{\partial n} S_{2,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right) \\ &\quad - \frac{1}{2} H_{1,0}\left(\frac{1}{2}\right) S_2\left(-\frac{1}{2}; n\right) + \frac{1}{2} H_{-\frac{1}{2},0}\left(\frac{1}{4}\right) S_2\left(\frac{1}{2}; n\right) \\ &\quad + H_0\left(\frac{1}{2}\right) S_{2,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right) + \frac{1}{2} H_0\left(\frac{1}{4}\right) S_{2,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right) \end{aligned}$$

$$\begin{aligned}
& -S_{3,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right) + \frac{1}{2}H_{\frac{1}{2}}\left(\frac{1}{4}\right)H_{0,-1,0}\left(\frac{1}{2}\right) + \frac{1}{2}H_{\frac{3}{4}}\left(\frac{1}{4}\right)H_{0,1,0}\left(\frac{1}{2}\right) \\
& + \frac{1}{2}H_{-\frac{1}{2},0,-1,0}\left(\frac{1}{4}\right) - \frac{1}{6}H_{0,0,-1,0}\left(\frac{1}{4}\right) - \frac{1}{2}H_{\frac{1}{2},0,-1,0}\left(\frac{1}{4}\right) \\
& - \frac{1}{2}H_0\left(\frac{1}{2}\right)H_{\frac{3}{4}}\left(\frac{1}{4}\right)S_2\left(\frac{1}{2}; n\right) - \frac{1}{6}H_0\left(\frac{1}{4}\right)S_3\left(-\frac{1}{4}; n\right) \\
& - \frac{1}{2}S_2\left(-\frac{1}{2}; n\right)S_2\left(\frac{1}{2}; n\right).
\end{aligned}$$

Using all the relations we can reduce the number of basis sums at depth $d = 2$ to 3 by introducing differentiation. In our case the basis sum are:

$$S_{3,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right), S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right), S_{3,3}\left(-\frac{1}{2}, \frac{1}{2}; n\right)$$

Note that we introduced the letters $(2, \pm\frac{1}{2})$ and $(3, \pm\frac{1}{4})$, however these letters appear just in sums of depth 2 with weight 3 and are only used to express sums of weight 4.

3.6.3 Duplication Relations

As for harmonic sums we have a duplication relation:

Theorem 3.6.3 (Duplication Relation). For $a_i \in \mathbb{N}$, $b_i \in \mathbb{R}^+$ and $n \in \mathbb{N}$ we have

$$\sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2n) = \frac{1}{2^{\sum_{i=1}^m a_i - m}} S_{a_m, \dots, a_1}(b_m^2, \dots, b_1^2; n).$$

where we sum on the left hand side over the 2^m possible combinations concerning \pm .

Proof. We proceed by induction on m . For $m = 1$ we get

$$\begin{aligned}
S_a(-b, 2n) &= \sum_{i=1}^{2n} \frac{(-b)^i}{i^a} = \sum_{i=1}^n \left(\frac{b^{2i}}{(2i)^a} - \frac{b^{2i-1}}{(2i-1)^a} \right) = \frac{1}{2^a} S_a(b^2; n) - \sum_{i=1}^n \frac{b^{2i-1}}{(2i-1)^a} \\
&= \frac{1}{2^a} S_a(b^2; n) - \sum_{i=1}^n \left(\frac{b^{2i}}{(2i)^a} + \frac{b^{2i-1}}{(2i-1)^a} - \frac{b^{2i}}{(2i)^a} \right) \\
&= \frac{1}{2^a} S_a(b^2; n) - S_a(b; 2n) + \frac{1}{2^a} S_a(b^2; n) \\
&= \frac{1}{2^{a-1}} S_a(b^2, n) - S_a(b; 2n).
\end{aligned}$$

Now suppose the theorem holds for m :

$$\begin{aligned}
& \sum S_{a_{m+1}, \dots, a_1}(\pm b_{m+1}, \dots, \pm b_1; 2n) = \\
& = \sum_{i=1}^n \left(\frac{(\pm b_{m+1}^{2i})}{(2i)^{a_{m+1}}} \sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2i) \right. \\
& \quad \left. + \frac{\pm b_{m+1}^{2i-1}}{(2i-1)^{a_{m+1}}} \sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2i+1) \right)
\end{aligned}$$

$$\begin{aligned}
&= 2 \sum_{i=1}^n \frac{(b^2)^i}{(2i)^{a_{m+1}}} \sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2i) \\
&= 2 \sum_{i=1}^n \frac{(b^2)^i}{(2i)^{a_{m+1}}} \frac{1}{2^{\sum_{i=1}^m a_i - m}} S_{a_m, \dots, a_1}(b_m^2, \dots, b_1^2; i) \\
&= \frac{1}{2^{\sum_{i=1}^{m+1} a_i - (m+1)}} S_{a_{m+1}, a_m, \dots, a_1}(\pm b_{m+1}, \pm b_m, \dots, \pm b_1; n).
\end{aligned}$$

□

Example 3.6.4 (Example 3.6.2 continued). *The duplication relations are*

$$\begin{aligned}
S_{3,3}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= -S_{3,3}\left(-\frac{1}{2}, -\frac{1}{2}; 2n\right) - S_{3,3}\left(-\frac{1}{2}, \frac{1}{2}; 2n\right) \\
&\quad + \frac{1}{16} S_{3,3}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{3,3}\left(\frac{1}{2}, -\frac{1}{2}; 2n\right) \\
S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= -S_{1,1}\left(-\frac{1}{2}, -\frac{1}{2}; 2n\right) - S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; 2n\right) \\
&\quad + S_{1,1}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{1,1}\left(\frac{1}{2}, -\frac{1}{2}; 2n\right) \\
S_{3,1}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= -S_{3,1}\left(-\frac{1}{2}, -\frac{1}{2}; 2n\right) - S_{3,1}\left(-\frac{1}{2}, \frac{1}{2}; 2n\right) \\
&\quad + \frac{1}{4} S_{3,1}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{3,1}\left(\frac{1}{2}, -\frac{1}{2}; 2n\right) \\
S_{1,3}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= -S_{1,3}\left(-\frac{1}{2}, -\frac{1}{2}; 2n\right) - S_{1,3}\left(-\frac{1}{2}, \frac{1}{2}; 2n\right) \\
&\quad + \frac{1}{4} S_{1,3}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{1,3}\left(\frac{1}{2}, -\frac{1}{2}; 2n\right).
\end{aligned}$$

Note that from duplication we do not get a further reduction in this case. We would have to introduce new sums of the same depth and weight to express the basis sums from Example 3.6.2.

3.6.4 Examples for Specific Index Sets

In this subsection we want to present the numbers of basis sums for specific index sets at special depths or weights. In the Tables 3.1, 3.2 and 3.3 we summarize the number of algebraic basis sums at the possible index sets at depths 2, 3, 4 respectively. To illustrate how these tables are to be understood we take a closer look at the depth $d = 3$ example with the index set $\{(a_1, a_1, a_2), (x_1, x_2, x_3)\}$; here, e.g., $\{(a_1, a_1, a_2), (x_1, x_2, x_3)\}$ stands for a multiset and each element is allowed to be taken once to build all the possible S-sums. There we obtain the 18 sums:

$$\begin{aligned}
&S_{a_1, a_1, a_2}(x_1, x_2, x_3; n), S_{a_1, a_1, a_2}(x_1, x_3, x_2; n), S_{a_1, a_1, a_2}(x_2, x_1, x_3; n), \\
&S_{a_1, a_1, a_2}(x_2, x_3, x_1; n), S_{a_1, a_1, a_2}(x_3, x_1, x_2; n), S_{a_1, a_1, a_2}(x_3, x_2, x_1; n), \\
&S_{a_1, a_2, a_1}(x_1, x_2, x_3; n), S_{a_1, a_2, a_1}(x_1, x_3, x_2; n), S_{a_1, a_2, a_1}(x_2, x_1, x_3; n), \\
&S_{a_1, a_2, a_1}(x_2, x_3, x_1; n), S_{a_1, a_2, a_1}(x_3, x_1, x_2; n), S_{a_1, a_2, a_1}(x_3, x_2, x_1; n),
\end{aligned}$$

Index set	sums	basis sums	dependent sums
$\{a_1, a_1\}, \{x_1, x_1\}$	1	0	1
$\{a_1, a_1\}, \{x_1, x_2\}$	2	1	1
$\{a_1, a_2\}, \{x_1, x_1\}$	2	1	1
$\{a_1, a_2\}, \{x_1, x_2\}$	4	2	2

Table 3.1: Number of basis sums for different index sets at depth 2.

Index set	sums	basis sums	dependent sums
$\{a_1, a_1, a_1\}, \{x_1, x_1, x_1\}$	1	0	1
$\{a_1, a_1, a_1\}, \{x_1, x_1, x_2\}$	3	1	2
$\{a_1, a_1, a_1\}, \{x_1, x_2, x_3\}$	6	2	4
$\{a_1, a_1, a_2\}, \{x_1, x_1, x_1\}$	3	1	2
$\{a_1, a_1, a_2\}, \{x_1, x_1, x_2\}$	9	3	6
$\{a_1, a_1, a_2\}, \{x_1, x_2, x_3\}$	18	6	12
$\{a_1, a_2, a_3\}, \{x_1, x_1, x_1\}$	6	2	4
$\{a_1, a_2, a_3\}, \{x_1, x_1, x_2\}$	18	6	12
$\{a_1, a_2, a_3\}, \{x_1, x_2, x_3\}$	36	12	24

Table 3.2: Number of basis sums for different index sets at depth 3.

$$\begin{aligned} & S_{a_2, a_1, a_1}(x_1, x_2, x_3; n), S_{a_2, a_1, a_1}(x_1, x_3, x_2; n), S_{a_2, a_1, a_1}(x_2, x_1, x_3; n), \\ & S_{a_2, a_1, a_1}(x_2, x_3, x_1; n), S_{a_2, a_1, a_1}(x_3, x_1, x_2; n), S_{a_2, a_1, a_1}(x_3, x_2, x_1; n). \end{aligned}$$

Using relations of the form

$$\begin{aligned} S_{a_1, a_1, a_2}(x_1, x_2, x_3; n) &= S_{a_2}(x_3; n) S_{a_1, a_1}(x_1, x_2; n) + S_{a_1, a_1 + a_2}(x_1, x_2 x_3; n) \\ &\quad - S_{a_1}(x_1; n) S_{a_2, a_1}(x_3, x_2; n) - S_{a_2, 2a_1}(x_3, x_1 x_2; n) + S_{a_2, a_1, a_1}(x_3, x_2, x_1; n) \end{aligned}$$

we can express all these 18 sums using the following 6 basis sums (with the price of introducing additional S-sums of lower depth subject to the relations given by the quasi shuffle algebra):

$$\begin{aligned} & S_{a_2, a_1, a_1}(x_1, x_2, x_3; n), S_{a_2, a_1, a_1}(x_1, x_3, x_2; n), S_{a_2, a_1, a_1}(x_2, x_1, x_3; n), \\ & S_{a_2, a_1, a_1}(x_2, x_3, x_1; n), S_{a_2, a_1, a_1}(x_3, x_1, x_2; n), S_{a_2, a_1, a_1}(x_3, x_2, x_1; n). \end{aligned}$$

In Table 3.4 we summarize the number of algebraic basis sums at specified weights for arbitrary indices in the x_i , while in Table 3.5 we summarize the number of algebraic and differential bases sums for $x_i \in \{1, -1, 1/2, -1/2, 2, -2\}$ and where each of the indices $\{1/2, -1/2, 2, -2\}$ is allowed to appear just once in each sum. To illustrate how these tables are to be understood we take a closer look at two examples. At weight $w = 3$ with index set $\{x_1, x_2, x_3\}$, we consider the 19 sums:

$$\begin{aligned} & S_3(x_1 x_2 x_3; n), S_{1,2}(x_1, x_2 x_3; n), S_{1,2}(x_2, x_1 x_3; n), S_{1,2}(x_1 x_2, x_3; n), S_{1,2}(x_3, x_1 x_2; n), \\ & S_{1,2}(x_1 x_3, x_2; n), S_{1,2}(x_2 x_3, x_1; n), S_{2,1}(x_1, x_2 x_3; n), S_{2,1}(x_2, x_1 x_3; n), S_{2,1}(x_1 x_2, x_3; n), \\ & S_{2,1}(x_3, x_1 x_2; n), S_{2,1}(x_1 x_3, x_2; n), S_{2,1}(x_2 x_3, x_1; n), S_{1,1,1}(x_1, x_2, x_3; n), S_{1,1,1}(x_1, x_3, x_2; n), \\ & S_{1,1,1}(x_2, x_1, x_3; n), S_{1,1,1}(x_2, x_3, x_1; n), S_{1,1,1}(x_3, x_1, x_2; n), S_{1,1,1}(x_3, x_2, x_1; n). \end{aligned}$$

Index set	sums	basis sums	dependent sums
$\{a_1, a_1, a_1, a_1\}, \{x_1, x_1, x_1, x_1\}$	1	0	1
$\{a_1, a_1, a_1, a_1\}, \{x_1, x_1, x_1, x_2\}$	4	1	3
$\{a_1, a_1, a_1, a_1\}, \{x_1, x_1, x_2, x_2\}$	6	1	5
$\{a_1, a_1, a_1, a_1\}, \{x_1, x_1, x_2, x_3\}$	12	3	9
$\{a_1, a_1, a_1, a_1\}, \{x_1, x_2, x_3, x_4\}$	24	6	18
$\{a_1, a_1, a_1, a_2\}, \{x_1, x_1, x_1, x_1\}$	4	1	3
$\{a_1, a_1, a_1, a_2\}, \{x_1, x_1, x_1, x_2\}$	16	4	12
$\{a_1, a_1, a_1, a_2\}, \{x_1, x_1, x_2, x_2\}$	24	6	18
$\{a_1, a_1, a_1, a_2\}, \{x_1, x_1, x_2, x_3\}$	48	12	36
$\{a_1, a_1, a_1, a_2\}, \{x_1, x_2, x_3, x_4\}$	96	24	72
$\{a_1, a_1, a_2, a_2\}, \{x_1, x_1, x_1, x_1\}$	6	1	5
$\{a_1, a_1, a_2, a_2\}, \{x_1, x_1, x_1, x_2\}$	24	6	18
$\{a_1, a_1, a_2, a_2\}, \{x_1, x_1, x_2, x_2\}$	36	8	28
$\{a_1, a_1, a_2, a_2\}, \{x_1, x_1, x_2, x_3\}$	72	18	54
$\{a_1, a_1, a_2, a_2\}, \{x_1, x_2, x_3, x_4\}$	144	36	108
$\{a_1, a_1, a_2, a_3\}, \{x_1, x_1, x_1, x_1\}$	12	3	9
$\{a_1, a_1, a_2, a_3\}, \{x_1, x_1, x_1, x_2\}$	48	12	36
$\{a_1, a_1, a_2, a_3\}, \{x_1, x_1, x_2, x_2\}$	72	18	54
$\{a_1, a_1, a_2, a_3\}, \{x_1, x_1, x_2, x_3\}$	144	36	108
$\{a_1, a_1, a_2, a_3\}, \{x_1, x_2, x_3, x_4\}$	288	72	216
$\{a_1, a_2, a_3, a_4\}, \{x_1, x_1, x_1, x_1\}$	24	6	18
$\{a_1, a_2, a_3, a_4\}, \{x_1, x_1, x_1, x_2\}$	96	24	72
$\{a_1, a_2, a_3, a_4\}, \{x_1, x_1, x_2, x_2\}$	144	36	108
$\{a_1, a_2, a_3, a_4\}, \{x_1, x_1, x_2, x_3\}$	288	72	216
$\{a_1, a_2, a_3, a_4\}, \{x_1, x_2, x_3, x_4\}$	576	144	432

Table 3.3: Number of basis sums for different index sets at depth 4.

weight	index set	sums	basis sums	dependent sums
2	$\{x_1, x_1\}$	2	1	1
	$\{x_1, x_2\}$	3	3	1
3	$\{x_1, x_1, x_1\}$	6	3	3
	$\{x_1, x_1, x_2\}$	12	6	6
	$\{x_1, x_2, x_3\}$	19	9	10
4	$\{x_1, x_1, x_1, x_1\}$	20	8	12
	$\{x_1, x_1, x_1, x_2\}$	50	20	30
	$\{x_1, x_1, x_2, x_2\}$	64	24	40
	$\{x_1, x_1, x_2, x_3\}$	106	40	66
	$\{x_1, x_2, x_3, x_4\}$	175	64	111
5	$\{x_1, x_1, x_1, x_1, x_1\}$	70	25	45
	$\{x_1, x_1, x_1, x_1, x_2\}$	210	70	140
	$\{x_1, x_1, x_1, x_2, x_2\}$	325	105	220
	$\{x_1, x_1, x_1, x_2, x_3\}$	555	175	380
	$\{x_1, x_1, x_2, x_2, x_3\}$	725	225	500
	$\{x_1, x_1, x_2, x_3, x_4\}$	1235	375	860
	$\{x_1, x_2, x_3, x_4, x_5\}$	2101	625	1476
6	$\{x_1, x_1, x_1, x_1, x_1, x_1\}$	252	75	177
	$\{x_1, x_1, x_1, x_1, x_1, x_2\}$	882	252	630
	$\{x_1, x_1, x_1, x_1, x_2, x_2\}$	1596	438	1158
	$\{x_1, x_1, x_1, x_2, x_2, x_2\}$	1911	522	1389
	$\{x_1, x_1, x_1, x_1, x_2, x_3\}$	2786	756	2030
	$\{x_1, x_1, x_1, x_2, x_2, x_3\}$	4431	1176	3255
	$\{x_1, x_1, x_2, x_2, x_3, x_3\}$	5886	1539	4347
	$\{x_1, x_1, x_1, x_2, x_3, x_4\}$	7721	2016	5705
	$\{x_1, x_1, x_2, x_2, x_3, x_4\}$	10251	2646	7605
	$\{x_1, x_1, x_2, x_3, x_4, x_5\}$	17841	4536	13305
	$\{x_1, x_2, x_3, x_4, x_5, x_6\}$	31031	7776	23255

Table 3.4: Number of basis sums for different index sets up to weight 6.

Using relations of the form

$$\begin{aligned}
S_{1,2}(x_2x_3, x_1; n) &= S_1(x_2x_3; n) S_2(x_1; n) + S_3(x_1x_2x_3; n) - S_{2,1}(x_1, x_2x_3; n), \\
S_{1,1,1}(x_1, x_2, x_3; n) &= -S_1(x_3; n) S_{1,1}(x_2, x_1; n) + S_1(x_1; n) S_{1,1}(x_2, x_3; n) \\
&\quad + S_{2,1}(x_1x_2, x_3; n) - S_{2,1}(x_2x_3, x_1; n) + S_{1,1,1}(x_3, x_2, x_1; n)
\end{aligned}$$

we can express all these 19 sums using the following 9 basis sums:

$$\begin{aligned}
&S_3(x_1x_2x_3; n), S_{2,1}(x_1, x_2x_3; n), S_{2,1}(x_2, x_1x_3; n), S_{2,1}(x_1x_2, x_3; n), S_{2,1}(x_3, x_1x_2; n), \\
&S_{2,1}(x_1x_3, x_2; n), S_{2,1}(x_2x_3, x_1; n), S_{1,1,1}(x_3, x_1, x_2; n), S_{1,1,1}(x_3, x_2, x_1; n).
\end{aligned}$$

At weight $w = 2$ with index set $\{1, -1, 1/2, -1/2, 2, -2\}$, where each of the indices $\{1/2, -1/2, 2, -2\}$ is allowed to appear just once, we consider the 38 sums:

$$S_{-2}(n), S_2(n), S_{-1,-1}(n), S_{-1,1}(n), S_{1,-1}(n), S_{1,1}(n), S_2(-2; n), S_2\left(-\frac{1}{2}; n\right),$$

$$\begin{aligned}
& S_2\left(\frac{1}{2}; n\right), S_2(2; n), S_{1,1}(-2, -1; n), S_{1,1}\left(-2, -\frac{1}{2}; n\right), S_{1,1}\left(-2, \frac{1}{2}; n\right), S_{1,1}(-2, 1; n), \\
& S_{1,1}(-2, 2; n), S_{1,1}(-1, -2; n), S_{1,1}\left(-1, -\frac{1}{2}; n\right), S_{1,1}\left(-1, \frac{1}{2}; n\right), S_{1,1}(-1, 2; n), \\
& S_{1,1}\left(-\frac{1}{2}, -2; n\right), S_{1,1}\left(-\frac{1}{2}, -1; n\right), S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right), S_{1,1}\left(-\frac{1}{2}, 1; n\right), S_{1,1}\left(-\frac{1}{2}, 2; n\right), \\
& S_{1,1}\left(\frac{1}{2}, -2; n\right), S_{1,1}\left(\frac{1}{2}, -1; n\right), S_{1,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right), S_{1,1}\left(\frac{1}{2}, 1; n\right), S_{1,1}\left(\frac{1}{2}, 2; n\right), \\
& S_{1,1}(1, -2; n), S_{1,1}\left(1, -\frac{1}{2}; n\right), S_{1,1}\left(1, \frac{1}{2}; n\right), S_{1,1}(1, 2; n), S_{1,1}(2, -2; n), S_{1,1}(2, -1; n), \\
& S_{1,1}\left(2, -\frac{1}{2}; n\right), S_{1,1}\left(2, \frac{1}{2}; n\right), S_{1,1}(2, 1; n).
\end{aligned}$$

Using relations of the form

$$\begin{aligned}
S_{1,1}\left(-\frac{1}{2}, 2; n\right) &= -\frac{\partial}{\partial n} S_{-1}(n) + H_{-1,0}(1) + S_1\left(-\frac{1}{2}; n\right) S_1(2; n) - S_{1,1}\left(2, -\frac{1}{2}; n\right) \\
S_{1,1}\left(-\frac{1}{2}, -2; n\right) &= -\frac{\partial}{\partial n} S_1(n) - H_{1,0}(1) + S_1(-2; n) S_1\left(-\frac{1}{2}; n\right) - S_{1,1}\left(-2, -\frac{1}{2}; n\right)
\end{aligned}$$

we can express all these 38 sums using the following 17 basis sums:

$$\begin{aligned}
& S_{1,-1}(n), S_{1,1}\left(-2, -\frac{1}{2}; n\right), S_{1,1}\left(-2, \frac{1}{2}; n\right), S_{1,1}(-2, 2; n), S_{1,1}(-1, -2; n), \\
& S_{1,1}\left(-1, -\frac{1}{2}; n\right), S_{1,1}\left(-1, \frac{1}{2}; n\right), S_{1,1}(-1, 2; n), S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right), S_{1,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right), \\
& S_{1,1}(1, -2; n), S_{1,1}\left(1, -\frac{1}{2}; n\right), S_{1,1}\left(1, \frac{1}{2}; n\right), S_{1,1}(1, 2; n), S_{1,1}(2, -2; n), \\
& S_{1,1}\left(2, -\frac{1}{2}; n\right), S_{1,1}\left(2, \frac{1}{2}; n\right).
\end{aligned}$$

Note that we have

$$\begin{aligned}
N_D(w) &= N_S(w) - N_S(w-1) \\
N_{AD}(w) &= N_A(w) - N_A(w-1)
\end{aligned}$$

where $N_S(w)$, $N_D(w)$ and $N_{AD}(w)$ are the number of sums, the number algebraic basis sums and the number of basis sums using algebraic and differential relations at weight w respectively.

3.7 S-Sums at Infinity

Of course not all S-sums are finite at infinity, since for example $\lim_{n \rightarrow \infty} S_2(2; n)$ does not exist. In fact, we have the following theorem that extends Lemma 2.7.1 which is used in the proof of the theorem:

weight	sums	a-basis sums	d-basis sums	ad-basis sums
1	6	6	6	6
2	38	23	32	17
3	222	120	184	97
4	1206	654	984	543
5	6150	3536	4944	2882
6	29718	18280	23568	14744

Table 3.5: Number of basis sums up to weight 6 with index set $\{1, -1, 1/2, -1/2, 2, -2\}$. Each of the indices $\{1/2, -1/2, 2, -2\}$ is allowed to appear just once in each sum.

Theorem 3.7.1. *Let $a_1, a_2, \dots, a_k \in \mathbb{N}$ and $x_1, x_2, \dots, x_k \in \mathbb{R}^*$ for $k \in \mathbb{N}$. The S-sum $S_{a_1, a_2, \dots, a_k}(x_1, x_2, \dots, x_k; n)$ is absolutely convergent, when $n \rightarrow \infty$, if and only if one of the following conditions holds:*

1. $|x_1| < 1 \wedge |x_1 x_2| \leq 1 \wedge \dots \wedge |x_1 x_2 \cdots x_k| \leq 1$
2. $a_1 > 1 \wedge |x_1| = 1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_k| \leq 1$.

In addition the S-sum is conditional convergent (convergent but not absolutely convergent) if and only if

3. $a_1 = 1 \wedge x_1 = -1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_k| \leq 1$.

Proof. First we want to show that the S-sum converges absolutely if either condition 1 or condition 2 holds. Therefore we proceed by induction on the depth k . Here we prove the slightly more general case of S-sums, where we allow the last index a_k to equal zero. Note that we extend the definition of S-sums in the obvious way. For $k = 1$ the statement is obvious in both cases. Now let us look at the first condition and assume that the statement holds for depth $k - 1$: We distinguish two cases. First let $|x_k| < 1$:

$$\begin{aligned} \sum_{i=1}^n \left| \frac{x_1^i}{i^{a_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) \right| &\leq S_{a_1, a_2, \dots, a_k}(|x_1|, |x_2|, \dots, |x_k|; n) \\ &\leq S_{a_1, a_2, \dots, a_{k-1}-1}(|x_1|, |x_2|, \dots, |x_{k-1}|; n). \end{aligned}$$

If $a_{k-1} - 1 = 0$ we extend the definition of S-sums in the obvious way. The last sum is of depth $k - 1$ and it converges absolutely since $|x_1| < 1 \wedge |x_1 x_2| \leq 1 \wedge \dots \wedge |x_1 x_2 \cdots x_{k-1}| \leq 1$ and due to the induction hypothesis. Thus $S_{a_1, a_2, \dots, a_k}(x_1, x_2, \dots, x_k; n)$ converges absolutely since the partial sums are bounded.

For $|x_k| > 1$ we get:

$$\sum_{i=1}^n \left| \frac{x_1^i}{i^{a_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) \right| \leq S_{a_1, a_2, \dots, a_k}(|x_1|, |x_2|, \dots, |x_k|; n)$$

$$\leq S_{a_1, a_2, \dots, a_{k-1}-1}(|x_1|, |x_2|, \dots, |x_{k-2}|, |x_{k-1}x_k|; n).$$

The last sum is of depth $k - 1$ and it converges absolutely since $|x_1| < 1 \wedge |x_1x_2| \leq 1 \wedge \dots \wedge |x_1x_2 \cdots x_{k-2}| \leq 1 \wedge |x_1x_2 \cdots x_{k-1}x_k| \leq 1$ and due to the induction hypothesis. Hence $S_{a_1, a_2, \dots, a_k}(x_1, x_2, \dots, x_k; n)$ converges absolutely.

Let us look at the second condition. For the special case $k = 2$ and $a_1 > 2$ we get:

$$\sum_{i=1}^n \left| \frac{1}{i^{a_1}} S_{a_2}(x_2; i) \right| \leq S_{a_1, a_2}(1, |x_2|; n) \leq S_{a_1-1}(1; n) = S_{a_1-1}(n).$$

$S_{a_1, a_2}(1, x_2; n)$ converges absolutely since $S_{a_1-1}(n)$ converges (base case). For $k = 2$ and $a_1 = 2$ we get

$$\sum_{i=1}^n \left| \frac{1}{i^2} S_{a_2}(x_2; i) \right| \leq S_{2, a_2}(1, 1; n) = S_{2, a_2}(n).$$

$|S_{2, a_2}(1, x_2; n)|$ converges absolutely since $S_{2, a_2}(n)$ converges (see Lemma 2.7.1). Assume now that the second condition holds for depth $k - 1$ with $k \geq 3$: We distinguish two cases. First let $|x_k| < 1$:

$$\begin{aligned} \sum_{i=1}^n \left| \frac{x_1^i}{i^{a_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) \right| &\leq S_{a_1, a_2, \dots, a_k}(1, |x_2|, \dots, |x_k|; n) \\ &\leq S_{a_1, a_2, \dots, a_{k-1}-1}(1, |x_2|, \dots, |x_{k-1}|; n). \end{aligned}$$

The last sum is of depth $k - 1$ and it converges absolutely since $a_1 > 1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_{k-1}| \leq 1$ and due to the induction hypothesis. Therefore $S_{a_1, a_2, \dots, a_k}(x_1, x_2, \dots, x_k; n)$ converges absolutely.

For $|x_k| > 1$ we get:

$$\begin{aligned} \sum_{i=1}^n \left| \frac{x_1^i}{i^{a_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) \right| &\leq S_{a_1, a_2, \dots, a_k}(1, |x_2|, \dots, |x_k|; n) \\ &\leq S_{a_1, a_2, \dots, a_{k-1}-1}(1, |x_2|, \dots, |x_{k-2}|, |x_{k-1}x_k|; n). \end{aligned}$$

The last sum is of depth $k - 1$ and it converges absolutely since $a_1 > 1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_{k-2}| \leq 1 \wedge |x_2 \cdots x_{k-1}x_k| \leq 1$ and due to the induction hypothesis. Consequently $S_{a_1, a_2, \dots, a_k}(x_1, x_2, \dots, x_k; n)$ converges absolutely.

Let us now look at the third condition: Note, that it can be seen easily, that the considered sums are not absolutely convergent. To show that they are conditional convergent, we again proceed by induction on the depth k . For $k = 1$ the statement is obvious. We assume that it holds for depth k and we consider

$$S_{1, a_1, \dots, a_k}(-1, x_1, \dots, x_k; n) = \sum_{i=1}^n \frac{(-1)^i}{i} S_{a_1, \dots, a_k}(x_1, \dots, x_k; i).$$

If $|x_1| < 1$ or $|x_1| = 1$ and $a_1 > 1$ the sum $S_{a_1, \dots, a_k}(x_1, \dots, x_k; i)$ is convergent for $i \rightarrow \infty$ due to condition 1 respectively 2, while if $x_1 = -1$ and $a_1 = 1$ the sum $S_{a_1, \dots, a_k}(x_1, \dots, x_k; i)$ is convergent for $i \rightarrow \infty$ due to the induction hypothesis and hence the sum $S_{1, a_1, \dots, a_k}(-1, x_1, \dots, x_k; n)$ converges in these cases for $n \rightarrow \infty$. The last case we have to consider is $x_1 = 1$ and $a_1 = 1$: if $a_i = 1$ and $x_i = 1$ for all $1 \leq i \leq k$ then we are in fact considering the sum $S_{-1, 1, \dots, 1}(n)$ which is convergent for $n \rightarrow \infty$ due to Lemma 2.7.1. Now suppose that not for all i we have $a_i = 1$ and $x_i = 1$. Let d be the smallest index such that $a_d \neq 1$ or $x_d \neq 1$, i.e., we consider the case

$$S_{1, 1, \dots, 1, a_d, \dots, a_k}(-1, 1, \dots, 1, x_d, \dots, x_k; n) = \sum_{i=0}^n \frac{(-1)^i}{i} S_{1, \dots, 1, a_d, \dots, a_k}(1, \dots, 1, x_d, \dots, x_k; i).$$

Similar as for harmonic sums we can extract the leading ones of the S-sum $S_{1, \dots, 1, a_d, \dots, a_k}(1, \dots, 1, x_d, \dots, x_k; i)$ and end up in a univariate polynomial in $S_1(n)$ with coefficients in S-sums which are convergent for $i \rightarrow \infty$ due to condition 1 or 2 or due to the induction hypothesis (compare Remark 2.1.5 and Section 2.4.2). Hence we can write

$$S_{1, \dots, 1, a_d, \dots, a_k}(1, \dots, 1, x_d, \dots, x_k; i) = \sum_{j=0}^{d-1} S_1(i)^j c_j(i),$$

where the $c_j(i)$ are convergent $i \rightarrow \infty$. For $p \in \mathbb{N}$, $S_1(i)^p$ diverges for $i \rightarrow \infty$, but the divergence is of order $\log(i)^p$ (see Lemma 2.8.19). Hence $\frac{S_1(i)^j}{i} c_j(i)$ tends to zero for $i \rightarrow \infty$ and thus

$$S_{1, 1, \dots, 1, a_d, \dots, a_k}(-1, 1, \dots, 1, x_d, \dots, x_k; n) = \sum_{j=0}^{d-1} \sum_{i=1}^n (-1)^i \frac{S_1(i)^j}{i} c_j(i)$$

converges for $n \rightarrow \infty$.

If non of the three conditions holds i.e.,

$$(a_1 = 1 \wedge x_1 = 1) \vee |x_1| > 1 \vee |x_1 x_2| > 1 \vee \dots \vee |x_1 x_2 \dots x_k| > 1$$

we show that the S-sum diverges. To see that the S-sum diverges if non of the three conditions holds we use the integral representation of Theorem 3.4.3. If $a_1 = 1 \wedge x_1 = 1$, the innermost integral

$$\int_0^1 \frac{y^n - 1}{y - 1} dy$$

in the integral representation of Theorem 3.4.3 diverges for $n \rightarrow \infty$ and hence the S-sum diverges.

If $|x_1| > 1 \vee |x_1 x_2| > 1 \vee \dots \vee |x_1 x_2 \dots x_k| > 1$ then the absolute value of z the upper integration limit of the innermost integral

$$\int_0^z \frac{y^n - 1}{y - 1}$$

exceeds 1 and hence the absolute value of the integral tends to infinity for $n \rightarrow \infty$ and the S-sum diverges. \square

3.7.1 Relations between S-Sums at Infinity

In this section we will state several types of relations between the values of S-sums at infinity which are of importance in the following chapters.

- The first type of relations originates from the algebraic relations of S-sums, see Section 3.6.1. These relations remain valid when we consider them at infinity. We will refer to these relations as the quasi shuffle or stuffle relations.
- The duplication relations from Section 3.6.3 remain valid if we consider sums which are finite at infinity, since it makes no difference whether the argument is ∞ or $2 \cdot \infty$.
- We can generalize the relation form [85] (see Section 2.7.1) for harmonic sums to S-sums. For convergent sums we have:

$$\begin{aligned} & S_{m_1, \dots, m_p}(x_1, \dots, x_p; \infty) S_{k_1, \dots, k_q}(y_1, \dots, y_p; \infty) = \\ & \lim_{n \rightarrow \infty} \sum_{i=1}^n \frac{y_1^i S_{m_1, \dots, m_p}(x_1, \dots, x_p; n-i) S_{k_2, \dots, k_q}(y_2, \dots, y_p; i)}{i^{k_1}}. \end{aligned}$$

Using

$$\begin{aligned} & \lim_{n \rightarrow \infty} \sum_{i=1}^n \frac{y_1^i S_{m_1, \dots, m_p}(x_1, \dots, x_p; n-i) S_{k_2, \dots, k_q}(y_2, \dots, y_p; i)}{i^{k_1}} = \\ & \sum_{a=1}^{k_1} \binom{k_1 + m_1 - 1 - a}{m_1 - 1} \sum_{i=1}^n \frac{x_1^i}{i^{m_1 + k_1 - a}} \\ & \quad \frac{\sum_{j=1}^i \left(\frac{y_1}{x_1}\right)^j S_{m_2, \dots, m_p}(x_2, \dots, x_p; i-j) S_{k_2, \dots, k_q}(y_2, \dots, y_p; j)}{j^a} \\ & + \sum_{a=1}^{m_1} \binom{k_1 + m_1 - 1 - a}{m_1 - 1} \sum_{i=1}^n \frac{y_1^i}{i^{m_1 + k_1 - a}} \\ & \quad \frac{\sum_{j=1}^i \left(\frac{x_1}{y_1}\right)^j S_{k_2, \dots, k_q}(y_2, \dots, y_p; i-j) S_{m_2, \dots, m_p}(x_2, \dots, x_p; j)}{j^a} \end{aligned}$$

we can rewrite the right hand side in terms of S-sums. We will refer to these relations as the shuffle relations since one could also obtain them from the shuffle algebra of multiple polylogarithms.

3.7.2 S-Sums of Roots of Unity at Infinity

In this section we look at the values of infinite S-sums at roots of unity (compare [8]). We define

$$\sigma_{k_1, \dots, k_m}(x_1, \dots, x_m) := \lim_{n \rightarrow \infty} S_{k_1, \dots, k_m}(x_1, \dots, x_m; n),$$

with $S_{k_1, \dots, k_m}(x_1, \dots, x_m; n)$ a S-sum, $k_1 \neq 1$ for $x_1 = 1$ and x_j is a l -th root of unity ($l \geq 1$), i.e., $x_j \in \{e_l | e_l^l = 1, e_l \in \mathbb{C}\}$.

We seek the relations between the sums of $w = 1, 2$. They can be expressed in terms of polylogarithms by :

$$\sigma_w(x) = \text{Li}_w(x), \quad w \in \mathbb{N}, w \geq 1 \quad (3.27)$$

$$\sigma_1(x) = \text{Li}_1(x) = -\ln(1-x) \quad (3.28)$$

$$\sigma_{1,1}(x, y) = \text{Li}_2(x) + \frac{1}{2} \ln^2(1-x) + \text{Li}_2\left(-\frac{x(1-y)}{1-x}\right) \quad (3.29)$$

and $*$ denotes complex conjugation. At weight $w = 1$ we use the suitable relations from Section 3.7.1 together with relations due to complex conjugation (indicated by $*$)

$$\sigma_1(e_j^k)^* = \sigma_1(e_j^{j-k}) = \sigma_1(e_j^k) - \frac{j-2k}{j} \pi.$$

In addition we extend Proposition 2.3 of Ref. [43], where we consider S-sums $S_{k_1, \dots, k_m}(x_1, \dots, x_m; n)$ with $n \in \mathbb{N}_0, k_i \in \mathbb{N}, x_i \in \mathbb{C}, |x_i| \leq 1$. Let $l \in \mathbb{N}$ and

$$y_i^l = x_i \quad (3.30)$$

then [8, (6.12)]

$$S_{k_1, \dots, k_m}(x_1, \dots, x_m; n) = \prod_{j=1}^m l^{k_j-1} \sum_{y_i^l = x_i} S_{k_1, \dots, k_m}(y_1, \dots, y_m; ln) . \quad (3.31)$$

Here the sum is over the l th roots of x_i for $i \in \{1, \dots, m\}$. Equation (3.31) is called *distribution relation*. It follows from the Vieta's theorem for (3.30) and properties of symmetric polynomials [56]. If $x_1 \neq 1$ for $k_1 = 1$ the limit

$$\sigma_{k_1, \dots, k_m}(x_1, \dots, x_m) = \lim_{N \rightarrow \infty} S_{k_1, \dots, k_m}(x_1, \dots, x_m; N) \quad (3.32)$$

l	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
basis	0	1	2	2	3	3	4	3	4	4	6	4	7	5	6	5	9	5	10	6
new	0	1	2	0	2	0	3	1	2	0	5	1	6	0	2	2	8	0	9	2

Table 3.6: The number of the basis elements spanning the $w = 1$ S-sums at l th roots of unity up to 20.

exists. One may apply (3.31,3.32) to roots of unity x_j and y_j , i.e., $x_j = \exp(2\pi i n_j/m_j)$ and $y_j^k = \exp(2\pi i k n_j/(m_j l)), k \in \{1, \dots, (l-1)\}, n_j, m_j \in \mathbb{N}$ and i the imaginary unit.

We combined all these relations together with the relations from Section 3.7.1 and solved the corresponding linear systems using computer algebra methods and derived the representations for the dependent sums analytically in Table 3.6 we summarize the number of basis elements. The new elements contributing at the respective level of cyclotomy for $l \leq 20$ are :

$$\begin{array}{ll}
l = 1 & - \\
l = 2 & \sigma_1(e_2) \\
l = 3 & \sigma_1(e_3), \pi \\
l = 4 & - \\
l = 5 & \sigma_1(e_5), \sigma_1(e_5^2) \\
l = 6 & - \\
l = 7 & \sigma_1(e_7^k)|_{k=1}^3 \\
l = 8 & \sigma_1(e_8) \\
l = 9 & \sigma_1(e_9), \sigma_1(e_9^2) \\
l = 10 & - \\
l = 11 & \sigma_1(e_{11}^k)|_{k=1}^5 \\
l = 12 & \sigma_1(e_{12}) \\
l = 13 & \sigma_1(e_{13}^k)|_{k=1}^6 \\
l = 14 & - \\
l = 15 & \sigma_1(e_{15}), \sigma_1(e_{15}^2) \\
l = 16 & \sigma_1(e_{16}), \sigma_1(e_{16}^3) \\
l = 17 & \sigma_1(e_{17}^k)|_{k=1}^8 \\
l = 18 & - \\
l = 19 & \sigma_1(e_{19}^k)|_{k=1}^9 \\
l = 20 & \sigma_1(e_{20}), \sigma_1(e_{20}^3) .
\end{array}$$

At weight $w = 2$ we use again the suitable relations from Section 3.7.1 together with the distribution relations (3.31) and the relations due to complex conjugation:

$$\begin{aligned}
\sigma_2(e_j^k)^* &= \sigma_2(e_j^{j-k}) = \sigma_2(e_j^k) - \frac{6k^2 - 6jk + j^2}{3j^2} \pi^2 \\
\sigma_{1,1}(e_j^k, e_j^{j-k}) &= \sigma_2(e_j^k) + \frac{1}{2} \sigma_1(e_j^k)^2.
\end{aligned}$$

In addition we use the relations

$$\sigma_{1,1}(x, 1) = \sigma_2(x) + \frac{1}{2} \sigma_1(x)^2$$

and

$$\sigma_{1,1}(e_j^k, e_j^l) = \sigma_2(e_j^k) + \frac{1}{2} \sigma_1(e_j^k)^2 + \sigma_2\left(-\frac{e_j^k(1-e_j^l)}{1-e_j^k}\right),$$

l	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Li ₂ basis	1	1	2	2	3	2	4	3	4	3	6	3	7	4	5	5	9	4	10	5
Li ₂ new	1	0	1	1	2	0	3	1	2	0	5	0	6	0	1	2	8	0	9	1
basis	1	2	3	3	5	5	8	7	10	10	16	12	21	17	21	21	33	23	40	29
new	1	0	1	1	2	1	4	3	5	4	10	5	14	8	12	12	24	11	30	16

Table 3.7: The number of the basis elements spanning the dilogarithms respectively the weight $w = 2$ S-sums at l th roots of unity up to 20.

for $-\frac{e_j^k(1-e_j^l)}{1-e_j^k} = 1$ or $-\frac{e_j^k(1-e_j^l)}{1-e_j^k} = \frac{z}{1+z}$ for a j -th root of unity z , since then

$$\sigma_2\left(\frac{z}{1+z}\right) = \sigma_2(z) - \frac{1}{2}\sigma_2(z^2) - \frac{1}{2}(\sigma_1(z) - \sigma_1(z^2))^2.$$

The new basis elements spanning the dilogarithms of the l th roots of unity for $l \leq 20$ are :

$$\begin{array}{ll}
l = 1 & - \\
l = 2 & - \\
l = 3 & \sigma_2(e_3) \\
l = 4 & \sigma_2(e_4) \\
l = 5 & \sigma_2(e_5), \sigma_2(e_5^2) \\
l = 6 & - \\
l = 7 & \sigma_2(e_7^k) \Big|_{k=1}^3 \\
l = 8 & \sigma_2(e_8) \\
l = 9 & \sigma_2(e_9), \sigma_2(e_9^2) \\
l = 10 & - \\
l = 11 & \sigma_2(e_{11}^k) \Big|_{k=1}^5 \\
l = 12 & \sigma_2(e_{12}) \\
l = 13 & \sigma_2(e_{13}^k) \Big|_{k=1}^6 \\
l = 14 & - \\
l = 15 & \sigma_2(e_{15}) \\
l = 16 & \sigma_2(e_{16}), \sigma_2(e_{16}^3) \\
l = 17 & \sigma_2(e_{17}^k) \Big|_{k=1}^8 \\
l = 18 & - \\
l = 19 & \sigma_2(e_{19}^k) \Big|_{k=1}^9 \\
l = 20 & \sigma_2(e_{20}) .
\end{array}$$

In Table 3.7 we summarize the number of basis elements found at $w = 2$ using the mentioned relations. We also list the number of basis elements for the class of dilogarithms at roots of unity, and in both cases the number of new elements beyond those being obtained at $w = 1$ at the same value of l .

At $w = 2$ the respective new basis elements are :

$$\begin{array}{ll}
l = 1 & \sigma_2 \\
l = 2 & - \\
l = 3 & \sigma_2(e_3) \\
l = 4 & \sigma_2(e_4) \\
l = 5 & \sigma_2(e_5)\sigma_2(e_5^2) \\
l = 6 & \sigma_{1,1}(e_3, e_2) \\
l = 7 & \sigma_2(e_7^k) \Big|_{k=1}^3, \sigma_{1,1}(e_7, e_7^2) \\
l = 8 & \sigma_2(e_8), \sigma_{1,1}(e_8, e_4), \sigma_{1,1}(e_8, e_8^3)
\end{array}$$

$$\begin{aligned}
l = 9 & \quad \sigma_2(e_9), \sigma_2(e_9^2), \sigma_{1,1}(e_9, e_9^2), \sigma_{1,1}(e_9, e_3), \sigma_{1,1}(e_9^2, e_3) \\
l = 10 & \quad \sigma_{1,1}(e_5, e_2), \sigma_{1,1}(e_5^2, e_2), \sigma_{1,1}(e_{10}, e_5), \sigma_{1,1}(e_{10}, e_{10}^3) \\
l = 11 & \quad \sigma_2(e_{11}^k) \Big|_{k=1}^5, \sigma_{1,1}(e_{11}, e_{11}^k) \Big|_{k=2}^4, \sigma_{1,1}(e_{11}^2, e_{11}^k) \Big|_{k=3}^4, \text{ etc.}
\end{aligned}$$

3.8 Asymptotic Expansion of S-Sums

In Section 2.8 we introduced an algorithm to compute the asymptotic expansions of harmonic sums. In this section we seek expansions of S-sums and try to generalize the algorithm for harmonic sums to S-sums to the extent that is possible.

3.8.1 Asymptotic Expansions of Harmonic Sums $S_1(c; n)$ with $c \geq 1$

Since $\frac{1}{c-x}$ is not continuous in $[0, 1]$ for $0 < c \leq 1$, we cannot use the strategy mentioned in Section 2.8.2 to find an asymptotic representation of $\int_0^1 \frac{x^n - 1}{c-x} dx = S_1(c; n)$. For $S_1(n)$ see Lemma 2.8.19. To compute the asymptotic expansion of $S_1(c; n)$ with $c > 1$ one may represent it using the Euler-Maclaurin formula [38, 58]:

$$S_1(c; n) = \bar{S}_1(c; n) + S_1(n)$$

where

$$\begin{aligned}
\bar{S}_1(c; n) & := \sum_{i=1}^n \frac{c^i - 1}{i} \\
& = -\frac{1}{2} \left[\log(c) + \frac{c^{n+1} - 1}{n+1} \right] - \gamma - \log(\log(c)) - \log(n+1) \\
& \quad + \text{Ei}(\log(c)(n+1)) + \sum_{j=1}^m \frac{B_{2j}}{(2j)!} \left[\frac{d^{2j-1}}{di^{2j-1}} \left(\frac{c^i - 1}{i} \right) \right] \Big|_0^{n+1} + R_k(c, n);
\end{aligned}$$

here $\text{Ei}(z)$ is the exponential integral [40, 68],

$$\int_0^x \frac{c^t - 1}{t} dt = \text{Ei}(x \log(c)) - \gamma - \log(x) - \log(\log(c)),$$

B_k are the Bernoulli numbers [16, 75, 66],

$$B_n = \sum_{k=0}^n \binom{n}{k} B_k, \quad B_0 = 1,$$

and $R_k(c, n)$ stand for the rest term. The derivatives are given in closed form by

$$\frac{d^j}{di^j} \left(\frac{c^i - 1}{i} \right) = \frac{c^i}{i} \sum_{k=0}^j \frac{\log^{j-k}(c)}{i^k} (-1)^k \frac{\Gamma(j+1)}{\Gamma(j+1-k)} - (-1)^j \frac{\Gamma(j+1)}{i^{j+1}}$$

$$\lim_{i \rightarrow 0} \frac{d^j}{di^j} \left(\frac{c^i - 1}{i} \right) = \frac{\log^{j+1}(c)}{j+1}.$$

The asymptotic representation for $S_1(c; n)$ with $c > 1$ can now be derived using

$$\text{Ei}(t) \sim \exp(t) \sum_{k=1}^{\infty} \frac{\Gamma(k)}{t^k}.$$

3.8.2 Computation of Asymptotic Expansions of S-Sums

In this section we extend the algorithm of Section 2.8 to S-Sums $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ with $b_i \in [-1, 0) \cup (0, 1]$. Analyzing Section 3.4.1 it is easy to see that these sums can be represented using Mellin transforms of the form

$$M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c \pm x}, n\right)$$

with $m_i \in \mathbb{R} \setminus ((-1, 0) \cup (0, 1))$ and $|c| \geq 1$. Analyzing the product of S-sums it is straightforward to see that the subclass of S-Sums we are considering here are closed under multiplication, in the sense that the product can be expressed as a linear combination of S-sums of this subclass. In the following we state several necessary facts which are more or less extensions of lemmas from Section 2.8. The two subsequent lemmas are generalizations of Lemma 2.8.14 and Lemma 2.8.15, respectively, and the proofs of the lemmas follow using similar arguments as used in the proof of Lemma 2.8.14.

Lemma 3.8.1. *Let $H_{m_1, m_2, \dots, m_k}(x)$ be a multiple polylogarithm with $m_i \in \mathbb{R} \setminus (0, 1]$ for $1 \leq i \leq k$. Then*

$$H_{m_1, m_2, \dots, m_k}(x), \frac{H_{m_1, m_2, \dots, m_k}(x)}{c + x}$$

and

$$\frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{c - x}$$

are analytic for $|c| \geq 1$ and $x \in (0, 1]$.

Lemma 3.8.2. *Let $H_{m_1, m_2, \dots, m_k}(x)$ be a multiple polylogarithm with $m_i \in \mathbb{R} \setminus ((-1, 0) \cup (0, 1))$ for $1 \leq i \leq k$, and $m_k \neq 0$. Then*

$$\frac{H_{m_1, m_2, \dots, m_k}(1 - x)}{c + x}$$

and

$$\frac{H_{m_1, m_2, \dots, m_k}(1-x)}{c-x}$$

are analytic for $|c| \geq 1$ and $x \in (0, 1]$.

The proof of the subsequent lemma is analogue to the proof of Lemma 2.8.16.

Lemma 3.8.3 (Compare Lemma 2.8.16). *Let $H_m(x) = H_{m_1, m_2, \dots, m_k}(x)$ and $H_b(x) = H_{b_1, b_2, \dots, b_l}(x)$ be a multiple polylogarithm with $m_i \in \mathbb{R} \setminus (0, 1]$ for $1 \leq i \leq k$ and $b_i \in \mathbb{R} \setminus ((-1, 0) \cup (0, 1))$ for $1 \leq i \leq l$ where $b_l \neq 0$. Then we have*

$$M\left(\frac{H_m(x)}{1-x}, n\right) = \int_0^1 \frac{x^n(H_m(x) - H_m(1))}{1-x} dx - \int_0^1 \frac{H_m(x) - H_m(1)}{1-x} dx - S_1(n) H_m(1),$$

and

$$M\left(\frac{H_b(1-x)}{1-x}, n\right) = \int_0^1 \frac{x^n H_b(1-x)}{1-x} dx - H_{0, b}(1)$$

where

$$\int_0^1 \frac{H_m(x) - H_m(1)}{1-x} dx, H_m(1) \text{ and } H_{0, b}(1)$$

are finite constants.

Remark 3.8.4. *Combining Lemma 3.8.1, Lemma 3.8.2 and 3.8.3 we are able to find the asymptotic expansion of Mellin transforms (see Section 3.4.1) of the form*

$$M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c \pm x}, n\right) \text{ and } M\left(\frac{H_{b_1, b_2, \dots, b_l}(1-x)}{c \pm x}, n\right)$$

where $|c| > 1$, $m_i \in \mathbb{R} \setminus (0, 1]$, $b_i \in \mathbb{R} \setminus (-1, 0) \cup (0, 1)$ and $b_l \neq 0$ using the method presented in the beginning of Section 2.8, or using repeated integration by parts.

Lemma 3.8.5. [Compare Lemma 3.4.14]

1. *If an \bar{S} -sum $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ has no trailing ones, i.e., $a_k \neq 1$ or $b_k \neq 1$ then the most complicated multiple polylogarithm in the inverse Mellin transform of $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ has no trailing ones.*
2. *If an \bar{H} -multiple polylogarithm $H_{m_1, m_2, \dots, m_k}(x)$ has no trailing ones, i.e., $m_k \neq 1$ then the most complicated S-sum in the Mellin transform of $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ has no trailing ones.*

Proof. The statements follow immediately from Algorithm 3 and Algorithm 2 respectively. \square

Remark 3.8.6. *According to the previous lemma we know that if $H_{m_1, m_2, \dots, m_k}(x)$ is the most complicated multiple polylogarithm in the inverse Mellin transform of an S-sum*

$S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ with $b_i \in [-1, 0) \cup (0, 1]$ then $m_k \neq 1$. Due to Remark 3.8.4 we can expand the resulting integrals asymptotically (either we can handle it directly, or we have to transform the argument of the multiple polylogarithm). A S -sum with trailing ones might lead to a multiple polylogarithm with trailing ones, however $\frac{H_{m_1, m_2, \dots, m_{k-1}, 1}(x)}{c \pm x}$ is not analytic at 1 and hence we cannot use the strategy mentioned in Section 2.8.2 to find an asymptotic representation of such integrals. Fortunately we can always extract trailing ones such that we end up in a univariate polynomial in $S_1(n)$ with coefficients in the S -sums without trailing ones (this is possible due to the quasi shuffle algebra property). Hence we only need to deal with powers of $S_1(n)$ and harmonic sums without trailing ones.

We are now prepared to extend the algorithm presented in Section 2.8.3 to compute asymptotic expansions for harmonic sums to an algorithm which computes asymptotic expansions of S -sums $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ with $b_i \in [-1, 1]$ and $b_i \neq 0$. We can proceed as follows:

- if $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ has trailing ones, i.e., $a_k = b_k = 1$, we first extract them such that we end up in a univariate polynomial in $S_1(n)$ with coefficients in the S -sums without trailing ones; apply the following items to each of the S -sums without trailing ones;
- suppose now $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ has no trailing ones, i.e., $a_k \neq 1 \neq b_k$; let $\frac{H_{m_1, m_2, \dots, m_k}(x)}{c+sx}$ be the most complicated weighted multiple polylogarithm in the inverse Mellin transform of $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$; express $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ as

$$S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n) = M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c+sx}, n\right) + T; \quad (3.33)$$

note that T is an expression in S -sums (which are less complicated than $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$) and constants;

- we proceed by expanding $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c+sx}, n\right)$ in (3.33);

all $m_i \neq 1$: expand $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c+sx}, n\right)$ directly see Remark 3.8.4

not all $m_i \neq 1$:

- transform $x \rightarrow 1-x$ in $H_m(x)$; expand all products; now we can rewrite

$$M\left(\frac{H_m(x)}{c+sx}, n\right) = \sum_{i=1}^p d_i M\left(\frac{H_{b_i}(1-x)}{c+sx}, n\right) + d \quad \text{with } d, d_i \in \mathbb{R} \quad (3.34)$$

– for each Mellin transform $M\left(\frac{H_{b_1, \dots, b_j(1-x)}}{c+sx}, n\right)$ do

$b_j \neq 0$: expand $\int_0^1 \frac{x^n H_b(1-x)}{c+sx}$ see Remark 3.8.4

$b_j = 0$: transform back $1-x \rightarrow x$ in $H_b(1-x)$; expand all products;
write

$$M\left(\frac{H_b(1-x)}{c+sx}, n\right) = \sum_{i=1}^p e_i M\left(\frac{H_{g_i}(x)}{c+sx}, n\right) + e \quad (3.35)$$

with $e, e_i \in \mathbb{R}$ and perform the Mellin transforms $M\left(\frac{H_{g_i}(x)}{c+sx}, n\right)$

- replace $M\left(\frac{H_{m_1, m_2, \dots, m_l}(x)}{c+sx}, n\right)$ in equation (3.33) by the result of this process
- expand the powers of $S_1(n)$ using Lemma 2.8.19
- for all harmonic sums that remain in equation (3.33) apply the above points; since these harmonic sums are less complicated this process will terminate.

Some remarks are in place: Since $a_k \neq 1$ in equation (3.33), we know due to Lemma 3.8.5 that $m_l \neq 0$ in equation (3.33). If not all $m_i \neq 1$ in equation (3.33), we have to transform $x \rightarrow 1-x$ in $H_{m_1, m_2, \dots, m_l}(x)$ from Section 3.2. It is easy to see that the single multiple polylogarithm at argument x with weight l , which will pop up, will not have trailing zeroes since $m_l \neq 1$. Therefore the S-sums which will appear in equation (3.35) are less complicated (i.e., smaller in the sense of Definition 3.4.13) than $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ of (3.33) and hence this algorithm will eventually terminate.

Example 3.8.7.

$$\begin{aligned} S_{2,1}\left(\frac{1}{3}, \frac{1}{2}; n\right) &\sim -S_{1,2}\left(\frac{1}{6}, 3; \infty\right) + S_1\left(\frac{1}{2}; \infty\right) \left(-S_2\left(\frac{1}{6}; \infty\right) + S_2\left(\frac{1}{3}; \infty\right) + \frac{1}{6^n} \left(-\frac{1464}{625n^5}\right.\right. \\ &\quad \left.\left. + \frac{126}{125n^4} - \frac{12}{25n^3} + \frac{1}{5n^2} + 33\frac{2^{n-1}}{n^5} - 9\frac{2^{n-1}}{n^4} + 3\frac{2^{n-1}}{n^3} - \frac{2^{n-1}}{n^2}\right)\right) \\ &\quad + \frac{1}{6^n} \left(-\frac{4074}{3125n^5} + \frac{366}{625n^4} - \frac{42}{125n^3} + \frac{6}{25n^2} - \frac{1}{5n}\right) S_2\left(\frac{1}{2}; \infty\right) \\ &\quad + S_1\left(\frac{1}{6}; \infty\right) S_2\left(\frac{1}{2}; \infty\right) + S_3\left(\frac{1}{2}; \infty\right) + \frac{1}{6^n} \left(\frac{642}{125n^5} - \frac{28}{25n^4} + \frac{1}{5n^3}\right) \\ &\quad + \frac{1}{6^n} \left(\frac{2037}{3125n^5} - \frac{183}{625n^4} + \frac{21}{125n^3} - \frac{3}{25n^2} + \frac{1}{10n}\right) \zeta_2 + \frac{1}{6^n} \left(-\frac{2037}{3125n^5}\right. \\ &\quad \left. + \frac{183}{625n^4} - \frac{21}{125n^3} + \frac{3}{25n^2} - \frac{1}{10n}\right) \log^2(2) + \frac{1}{6^n} \left(\frac{1464}{625n^5} - \frac{126}{125n^4} + \frac{12}{25n^3}\right. \\ &\quad \left. - \frac{1}{5n^2}\right) \log(2), \quad x \rightarrow \infty. \end{aligned}$$

In order to extend this algorithm to a slightly wider class, we state the following lemma.

Lemma 3.8.8. *Let $H_{m_1, m_2, \dots, m_k}(x)$ be a multiple polylogarithm with $m_i \in \mathbb{R} \setminus (-1, 1] \cup \{0\}$ for $1 \leq i \leq k$ and $0 < c < 1$. Then*

$$\begin{aligned} M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c-x}, n\right) &= \\ & \frac{1}{c^n} \int_0^1 \frac{x^n (H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c))}{c-x} dx \\ & + H_{m_1, c, m_2, \dots, m_k}(c) + H_{m_1, m_2, c, \dots, m_k}(c) + \dots + H_{m_1, m_2, \dots, m_k, c}(c) \\ & + H_{m_2, \dots, m_k}(c) H_{0, m_1-c}(1-c) + H_{m_3, \dots, m_k}(c) H_{0, m_1-c, m_2-c}(1-c) \\ & + \dots + H_{m_k}(c) H_{0, m_1-c, \dots, m_{k-1}-c}(1-c) + H_{0, m_1-c, \dots, m_k-c}(1-c) \\ & - S_{1, \{\frac{1}{c}\}}(n) H_{m_1, m_2, \dots, m_k}(c). \end{aligned}$$

Proof. We have

$$\begin{aligned} M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c-x}, n\right) &= \int_0^1 \frac{\left(\frac{x}{c}\right)^n - 1}{c-x} H_{m_1, m_2, \dots, m_k}(x) dx = \\ &= \int_0^1 \frac{\left(\frac{x}{c}\right)^n (H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c))}{c-x} dx \\ & \quad + \int_0^1 \frac{\left(\frac{x}{c}\right)^n H_{m_1, m_2, \dots, m_k}(c) - H_{m_1, m_2, \dots, m_k}(x)}{c-x} dx \\ &= \int_0^1 \frac{\left(\frac{x}{c}\right)^n (H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c))}{c-x} dx \\ & \quad + \underbrace{H_{m_1, m_2, \dots, m_k}(c) \int_0^1 \frac{\left(\frac{x}{c}\right)^n - 1}{c-x} dx}_{A:=} \\ & \quad - \underbrace{\int_0^1 \frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c)}{c-x} dx}_{B:=}. \end{aligned}$$

with

$$\begin{aligned} A &= -S_1\left(\frac{1}{c}; n\right) H_{m_1, m_2, \dots, m_k}(c) \\ B &= \underbrace{\int_0^c \frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c)}{c-x} dx}_{B_1:=} \\ & \quad + \underbrace{\int_c^1 \frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c)}{c-x} dx}_{B_2:=} \end{aligned}$$

where

$$\begin{aligned}
B_1 &= -\mathbf{H}_{m_1, c, m_2, \dots, m_k}(c) - \dots - \mathbf{H}_{m_1, m_2, \dots, m_k, c}(c) \\
B_2 &= \int_0^{1-c} \frac{\mathbf{H}_{m_1, m_2, \dots, m_k}(x+c) - \mathbf{H}_{m_1, m_2, \dots, m_k}(c)}{-x} dx \\
&= -\int_0^{1-c} \frac{\mathbf{H}_{m_2, \dots, m_k}(c) \mathbf{H}_{m_1-c}(x) + \dots + \mathbf{H}_{m_1-c, \dots, m_k-c}(x)}{x} dx \\
&= -\mathbf{H}_{m_2, \dots, m_k}(c) \mathbf{H}_{0, m_1-c}(1-c) - \mathbf{H}_{m_3, \dots, m_k}(c) \mathbf{H}_{0, m_1-c, m_2-c}(1-c) \\
&\quad - \dots - \mathbf{H}_{m_k}(c) \mathbf{H}_{0, m_1-c, \dots, m_{k-1}-c}(1-c) - \mathbf{H}_{0, m_1-c, \dots, m_k-c}(1-c);
\end{aligned}$$

thus the lemma follows. \square

Remark 3.8.9. Using this lemma we can extend the presented algorithm to \bar{S} -sums $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ provided that if $|b_1| > 1$, we have that $|b_i| < 1$ for $2 < i < k$.

Chapter 4

Cyclotomic Harmonic Sums

In Chapter 3 we already generalized harmonic sums and worked with S-sums, whereas in this chapter we want to extend harmonic sums into a different direction that leads to *cyclotomic harmonic sums* (compare [8, 4]). Most of the facts that we will present here were already published in [8], however here we will work out the theoretic background in detail. For instance the theorems are supplemented by proofs, the algorithms mentioned in [8] are worked out in detail and more examples are given. Note that all methods presented in this chapter can be applied also for harmonic sums and harmonic polylogarithms.

4.1 Definition and Structure of Cyclotomic Harmonic Sums

Definition 4.1.1 (Cyclotomic Harmonic Sums). *Let $a_i, k \in \mathbb{N}, b_i, n \in \mathbb{N}_0$ and $c_i \in \mathbb{Z}^*$ for $i \in \{1, 2, \dots, k\}$. We define*

$$\begin{aligned} S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n) &= \\ &= \sum_{i_1 \geq i_2, \dots, i_k \geq 1} \frac{\text{sign}(c_1)^{i_1}}{(a_1 i_1 + b_1)^{|c_1|}} \frac{\text{sign}(c_2)^{i_2}}{(a_2 i_2 + b_2)^{|c_2|}} \cdots \frac{\text{sign}(c_k)^{i_k}}{(a_k i_k + b_k)^{|c_k|}} \\ &= \sum_{i_1=1}^n \frac{\text{sign}(c_1)^{i_1}}{(a_1 i_1 + b_1)^{|c_1|}} \sum_{i_2=1}^{i_1} \frac{\text{sign}(c_2)^{i_2}}{(a_2 i_2 + b_2)^{|c_2|}} \cdots \sum_{i_k=1}^{i_{k-1}} \frac{\text{sign}(c_k)^{i_k}}{(a_k i_k + b_k)^{|c_k|}}. \end{aligned}$$

k is called the *depth* and $w = \sum_{i=0}^k |c_i|$ is called the *weight* of the cyclotomic harmonic sum $S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n)$.

4.1.1 Product

In the following we will see that as for harmonic sums and S-sums it is possible to express the product of cyclotomic harmonic sums with the same upper summation limit as linear combination of single cyclotomic harmonic sums. Hence cyclotomic harmonic sums form a quasi shuffle algebra. We start with the subsequent lemma.

Lemma 4.1.2. *Let $a_1, a_2, c_1, c_2 \in \mathbb{N}, b_1, b_2, i \in \mathbb{N}_0$. If $a_1 b_2 \neq a_2 b_1$, we have*

$$\begin{aligned} \frac{1}{(a_1 i + b_1)^{c_1} (a_2 i + b_2)^{c_2}} &= \\ &(-1)^{c_1} \sum_{j=1}^{c_1} (-1)^j \binom{c_1 + c_2 - j - 1}{c_2 - 1} \frac{a_1^{c_2} a_2^{c_1 - j}}{(a_1 b_2 - a_2 b_1)^{c_1 + c_2 - j}} \frac{1}{(a_1 i + b_1)^j} \\ &+ (-1)^{c_2} \sum_{j=1}^{c_2} (-1)^j \binom{c_1 + c_2 - j - 1}{c_1 - 1} \frac{a_1^{c_2 - j} a_2^{c_1}}{(a_2 b_1 - a_1 b_2)^{c_1 + c_2 - j}} \frac{1}{(a_2 i + b_2)^j}, \end{aligned}$$

and if $a_1 b_2 = a_2 b_1$, we have

$$\frac{1}{(a_1 i + b_1)^{c_1} (a_2 i + b_2)^{c_2}} = \left(\frac{a_1}{a_2}\right)^{c_2} \frac{1}{(a_1 i + b_1)^{c_1 + c_2}}.$$

Having this lemma in mind we find the following product formulas.

Theorem 4.1.3. *Let $a_i, d_i, k, l, n \in \mathbb{N}, b_i, e_i \in \mathbb{N}_0$ and $c_i, f_i \in \mathbb{Z}^*$. If $a_1 e_1 \neq d_1 b_1$ we have*

$$\begin{aligned} &S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(n) = \\ &\sum_{i=1}^n \frac{\text{sign}(c_1)^i}{(a_1 i + b_1)^{|c_1|}} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(i) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(i) \\ &+ \sum_{i=1}^n \frac{\text{sign}(f_1)^i}{(d_1 i + e_1)^{|f_1|}} S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i) \\ &- \sum_{i=1}^n \left((-1)^{|c_1|} \sum_{j=1}^{|c_1|} (-1)^j \binom{|c_1| + |f_1| - j - 1}{|f_1| - 1} \frac{a_1^{|f_1|} d_1^{|c_1| - j}}{a_1 e_1 - d_1 b_1} \frac{1}{(a_1 i + b_1)^j} \right. \\ &\quad \left. + (-1)^{|f_1|} \sum_{j=1}^{|f_1|} (-1)^j \binom{|c_1| + |f_1| - j - 1}{|f_1| - 1} \frac{a_1^{|f_1| - j} d_1^{|c_1|}}{d_1 b_1 - a_1 e_1} \frac{1}{(d_1 i + e_1)^j} \right) \\ &S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i), \end{aligned}$$

and if $a_1 e_1 = d_1 b_1$, we have

$$S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(n) =$$

$$\begin{aligned}
& \sum_{i=1}^n \frac{\text{sign}(c_1)^i}{(a_1 i + b_1)^{|c_1|}} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(i) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(i) \\
& + \sum_{i=1}^n \frac{\text{sign}(f_1)^i}{(d_1 i + e_1)^{|f_1|}} S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i) \\
& - \left(\frac{a_1}{d_1} \right)^{|f_1|} \sum_{i=1}^n \frac{(\text{sign}(c_1) \text{sign}(f_1))^i}{(a_1 i + b_1)^{|c_1| + |f_1|}} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i).
\end{aligned}$$

Proof. From the identity

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} = \sum_{i=1}^n \sum_{j=1}^i a_{ij} + \sum_{j=1}^n \sum_{i=1}^j a_{ij} - \sum_{i=1}^n a_{ii}$$

we get immediately

$$\begin{aligned}
& S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(n) = \\
& \sum_{i=1}^n \frac{\text{sign}(c_1)^i}{(a_1 i + b_1)^{|c_1|}} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(i) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(i) \\
& + \sum_{i=1}^n \frac{\text{sign}(f_1)^i}{(d_1 i + e_1)^{|f_1|}} S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i) \\
& - \sum_{i=1}^n \frac{(\text{sign}(c_1) \text{sign}(f_1))^i}{(a_1 i + b_1)^{|c_1|} (d_1 i + e_1)^{|f_1|}} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i).
\end{aligned}$$

Using Lemma 4.1.2 we get the results. \square

Extracting Leading or Trailing Ones.

We say that a cyclotomic harmonic sum $S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)$ has leading or trailing ones, if $c_1 = 1$ or $c_k = 1$, respectively. If $c_i = 1$ for $1 \leq i \leq j < k$ and $c_{j+1} \neq 1$, we say that the sum has j -leading ones, analogously, if $c_i = 1$ for $1 < j \leq i \leq k$ and $c_{j-1} \neq 1$, we say that the sum has $k - j + 1$ -trailing ones. In addition, we call a cyclotomic harmonic sum $S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)$ which has only ones i.e., $c_i = 1$ for $1 \leq i \leq k$ a *linear* cyclotomic harmonic sum.

As for harmonic sums we can use the product of the cyclotomic harmonic sums to single out leading or trailing ones: we consider the sum

$$S_{(a_1, b_1, 1), (a_2, b_2, 1), \dots, (a_j, b_j, 1), (a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n)$$

with $c_{j+1} \neq 1$, i.e., this sum has j -leading ones. Let p be the expansion of

$$S_{(a_1, b_1, 1), (a_2, b_2, 1), \dots, (a_j, b_j, 1)}(n) S_{(a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n)$$

using Theorem 4.1.3. The only cyclotomic harmonic sum with j -leading ones in p is $S_{(a_1, b_1, 1), \dots, (a_j, b_j, 1), (a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n)$, all the other sums in p have less leading ones. Now define

$$q := p - S_{(a_1, b_1, 1), \dots, (a_j, b_j, 1), (a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n),$$

i.e., all the cyclotomic harmonic sums in q have less than j -leading ones. We can now write

$$\begin{aligned} & S_{(a_1, b_1, 1), \dots, (a_j, b_j, 1), (a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n) \\ &= S_{(a_1, b_1, 1), \dots, (a_j, b_j, 1)}(n) S_{(a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n) - q; \end{aligned}$$

in this way we can express $S_{(a_1, b_1, 1), \dots, (a_j, b_j, 1), (a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n)$ using sums with less than j -leading ones and $S_{(a_1, b_1, 1), \dots, (a_j, b_j, 1)}(n)$. Applying the same strategy to the remaining sums with leading ones which are not *linear* cyclotomic harmonic sums we can eventually decompose the cyclotomic harmonic sum $S_{(a_1, b_1, 1), (a_2, b_2, 1), \dots, (a_j, b_j, 1), (a_{j+1}, b_{j+1}, c_{j+1}), \dots, (a_k, b_k, c_k)}(n)$ in a multivariate polynomial in *linear* cyclotomic harmonic sum with coefficients in the cyclotomic harmonic sums without leading ones.

Example 4.1.4.

$$\begin{aligned} S_{(2,1,1), (3,2,1), (1,0,2)}(n) &= -S_{(1,0,1)}(n) + \frac{1}{2}S_{(1,0,2)}(n) + \frac{1}{2}S_{(1,0,2)}(n)S_{(2,1,1)}(n) \\ &+ 2S_{(2,1,1)}(n) - \frac{5}{2}S_{(1,0,2), (2,1,1)}(n) - S_{(2,1,1)}(n)S_{(1,0,2), (3,2,1)}(n) \\ &+ 3S_{(1,0,2), (3,2,1)}(n) - \frac{3}{4}S_{(2,1,1), (1,0,1)}(n) + S_{(1,0,2)}(n)S_{(2,1,1), (3,2,1)}(n) \\ &+ \frac{9}{4}S_{(2,1,1), (3,2,1)}(n) + S_{(1,0,2), (3,2,1), (2,1,1)}(n). \end{aligned}$$

Remark 4.1.5. We can always decompose a cyclotomic harmonic sum $S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)$ in a multivariate polynomial in linear cyclotomic harmonic sums with coefficients in the cyclotomic harmonic sums without leading ones. Note, that in a similar way it is possible to extract trailing ones. Hence we can also decompose a cyclotomic harmonic sum $S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)$ in a multivariate polynomial in linear cyclotomic harmonic sums with coefficients in the cyclotomic harmonic sums without trailing ones. Clearly, restricting to harmonic sums we get just the results stated in Section 2.1.

Example 4.1.6.

$$S_{(1,0,2), (2,1,1), (3,2,1)}(n) = -\frac{3}{4}S_{(1,0,1)}(n) + \frac{1}{2}S_{(1,0,2)}(n) + S_{(1,0,2)}(n)S_{(3,2,1)}(n)$$

$$\begin{aligned}
& + \frac{9}{4} S_{(3,2,1)}(n) - 2S_{(1,0,1),(3,2,1)}(n) - S_{(3,2,1)}(n)S_{(2,1,1),(1,0,2)}(n) \\
& - 2S_{(2,1,1),(1,0,2)}(n) + S_{(1,0,2)}(n)S_{(2,1,1),(3,2,1)}(n) + 4S_{(2,1,1),(3,2,1)}(n) \\
& + 2S_{(3,2,1),(1,0,2)}(n) + S_{(3,2,1),(2,1,1),(1,0,2)}(n).
\end{aligned}$$

4.1.2 Synchronization

In this subsection we consider cyclotomic harmonic sums with upper summation limit $n + c$, kn and $kn + c$ for $c \in \mathbb{Z}$ and $k \in \mathbb{N}$.

Lemma 4.1.7. *Let $a_i, n, k, c \in \mathbb{N}$, $b_i \in \mathbb{N}_0$ and $c_i \in \mathbb{Z}^*$ for $i \in (1, 2, \dots, k)$. Then for $n \geq 0$,*

$$\begin{aligned}
S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n + c) &= S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n) \\
&+ \sum_{j=1}^c \frac{\text{sign}(c_1)^{j+n} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n + j)}{(a_1(j + n) + b_1)^{|c_1|}},
\end{aligned}$$

and for $n \geq c$,

$$\begin{aligned}
S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n - c) &= S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n) \\
&+ \sum_{j=1}^c \frac{\text{sign}(c_1)^{j+n-c} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n - c + j)}{(a_1(j + n - c) + b_1)^{|c_1|}}.
\end{aligned}$$

Given a cyclotomic harmonic sum of the form $S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n + c)$ with $c \in \mathbb{Z}$, we can apply the previous lemma recursively in order to synchronize the upper summation limit of the arising cyclotomic harmonic sums to n .

Lemma 4.1.8. *For $a, k \in \mathbb{N}$, $b \in \mathbb{N}_0$, $c \in \mathbb{Z}^*$, $k \geq 2$:*

$$S_{(a,b,c)}(k \cdot n) = \sum_{i=0}^{k-1} \text{sign}(c)^i S_{(k \cdot a, b - a \cdot i, \text{sign}(c)^k |c|)}(n).$$

Proof.

$$\begin{aligned}
S_{(a,b,c)}(x, k \cdot n) &= \sum_{j=1}^{k \cdot n} \frac{\text{sign}(c)^j}{(aj + b)^{|c|}} = \\
&= \sum_{j=1}^n \frac{\text{sign}(c)^{kj}}{(a(k \cdot j) + b)^{|c|}} + \sum_{j=1}^n \frac{\text{sign}(c)^{kj-1}}{(a(k \cdot j - 1) + b)^{|c|}} + \cdots + \sum_{j=1}^n \frac{\text{sign}(c)^{kj-(k-1)}}{(a(k \cdot j - (k-1)) + b)^{|c|}} \\
&= \sum_{j=1}^n \frac{\text{sign}(c)^{kj}}{((ak)j + b)^{|c|}} + \sum_{j=1}^n \frac{\text{sign}(c)^{kj} \text{sign}(c)^{-1}}{((ak)j + (b - a))^{|c|}} + \cdots + \sum_{j=1}^n \frac{\text{sign}(c)^{kj} \text{sign}(c)^{-(k-1)}}{((ak)j + (b - (k-1)a))^{|c|}}
\end{aligned}$$

$$= \sum_{i=0}^{k-1} \text{sign}(c)^i S_{(k \cdot a, b - a \cdot i, \text{sign}(c)^k |c|)}(n).$$

□

Theorem 4.1.9. For $a_i, m \in \mathbb{N}, b_i, k \in \mathbb{N}_0, c_i \in \mathbb{Z}^*, k \geq 2$:

$$S_{(a_m, b_m, c_m), (a_{m-1}, b_{m-1}, c_{m-1}), \dots, (a_1, b_1, c_1)}(k \cdot n) = \sum_{i=0}^{m-1} \sum_{j=1}^n \frac{S_{(a_{m-1}, b_{m-1}, c_{m-1}), \dots, (a_1, b_1, c_1)}(k \cdot j - i) \text{sign}(c_m)^{k \cdot j - i}}{(a_m(k \cdot j - i) + b_1)^{|c_m|}}.$$

After applying Theorem 4.1.9 we can synchronize the cyclotomic harmonic sums in the inner sum with upper summation limit $k \cdot j - i$ to upper the summation limit $k \cdot j$. Now we can apply Theorem 4.1.9 to these sums. Repeated application of this procedure leads eventually to cyclotomic harmonic sums with upper summation limit n .

4.2 Definition and Structure of Cyclotomic Harmonic Polylogarithms

In Definition 2.2.1 we defined harmonic polylogarithms and in Definition 3.1.2 we already extended harmonic polylogarithms to multiple polylogarithms by extending the considered alphabet. In this section we will extend the harmonic polylogarithms from Definition 2.2.1 into an other direction, i.e., we will end up with cyclotomic harmonic polylogarithms. We start by defining the following auxiliary function: For $a \in \mathbb{N}$ and $b \in \mathbb{N}, b < \varphi(a)$ (here $\varphi(b)$ denotes Euler’s totient function [39, 84]) we define

$$f_a^b : (0, 1) \mapsto \mathbb{R}$$

$$f_a^b(x) = \begin{cases} \frac{1}{x}, & \text{if } a = b = 0 \\ \frac{x^b}{\Phi_a(x)}, & \text{otherwise,} \end{cases}$$

where $\Phi_a(x)$ denotes the a th cyclotomic polynomial [54]:

$$\Phi_a(x) = \frac{x^a - 1}{\prod_{d|a, d < a} \Phi_d(x)}. \tag{4.1}$$

The first cyclotomic polynomials are given by

$$\begin{aligned} \Phi_1(x) &= x - 1 \\ \Phi_2(x) &= x + 1 \end{aligned}$$

$$\begin{aligned}
\Phi_3(x) &= x^2 + x + 1 \\
\Phi_4(x) &= x^2 + 1 \\
\Phi_5(x) &= x^4 + x^3 + x^2 + x + 1 \\
\Phi_6(x) &= x^2 - x + 1 \\
\Phi_7(x) &= x^6 + x^5 + x^4 + x^3 + x^2 + x + 1 \\
\Phi_8(x) &= x^4 + 1 \\
\Phi_9(x) &= x^6 + x^3 + 1 \\
\Phi_{10}(x) &= x^4 - x^3 + x^2 - x + 1 \\
\Phi_{11}(x) &= x^{10} + x^9 + x^8 + x^7 + x^6 + x^5 + x^4 + x^3 + x^2 + x + 1 \\
\Phi_{12}(x) &= x^4 - x^2 + 1, \text{ etc.}
\end{aligned}$$

Now we are ready to define cyclotomic polylogarithms:

Definition 4.2.1 (Cyclotomic Harmonic Polylogarithms). *Let $m_i = (a_i, b_i) \in \mathbb{N}^2$, $b_i < \varphi(a_i)$; we define for $x \in (0, 1)$:*

$$\begin{aligned}
H(x) &= 1, \\
H_{m_1, \dots, m_k}(x) &= \begin{cases} \frac{1}{k!} (\log x)^k, & \text{if } m_i = (0, 0) \text{ for } 1 \leq i \leq k \\ \int_0^x f_{a_1}^{b_1}(y) H_{m_2, \dots, m_k}(y) dy, & \text{otherwise.} \end{cases}
\end{aligned}$$

The length k of the vector $\mathbf{m} = (m_1, \dots, m_k)$ is called the weight of the cyclotomic harmonic polylogarithm $H_{\mathbf{m}}(x)$.

Example 4.2.2.

$$\begin{aligned}
H_{(5,3)}(x) &= \int_0^x \frac{y^3}{\Phi_5(y)} dy = \int_0^x \frac{y^3}{y^4 + y^3 + y^2 + y + 1} dy \\
H_{(3,1),(2,0),(5,2)}(x) &= \int_0^x \frac{y}{\Phi_3(y)} \int_0^y \frac{1}{\Phi_2(z)} \int_0^z \frac{w^2}{\Phi_5(w)} dw dz dy \\
H_{(0,0),(2,0),(1,0)}(x) &= \int_0^x \frac{1}{y} \int_0^y \frac{1}{z+1} \int_0^z \frac{1}{w-1} dw dz dy = -H_{0,-1,1}(x).
\end{aligned}$$

A cyclotomic harmonic polylogarithm $H_{\mathbf{m}}(x) = H_{m_1, \dots, m_w}(x)$ is an analytic functions for $x \in (0, 1)$. For the limits $x \rightarrow 0$ and $x \rightarrow 1$ we have (compare Section 2.2):

- It follows from the definition that if $m_v \neq (0, 0)$ for all v with $1 \leq v \leq w$, then $H_{\mathbf{m}}(0) = 0$.
- If $m_1 \neq (1, 0)$ or if $m_1 = (1, 0)$ and $m_v = (0, 0)$ for all v with $1 < v \leq w$, then $H_{\mathbf{m}}(1)$ is finite.

- If $m_1 = (1, 0)$ and $m_v \neq (0, 0)$ for some v with $1 < v \leq w$, $\lim_{x \rightarrow 1^-} H_m(x)$ behaves as a combination of powers of $\log(1 - x)$.

We define $H_m(0) := \lim_{x \rightarrow 0^+} H_m(x)$ and $H_m(1) := \lim_{x \rightarrow 1^-} H_m(x)$ if the limits exist.

Remark 4.2.3. For the derivatives we have for all $x \in (0, 1)$ that

$$\frac{d}{dx} H_{(m_1, n_1), (m_2, n_2), \dots, (m_k, n_k)}(x) = f_{m_1}^{n_1}(x) H_{(m_2, n_2), \dots, (m_k, n_k)}(x).$$

Remark 4.2.4. For harmonic polylogarithms we considered the alphabet $\{-1, 0, 1\}$. The letters -1 and 0 correspond to $(2, 0)$ and $(0, 0)$ respectively. The letter 1 corresponds to $(1, 0)$. However 1 indicates an iteration of $\frac{1}{1-x}$ while $(1, 0)$ indicates an iteration of $\frac{1}{x-1}$; hence there is a change of sign. From now on we will sometimes mix both notations in the obvious way:

Example 4.2.5.

$$H_{(0,0), -1, (1,0), (3,1)}(x) = -H_{0, -1, 1, (3,1)}(x) = H_{(0,0), (2,0), (1,0), (3,1)}(x).$$

Remark 4.2.6. Again the product of two cyclotomic harmonic polylogarithms of the same argument can be expressed using the formula (compare (2.3))

$$H_p(x) H_q(x) = \sum_{r=p \sqcup q} H_r(x) \tag{4.2}$$

in which $p \sqcup q$ represent all merges of p and q in which the relative orders of the elements of p and q are preserved. Hence cyclotomic harmonic polylogarithms form a shuffle algebra.

The number of basis elements spanning the shuffle algebra are given by

$$N^{\text{basic}}(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) M^d, w \geq 1 \tag{4.3}$$

basis elements according to the 1st Witt formula [87]. Here μ denotes the Möbius function [61, 46]. The number of basic cyclotomic harmonic polylogarithms in dependence of w and M is given in Table 4.1. It applies to any alphabet containing M letters.

Example 4.2.7. We consider the alphabet $\{(0, 0), (2, 0), (4, 1), (5, 3)\}$ at weight two. We obtain the 6 basis cyclotomic harmonic polylogarithms

$$H_{(2,0), (0,0)}(x), H_{(4,1), (0,0)}(x), H_{(4,1), (2,0)}(x), H_{(5,3), (0,0)}(x), H_{(5,3), (2,0)}(x), H_{(5,3), (4,1)}(x),$$

together with the relations

$$H_{(0,0), (0,0)}(x) = \frac{1}{2} H_{(0,0)}(x)^2,$$

weight	Number of letters						
	2	3	4	5	6	7	8
1	2	3	4	5	6	7	8
2	1	3	6	10	15	21	28
3	2	8	20	40	70	112	168
4	3	18	60	150	315	588	1008
5	6	48	204	624	1554	3360	6552
6	9	116	670	2580	7735	19544	43596
7	18	312	2340	11160	39990	117648	299592
8	30	810	8160	48750	209790	729300	2096640

Table 4.1: Number of basic cyclotomic harmonic polylogarithms in dependence of the number of letters and weight.

$$\begin{aligned}
 H_{(0,0),(2,0)}(x) &= H_{(0,0)}(x)H_{(2,0)}(x) - H_{(2,0),(0,0)}(x), \\
 H_{(0,0),(4,1)}(x) &= H_{(0,0)}(x)H_{(4,1)}(x) - H_{(4,1),(0,0)}(x), \\
 H_{(0,0),(5,3)}(x) &= H_{(0,0)}(x)H_{(5,3)}(x) - H_{(5,3),(0,0)}(x), \\
 H_{(2,0),(2,0)}(x) &= \frac{1}{2}H_{(2,0)}(x)^2, \\
 H_{(2,0),(4,1)}(x) &= H_{(2,0)}(x)H_{(4,1)}(x) - H_{(4,1),(2,0)}(x), \\
 H_{(2,0),(5,3)}(x) &= H_{(2,0)}(x)H_{(5,3)}(x) - H_{(5,3),(2,0)}(x), \\
 H_{(4,1),(4,1)}(x) &= \frac{1}{2}H_{(4,1)}(x)^2, \\
 H_{(4,1),(5,3)}(x) &= H_{(4,1)}(x)H_{(5,3)}(x) - H_{(5,3),(4,1)}(x), \\
 H_{(5,3),(5,3)}(x) &= \frac{1}{2}H_{(5,3)}(x)^2.
 \end{aligned}$$

4.3 Identities between Cyclotomic Harmonic Polylogarithms of Related Arguments

4.3.1 $\frac{1}{x} \rightarrow x$

First we consider just cyclotomic harmonic polylogarithms with indices not equal to $(1, 0)$. Proceeding recursively on the weight w of the cyclotomic harmonic polylogarithm we have for $0 < x < 1$:

$$H_{(0,0)}\left(\frac{1}{x}\right) = -H_{(0,0)}(x),$$

and in addition, for $a \in \mathbb{N}, b \in \mathbb{N}_0, a > 1, b < \varphi(a)$ we can use

$$\int_0^{\frac{1}{x}} \frac{y^b}{\Phi_a(y)} dy = H_{(a,b)}(1) - \int_{\frac{1}{x}}^1 \frac{y^b}{\Phi_a(y)} dy = H_{(a,b)}(1) + \int_x^1 \frac{\frac{1}{y^b}}{y^2 \Phi_a(\frac{1}{y})} dy. \tag{4.4}$$

At this point we can perform a partial fraction decomposition on the integrand and finally rewrite the resulting integrals in terms of cyclotomic harmonic polylogarithms at x and 1. Now let us look at higher weights $w > 1$. We consider $H_{m_1, m_2, \dots, m_w}(\frac{1}{x})$ and suppose that we can already apply the transformation for cyclotomic harmonic polylogarithms of weight $< w$. For $(a, b) \neq (1, 0)$ we get:

$$\begin{aligned} H_{(0,0), m_2, \dots, m_w} \left(\frac{1}{x} \right) &= H_{(0,0), m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t^2(1/t)} H_{m_2, \dots, m_w} \left(\frac{1}{t} \right) dt \\ &= H_{(0,0), m_2, \dots, m_w}(1) + \int_x^1 \frac{1}{t} H_{m_2, \dots, m_w} \left(\frac{1}{t} \right) dt \\ H_{(a,b), m_2, \dots, m_w} \left(\frac{1}{x} \right) &= H_{(a,b), m_2, \dots, m_w}(1) + \int_x^1 \frac{\frac{1}{y^b}}{y^2 \Phi_a(\frac{1}{y})} H_{m_2, \dots, m_w} \left(\frac{1}{y} \right) dy. \end{aligned}$$

At this point we again have to perform a partial fraction decomposition on the integrand and since we know the transformation for weights $< w$ we can apply it to $H_{m_2, \dots, m_w}(\frac{1}{t})$ and finally we obtain the required weight w identity by using the definition of the cyclotomic harmonic polylogarithms.

The index $(1, 0)$ in the index set leads to a branch point at 1 and a branch cut discontinuity in the complex plane for $x \in (1, \infty)$. This corresponds to the branch point at $x = 1$ and the branch cut discontinuity in the complex plane for $x \in (1, \infty)$ of $\log(1-x) = H_{(1,0)}(x)$. However the analytic properties of the logarithm are well known and we can set for $0 < x < 1$ for instance

$$H_{(1,0)} \left(\frac{1}{x} \right) = H_{(1,0)}(x) - H_{(0,0)}(x) + i\pi \quad (4.5)$$

by approaching the argument $\frac{1}{x}$ from the lower half complex plane. The strategy now is as follows: if a cyclotomic harmonic polylogarithm has leading $(1, 0)$, we remove them and end up with cyclotomic harmonic polylogarithms without leading $(1, 0)$ and powers of $H_{(1,0)}(\frac{1}{x})$. We know how to deal with the cyclotomic harmonic polylogarithms without leading $(1, 0)$ due to the previous part of this section and for the powers of $H_{(1,0)}(\frac{1}{x})$ we can use (4.5).

Example 4.3.1.

$$\begin{aligned} H_{(3,1),(5,2)}(x) &= (H_{(5,0)}(1) + H_{(5,2)}(1)) \left(-H_{(0,0)} \left(\frac{1}{x} \right) \right) \\ &\quad - (H_{(5,0)}(1) + H_{(5,2)}(1)) \left(H_{(3,0)}(1) - H_{(3,0)} \left(\frac{1}{x} \right) \right) \\ &\quad - (H_{(5,0)}(1) + H_{(5,2)}(1)) \left(H_{(3,1)}(1) - H_{(3,1)} \left(\frac{1}{x} \right) \right) \\ &\quad + H_{(0,0),(5,0)} \left(\frac{1}{x} \right) - H_{(3,0),(5,0)} \left(\frac{1}{x} \right) - H_{(3,1),(5,0)} \left(\frac{1}{x} \right) \\ &\quad - H_{(0,0),(5,0)}(1) + H_{(3,0),(5,0)}(1) + H_{(3,1),(5,0)}(1) + H_{(3,1),(5,2)}(1). \end{aligned}$$

4.3.2 $\frac{1-x}{1+x} \rightarrow x$

We restrict the index set now to letters out of $\{1, 0, -1, (4, 0), (4, 1)\}$, and proceed recursively on the weight w of the cyclotomic harmonic polylogarithm. For the base cases we have

$$\mathbf{H}_{-1}\left(\frac{1-x}{1+x}\right) = \mathbf{H}_{-1}(1) - \mathbf{H}_{-1}(x) \tag{4.6}$$

$$\mathbf{H}_0\left(\frac{1-x}{1+x}\right) = -\mathbf{H}_1(x) + \mathbf{H}_{-1}(x) \tag{4.7}$$

$$\mathbf{H}_1\left(\frac{1-x}{1+x}\right) = -\mathbf{H}_{-1}(1) - \mathbf{H}_0(x) + \mathbf{H}_{-1}(x) \tag{4.8}$$

$$\mathbf{H}_{(4,0)}\left(\frac{1-x}{1+x}\right) = \mathbf{H}_{(4,0)}(1) + \mathbf{H}_{(4,0)}(x) \tag{4.9}$$

$$\mathbf{H}_{(4,1)}\left(\frac{1-x}{1+x}\right) = -\mathbf{H}_{(4,1)}(1) - \mathbf{H}_{-1}(x) + \mathbf{H}_{(4,1)}(x). \tag{4.10}$$

Now let us look at higher weights $w > 1$. We consider $\mathbf{H}_{m_1, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right)$ with $m_i \in \{1, 0, -1, (4, 0), (4, 1)\}$ and suppose that we can already apply the transformation for harmonic polylogarithms of weight $< w$. If $m_1 = 1$, we can remove leading ones and end up with harmonic polylogarithms without leading ones and powers of $\mathbf{H}_1\left(\frac{1-x}{1+x}\right)$. For the powers of $\mathbf{H}_1\left(\frac{1-x}{1+x}\right)$ we can use (4.8); therefore, only the cases in which the first index $m_1 \neq 1$ are to be considered. We get (compare [73] and Sections 2.3.2 and 3.2.3):

$$\begin{aligned} \mathbf{H}_{-1, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= \mathbf{H}_{-1, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ \mathbf{H}_{0, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= \mathbf{H}_{0, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1-t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ &\quad - \int_0^x \frac{1}{1-t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1+t}{1+t}\right) dt \\ \mathbf{H}_{(4,0), m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= \mathbf{H}_{(4,0), m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t^2} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ \mathbf{H}_{(4,1), m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= \mathbf{H}_{(4,1), m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ &\quad + \int_0^x \frac{t}{1+t^2} \mathbf{H}_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt. \end{aligned}$$

Since we know the transform for weights $< w$ we can apply it to $\mathbf{H}_{m_2, \dots, m_w}\left(\frac{1+t}{1+t}\right)$ and finally we obtain the required weight w identity by using the definition of the cyclotomic harmonic polylogarithms.

4.4 Power Series Expansion of Cyclotomic Harmonic Polylogarithms

In order to be able to compute the power series expansion of cyclotomic harmonic polylogarithms, we state the following lemma.

Lemma 4.4.1. *Let $\Phi_n(x)$ be the n -th cyclotomic polynomial and let $\sum_{i \geq 0} f_i x^i$ be the power series expansion of $f(x) := \frac{1}{\Phi_n(x)}$ about zero. Then the sequence $(f_i)_{i \geq 0}$ is periodic with period n . For $0 \leq i < n$ the i -th coefficient f_i equals the coefficient of x^i in $-\prod_{d|n, d < n} \Phi_d(x)$.*

Proof. We have that

$$f(x) = \frac{1}{\Phi_n(x)} = \frac{\prod_{d|n, d < n} \Phi_d(x)}{x^n - 1},$$

hence

$$\begin{aligned} \prod_{d|n, d < n} \Phi_d(x) &= (x^n - 1)f(x) = (x^n - 1) \sum_{i \geq 0} f_i x^i = \sum_{i \geq 0} f_i x^{n+i} - \sum_{i \geq 0} f_i x^i \\ &= \sum_{i \geq 0} f_i x^{n+i} - \sum_{i=0}^{n-1} f_i x^i - \sum_{i \geq 0} f_{n+i} x^{n+i} \\ &= \sum_{i \geq 0} (f_i - f_{n+i}) x^{n+i} - \sum_{i=0}^{n-1} f_i x^i. \end{aligned}$$

Since the degree of $\prod_{d|n, d < n} \Phi_d(x)$ is $n - \varphi(n) < n$, we get that $f_{n+i} - f_n = 0$ and hence the sequence $(f_i)_{i \geq 0}$ is periodic with period n . \square

In general, the cyclotomic harmonic polylogarithms $H_m(x)$ do not have a regular Taylor series expansion. This is due to the effect that trailing zeroes, *i.e.*, the letter $(0, 0)$ in the index set may cause powers of $\log(x)$. Hence the proper expansion is one in terms of both x and $\log(x)$. We first look at the cyclotomic harmonic polylogarithms of depth one. Let $a, b \in \mathbb{N}$; and $0 < x < 1$; due to the previous lemma we can write

$$\frac{1}{\Phi_a(x)} = \sum_{q=0}^{a-1} f_q \sum_{i=0}^{\infty} x^{ai+q}.$$

Hence we get

$$H_{(a,b)}(x) = \int_0^x \frac{y^b}{\Phi_a(y)} dy = \sum_{q=0}^{a-1} f_q \int_0^x \sum_{i=0}^{\infty} y^{ai+q+b}$$

$$\begin{aligned}
&= \sum_{q=0}^{a-1} f_q \sum_{i=0}^{\infty} \frac{x^{ai+q+b+1}}{ai+q+b+1} \\
&= \sum_{q=0}^{a-1} f_q \sum_{i=1}^{\infty} \frac{x^{ai+q-a+b+1}}{ai+q-a+b+1}.
\end{aligned}$$

Remark 4.4.2. If $z = ka$ for some $k \in \mathbb{N}$ we can write this as well in the form:

$$H_{(a,b)}(x) = \sum_{j=1}^k \sum_{q=0}^{a-1} f_q \sum_{i=1}^{\infty} \frac{x^{zi+a(j-1)+q-z+b+1}}{zi+a(j-1)+q-z+b+1}.$$

Lemma 4.4.3. Let $H_m(x)$ be a cyclotomic harmonic polylogarithm with depth d . We assume that its power series expansion is of the form

$$H_m(x) = \sum_{j=1}^w \sum_{i=1}^{\infty} \frac{x^{zi+c_j}}{(zi+c_j)^{g_j}} S_{n_j}(i)$$

for $x \in (0, 1)$, $w, g_j \in \mathbb{N}$ and $c_j \in \mathbb{Z}$. We can get the depth $d+1$ expansion of $H_{(a,b),m}(x)$ provided that $a = 0$ or $ak = z$ for some $k \in \mathbb{N}$ using

$$\begin{aligned}
H_{(0,0),m}(x) &= \sum_{i=1}^{\infty} \frac{x^{zi+c_j}}{(zi+c_j)^{g_j+1}} S_{n_j}(i) \\
H_{(a,b),m}(x) &= \sum_{j=1}^w \sum_{q=0}^{z-1} f_q \sum_{i=1}^{\infty} \frac{x^{zi+q+b+c_j+1}}{(zi+q+b+c_j+1)} S_{(z,c_j,g_j),n_j}(i)
\end{aligned}$$

where

$$\frac{1}{\Phi_a(x)} = \sum_{q=0}^{z-1} f_q \sum_{p=0}^{\infty} x^{zp+q}.$$

Proof. We start with $H_{(0,0),m}(x)$. We have to consider w integrals of the form

$$\begin{aligned}
\int_0^x \frac{1}{y} \sum_{i=1}^{\infty} \frac{y^{zi+c}}{(zi+c)^g} S_n(i) dy &= \sum_{i=1}^{\infty} \frac{1}{(zi+c)^g} S_n(i) \int_0^x y^{zi+c-1} dy \\
&= \sum_{i=1}^{\infty} \frac{1}{(zi+c)^g} S_n(i) \frac{x^{zi+c}}{zi+c} dy \\
&= \sum_{i=1}^{\infty} \frac{x^{zi+c}}{(zi+c)^{g+1}} S_n(i).
\end{aligned}$$

For $H_{(a,b),m}(x)$ with $ak = z$ we have to consider w integrals of the type

$$\int_0^x \frac{y^b}{\Phi_a(y)} \sum_{i=1}^{\infty} \frac{y^{zi+c}}{(zi+c)^g} S_n(i) dy.$$

We use Lemma 4.4.1 and write

$$\frac{1}{\Phi_a(x)} = \sum_{q=0}^{z-1} f_q \sum_{p=0}^{\infty} x^{zp+q}.$$

Now we get

$$\begin{aligned} \int_0^x \frac{y^b}{\Phi_a(y)} \sum_{i=1}^{\infty} \frac{y^{zi+c}}{(zi+c)^g} S_n(i) dy &= \int_0^x y^b \sum_{q=0}^{z-1} f_q \sum_{p=0}^{\infty} y^{zp+q} \sum_{i=1}^{\infty} \frac{y^{zi+c}}{(zi+c)^g} S_n(i) dy \\ &= \sum_{q=0}^{z-1} f_q \int_0^x \sum_{p=0}^{\infty} y^{zp+q+b} \sum_{i=0}^{\infty} \frac{y^{zi+z+c}}{(zi+z+c)^g} S_n(i+1) dy \\ &= \sum_{q=0}^{z-1} f_q \int_0^x \sum_{i=0}^{\infty} \sum_{p=0}^i y^{z(i-p)+q+b} \frac{y^{zp+z+c}}{(zp+z+c)^g} S_n(p+1) dy \\ &= \sum_{q=0}^{z-1} f_q \int_0^x \sum_{i=0}^{\infty} y^{zi+q+b+c+z} S_{(z,c,g),n}(i+1) dy \\ &= \sum_{q=0}^{z-1} f_q \sum_{i=0}^{\infty} \frac{x^{zi+q+b+c+z+1}}{zi+q+b+c+z+1} S_{(z,c,g),n}(i+1) dy \\ &= \sum_{q=0}^{z-1} f_q \sum_{i=1}^{\infty} \frac{x^{zi+q+b+c+1}}{zi+q+b+c+1} S_{(z,c,g),n}(i) dy. \end{aligned}$$

□

Remark 4.4.4. Using the above strategy we can get the expansion of a cyclotomic harmonic polylogarithm $H_{(a_d, b_d), (a_{d-1}, b_{d-1}), \dots, (a_1, b_1)}(x)$ up to arbitrary weight d . If we set z equal to the least common multiple of the a_i which are not zero (this is possible due to Lemma 4.4.2) we can guarantee that the induction step works.

Example 4.4.5.

$$\begin{aligned} H_{(3,1), (1,0)}(x) &= \sum_{i=1}^{\infty} \frac{x^{3i+1} S_{(3,1,1)}(i)}{3i+1} - \sum_{i=1}^{\infty} \frac{x^{3i+1} S_{(3,2,1)}(i)}{3i+1} + \sum_{i=1}^{\infty} \frac{x^{3i+2} S_{(3,2,1)}(i)}{3i+2} \\ &\quad - \frac{1}{3} \sum_{i=1}^{\infty} \frac{x^{3i} S_{(3,1,1)}(i)}{i} - \frac{1}{3} \sum_{i=1}^{\infty} \frac{S_1(i) x^{3i+2}}{3i+2} + \frac{1}{3} \sum_{i=1}^{\infty} \frac{S_1(i) x^{3i+3}}{3i+3} \\ &\quad + \frac{3}{2} \sum_{i=1}^{\infty} \frac{x^{3i+1}}{3i+1} - \sum_{i=1}^{\infty} \frac{x^{3i+1}}{(3i+1)^2} - \sum_{i=1}^{\infty} \frac{x^{3i+1}}{3i+2} + \frac{1}{2} \sum_{i=1}^{\infty} \frac{x^{3i+2}}{3i+2} \\ &\quad - \sum_{i=1}^{\infty} \frac{x^{3i+2}}{(3i+2)^2} - \sum_{i=1}^{\infty} \frac{x^{3i}}{3i+1}. \end{aligned}$$

4.4.1 Asymptotic Behavior of Extended Harmonic Polylogarithms

Combining Section 4.3.1 together with the power series expansion of cyclotomic harmonic polylogarithms we can determine the asymptotic behavior of cyclotomic harmonic polylogarithms. Let us look at the cyclotomic harmonic polylogarithm $H_m(x)$ and define $y := \frac{1}{x}$. Using Section 4.3.1 on $H_m\left(\frac{1}{y}\right) = H_m(x)$ we can rewrite $H_m(x)$ in terms of cyclotomic harmonic polylogarithms at argument y together with some constants. Now we can get the power series expansion of the harmonic polylogarithms at argument y about 0 easily using the previous part of this Section. Since sending x to infinity corresponds to sending y to zero, we get the asymptotic behavior of $H_m(x)$.

Example 4.4.6.

$$\begin{aligned}
H_{(3,0),(3,1)}(x) &= -H_{(0,0)}(x) \left(\sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-2}}{3i-2} - \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-1}}{3i-1} \right) \\
&\quad - H_{(3,0)}(1) \left(- \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-2}}{3i-2} + \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-1}}{3i-1} + H_{(3,0)}(1) \right) \\
&\quad + \frac{1}{3} \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i} S_{(3,1,1)}(i)}{i} - \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-1} S_{(3,1,1)}(i)}{3i-1} \\
&\quad + \frac{1}{3} \sum_{i=1}^{\infty} \frac{S_1(i) \left(\frac{1}{x}\right)^{3i+1}}{3i+1} - \frac{1}{3} \sum_{i=1}^{\infty} \frac{S_1(i) \left(\frac{1}{x}\right)^{3i+2}}{3i+2} - \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-2}}{(3i-2)^2} \\
&\quad - \frac{1}{2} \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-1}}{3i-1} + \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-1}}{(3i-1)^2} + \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i}}{3i+1} - \frac{1}{2} \sum_{i=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3i-1}}{3i+1} \\
&\quad - H_{(3,0),(0,0)}(1) + H_{(3,0),(3,0)}(1) + 2H_{(3,0),(3,1)}(1).
\end{aligned}$$

4.4.2 Values of Cyclotomic Harmonic Polylogarithms at 1 Expressed by Cyclotomic Harmonic Sums at Infinity

As worked out in the previous part of this section, the expansion of the cyclotomic harmonic polylogarithms without trailing zeros is a combination of sums of the form:

$$\sum_{i=1}^{\infty} x^{ai+b} \frac{S_n(i)}{(ai+b)^c}, \quad a, b, c \in \mathbb{N}.$$

For $x \rightarrow 1$ these sums turn into cyclotomic harmonic sums at infinity if $c \neq 1$:

$$\sum_{i=1}^{\infty} x^{ai+b} \frac{S_n(i)}{(ai+b)^c} \rightarrow S_{(a,b,c),n}(\infty).$$

Hence the values of cyclotomic harmonic polylogarithms at one are related to the values of the cyclotomic harmonic sums at infinity.

Example 4.4.7.

$$H_{(0,0),(3,2)}(1) = \frac{1}{9}S_{(1,0,2)}(\infty) - S_{(3,1,2)}(\infty).$$

If $c = 1$, these sums turn into

$$\sum_{i=1}^{\infty} x^{ai+b} \frac{S_n(i)}{(ai+b)}.$$

Sending x to one gives:

$$\lim_{x \rightarrow 1} \sum_{i=1}^{\infty} x^{ai+b} \frac{S_n(i)}{(ai+b)} = \infty$$

We see that these limits do not exist: this corresponds to the infiniteness of the cyclotomic harmonic sums with leading ones: $\lim_{k \rightarrow \infty} S_{(a,b,1),n}(k) = \infty$.

4.5 Integral Representation of Cyclotomic Harmonic Sums

In this section we look at integral representations of cyclotomic harmonic sums. It will turn out that we can find representations in form of Mellin-type transforms of cyclotomic polylogarithms. The integral representation of cyclotomic harmonic sums of depth one can be derived easily:

Lemma 4.5.1. *Let $a, c \in \mathbb{N}, b \in \mathbb{N}_0, d \in \{1, -1\}$ and $n \in \mathbb{N}$; then*

$$\begin{aligned} S_{(a,b,1)}(d; n) &= \int_0^1 \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - d} dx_1 \\ S_{(a,b,2)}(d; n) &= \int_0^1 \frac{1}{x_2} \int_0^{x_2} \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - d} dx_1 dx_2 \\ S_{(a,b,c)}(d; n) &= \int_0^1 \frac{1}{x_c} \int_0^{x_c} \frac{1}{x_{c-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - d} dx_1 \cdots dx_c. \end{aligned}$$

Let us now look at the integral representation of cyclotomic harmonic sums of higher depths. We consider the sum $S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n)$ and apply Lemma 4.5.1 to the innermost sum ($a = a_k, b = b_k, c = |c_k|, d = \text{sign}(c_k)$). One now may perform the next sum in the same way, provided $a_{k-1} \nmid a_k$. At this point we may need the fact:

$$\sum_{i=1}^n \frac{(dy^a)^i}{(ai+b)^c} = \frac{1}{y^b} \int_0^y \frac{1}{x_c} \int_0^{x_c} \frac{1}{x_{c-1}} \cdots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - d} dx_1 \cdots dx_c$$

for $n, a, b, c, k \in \mathbb{N}, d = \pm 1$ and $y \in \mathbb{R}$. If $a_{k-1} \nmid a_k$, one transforms the integration variables such that the next denominator can be generated, etc. In this way, the sum

$S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n)$ can be represented in terms of linear combinations of Poincaré-iterated integrals. Evidently, the representation of the cyclotomic harmonic sum $S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(n)$ in terms of a (properly regularized) Mellin transform will be related to the Mellin variable kn , with k being the least common multiple of a_1, \dots, a_k .

Let us illustrate the principle steps in case of the following example (compare [8]):

$$S_{(3,2,2), (2,1,-1)}(n) = \sum_{k=1}^n \frac{1}{(3k+2)^2} \sum_{l=1}^k \frac{(-1)^l}{(2l+1)} .$$

The first sum yields

$$S_{(3,2,2), (2,1,-1)}(n) = \sum_{k=1}^n \int_0^1 \frac{1}{(3k+2)^2} \frac{x^2((-x^2)^k - 1)}{x^2 + 1} dx .$$

Setting $x = y^3$ one obtains

$$\begin{aligned} S_{(3,2,2), (2,1,-1)}(n) &= 12 \int_0^1 \frac{y^8}{y^6 + 1} \sum_{k=1}^n \frac{(-y^6)^k - 1}{(6k+4)^2} dy \\ &= 12 \int_0^1 \frac{y^4}{y^6 + 1} \left\{ \int_0^y \frac{1}{z} \int_0^z t^9 \frac{(-t^6)^n - 1}{t^6 + 1} dt dz \right. \\ &\quad \left. - y^4 \int_0^1 \frac{1}{z} \int_0^z t^9 \frac{t^{6n} - 1}{t^6 - 1} dt dz \right\} dy \\ &= 12 \int_0^1 \frac{y^4}{y^6 + 1} \int_0^y \frac{1}{z} \int_0^z t^9 \frac{(-t^6)^n - 1}{t^6 + 1} dt dz dy \\ &\quad - (4 - \pi) \int_0^1 \frac{1}{z} \int_0^z t^9 \frac{t^{6n} - 1}{t^6 - 1} dt dz \Big\} . \end{aligned} \tag{4.11}$$

In general, the polynomials

$$x_1^a \pm 1$$

in Lemma 4.5.1 are either cyclotomic or decompose into products of cyclotomic polynomials in other cases. All factors divide $(x^a)^l - 1$, resp. $(-x^a)^l - 1$. We remark that (4.11) is not yet written in terms of a Mellin transform. This can be achieved using partial fractioning and integration by parts (for details we refer to the next sections):

$$\begin{aligned} S_{(3,2,2), (2,1,-1)}(n) &= \\ &= \frac{1}{6} (4 - \pi) \int_0^1 x^3 (x^{6n} - 1) [6 + f_1^0(x) - f_2^0(x) - 2f_3^0(x) \\ &\quad - f_3^1(x) - 2f_6^0(x) + f_6^1(x)] H_{(0,0)}(x) dx \end{aligned}$$

$$\begin{aligned}
 & -2 \int_0^1 x^3 [(-1)^n x^{6n} - 1] [3 - f_4^0(x) - 2f_{12}^0(x) + 2f_{12}^2(x)] H_{(0,0)}(x) dx \\
 & -\frac{4}{3} [H_{(0,0),(4,0)}(1) - H_{(0,0),(12,0)}(1) + 2H_{(0,0),(12,2)}(1)] \int_0^1 x^3 [(-1)^n x^{6n} - 1] \\
 & \quad \times [3 - f_4^0(x) - 2f_{12}^0(x) + 2f_{12}^2(x)] dx \\
 & +\frac{4}{3} \int_0^1 x^3 [(-1)^n x^{6n} - 1] [H_{(0,0),(4,0)}(x) - H_{(0,0),(12,0)}(x) + 2H_{(0,0),(12,2)}(x)] \\
 & \quad \times [3 - f_4^0(x) - 2f_{12}^0(x) + 2f_{12}^2(x)] dx .
 \end{aligned}$$

4.5.1 Mellin Transform of Cyclotomic Harmonic Polylogarithms

In this subsection we look at the Mellin transformation of cyclotomic polylogarithms. Therefore we extend the Mellin transform to cyclotomic harmonic polylogarithms (compare [8]).

Definition 4.5.2. *Let $h(x)$ be a cyclotomic harmonic polylogarithm, $n, k \in \mathbb{N}; p \in \mathbb{N}^*$ with $p < k$ and $a \in \mathbb{N}, a > 1$. We extend the Mellin-transform as follows:*

$$\begin{aligned}
 M(h(x), kn + p) &= \int_0^1 x^{kn+p} h(x) dx, \\
 M\left(\frac{h(x)}{\Phi_a(x)}, kn + p\right) &= \int_0^1 \frac{x^{kn+p} h(x)}{\Phi_a(x)} dx, \\
 M\left(\frac{h(x)}{x-1}, kn + p\right) &= \int_0^1 \frac{(x^{kn+p} - 1)h(x)}{x-1} dx.
 \end{aligned}$$

We cannot compute the Mellin transformation

$$M(H_{(a_1,b_1),(a_2,b_2),\dots}(x), kn + p)$$

of a cyclotomic polylogarithm $H_{(a_1,b_1),(a_2,b_2),\dots}(x)$ for general $n \in \mathbb{N}$. However we will always be able to calculate the Mellin transformation of

$$M(H_{(a_1,b_1),(a_2,b_2),\dots}(x), kn + p),$$

where $k \in \mathbb{N}$ is a multiple of the least common multiple of a_1, a_2, \dots and $p \in \mathbb{N}$. It will turn out that these Mellin transforms of cyclotomic polylogarithms can be expressed using cyclotomic harmonic sums. The following lemma will be needed several times in this subsection.

Lemma 4.5.3. *Let $a, k, v, n \in \mathbb{N}, p \in \mathbb{N}_0$ and $0 < x < 1$. If $va = k$, we have*

$$\frac{x^{kn+p} - x^p}{\Phi_a(x)} = - \sum_{j=0}^{a-1} f_j \sum_{t=0}^{v-1} \sum_{s=0}^{n-1} x^{at+ks+j+p},$$

and if $a = 2k$ we have

$$\frac{x^{kn+p} - (-1)^n x^p}{\Phi_a(x)} = - \sum_{j=0}^{k-1} f_j \sum_{s=0}^{n-1} (-1)^{n+s} x^{ks+j+p},$$

where f_j are the coefficients of the power series expansion of $f(x) := \frac{1}{\Phi_a(x)}$ about zero, i.e., $f(x) = \sum_{j=0}^{\infty} f_j x^j$ (see Lemma 4.4.1).

Proof. Due to Lemma 4.4.1 we get

$$\begin{aligned} \frac{x^{kn+p} - x^p}{\Phi_a(x)} &= (x^{kn+p} - x^p) \sum_{j=0}^{a-1} f_j \sum_{t=0}^{\infty} x^{at+j} \\ &= x^p \sum_{j=0}^{a-1} f_j \sum_{t=0}^{\infty} (x^{at+j+kn} - x^{at+j}) \\ &= x^p \sum_{j=0}^{a-1} f_j x^j \sum_{t=0}^{\infty} (x^{a(t+vn)} - x^{at}) \\ &= -x^p \sum_{j=0}^{a-1} f_j x^j \sum_{t=0}^{vn-1} x^{at} \\ &= - \sum_{j=0}^{a-1} f_j \sum_{t=0}^{v-1} \sum_{s=0}^{n-1} x^{at+ks+j+p} \end{aligned}$$

and if $a = 2k$ we get

$$\begin{aligned} \frac{x^{kn+p} - (-1)^n x^p}{\Phi_a(x)} &= \sum_{j=0}^{\frac{a}{2}-1} f_j \sum_{s=0}^{\infty} x^{\frac{a}{2}i+j} (-1)^i (x^{kn+p} - (-1)^n x^p) \\ &= -x^p \sum_{j=0}^{k-1} f_j x^j \sum_{s=0}^{\infty} (-1)^i (x^{k(n+s)} - (-1)^n x^{ks}) \\ &= - \sum_{j=0}^{k-1} f_j \sum_{s=0}^{n-1} (-1)^{n+s} x^{ks+j+p}. \end{aligned}$$

□

Now we can look at the depth one cases.

Lemma 4.5.4. *Let $k, a, n \in \mathbb{N}, b, p \in \mathbb{N}_0$ with $a > 1, a|k$. We have*

$$\begin{aligned} M(\mathbb{H}_{(0,0)}(x), k, n+p) &= -\frac{1}{(kn+p+1)^2}, \\ M(\mathbb{H}_{(1,0)}(x), k, n+p) &= -\frac{S_1(kn+p+1)}{kn+p+1} \end{aligned}$$

$$\begin{aligned}
&= -\frac{1}{kn+p+1} \left(S_1(p+1) + \sum_{i=0}^{n-1} \sum_{t=0}^{k-1} \frac{1}{ki+t+p+2} \right), \\
M(H_{(a,b)}(x), k n + p) &= \frac{1}{kn+p+1} \left(H_{(a,b)}(1) - H_{(a,p+b+1)}(1) \right. \\
&\quad \left. + \sum_{j=0}^{a-1} f_j \sum_{t=0}^{\frac{k}{a}-1} \sum_{s=0}^{n-1} \frac{1}{at+ks+j+p+b+2} \right)
\end{aligned}$$

where f_j are the coefficients of the power series expansion of $f(x) := \frac{1}{\Phi_a(x)}$ about zero, i.e., $f(x) = \sum_{j=0}^{\infty} f_j x^j$ (see Lemma 4.4.1).

Proof. We give a proof of the first and third identity:

$$\begin{aligned}
M(H_{(0,0)}(x), k n + p) &= \int_0^1 x^{kn+p} H_{(0,0)}(x) dx = - \int_0^1 \frac{x^{kn+p+1}}{kn+p+1} \frac{1}{x} dx \\
&= -\frac{1}{(kn+p+1)^2}.
\end{aligned}$$

Using integration by parts and Lemma 4.5.3 we get

$$\begin{aligned}
M(H_{(a,b)}(x), k n + p) &= \int_0^1 x^{kn+p} H_{(a,b)}(x) dx = \\
&= \frac{1}{kn+p+1} H_{(a,b)}(1) - \int_0^1 \frac{x^{kn+p+b+1}}{(kn+p+1)\Phi_a(x)} dx \\
&= \frac{1}{kn+p+1} \left(H_{(a,b)}(1) - H_{(a,p+b+1)}(1) \right. \\
&\quad \left. - \int_0^1 \frac{x^{kn+p+b+1} - x^{p+b+1}}{\Phi_a(x)} dx \right) \\
&= \frac{1}{kn+p+1} \left(H_{(a,b)}(1) - H_{(a,p+b+1)}(1) \right. \\
&\quad \left. + \sum_{j=0}^{a-1} f_j \sum_{t=0}^{\frac{k}{a}-1} \sum_{s=0}^{n-1} \int_0^1 x^{at+ks+j+p+b+1} dx \right) \\
&= \frac{1}{kn+p+1} \left(H_{(a,b)}(1) - H_{(a,p+b+1)}(1) \right. \\
&\quad \left. + \sum_{j=0}^{a-1} f_j \sum_{t=0}^{\frac{k}{a}-1} \sum_{s=0}^{n-1} \frac{1}{at+ks+j+p+b+2} \right).
\end{aligned}$$

□

For higher weights we need the following lemma.

Lemma 4.5.5. *Let $k, a \in \mathbb{N}, b, p \in \mathbb{N}_0$ with $a > 1, a|k$ and $b < \varphi(a)$. We have*

$$\begin{aligned} M(H_{(0,0),m}(x), k n + p) &= \frac{1}{k n + p + 1} \left(H_{(0,0),m}(1) - M(H_m(x), k n + p) \right) \\ M(H_{(1,0),m}(x), k n + p) &= \frac{-1}{k n + p + 1} \left(\int_0^1 \frac{x^{p+1} - 1}{x - 1} H_m(x) dx \right. \\ &\quad \left. + \sum_{i=0}^{n-1} \sum_{l=0}^{k-1} M(H_m(x), k i + l + p + 1) \right) \\ M(H_{(a,b),m}(x), k n + p) &= \frac{1}{k n + p + 1} \left(H_{(a,b),m}(1) - H_{(a,p+b+1),m}(1) \right. \\ &\quad \left. + \sum_{i=0}^{n-1} \sum_{j=0}^{a-1} f_j \sum_{l=0}^{\frac{k}{a}-1} M(H_m(x), k i + j + b + p + 1 + a l) \right), \end{aligned}$$

where f_j are the coefficients of the power series expansion of $f(x) := \frac{1}{\Phi_a(x)}$ about zero i.e., $f(x) = \sum_{j=0}^{\infty} f_j x^j$ (see Lemma 4.4.1).

Proof. We just give a proof of the third identity using integration by parts and Lemma 4.5.3:

$$\begin{aligned} M(H_{(a,b),m}(x), k n + p) &= \frac{1}{k n + p + 1} \left(H_{(a,b),m}(1) - \int_0^1 \frac{x^{kn+p+b+1}}{\Phi_a(x)} H_m(x) dx \right) \\ &= \frac{1}{k n + p + 1} \left(H_{(a,b),m}(1) - \int_0^1 \frac{x^{p+b+1}}{\Phi_a(x)} H_m(x) dx \right. \\ &\quad \left. - \int_0^1 \frac{x^{kn+p+b+1} - x^{p+b+1}}{\Phi_a(x)} H_m(x) dx \right) \\ &= \frac{1}{k n + p + 1} \left(H_{(a,b),m}(1) - H_{(a,p+b+1),m}(1) \right. \\ &\quad \left. + \sum_{j=0}^{a-1} f_j \sum_{t=0}^{\frac{k}{a}-1} \sum_{s=0}^{n-1} \frac{1}{at + ks + j + p + b + 2} \right). \end{aligned}$$

□

We can even handle slightly more cases as mentioned in the beginning of this subsection:

Lemma 4.5.6. *Let $k, n \in \mathbb{N}, b, p \in \mathbb{N}_0$. We have*

$$M(H_{(2k,b)}(x), k n + p) = \frac{1}{k n + p + 1} \left(H_{(2k,b)}(1) - (-1)^n H_{(2k,p+b+1)}(1) \right)$$

$$\begin{aligned}
& +(-1)^n \sum_{j=0}^{k-1} f_j \sum_{t=0}^{n-1} (-1)^t \frac{1}{kt+j+p+b+2} \Big) \\
M(\mathbf{H}_{(2k,b),m}(x), kn+p) &= \frac{1}{kn+p+1} \left(\mathbf{H}_{(2k,b),m}(1) - (-1)^n \mathbf{H}_{(2k,p+b+1),m}(1) \right. \\
& \left. +(-1)^n \sum_{j=0}^{k-1} f_j \sum_{t=0}^{n-1} (-1)^t M(\mathbf{H}_m(x), kt+j+p+b+1) \right)
\end{aligned}$$

where f_j are the coefficients of the power series expansion of $f(x) := \frac{1}{\Phi_{2k}(x)}$ about zero, i.e., $f(x) = \sum_{j=0}^{\infty} f_j x^j$ (see Lemma 4.4.1).

Proof. The proof follows using integration by parts and Lemma 4.5.3. \square

Combining the Lemmas 4.5.4, 4.5.5 and 4.5.6 we can compute the desired Mellin transformations of cyclotomic polylogarithms up to arbitrary weight. Using the following lemma we can as well compute the Mellin transformation of cyclotomic polylogarithms weighted by cyclotomic polynomials.

Lemma 4.5.7. For $a, k, n \in \mathbb{N}, p \in \mathbb{N}_0$ we have

$$\begin{aligned}
M\left(\frac{\mathbf{H}_m(x)}{\Phi_1(x)}, kn+p\right) &= -(kn+p) M(\mathbf{H}_{(1,0),m}(x), kn+p) \\
M\left(\frac{\mathbf{H}_m(x)}{\Phi_a(x)}, kn+p\right) &= \mathbf{H}_{(a,0),m}(1) - (kn+p) M(\mathbf{H}_{(a,0),m}(x), kn+p-1).
\end{aligned}$$

Proof. The proof follows immediately by integration by parts. \square

Example 4.5.8.

$$\begin{aligned}
M(\mathbf{H}_{(4,1),(2,0)}(x), 4n+1) &= n \left(-\frac{\mathbf{S}_{(1,0,2)}(\infty)}{32n+16} + \frac{\mathbf{S}_{(2,-1,1)}(\infty)}{16n+8} - \frac{\mathbf{S}_{(2,1,1)}(\infty)}{16n+8} - \frac{\mathbf{S}_{(2,1,2)}(\infty)}{8n+4} \right. \\
& - \frac{\mathbf{S}_{(4,-1,1)}(\infty)}{8n+4} - \frac{7n\mathbf{S}_{(4,1,1)}(\infty)}{12n+6} + \frac{\mathbf{S}_{(4,1,2)}(\infty)}{2n+1} + \frac{17n\mathbf{S}_{(4,3,1)}(\infty)}{24n+12} + \frac{\mathbf{S}_{(4,3,2)}(\infty)}{2n+1} \\
& + \frac{\mathbf{S}_{(1,0,1),(1,0,1)}(\infty)}{32n+16} - \frac{\mathbf{S}_{(1,0,1),(2,1,1)}(\infty)}{16n+8} - \frac{\mathbf{S}_{(2,1,1),(1,0,1)}(\infty)}{16n+8} + \frac{\mathbf{S}_{(2,1,1),(2,1,1)}(\infty)}{8n+4} \\
& - \frac{\mathbf{S}_{(4,1,1),(4,1,1)}(\infty)}{2n+1} + \frac{\mathbf{S}_{(4,1,1),(4,3,1)}(\infty)}{2n+1} + \frac{\mathbf{S}_{(4,3,1),(4,1,1)}(\infty)}{2n+1} - \frac{\mathbf{S}_{(4,3,1),(4,3,1)}(\infty)}{2n+1} \\
& - \frac{\mathbf{S}_{(2,1,1)}(n)}{24n+12} + \frac{\mathbf{S}_{(4,1,1)}(n)}{4n+2} - \frac{\mathbf{S}_{(4,3,1)}(n)}{6n+3} - \frac{\mathbf{S}_{(1,0,1),(2,1,1)}(n)}{32n+16} + \frac{\mathbf{S}_{(1,0,1),(4,1,1)}(n)}{16n+8} \\
& + \frac{\mathbf{S}_{(1,0,1),(4,3,1)}(n)}{16n+8} + \frac{\mathbf{S}_{(2,1,1),(1,0,1)}(n)}{32n+16} + \frac{\mathbf{S}_{(2,1,1),(2,1,1)}(n)}{16n+8} - \frac{\mathbf{S}_{(2,1,1),(4,1,1)}(n)}{8n+4} \\
& \left. - \frac{\mathbf{S}_{(2,1,1),(4,3,1)}(n)}{8n+4} - \frac{\mathbf{S}_{1,1}(n)}{64n+32} + \frac{1}{12n+6} \right).
\end{aligned}$$

4.5.2 Differentiation of Cyclotomic Harmonic Sums

We already considered the differentiation of harmonic sums with respect to the upper summation limit. In a similar way, we can differentiate cyclotomic harmonic sums since they can be represented as linear combinations of Mellin transforms of cyclotomic harmonic polylogarithms, as has been illustrated in Section 4.5.1. Based on this representation, the differentiation of these sums can be expressed in the following format:

$$\frac{\partial^m}{\partial n^m} S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n) = \sum_{i=1}^s e_i \int_0^1 x^{ln} l^m H_0(x)^m (f_{\alpha_i}^{\beta_i}(x))^{u_i} H_{g_i}(x) dx, \quad (4.12)$$

where $m, \alpha_i, \beta_i, u_i \in \mathbb{N}$ and $l, e_i \in \mathbb{Z}$. The product $H_0(x)^m H_{g_i}(x)$ may be transformed into a linear combination of cyclotomic harmonic polylogarithms following Section 4.2. Finally, using the inverse Mellin transform, the derivative (4.12) of a cyclotomic harmonic sum w.r.t. n is given as a polynomial expression in terms of cyclotomic harmonic sums and cyclotomic harmonic polylogarithms at $x = 1$. Together with the previous sections, the derivative (4.12) can be expressed as a polynomial expression with rational coefficients in terms of cyclotomic harmonic sums and their values at $n \rightarrow \infty$.

Example 4.5.9. *We start with the integral representation:*

$$\begin{aligned} S_{(2,1,2)}(n) &= -\frac{1}{2} \int_0^1 \frac{(x^{2n} - 1)H_{(0,0)}(x)}{x - 1} dx + \frac{1}{2} \int_0^1 \frac{x^{2n}H_{(0,0)}(x)}{x + 1} dx \\ &\quad - \int_0^1 x^{2n}H_{(0,0)}(x) dx + \frac{1}{4}S_2(\infty) - 1. \end{aligned}$$

Differentiation with respect to n leads to

$$\begin{aligned} \frac{\partial}{\partial n} S_{(2,1,2)}(n) &= -\frac{1}{2} \int_0^1 \frac{2x^{2n}H_{(0,0)}(x) H_{(0,0)}(x)}{x - 1} dx + \frac{1}{2} \int_0^1 \frac{2x^{2n}H_{(0,0)}(x) H_{(0,0)}(x)}{x + 1} dx \\ &\quad - \int_0^1 2x^{2n}H_{(0,0)}(x) H_{(0,0)}(x) dx + \frac{1}{4}S_2(\infty) - 1. \end{aligned}$$

After expanding the products of the cyclotomic harmonic polylogarithms and performing the Mellin transforms we end up with

$$\frac{\partial}{\partial n} S_{(2,1,2)}(n) = -4S_{(2,1,3)}(n) + \frac{7}{4}S_{(1,0,3)}(\infty) + 2S_{(2,1,3)}(\infty) - 2.$$

4.6 Relations between Cyclotomic Harmonic Sums

4.6.1 Algebraic Relations

We already mentioned in Section 4.1 that cyclotomic harmonic sums form a quasi shuffle algebra. We will now take a closer look at the quasi shuffle algebra property. Therefore we will define the following set:

$$\mathcal{C}(n) = \{q(s_1, \dots, s_r) \mid r \in \mathbb{N}; s_i \text{ a cyclotomic harmonic sum at } n; q \in \mathbb{R}[x_1, \dots, x_r]\}.$$

From Section 4.1 we know that we can always expand a product of cyclotomic harmonic sums into a linear combination of cyclotomic harmonic sums. For two cyclotomic harmonic sums s_1 and s_2 let $L(s_1, s_2)$ denote the expansion of $s_1 s_2$ into a linear combination of cyclotomic harmonic sums. Now we can define the ideal \mathcal{I} on $\mathcal{C}(n)$:

$$\mathcal{I}(n) = \{s_1 s_2 - L(s_1, s_2) \mid s_i \text{ a cyclotomic harmonic sum at } n\}.$$

By construction $\mathcal{C}(n)/\mathcal{I}$ is a quasi shuffle algebra with alphabet

$$A_C := \{(a, b, \pm c) \mid a, c \in \mathbb{N}; b \in \mathbb{N}_0, b < a\}.$$

We define the degree of a letter $(a, b, \pm c) \in A_C$ as $|(a, b, \pm c)| := c$. For $a_1, a_2 \in \mathbb{N}; c_1, c_2 \in \mathbb{N}; b_1, b_2 \in \mathbb{N}_0, b_i < a_i$ and $c_3 \in \mathbb{Z}^*$ we order the letters in A_C by

$$\begin{aligned} (a_1, b_1, \pm c_1) &< (a_2, b_2, \pm c_2) && \text{if } c_1 < c_2 \\ (a_1, b_1, -c_1) &< (a_2, b_2, c_1) \\ (a_1, b_1, c_3) &< (a_2, b_2, c_3) && \text{if } a_1 < a_2 \\ (a_1, b_1, c_3) &< (a_1, b_2, c_3) && \text{if } b_1 < b_2 \end{aligned}$$

and extend this order lexicographically to words. Using this order it can be shown analogously to [1, 49] that the quasi shuffle algebra $\mathcal{C}(n)/\mathcal{I}$ is the free polynomial algebras on the *Lyndon* words with alphabet A_C . Hence the number of algebraic independent sums in $\mathcal{S}(n)/\mathcal{I}$ which we also call basis sums is the number of *Lyndon* words. If we consider for example an index set with 4 letters, say

$$\{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$$

and we look for the number of basis sums where the index α_i appears n_i times, we can use the second Witt formula (2.12):

$$\frac{1}{n} \sum_{d|n} \mu(d) \frac{\left(\frac{n}{d}\right)!}{\left(\frac{n_1}{d}\right)! \cdots \left(\frac{n_4}{d}\right)!}, \quad n = \sum_{i=1}^4 n_i.$$

For a specific alphabet we can count as well the number of basis sums at a certain weight. For the alphabet

$$\left\{ \frac{1}{k}, \frac{(-1)^k}{k}, \frac{1}{2k+1}, \frac{(-1)^k}{2k+1} \right\}$$

the number of basis sums at $w \geq 1$ is given by

$$N_A(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 5^d.$$

This is due to the fact that the cyclotomic harmonic sums of weight w with alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(2k+1)\}$ can be viewed as the words of length w out of an alphabet with the five letters $\{0, (1, 0, 1), (1, 0, -1), (2, 1, 1), (2, 1, -1)\}$ and that the number of *Lyndon* words of length n over an alphabet of length q is given by the first Witt formula (2.13).

We can use an analogous method of the method presented in [1, 19] for harmonic sums to find the basis sums together with the relations for the dependent sums; compare Section 2.6.1. Here we want to give an example for cyclotomic harmonic sums at weight $w = 2$.

Example 4.6.1. *We consider the alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(2k+1)\}$. At weight $w = 2$ we have for instance the 10 basis sums:*

$$\begin{aligned} & S_{(1,0,-2)}(n), S_{(1,0,2)}(n), S_{(2,1,-2)}(n), S_{(2,1,2)}(n), S_{(1,0,-1),(1,0,1)}(n), S_{(1,0,-1),(2,1,1)}(n), \\ & S_{(1,0,-1),(2,1,-1)}(n), S_{(1,0,1),(2,1,1)}(n), S_{(2,1,-1),(1,0,1)}(n), S_{(2,1,-1),(2,1,1)}(n) \end{aligned}$$

together with the relations for the remaining sums:

$$\begin{aligned} S_{(2,1,1),(2,1,1)}(n) &= \frac{1}{2} S_{(2,1,1)}(n)^2 + \frac{1}{2} S_{(2,1,2)}(n) \\ S_{(2,1,1),(1,0,1)}(n) &= S_{(2,1,1)}(n) S_{(1,0,1)}(n) + S_{(1,0,1)}(n) - 2S_{(2,1,1)}(n) \\ &\quad - S_{(1,0,1),(2,1,1)}(n) \\ S_{(1,0,1),(1,0,1)}(n) &= \frac{1}{2} S_{(1,0,1)}(n)^2 + \frac{1}{2} S_{(1,0,2)}(n) \\ S_{(2,1,1),(2,1,-1)}(n) &= S_{(2,1,-2)}(n) + S_{(2,1,-1)}(n) S_{(2,1,1)}(n) - S_{(2,1,-1),(2,1,1)}(n) \\ S_{(2,1,1),(1,0,-1)}(n) &= S_{(2,1,1)}(n) S_{(1,0,-1)}(n) + S_{(1,0,-1)}(n) - 2S_{(2,1,-1)}(n) \\ &\quad - S_{(1,0,-1),(2,1,1)}(n) \\ S_{(1,0,1),(2,1,-1)}(n) &= S_{(1,0,-1)}(n) + S_{(1,0,1)}(n) S_{(2,1,-1)}(n) - 2S_{(2,1,-1)}(n) \end{aligned}$$

$$\begin{aligned}
& -S_{(2,1,-1),(1,0,1)}(n) \\
S_{(1,0,1),(1,0,-1)}(n) &= S_{(1,0,-2)}(n) + S_{(1,0,-1)}(n) S_{(1,0,1)}(n) - S_{(1,0,-1),(1,0,1)}(n) \\
S_{(2,1,-1),(2,1,-1)}(n) &= \frac{1}{2}S_{(2,1,-1)}(n)^2 + \frac{1}{2}S_{(2,1,2)}(n) \\
S_{(2,1,-1),(1,0,-1)}(n) &= S_{(1,0,1)}(n) + S_{(1,0,-1)}(n) S_{(2,1,-1)}(n) - 2S_{(2,1,1)}(n) \\
& -S_{(1,0,-1),(2,1,-1)}(n) \\
S_{(1,0,-1),(1,0,-1)}(n) &= \frac{1}{2}S_{(1,0,-1)}(n)^2 + \frac{1}{2}S_{(1,0,2)}(n).
\end{aligned}$$

Hence we can use the 10 basis sums together with sums of lower weight to express all sums of weight $w = 2$. Note that the sums of lower weight in this example are not yet reduced to a basis.

4.6.2 Differential Relations

In Section 4.5.2 we described the differentiation of cyclotomic harmonic sums with respect to the upper summation limit. The differentiation leads to new relation. For instance we find

$$\frac{\partial}{\partial n} S_{(2,1,2)}(n) = -4S_{(2,1,3)}(n) + \frac{7}{4}S_{(1,0,3)}(\infty) + 2S_{(2,1,3)}(\infty) - 2.$$

Continuing the Example 4.6.1 we get

Example 4.6.2 (Example 4.6.1 continued). *From differentiation we get the additional relations*

$$\begin{aligned}
S_{(1,0,-2)}(n) &= -\frac{\partial}{\partial n} S_{(1,0,-1)}(n) + \frac{1}{4}S_{(1,0,2)}(\infty) - S_{(2,1,2)}(\infty) - 1 \\
S_{(1,0,2)}(n) &= S_{(1,0,2)}(\infty) - \frac{\partial}{\partial n} S_{(1,0,1)}(n) \\
S_{(2,1,-2)}(n) &= -\frac{1}{2}\frac{\partial}{\partial n} S_{(2,1,-1)}(n) + S_{(4,1,2)}(\infty) - S_{(4,3,2)}(\infty) - \frac{1}{9} \\
S_{(2,1,2)}(n) &= -\frac{1}{2}\frac{\partial}{\partial n} S_{(2,1,1)}(n) + \frac{3}{8}S_{(1,0,2)}(\infty) + \frac{1}{2}S_{(2,1,2)}(\infty) - \frac{1}{2}.
\end{aligned}$$

Hence we could reduce the number of basis sums at weight $w = 2$ to 6 by introducing differentiation. The basis sums are:

$$\begin{aligned}
& S_{(1,0,-1),(1,0,1)}(n), S_{(1,0,-1),(2,1,-1)}(n), S_{(1,0,-1),(2,1,1)}(n), S_{(1,0,1),(2,1,1)}(n), \\
& S_{(2,1,-1),(1,0,1)}(n), S_{(2,1,-1),(2,1,1)}(n).
\end{aligned}$$

Note that we collect the derivatives in

$$S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)^{(D)} = \left\{ \frac{\partial^N}{\partial n^N} S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n); N \in \mathbb{N} \right\}.$$

and identify an appearance of a derivative of a cyclotomic harmonic sum with the cyclotomic harmonic sum itself. For a motivation see also Section 2.6.2.

4.6.3 Multiple Argument Relations

For harmonic sums we found duplication relations. For cyclotomic harmonic sums we can even look at upper summation limits of the form kn with $k \in \mathbb{N}$, as the synchronization of Section 4.1 suggests: We can always synchronize a cyclotomic harmonic sum with upper summation limit kn with $k \in \mathbb{N}$ to sums with upper summation limit n . This leads again to new relations for example we have

$$S_{(2,1,2)}(3n) = \frac{1}{9}S_{(2,1,2)}(n) + S_{(6,1,2)}(n) + S_{(6,5,2)}(n) - \frac{1}{(6n+3)^2} - \frac{1}{(6n+5)^2} + \frac{34}{225}.$$

In the following subsection we consider duplication relations in detail.

Duplication Relations

Unlike for harmonic sums, where we had just one type of duplication relations, there are two different types of duplication relations for cyclotomic harmonic sums. We summarize them in the following theorems; compare [8].

Theorem 4.6.3. *We have the following relation:*

$$\sum S_{(a_m, b_m, \pm c_m), (a_{m-1}, b_{m-1}, \pm c_{m-1}), \dots, (a_1, b_1, \pm c_1)}(2n) = 2^m S_{(2a_m, b_m, c_m), \dots, (2a_1, b_1, c_1)}(n)$$

where we sum on the left hand side over the 2^m possible combinations concerning \pm .

Proof. We proceed by induction on m . Let $m = 1$:

$$\begin{aligned} S_{(a_1, b_1, c_1)}(2n) + S_{(a_1, b_1, -c_1)}(2n) &= \sum_{i=1}^{2n} \frac{1}{(a_1 i + b_1)^{c_1}} + \sum_{i=1}^{2n} \frac{(-1)^i}{(a_1 i + b_1)^{c_1}} \\ &= \sum_{i=1}^n \left(\frac{1}{(a_1 2i + b_1)^{c_1}} + \frac{1}{(a_1 (2i - 1) + b_1)^{c_1}} \right) \\ &\quad + \sum_{i=1}^n \left(\frac{1}{(a_1 2i + b_1)^{c_1}} - \frac{1}{(a_1 (2i - 1) + b_1)^{c_1}} \right) \end{aligned}$$

$$= 2 \sum_{i=1}^n \frac{1}{(2a_1 i + b_1)^{c_1}} = 2S_{(2a_1, b_1, c_1)}(n).$$

In the following we use the abbreviation:

$$A(n) := \sum S_{(a_m, b_m, \pm c_m), \dots, (a_1, b_1, \pm c_1)}(n).$$

Now we assume that the theorem holds for m :

$$\begin{aligned} & \sum S_{(a_{m+1}, b_{m+1}, \pm c_{m+1}), \dots, (a_1, b_1, \pm c_1)}(2n) \\ &= \sum_{i=1}^{2n} \frac{1}{(a_{m+1}i + b_{m+1})^{c_{m+1}}} \sum S_{(a_m, b_m, \pm c_m), \dots, (a_1, b_1, \pm c_1)}(i) \\ &+ \sum_{i=1}^{2n} \frac{(-1)^i}{(a_{m+1}i + b_{m+1})^{c_{m+1}}} \sum S_{(a_m, b_m, \pm c_m), \dots, (a_1, b_1, \pm c_1)}(i) \\ &= \sum_{i=1}^{2n} \frac{A(i)}{(a_{m+1}i + b_{m+1})^{c_{m+1}}} + \sum_{i=1}^{2n} \frac{(-1)^i A(i)}{(a_{m+1}i + b_{m+1})^{c_{m+1}}} \\ &= \sum_{i=1}^n \left(\frac{A(2i)}{(2a_{m+1}i + b_{m+1})^{c_{m+1}}} + \frac{A(2i-1)}{((2i-1)a_{m+1} + b_{m+1})^{c_{m+1}}} \right) \\ &+ \sum_{i=1}^n \left(\frac{(-1)^{2i} A(2i)}{(2a_{m+1}i + b_{m+1})^{c_{m+1}}} + \frac{(-1)^{2i-1} A(2i-1)}{((2i-1)a_{m+1} + b_{m+1})^{c_{m+1}}} \right) \\ &= 2 \sum_{i=1}^n \frac{A(2i)}{(2a_{m+1}i + b_{m+1})^{c_{m+1}}} \\ &= 2 \sum_{i=1}^n \frac{1}{(2a_{m+1}i + b_{m+1})^{c_{m+1}}} 2^m S_{(2a_m, b_m, c_m), \dots, (2a_1, b_1, c_1)}(i) \\ &= 2^{m+1} S_{(2a_{m+1}, b_{m+1}, c_{m+1}), \dots, (2a_1, b_1, c_1)}(n). \end{aligned}$$

□

Similar to the previous relation we have the following theorem.

Theorem 4.6.4. *Let $d_i \in \{-1, 1\}$; we have the following relation:*

$$\begin{aligned} & \sum d_m d_{m-1} \cdots d_1 S_{(a_m, b_m, d_m c_m), (a_{m-1}, b_{m-1}, d_{m-1} c_{m-1}), \dots, (a_1, b_1, d_1 c_1)}(2n) \\ &= 2^m S_{(2a_m, b_m - a_m, c_m), \dots, (2a_1, b_1 - a_1, c_1)}(n), \end{aligned}$$

where we sum on the left hand side over the 2^m possible combinations concerning d_i .

Proof. We proceed by induction on m . Let $m = 1$:

$$\begin{aligned}
S_{(a_1, b_1, c_1)}(2n) - S_{(a_1, b_1, -c_1)}(2n) &= \sum_{i=1}^{2n} \frac{1}{(a_1 i + b_1)^{c_1}} + \sum_{i=1}^{2n} \frac{(-1)^i}{(a_1 i + b_1)^{c_1}} \\
&= \sum_{i=1}^n \left(\frac{1}{(a_1 2i + b_1)^{c_1}} + \frac{1}{(a_1 (2i - 1) + b_1)^{c_1}} \right) \\
&\quad - \sum_{i=1}^n \left(\frac{1}{(a_1 2i + b_1)^{c_1}} - \frac{1}{(a_1 (2i - 1) + b_1)^{c_1}} \right) \\
&= 2 \sum_{i=1}^n \frac{1}{((2i - 1)a_1 + b_1)^{c_1}} = 2S_{(2a_1, b_1 - a_1, c_1)}(n).
\end{aligned}$$

In the following we use the abbreviation:

$$A(n) := \sum d_m \cdots d_1 S_{(a_m, b_m, d_m c_m), \dots, (a_1, b_1, d_1 c_1)}(n).$$

Note that

$$\begin{aligned}
A(2n - 1) &= A(2n) - \sum d_m \cdots d_1 \frac{d_m^{2n} S_{(a_{m-1}, b_{m-1}, d_{m-1} c_{m-1}), \dots, (a_1, b_1, d_1 c_1)}(n)}{(a_m i + b_m)^{c_m}} \\
&= A(2n) - \sum d_{m-1} \cdots d_1 \frac{S_{(a_{m-1}, b_{m-1}, d_{m-1} c_{m-1}), \dots, (a_1, b_1, d_1 c_1)}(n)}{(a_m i + b_m)^{c_m}} \\
&\quad + \sum d_{m-1} \cdots d_1 \frac{S_{(a_{m-1}, b_{m-1}, d_{m-1} c_{m-1}), \dots, (a_1, b_1, d_1 c_1)}(n)}{(a_m i + b_m)^{c_m}} = A(2n).
\end{aligned}$$

Now we assume that the theorem holds for m . Then we conclude that

$$\begin{aligned}
&\sum d_{m+1} \cdots d_1 S_{(a_{m+1}, b_{m+1}, d_{m+1} c_{m+1}), \dots, (a_1, b_1, d_1 c_1)}(2n) \\
&= \sum_{i=1}^{2n} \frac{1}{(a_{m+1} i + b_{m+1})^{c_{m+1}}} \sum d_m \cdots d_1 S_{(a_m, b_m, d_m c_m), \dots, (a_1, b_1, d_1 c_1)}(i) \\
&\quad - \sum_{i=1}^{2n} \frac{(-1)^i}{(a_{m+1} i + b_{m+1})^{c_{m+1}}} \sum d_m \cdots d_1 S_{(a_m, b_m, d_m c_m), \dots, (a_1, b_1, d_1 c_1)}(i) \\
&= \sum_{i=1}^{2n} \frac{A(i)}{(a_{m+1} i + b_{m+1})^{c_{m+1}}} - \sum_{i=1}^{2n} \frac{(-1)^i A(i)}{(a_{m+1} i + b_{m+1})^{c_{m+1}}} \\
&= \sum_{i=1}^n \left(\frac{A(2i)}{((2a_{m+1} i + b_{m+1})^{c_{m+1}})} + \frac{A(2i - 1)}{((2i - 1)a_{m+1} + b_{m+1})^{c_{m+1}}} \right) \\
&\quad - \sum_{i=1}^n \left(\frac{(-1)^{2i} A(2i)}{((2a_{m+1} i + b_{m+1})^{c_{m+1}})} + \frac{(-1)^{2i-1} A(2i - 1)}{((2i - 1)a_{m+1} + b_{m+1})^{c_{m+1}}} \right) \\
&= 2 \sum_{i=1}^n \frac{A(2i - 1)}{((2i - 1)a_{m+1} + b_{m+1})^{c_{m+1}}} = 2 \sum_{i=1}^n \frac{A(2i)}{((2i - 1)a_{m+1} + b_{m+1})^{c_{m+1}}} \\
&= 2 \sum_{i=1}^n \frac{1}{(2a_{m+1} i + b_{m+1} - a_{m+1})^{c_{m+1}}} 2^m S_{(2a_m, b_m - a_m, c_m), \dots, (2a_1, b_1 - a_1, c_1)}(n)
\end{aligned}$$

$$= 2^{m+1} S_{(2a_{m+1}, b_{m+1}-a_{m+1}, c_{m+1}), \dots, (2a_1, b_1-a_1, c_1)}(n).$$

□

Examples for these relations are

$$\begin{aligned} S_{(2,1,2)}(2n) &= 2S_{(4,1,2)}(n) - S_{(2,1,-2)}(2n) \\ S_{(2,1,2)}(2n) &= S_{(2,1,-2)}(2n) + 2S_{(4,3,2)}(n) - \frac{2}{(4n+3)^2} + \frac{2}{9}. \end{aligned}$$

Example 4.6.5 (Example 2.6.4 continued). *At weight $w = 2$ with letters $\{(\pm 1)^k/k, (\pm 1)^k/(2k + 1)\}$ the duplication relations and the multiple integer relations do not lead to a further reduction of the basis.*

Remark 4.6.6. *As for differentiation, when we are counting basis elements, we identify an appearance of a cyclotomic harmonic sum $S_a(kn)$ with the cyclotomic harmonic sum $S_a(n)$.*

4.6.4 Number of Basis Elements for Specific Alphabets

In this section we look at the different number of basis sums that we get using combinations of several of the relations discussed in the previous sections. First we restrict to the alphabet

$$\left\{ \frac{(\pm 1)^k}{k}, \frac{(\pm 1)^k}{(2k + 1)} \right\}$$

and look for the number of basis sums. We conjecture the following formulas which we checked up to weight 5 and we summarize the concrete numbers in Table 4.2 up to weight 5:

$$\begin{aligned} N_S(w) &= 4 \cdot 5^{w-1} \\ N_A(w) &\stackrel{w \geq 1}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 5^d \\ N_D(w) &= N_S(w) - N_S(w-1) \stackrel{w \geq 1}{=} 16 \cdot 5^{w-2} \\ N_{H_1}(w) = N_{H_2}(w) = N_M(w) &= N_S(w) - 2^{w-1} = 4 \cdot 5^{w-1} - 2^{w-1} \\ N_{H_1H_2}(w) &= N_S(w) - (2 \cdot 2^{w-1} - 1) = 4 \cdot 5^{w-1} - (2 \cdot 2^{w-1} - 1) \\ N_{H_1M}(w) = N_{H_2M}(w) &= N_S(w) - 2 \cdot 2^{w-1} = 4 \cdot 5^{w-1} - 2 \cdot 2^{w-1} \\ N_{H_1H_2M}(w) &= N_S(w) - (3 \cdot 2^{w-1} - 1) = 4 \cdot 5^{w-1} - (3 \cdot 2^{w-1} - 1) \\ N_{AD}(w) &= N_A(w) - N_A(w-1) \\ &\stackrel{w \geq 2}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 5^d - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) 5^d \end{aligned}$$

w	N_S	N_A	N_D	N_{H_1}	$N_{H_1H_2}$	N_{H_1M}	$N_{H_1H_2M}$	N_{AD}	$N_{AH_1H_2M}$	$N_{DH_1H_2M}$	$N_{ADH_1H_2M}$
1	4	4	4	3	3	2	2	4	2	2	2
2	20	10	16	18	17	16	15	6	8	13	6
3	100	40	80	96	93	92	89	30	35	74	27
4	500	150	400	492	485	484	477	110	142	388	107
5	2500	624	2000	2484	2469	2468	2453	474	607	1976	465

Table 4.2: Number of basis cyclotomic harmonic sums concerning the alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(2k + 1)\}$ and different relations up to weight 5.

$$\begin{aligned}
 N_{AH_1H_2M}(w) &\stackrel{w \geq 1}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 5^d - \left(3 \cdot \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 2^d - 1\right) \\
 N_{DH_1H_2M}(w) &= N_{H_1H_2M}(w) - N_{H_1H_2M}(w - 1) \\
 &\stackrel{w \geq 1}{=} 16 \cdot 5^{w-2} - 3 \cdot 2^{w-2} \\
 N_{ADH_1H_2M}(w) &= N_{AH_1H_2M}(w) - N_{AH_1H_2M}(w - 1) \\
 &\stackrel{w \geq 2}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) (5^d - 3 \cdot 2^d) \\
 &\quad - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) (5^d - 3 \cdot 2^d)
 \end{aligned}$$

Here N_S counts the number of cyclotomic harmonic sums concerning the alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(2k + 1)\}$, while $N_A, N_D, N_{H_1}, N_{H_2}$ and N_M count the number of basis sums using algebraic, differential, the first duplication, the second duplication and the multiple integer relations respectively. All the other quantities count the number of basis sums with respect to combinations of different types of relations. For instance $N_{ADH_1H_2M}$ gives the number of basis cyclotomic harmonic sum using all previously mentioned relations.

Now we consider the number of basic cyclotomic harmonic sums concerning the alphabet

$$\left\{ \frac{(\pm 1)^k}{k}, \frac{(\pm 1)^k}{(3k + 1)}, \frac{(\pm 1)^k}{(3k + 2)} \right\}$$

up to weight 4. We conjecture the following formulas which we checked up to weight 4 and we summarize the concrete numbers in Table 4.3 up to weight 4:

$$\begin{aligned}
 N_S(w) &= 6 \cdot 7^{w-1} \\
 N_A(w) &\stackrel{w \geq 1}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 7^d \\
 N_D(w) &= N_S(w) - N_S(w - 1) \stackrel{w \geq 1}{=} 36 \cdot 7^{w-2} \\
 N_{H_1}(w) = N_M(w) &= N_S(w) - 2 \cdot 3^{w-1} = 6 \cdot 7^{w-1} - 2 \cdot 3^{w-1} \\
 N_{H_2}(w) &= N_S(w) - 2^{w-1} = 6 \cdot 7^{w-1} - 2^{w-1} \\
 N_{H_1H_2}(w) &= N_S(w) - (2^{w-1} + 2 \cdot 3^{w-1}) = 6 \cdot 7^{w-1} - 2 \cdot 3^{w-1} - 2^{w-1}
 \end{aligned}$$

w	N_S	N_A	N_D	N_{H_1}	N_{H_2}	$N_{H_1H_2}$	N_{AD}	$N_{H_1H_2M}$	$N_{AH_1H_2M}$	$N_{DH_1H_2M}$	$N_{ADH_1H_2M}$
1	6	6	6	4	5	3	6	2	2	2	2
2	42	21	36	36	40	34	15	29	15	27	13
3	294	112	252	276	290	272	91	255	95	226	80
4	2058	588	1764	2004	2050	1996	476	1943	550	1688	455

Table 4.3: Number of basis cyclotomic harmonic sums concerning the alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(3k + 1), (\pm 1)^k/(3k + 2)\}$ and different relations up to weight 4.

$$\begin{aligned}
 N_{H_1H_2M}(w) &= N_S(w) - (2^{w-1} + 4 \cdot 3^{w-1} - 1) = 6 \cdot 7^{w-1} - 4 \cdot 3^{w-1} - 2^{w-1} + 1 \\
 N_{AD}(w) &= N_A(w) - N_A(w-1) \\
 &\stackrel{w \geq 2}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 7^d - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) 7^d \\
 N_{AH_1H_2M}(w) &\stackrel{w \geq 1}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) (7^d - 2 \cdot 3^d - 2^d) + 1 \\
 N_{DH_1H_2M}(w) &= N_{H_1H_2M}(w) - N_{H_1H_2M}(w-1) \\
 &\stackrel{w \geq 1}{=} 36 \cdot 7^{w-2} - 8 \cdot 3^{w-2} - 2^{w-2} \\
 N_{ADH_1H_2M}(w) &= N_{AH_1H_2M}(w) - N_{AH_1H_2M}(w-1) \\
 &\stackrel{w \geq 2}{=} \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) (7^d - 2 \cdot 3^d - 2^d) \\
 &\quad - \frac{1}{w-1} \sum_{d|(w-1)} \mu\left(\frac{w-1}{d}\right) (7^d - 2 \cdot 3^d - 2^d).
 \end{aligned}$$

Finally in Table 4.4 and Table 4.5 we summarize the number of basis elements for different cyclotomies at weight $w = 1$ and $w = 2$ respectively. At weight $w = 1$ we conjecture the following counting relation for the basis elements which was tested up to $l = 300$. Let p_i be pairwise distinct primes > 2 , and let k_i be positive integers. The number $N(l)$ of basis elements at $w = 1$ and cyclotomy l are given by

$$N(l) = \begin{cases} l, & l = 1 \text{ or } l = 2^k \\ \prod_{i=1}^n (p_i - 1) p_i^{k_i - 1}, & l = \prod_{i=1}^n p_i^{k_i} \\ 2^k \cdot \prod_{i=1}^n (p_i - 1) p_i^{k_i - 1}, & l = 2^k \prod_{i=1}^n p_i^{k_i}. \end{cases}$$

For weight $w = 2$ we guessed explicit formulas for some of the columns:

$$\begin{aligned}
 N_S(l) &= 2 \cdot l(2 \cdot l + 1) \\
 N_A(l) &= \frac{1}{2} \sum_{d|2} \mu\left(\frac{2}{d}\right) (2l + 1)^d = l(2 \cdot l + 1) \\
 N_D(l) &= 2 \cdot l(2 \cdot l + 1) - 2 \cdot l = 4 \cdot l^2 \\
 N_{H_1H_2}(l) &= \frac{1}{4}(-1)^l(l + 1) + \frac{1}{4}(2 \cdot l + 1)(7 \cdot l - 1) \\
 N_{AD}(l) &= l(2 \cdot l + 1) - 2 \cdot l = 2 \cdot l^2 - l.
 \end{aligned}$$

l	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
sums	2	4	6	8	10	12	14	16	18	20	22	24	26	28	30	32	34	36	38	40
basis	1	2	2	4	4	4	6	8	6	8	10	8	12	12	8	16	16	12	18	16
new basis sums	1	1	1	3	3	1	5	6	4	3	9	3	11	5	3	12	15	4	17	9

Table 4.4: The number of the $w = 1$ cyclotomic harmonic sums up to $l = 20$ and the corresponding number of basis elements at fixed value of l , and the new basis elements in ascending sequence.

l	N_S	N_A	N_D	$N_{H_1H_2}$	N_M	N_{AD}	$N_{AH_1H_2M}$	$N_{DH_1H_2M}$	$N_{ADH_1H_2M}$
1	6	3	4	4	6	1	2	3	1
2	20	10	16	17	18	6	8	13	6
3	42	21	36	34	36	15	15	27	13
4	72	36	64	62	66	28	29	52	25
5	110	55	100	92	104	45	44	83	40
6	156	78	144	135	126	66	55	103	51
7	210	105	196	178	204	91	87	167	81
8	272	136	256	236	252	120	110	208	102
9	342	171	324	292	300	153	128	247	122
10	420	210	400	365	372	190	162	311	154
11	506	253	484	434	500	231	215	419	205
12	600	300	576	522	492	276	213	412	205
13	702	351	676	604	696	325	300	587	288
14	812	406	784	707	738	378	321	623	309
15	930	465	900	802	784	435	335	655	327
16	1056	528	1024	920	984	496	428	832	412
17	1190	595	1156	1028	1184	561	512	1007	496
18	1332	666	1296	1161	1098	630	474	927	462
19	1482	741	1444	1282	1476	703	639	1259	621
20	1640	820	1600	1430	1464	780	635	1244	619

Table 4.5: Number of basis elements of the $w = 2$ cyclotomic harmonic sums up to cyclotomy $l = 20$.

4.7 Cyclotomic Harmonic Sums at Infinity

Not all cyclotomic harmonic sums are finite at infinity, since for example $\lim_{n \rightarrow \infty} S_{(2,1,1)}(n)$ does not exist. In fact, we have the following lemma, compare Lemma 4.7.1:

Lemma 4.7.1. *Let $a_i, p \in \mathbb{N}, b_i \in \mathbb{N}_0$ and $c_i \in \mathbb{Z}^*$. The cyclotomic harmonic sum $S_{(a_1, b_1, c_1), \dots, (a_p, b_p, c_p)}(n)$ is convergent, when $n \rightarrow \infty$, if and only if $c_1 \neq 1$.*

4.7.1 Relations between Cyclotomic Harmonic Sums at Infinity

The values of the cyclotomic harmonic polylogarithms at argument $x = 1$ and, related to it, the associated cyclotomic harmonic sums at $n \rightarrow \infty$ occur in various relations of the finite cyclotomic harmonic sums and the Mellin transforms of cyclotomic harmonic polylogarithms; compare [8]. In this Section we investigate their relations and basis representations. The infinite cyclotomic harmonic sums extend the Euler-Zagier and

multiple zeta values [23, 32, 33, 50] (see also Section 2.7.1) and are related at lower weight and depth to other known special numbers. We define

$$\sigma_{(a_1,b_1,c_1),\dots,(a_l,b_l,c_l)} := \lim_{n \rightarrow \infty} S_{(a_1,b_1,c_1),\dots,(a_l,b_l,c_l)}(n).$$

We first consider the sums of weight $w = 1$ and $w = 2$ up to cyclotomy $l = 20$. Afterwards the relations of the infinite cyclotomic harmonic sums associated to the summands

$$\frac{1}{k^{l_1}}, \quad \frac{(-1)^k}{k^{l_2}}, \quad \frac{1}{(2k+1)^{l_3}}, \quad \frac{(-1)^k}{(2k+1)^{l_4}}, \tag{4.13}$$

with $l_i \in \mathbb{N}$ up to weight $w = 6$ are worked out.

We consider the following relations:

- The algebraic relations of cyclotomic harmonic sums (see Section 4.6.1) remain valid when we consider them at infinity. We will refer to these relations as the stuffle relations.
- The duplication relations from Section 4.6.3 remain valid if we consider sums which are finite at infinity, since it makes no difference whether the argument is ∞ or $2 \cdot \infty$.
- We can generalize the relation form [85] (see Section 2.7.1) for harmonic sums to cyclotomic harmonic sums. For not both $c_1 = 1$ and $f_1 = 1$ we have (compare [8]):

$$S_{(a_1,b_1,c_1),\dots,(a_k,b_k,c_k)}(\infty) S_{(d_1,e_1,f_1),\dots,(d_l,e_l,f_l)}(\infty) = \lim_{n \rightarrow \infty} \sum_{i=1}^n \frac{\text{sign}(f_1)^i S_{(a_1,b_1,c_1),\dots,(a_k,b_k,c_k)}(n-i) S_{(d_2,e_2,f_2),\dots,(d_l,e_l,f_l)}(i)}{(d_1 i + e_1)^{|f_1|}}$$

Using

$$\begin{aligned} & \sum_{i=1}^n \frac{S_{(a_1,b_1,c_1),\dots,(a_k,b_k,c_k)}(n-i) S_{(d_2,e_2,f_2),\dots,(d_l,e_l,f_l)}(i) \text{sign}(f_1)^i}{(d_1 i + e_1)^{|f_1|}} = \\ & \sum_{k=1}^{|f_1|} \binom{|c_1| + |f_1| - k - 1}{|c_1| - 1} a_1^{|f_1| - k} d_1^{|c_1|} \sum_{i=1}^n \frac{\text{sign}(c_1)^i}{(d_1 b_1 + a_1 e_1 + i a_1 d_1)^{|c_1| |f_1| - k}} \\ & \sum_{j=1}^{i-1} \frac{S_{(a_2,b_2,c_2),\dots,(a_k,b_k,c_k)}(i-j) S_{(d_2,e_2,f_2),\dots,(d_l,e_l,f_l)}(j) \left(\frac{\text{sign}(f_1)}{\text{sign}(c_1)}\right)^j}{(d_1 j + e_1)^k} \\ & + \sum_{k=1}^{|c_1|} \binom{|c_1| + |f_1| - k - 1}{c_2 - 1} a_1^{|f_1|} d_1^{|c_1| - k} \sum_{i=1}^n \frac{\text{sign}(f_1)^i}{(d_1 b_1 + a_1 e_1 + i a_1 d_1)^{|c_1| |f_1| - k}} \end{aligned}$$

$$\sum_{j=1}^{i-1} \frac{S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(i-j) S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(j) \left(\frac{\text{sign}(c_1)}{\text{sign}(f_1)} \right)^j}{(a_1 j + b_1)^k},$$

we can rewrite the right hand side in terms of cyclotomic harmonic sums. We will refer to these relations as the shuffle relations since one could also obtain them from the shuffle algebra of cyclotomic harmonic polylogarithms.

- The multiple argument relations from Section 4.6.3 remain valid if we consider sums which are finite at infinity, since it makes no difference whether the argument is ∞ or $k \cdot \infty$.

Cyclotomic Harmonic Sums up to Weight $w = 2$ at Infinity

We study the sums up to weight $w = 2$ and cyclotomy $l = 20$ ¹, based on the sets of sums using the letters

$$\frac{(\pm 1)^k}{(lk + m)^n}, \quad 1 \leq n \leq 2, 1 \leq l \leq 20, m < l. \quad (4.14)$$

We use the stuffle (quasi-shuffle) relations for the sums, the shuffle relations on the side of the associated cyclotomic harmonic polylogarithms, and the multiple argument relations for these sums. In some cases the latter request to include sums which are outside the above pattern. In these cases the corresponding relations are not accounted for.

At $w = 1$ the respective numbers of basis elements is summarized in Table 4.6. The independent sums at $w = 1$ up to $l = 6$ are :

$$\begin{aligned} & \sigma_{(1,0,1)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}, \sigma_{(3,1,1)}, \sigma_{(3,1,-1)}, \sigma_{(4,1,-1)}, \sigma_{(4,3,-1)}, \sigma_{(5,1,1)}, \sigma_{(5,1,-1)}, \\ & \sigma_{(5,2,-1)}, \sigma_{(5,3,-1)}, \sigma_{(6,1,-1)}, \end{aligned}$$

see [8] for equivalent representations. The dependent sums up to $l = 6$ are

$$\begin{aligned} \sigma_{(2,1,1)} &= -1 - \sigma_{(1,0,-1)} + \frac{1}{2}\sigma_{(1,0,1)} \\ \sigma_{(3,2,1)} &= -\frac{1}{2} - \frac{1}{3}\sigma_{(1,0,-1)} - \sigma_{(3,1,-1)} + \sigma_{(3,1,1)} \\ \sigma_{(3,2,-1)} &= \frac{1}{2} + \frac{2}{3}\sigma_{(1,0,-1)} + \sigma_{(3,1,-1)} \\ \sigma_{(4,1,1)} &= -\frac{1}{2} - \frac{3}{4}\sigma_{(1,0,-1)} + \frac{1}{4}\sigma_{(1,0,1)} + \frac{1}{2}\sigma_{(2,1,-1)} \\ \sigma_{(4,3,1)} &= -\frac{5}{6} - \frac{3}{4}\sigma_{(1,0,-1)} + \frac{1}{4}\sigma_{(1,0,1)} - \frac{1}{2}\sigma_{(2,1,-1)} \end{aligned}$$

¹Relations between colored nested infinite harmonic sums have been investigated also in Refs. [34, 35] recently.

l	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
sums	2	4	6	8	10	12	14	16	18	20	22	24	26	28	30	32	34	36	38	40
basis	2	3	4	5	6	6	8	9	8	10	12	10	14	14	11	17	18	14	20	18
new basis sums	2	1	2	2	4	1	6	4	4	3	10	2	12	5	3	8	16	4	18	6

Table 4.6: The number of the $w = 1$ cyclotomic harmonic sums at infinity up to $l = 20$, the basis elements at fixed value of l , and the new basis elements in ascending sequence.

$$\begin{aligned}
 \sigma_{(5,2,1)} &= \frac{1}{5}\sigma_{(1,0,-1)} + \sigma_{(5,1,1)} - \sigma_{(5,2,-1)} \\
 \sigma_{(5,3,1)} &= -\frac{1}{3} - \frac{1}{5}\sigma_{(1,0,-1)} - \sigma_{(5,1,-1)} + \sigma_{(5,1,1)} \\
 \sigma_{(5,4,1)} &= -\frac{7}{12} - \frac{2}{5}\sigma_{(1,0,-1)} - \sigma_{(5,1,-1)} + \sigma_{(5,1,1)} - \sigma_{(5,3,-1)} \\
 \sigma_{(5,4,-1)} &= \frac{7}{12} + \frac{4}{5}\sigma_{(1,0,-1)} + \sigma_{(5,1,-1)} - \sigma_{(5,2,-1)} + \sigma_{(5,3,-1)} \\
 \sigma_{(6,1,1)} &= -\frac{1}{6}\sigma_{(1,0,-1)} + \frac{1}{2}\sigma_{(3,1,-1)} + \frac{1}{2}\sigma_{(3,1,1)} \\
 \sigma_{(6,5,1)} &= -\frac{7}{10} - \frac{2}{3}\sigma_{(1,0,-1)} - \sigma_{(3,1,-1)} + \frac{1}{2}\sigma_{(3,1,1)} \\
 \sigma_{(6,5,-1)} &= \frac{2}{15} + \frac{4}{3}\sigma_{(2,1,-1)} - \sigma_{(6,1,-1)}, \text{ etc.}
 \end{aligned}$$

The following counting relations for the basis elements were tested up to $l = 700$ using computer algebra methods. Let p, p_i, q be pairwise distinct primes > 2 , and let k, k_i be positive integers. We conjecture that the number $N(l)$ of basis elements at $w = 1$ and cyclotomy l are given by

$$N(l) = \begin{cases} l + 1, & l = 1 \text{ or } l = 2^k \\ (p - 1)p^{k-1} + 2, & l = p^k \\ 2 \cdot N\left(2^{k-1} \prod_{i=1}^n p_i^{k_i}\right) - n - 1, & l = 2^k \prod_{i=1}^n p_i^{k_i} \\ (q - 1) \cdot N\left(\prod_{i=1}^n p_i^{k_i}\right) - n(q - 2) - q + 3, & l = q \prod_{i=1}^n p_i^{k_i} \\ q \cdot N\left(q^{k-1} \prod_{i=1}^n p_i^{k_i}\right) - (n + 2)(q - 1), & l = q^k \prod_{i=1}^n p_i^{k_i}, k > 1. \end{cases}$$

Let us now consider the case $w = 2$. Applying the relations given in the beginning of this section the results given in Table 4.7 are obtained for the number of basis elements. Again we solved the corresponding linear systems using computer algebra methods and derived the representations for the dependent sums analytically.

The number of the weight $w = 2$ infinite sums for cyclotomy l is

$$N_S(l) = 2l(2l + 1). \tag{4.15}$$

l	N_S	SH	A	A + SH	A + SH + H_1	A + SH + H_1 + H_2	A + SH + H_1 + H_2 + M
1	6	4	3	1	1	1	1
2	20	13	10	3	3	2	1
3	42	27	21	7	6	6	5
4	72	46	36	12	11	10	3
5	110	70	55	19	17	17	16
6	156	99	78	27	25	24	5
7	210	133	105	37	34	34	33
8	272	172	136	48	45	44	12
9	342	216	171	61	57	57	52
10	420	265	210	75	71	70	22
11	506	319	253	91	86	86	85
12	600	378	300	108	103	102	21
13	702	442	351	127	121	121	120
14	812	551	406	147	141	140	49
15	930	585	465	169	162	162	145
16	1056	664	528	192	185	184	50
17	1190	748	595	217	209	209	208
18	1332	837	666	243	235	234	63
19	1482	931	741	271	262	262	261
20	1640	1030	820	300	291	290	74

Table 4.7: Number of basis elements of the $w = 2$ cyclotomic harmonic sums at infinity up to cyclotomy $l = 20$ after applying the quasi-shuffle algebra of the sums (A), the shuffle algebra of the cyclotomic harmonic polylogarithms (SH), and the three multiple argument relations (H_1, H_2, M) of the sums.

One may guess, based on the results for $l \leq 20$, counting relations for the length of the bases listed in Table 4.7. We found for all but the last column:

$$\begin{aligned}
 N_A(l) &= l(2l + 1) \\
 N_{SH}(l) &= \frac{(5l + 3)l}{2} \\
 N_{A,SH}(l) &= \frac{6l^2 + 1 - (-1)^l}{8} \\
 N_{A,SH,H_1}(l) &= \frac{6l^2 - 4l + 7 - (-1)^l}{8} \\
 N_{A,SH,H_1,H_2}(l) &= \frac{6l^2 - 4l + 3(1 - (-1)^l)}{8} .
 \end{aligned}$$

Cyclotomic Harmonic Sums of Higher Weights at Infinity

First we consider the iterated summation of the terms

$$\frac{1}{k^{l_1}}, \quad \frac{(-1)^k}{k^{l_2}}, \quad \frac{1}{(2k + 1)^{l_3}}, \quad \frac{(-1)^k}{(2k + 1)^{l_4}},$$

with $l_i \in \mathbb{N}$. A corresponding sum $S_{(a_1, b_1, c_1), \dots, (a_l, b_l, c_l)}(n)$ diverges if it has leading ones, i.e., if $c_1 = 1$. However, these divergences can be regulated by polynomials in $\sigma_{(1,0,1)} = \lim_{n \rightarrow \infty} S_1(n)$ and cyclotomic harmonic sums, which are convergent for $n \rightarrow \infty$, very similar to the case of the usual harmonic sums; see Remark 2.1.5. In

weight	N_S	A	SH	A + SH	A + SH + H_1	A + SH + H_1 + H_2	A + SH + H_1 + H_2 + M
1	4	4	4	4	4	3	3
2	20	10	13	3	3	2	1
3	100	40	46	6	6	5	3
4	500	150	163	10	10	9	6
5	2500	624	650	21	21	19	13
6	12500	2580	2635	36	36	34	25

Table 4.8: Basis representations of the infinite cyclotomic harmonic sums over the alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(2k+1)\}$ after applying the stuffle (A), shuffle (SH) relations, their combination, and their application together with the three multiple argument relations (H_1, H_2, M).

Table 4.8 we present the number of basis elements obtained applying the respective relations up to weight $w = 6$. The representation of all sums were computed by means of computer algebra in explicit form. We derive the cumulative basis, quoting only the new elements in the next weight. For suitable integral representations over known functions we refer to [8]. One possible choice of basis elements is :

$w = 1$:

$$\sigma_{(1,0,1)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}$$

$w = 2$:

$$\sigma_{(2,1,-2)}$$

$w = 3$:

$$\sigma_{(1,0,3)}, \sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-2)}, \sigma_{(1,0,-1)}$$

$w = 4$:

$$\sigma_{(1,0,-1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(2,1,-4)}, \sigma_{(2,1,-3)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,-2)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)},$$

$$\sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,1)}$$

$w = 5$:

$$\sigma_{(1,0,5)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,-4)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,4)}, \sigma_{(2,1,-1)}$$

$$\sigma_{(2,1,-4)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-3)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,1)}, \sigma_{(1,0,-3)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,3)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-1)},$$

$$\sigma_{(2,1,-3)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,1)}, \sigma_{(1,0,-2)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,-2)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,-1)},$$

$$\sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,1)}, \sigma_{(1,0,1)}$$

$w = 6$:

$$\sigma_{(1,0,-5)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(2,1,-6)}$$

$$\sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,-2)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,1)},$$

$$\sigma_{(1,0,-2)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,1)}, \sigma_{(1,0,-2)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,1)},$$

$$\sigma_{(1,0,-2)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,3)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,1)},$$

$$\sigma_{(1,0,-3)}, \sigma_{(1,0,-1)}, \sigma_{(2,1,1)}, \sigma_{(1,0,1)}, \sigma_{(1,0,-3)}, \sigma_{(1,0,-1)}, \sigma_{(1,0,1)}, \sigma_{(2,1,1)},$$

$$\sigma_{(2,1,-3)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,-3)}, \sigma_{(2,1,-1)}, \sigma_{(2,1,-1)}, \sigma_{(1,0,-1)},$$

weight	N_S	A	SH	A + SH	A + SH + H_1	A + SH + H_1 + H_2	A + SH + H_1 + H_2 + M
1	6	6	6	6	5	4	4
2	42	21	27	7	6	6	5
3	294	112	131	17	16	16	15
4	2058	588	651	40	37	37	36

Table 4.9: Basis representations of the infinite cyclotomic harmonic sums over the alphabet $\{(\pm 1)^k/k, (\pm 1)^k/(3k+1), (\pm 1)^k/(3k+2)\}$ after applying the stuffle (A), shuffle (SH) relations, their combination, and their application together with the three multiple argument relations (H_1, H_2, M).

$$\begin{aligned} &\sigma_{(1,0,-3),(2,1,-1),(1,0,-1),(2,1,-1)}, \sigma_{(1,0,-3),(1,0,-1),(2,1,-1),(2,1,-1)}, \sigma_{(2,1,4),(1,0,-1),(2,1,-1)}, \\ &\sigma_{(1,0,4),(2,1,-1),(1,0,-1)}, \sigma_{(1,0,4),(1,0,-1),(2,1,-1)}, \sigma_{(2,1,-4),(1,0,-1),(2,1,1)}, \\ &\sigma_{(2,1,-4),(1,0,-1),(1,0,1)}, \sigma_{(1,0,-4),(2,1,-1),(2,1,1)}, \sigma_{(1,0,-4),(2,1,-1),(1,0,1)}, \\ &\sigma_{(1,0,-4),(1,0,-1),(2,1,-1)}, \sigma_{(2,1,-4),(2,1,-2)}, \sigma_{(2,1,-5),(2,1,-1)} \cdot \end{aligned}$$

As a further example of the infinite cyclotomic harmonic sums we consider the iterated summation of the terms

$$\frac{1}{k^{l_1}}, \quad \frac{(-1)^k}{k^{l_2}}, \quad \frac{1}{(3k+1)^{l_3}}, \quad \frac{(-1)^k}{(3k+1)^{l_4}}, \quad \frac{1}{(3k+2)^{l_4}}, \quad \frac{(-1)^k}{(3k+2)^{l_5}},$$

with $l_i \in \mathbb{N}$. In Table 4.9 we list the corresponding numbers of basis elements up to weight 4.

4.8 Asymptotic Expansion of Cyclotomic Harmonic Sums

In this section we want to generalize the algorithm for the computation of the asymptotic expansion of harmonic sums to cyclotomic harmonic sums. Again the integral representation of these sums will be the starting point. In the algorithm for the computation of the asymptotic expansion of harmonic sums the possibility to express a harmonic polylogarithm $H_m(x)$ in terms of harmonic polylogarithms at argument $1-x$ plays a decisive role. This remains true for cyclotomic harmonic polylogarithms. In the case of harmonic polylogarithms we had to extend the index set to $\{-1, 0, 1, 2\}$ in order to be able to perform this transformation. Since in general we cannot express a cyclotomic harmonic polylogarithm $H_m(x)$ in terms of cyclotomic harmonic polylogarithms at argument $1-x$, we will introduce a new set of functions which is closely related to cyclotomic harmonic polylogarithms and which we will call *shifted cyclotomic harmonic polylogarithms*.

4.8.1 Shifted Cyclotomic Harmonic Polylogarithms

In the following we present new additional aspects which can not be found in [8]. We start by defining the new auxiliary function g : For $a \in \mathbb{N}$ and $b \in \mathbb{N}$, $b < \varphi(a)$ we define

$$g_a^b : (0, 1) \mapsto \mathbb{R}$$

$$g_a^b(x) = \begin{cases} \frac{1}{1-x}, & \text{if } a = b = 0 \\ \frac{(1-x)^b}{\Phi_a(1-x)}, & \text{otherwise.} \end{cases}$$

Here $\Phi_a(x)$ denotes again the a th cyclotomic polynomial and φ denotes Euler's totient function. Now we are ready to define *shifted cyclotomic harmonic polylogarithms*:

Definition 4.8.1 (Shifted Cyclotomic Harmonic Polylogarithms). *Let $m_i = (a_i, b_i)$ where $a_i, b_i \in \mathbb{N}$ with $b_i < \varphi(a_i)$; we define for $x \in (0, 1)$:*

$$\widehat{H}(x) = 1,$$

$$\widehat{H}_{m_1, \dots, m_k}(x) = \begin{cases} \frac{(-1)^k}{k!} (\log x)^k, & \text{if } m_i = (1, 0) \text{ for } 1 \leq i \leq k \\ \int_0^x g_{a_1}^{b_1}(y) \widehat{H}_{m_2, \dots, m_k}(y) dy, & \text{otherwise.} \end{cases}$$

The length k of the vector \mathbf{m} is called the *weight* of the shifted cyclotomic harmonic polylogarithm $H_{\mathbf{m}}(x)$.

Example 4.8.2.

$$\widehat{H}_{(5,3)}(x) = \int_0^x \frac{(1-y)^3}{\Phi_5(1-y)} dy = \int_0^x \frac{(1-y)^3}{y^4 - 5y^3 + 10y^2 - 10y + 5} dy$$

$$\widehat{H}_{(3,1),(2,0),(5,2)}(x) = \int_0^x \frac{1-y}{\Phi_3(1-y)} \int_0^y \frac{1}{\Phi_2(1-z)} \int_0^z \frac{(1-w)^2}{\Phi_5(1-w)} dw dz dy$$

$$\widehat{H}_{(1,0),(0,0),(0,0)}(x) = \int_0^x \frac{1}{-y} \int_0^y \frac{1}{1-z} \int_0^z \frac{1}{1-w} dw dz dy = -H_{(0,0),(1,0),(1,0)}(x).$$

Remark 4.8.3. *Note that these functions are again analytic for $x \in (0, 1)$ and for the derivatives we have for all $x \in (0, 1)$ that*

$$\frac{d}{dx} \widehat{H}_{(a_1, b_1), (a_2, b_2), \dots, (a_k, b_k)}(x) = g_{a_1}^{b_1}(x) \widehat{H}_{(a_2, b_2), \dots, (a_k, b_k)}(x).$$

In the following we will see that shifted cyclotomic harmonic polylogarithms at argument $1 - x$ can be expressed in terms of cyclotomic harmonic polylogarithms at argument x together with constants. We proceed recursively on the weight w of the

shifted cyclotomic harmonic polylogarithm. In the base case we have for $x \in (0, 1)$ and $a, b \in \mathbb{N}, 1 < a, b < \varphi(a)$:

$$\widehat{H}_{(0,0)}(1-x) = -H_{(0,0)}(x) \quad (4.16)$$

$$\widehat{H}_{(1,0)}(1-x) = -H_{(1,0)}(x) \quad (4.17)$$

$$\widehat{H}_{(a,b)}(1-x) = H_{a,b}(1) - H_{(a,b)}(x). \quad (4.18)$$

Now let us look at higher weights $w > 1$. We consider $\widehat{H}_{m_1, m_2, \dots, m_w}(1-x)$ and suppose that we can already apply the transform for shifted cyclotomic harmonic polylogarithms of weight $< w$. If $m_1 = (0, 0)$, we can remove leading $(0, 0)$ and end up with shifted cyclotomic harmonic polylogarithms without leading $(0, 0)$ and powers of $\widehat{H}_{(0,0)}(1-x)$. For the powers of $H_{(0,0)}(1-x)$ we can use (4.16); therefore, only the cases in which the first index $m_1 \neq (0, 0)$ are to be considered. If $m_i = (1, 0)$ for all $1 < i \leq w$, we are in fact dealing with a power of $\widehat{H}_{(1,0)}(1-x)$ and hence we can use (4.17) to transform these cyclotomic harmonic polylogarithms. Now let us assume that not all $m_i = (1, 0)$. For $m_1 = (1, 0)$ we get:

$$\begin{aligned} \widehat{H}_{(1,0), m_2, \dots, m_w}(1-x) &= \int_0^{1-x} \frac{\widehat{H}_{m_2, \dots, m_w}(y)}{-y} dy \\ &= -\widehat{H}_{(1,0), m_2, \dots, m_w}(1) + \int_{1-x}^1 \frac{\widehat{H}_{m_2, \dots, m_w}(y)}{y} dy \\ &= -\widehat{H}_{(1,0), m_2, \dots, m_w}(1) + \int_0^x \frac{\widehat{H}_{m_2, \dots, m_w}(1-y)}{1-y} dy. \end{aligned}$$

For $m_1 = (a, b)$ with $a, b \in \mathbb{N}, 1 < a, b < \varphi(a)$ we get:

$$\begin{aligned} \widehat{H}_{(a,b), m_2, \dots, m_w}(1-x) &= \int_0^{1-x} \frac{(1-y)^b \widehat{H}_{m_2, \dots, m_w}(y)}{\Phi_a(1-y)} dy \\ &= \widehat{H}_{(a,b), m_2, \dots, m_w}(1) - \int_{1-x}^1 \frac{(1-y)^b \widehat{H}_{m_2, \dots, m_w}(y)}{\Phi_a(1-y)} dy \\ &= \widehat{H}_{(a,b), m_2, \dots, m_w}(1) - \int_0^x \frac{y^b \widehat{H}_{m_2, \dots, m_w}(1-y)}{\Phi_a(y)} dy. \end{aligned}$$

Since we know the transform for weights $< w$ we can apply it to $\widehat{H}_{m_2, \dots, m_w}(1-y)$ and finally we obtain the required weight w identity by using the definition of the cyclotomic harmonic polylogarithms.

Example 4.8.4.

$$\begin{aligned} \widehat{H}_{(5,2), (3,1)}(1-x) &= -H_{(3,1)}(1)H_{(5,2)}(x) + H_{(5,2), (3,1)}(x) + H_{(3,1)}(1)H_{(5,2)}(1) \\ &\quad - H_{(5,2), (3,1)}(1). \end{aligned}$$

Remark 4.8.5. For $a, b \in \mathbb{N}_0$ with $a > 1$ and $b < \phi(a)$ we have $\widehat{H}_{(a,b)}(1) = H_{(a,b)}(1)$. For the values of shifted cyclotomic harmonic polylogarithms at argument 1 of higher

weights we can use the above procedure to express them by cyclotomic harmonic polylogarithms at argument 1. Note that we can as well perform the reverse direction, i.e., we can find a combination of shifted cyclotomic harmonic polylogarithms at argument $1 - x$ together with some constants to express a cyclotomic harmonic polylogarithm $H_m(x)$.

Example 4.8.6.

$$\begin{aligned} H_{(3,1),(5,2)}(x) &= -H_{(5,2)}(1) \widehat{H}_{(3,1)}(1-x) + \widehat{H}_{(3,1),(5,2)}(1-x) + H_{(3,1)}(1) H_{(5,2)}(1) \\ &\quad - \widehat{H}_{(3,1),(5,2)}(1) \\ \widehat{H}_{(3,1),(5,2)}(1) &= H_{(3,1)}(1) H_{(5,2)}(1) - H_{(3,1),(5,2)}(1). \end{aligned}$$

4.8.2 Computation of Asymptotic Expansions of Cyclotomic Harmonic Sums

Before we can state an algorithm to compute the asymptotic expansions for cyclotomic harmonic sums, we have to extend the Lemmas 2.8.14, 2.8.15 and 2.8.16. Since the proofs of these lemmas can be easily extended we will omit them here.

Lemma 4.8.7. *Let $H_{m_1, m_2, \dots, m_k}(x)$ be a cyclotomic harmonic polylogarithm with $m_i \neq (1, 0)$ for $1 \leq i \leq k$ and let $a \in \mathbb{N}$, with $a > 1$. Then*

$$H_{m_1, m_2, \dots, m_k}(x), \frac{H_{m_1, m_2, \dots, m_k}(x)}{\Phi_a(x)}$$

and

$$\frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(1)}{1 - x}$$

are analytic for $x \in (0, \infty)$.

Lemma 4.8.8. *Let $\widehat{H}_{m_1, m_2, \dots, m_k}(x)$ be a shifted cyclotomic harmonic polylogarithm with $m_k \neq (1, 0)$ and let $a \in \mathbb{N}$. Then*

$$\frac{\widehat{H}_{m_1, m_2, \dots, m_k}(1-x)}{\Phi_a(x)}$$

is analytic for $x \in (0, 2)$.

Lemma 4.8.9. *Let $H_m(x) = H_{m_1, m_2, \dots, m_k}(x)$ be a cyclotomic harmonic polylogarithm with $m_1 \neq (1, 0)$ and let $\widehat{H}_b(x) = \widehat{H}_{b_1, b_2, \dots, b_l}(x)$ be a shifted cyclotomic harmonic polylogarithm with $b_l \neq (1, 0)$. Then we have*

$$\begin{aligned} M\left(\frac{H_m(x)}{x-1}, in + p\right) &= \int_0^1 \frac{x^{in+p}(H_m(x) - H_m(1))}{x-1} dx - \int_0^1 \frac{H_m(x) - H_m(1)}{x-1} dx \\ &\quad - S_1(in + p) H_m(1) \end{aligned}$$

and

$$M\left(\frac{\widehat{H}_b(1-x)}{x-1}, jn+p\right) = \int_0^1 \frac{x^{jn+p}\widehat{H}_b(1-x)}{x-1} dx + \widehat{H}_{(1,0),b}(1)$$

where

$$\int_0^1 \frac{H_m(x) - H_m(1)}{x-1} dx, H_m(1) \text{ and } \widehat{H}_{(1,0),b}(1)$$

are finite constants.

Remark 4.8.10. Combining Lemma 4.8.7, Lemma 4.8.8 and 4.8.9 we are able to expand Mellin transforms of the form

$$M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{\Phi_a(x)}, in+p\right) \text{ and } M\left(\frac{\widehat{H}_{b_1, b_2, \dots, b_l}(1-x)}{\Phi_a(x)}, jn+p\right)$$

where $m_r \neq (1, 0)$ for $1 \leq r \leq k$ and $b_l \neq (1, 0)$ and suitable i and j (see Section 4.5.1) following the method presented in Section 2.8.2, or using repeated integration by parts.

Remark 4.8.11. Analyzing the method to compute the inverse Mellin transform of cyclotomic harmonic sums presented in Section 4.5 we find out that the cyclotomic harmonic polylogarithms with highest weight in the inverse Mellin transform of a cyclotomic harmonic sum without trailing ones do not have trailing $(1, 0)$, while the cyclotomic harmonic polylogarithms with highest weight in the inverse Mellin transform of a cyclotomic harmonic sum with trailing ones have trailing $(1, 0)$.

Using the method presented in Section 4.8.1 we can always express a cyclotomic harmonic polylogarithm without trailing $(1, 0)$ at argument x using shifted cyclotomic harmonic polylogarithms at argument $1-x$ where the shifted cyclotomic harmonic polylogarithms with highest weight do not have trailing $(1, 0)$.

Now we are ready to state an algorithm to compute asymptotic expansions of cyclotomic harmonic sums assuming that we are able to expand linear cyclotomic harmonic sums (we will treat linear cyclotomic harmonic sums in the subsequent subsection). If we want to find the asymptotic expansions of a cyclotomic harmonic sum $S_{m_1, m_2, \dots, m_k}(n) = S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)$, we can proceed as follows:

- if $S_{m_1, m_2, \dots, m_k}(n)$ has trailing ones, i.e., $c_k = 1$ we first extract them (see Section 4.1.1); treat linear cyclotomic harmonic sums in the subsequent subsection; apply the following items to each of the cyclotomic harmonic sums without trailing ones;
- suppose now $S_{m_1, m_2, \dots, m_k}(n) = S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(n)$ has no trailing ones, i.e., $c_k \neq 1$; let $\frac{H_{q_1}(x)}{\Phi_{r_1}(x)}, \dots, \frac{H_{q_v}(x)}{\Phi_{r_v}(x)}$ be the weighted cyclotomic harmonic polylogarithms of highest weight in the inverse Mellin transform of $S_{m_1, m_2, \dots, m_k}(n)$ and

let $M\left(\frac{H_{q_1}(x)}{\Phi_{r_1}(x)}, l_1n + p_1\right), \dots, M\left(\frac{H_{q_v}(x)}{\Phi_{r_v}(x)}, l_vn + p_v\right)$ be the derived associated Mellin transforms; we can express $S_{m_1, m_2, \dots, m_k}(n)$ as

$$S_{m_1, m_2, \dots, m_k}(n) = c_1 M\left(\frac{H_{q_1}(x)}{\Phi_{r_1}(x)}, l_1n + p_1\right) + \dots + c_v M\left(\frac{H_{q_v}(x)}{\Phi_{r_v}(x)}, l_vn + p_v\right) + T, \quad (4.19)$$

where $c_i \in \mathbb{R}$ and T is an expression in cyclotomic harmonic sums (which have smaller weight than $S_{m_1, m_2, \dots, m_k}(n)$) and constants;

- we proceed by expanding each of the $M\left(\frac{H_{q_i}(x)}{\Phi_{r_i}(x)}, l_i n + p_i\right)$; let $M\left(\frac{H_{q_1, \dots, q_s}(x)}{\Phi_r(x)}, ln + p\right)$ be one of these Mellin transforms:

all $q_i \neq (1, 0)$: expand $M\left(\frac{H_{q_1, q_2, \dots, q_s}(x)}{\Phi_r(x)}, n\right)$ directly see Remark 4.8.10

not all $m_i \neq (1, 0)$:

- express $H_q(x)$ in terms of shifted cyclotomic harmonic polylogarithms at argument $1 - x$; expand all products; then we get

$$M\left(\frac{H_q(x)}{\Phi_r(x)}, ln + p\right) = \sum_{i=1}^t c_i M\left(\frac{\widehat{H}_{f_i}(1-x)}{\Phi_r(x)}, ln + p\right) + c \quad \text{with } c, c_i \in \mathbb{R} \quad (4.20)$$

- for each Mellin transform $M\left(\frac{\widehat{H}_{f_1, \dots, f_j}(1-x)}{\Phi_r(x)}, ln + p\right)$ do

$f_j \neq (1, 0)$: expand $M\left(\frac{\widehat{H}_{f_j}(1-x)}{\Phi_r(x)}, ln + p\right)$ as given in Remark 4.8.10

$f_j = (1, 0)$: express $\widehat{H}_{f_j}(1-x)$ by cyclotomic harmonic polylogarithms at x see Section 4.8.1; expand all products; hence we can write

$$M\left(\frac{\widehat{H}_{f_j}(1-x)}{\Phi_r(x)}, ln + p\right) = \sum_{i=1}^t d_i M\left(\frac{H_{g_i}(x)}{\Phi_r(x)}, ln + p\right) + d \quad (4.21)$$

with $d, d_i \in \mathbb{R}$ and perform the Mellin transforms $M\left(\frac{H_{g_i}(x)}{\Phi_r(x)}, ln + p\right)$; see Section 4.5.1

- replace the $M\left(\frac{H_{q_i}(x)}{\Phi_{r_i}(x)}, l_i n + p_i\right)$ in equation (4.19) by the results of this process
- for all nonlinear cyclotomic harmonic sums that remain in equation (4.19) apply the above points; since these cyclotomic harmonic sums have smaller weights than $S_{m_1, m_2, \dots, m_k}(n)$ this process will terminate

Some remarks are in place: Since $c_k \neq 1$ in equation (4.19), we know (see Remark 4.8.11) that the cyclotomic harmonic polylogarithms $H_{q_i}(x)$ in equation (4.19) do not have trailing index $(1, 0)$. Since the cyclotomic harmonic polylogarithms $H_{q_i}(x)$ do not have the trailing index $(1, 0)$, the shifted cyclotomic harmonic polylogarithms of highest weight in equation (4.20) will not have the trailing index $(1, 0)$ (see Remark 4.8.11). Therefore the nonlinear cyclotomic harmonic sums which will appear in equation (4.21) have smaller weight than $S_{m_1, m_2, \dots, m_k}(n)$ of (4.19) and hence this algorithm will eventually terminate.

Example 4.8.12. *Using the algorithm from above we compute the asymptotic expansion of $S_{(3,1,2),(1,0,1)}(n)$ up to order 3:*

$$\begin{aligned} & \frac{1}{972} \left(-\frac{1}{n^3} (120H_{(3,0),(0,0)}(1) + 60H_{(3,1),(0,0)}(1) - 60\zeta_2 + 67) + \frac{1}{n^2} (168H_{(3,0),(0,0)}(1) \right. \\ & + 84H_{(3,1),(0,0)}(1) - 84\zeta_2 + 81) + \frac{108}{n} (-2H_{(3,0),(0,0)}(1) - H_{(3,1),(0,0)}(1) + \zeta_2 - 1) \\ & - 162(-12H_{(3,0)}(1) - 6H_{(3,1)}(1) + 12 - 6H_{(3,0),(0,0)}(1) - 3H_{(3,1),(0,0)}(1) \\ & - 4H_{(3,0),(0,0),(1,0)}(1) - 6H_{(3,0),(1,0),(0,0)}(1) + 4H_{(3,0),(3,0),(0,0)}(1) + 2H_{(3,0),(3,1),(0,0)}(1) \\ & - 2H_{(3,1),(0,0),(1,0)}(1) - 6H_{(3,1),(1,0),(0,0)}(1) + 8H_{(3,1),(3,0),(0,0)}(1) + 4H_{(3,1),(3,1),(0,0)}(1) \\ & \left. + 3\zeta_2 - 2\zeta_3 - 3) \right) + \frac{1}{3} S_{(3,1,1)}(n) (2H_{(3,0),(0,0)}(1) + H_{(3,1),(0,0)}(1) - \zeta_2 - 6) \\ & + \frac{1}{3} S_{(3,2,1)}(n) (2H_{(3,0),(0,0)}(1) + H_{(3,1),(0,0)}(1) - \zeta_2 + 3) \\ & + \frac{1}{162} S_1(n) \left(-72H_{(3,0),(0,0)}(1) - 36H_{(3,1),(0,0)}(1) - \frac{11}{n^3} + \frac{15}{n^2} - \frac{18}{n} + 36\zeta_2 + 54 \right). \end{aligned}$$

In order to expand the remaining linear cyclotomic sums, i.e., $S_{(3,1,1)}(n)$, $S_{(3,2,1)}(n)$ and $S_1(n)$, we refer to the next section.

Asymptotic Expansion of *Linear* Cyclotomic Harmonic Sums

So far we do not know how to compute the asymptotic expansion of Mellin transforms of the form

$$M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{\Phi_a(x)}, in + p\right)$$

with $m_k = (1, 0)$.

Since the cyclotomic harmonic polylogarithms with highest weight in the inverse Mellin transform of a cyclotomic harmonic sum with trailing ones have trailing $(1, 0)$, we have to find a new method for these sums. From Section 2.8.2 we know how to compute the expansion of $S_{1, \dots, 1}(n)$ and in the following we will connect the computation of the asymptotic expansion of general linear cyclotomic sums to $S_{1, \dots, 1}(n)$.

We start with the weight $w = 1$ case, i.e., we consider the sum $S_{(a,b,1)}(n)$. If $b = 0$, we have

$$S_{(a,b,1)}(n) = \frac{1}{a} S_1(n),$$

and since we know the expansion of $S_1(n)$ we can handle this case. Now assume that $b \neq 0$. Then we have

$$S_{(a,b,1)}(n) = \sum_{i=1}^n \left(\frac{1}{ai+b} - \frac{1}{ai} \right) + \frac{1}{a} S_1(n).$$

The integral representation of

$$\sum_{i=1}^n \left(\frac{1}{ai+b} - \frac{1}{ai} \right)$$

yields (compare Lemma 4.5.1)

$$\begin{aligned} \sum_{i=1}^n \left(\frac{1}{ai+b} - \frac{1}{ai} \right) &= \int_0^1 \frac{x^{a-1} (x^b - 1) (x^{an} - 1)}{x^a - 1} dx \\ &= \int_0^1 x^{a-1} (x^{an} - 1) \frac{\Phi_b \prod_{d|a, d < a} \Phi_d}{\Phi_a \prod_{d|b, d < b} \Phi_d} dx \\ &= \int_0^1 x^{a-1} (x^{an} - 1) \frac{\Phi_b \prod_{d|a, 1 < d < a} \Phi_d}{\Phi_a \prod_{d|b, 1 < d < b} \Phi_d} dx. \end{aligned}$$

At this point we may perform a partial fraction decomposition (note that there is no factor of $(1-x)$ in the denominator) and split the integrals. We can already compute the asymptotic expansions of these integrals (see Remark 4.8.11) and since we know the expansion of $S_1(n)$ we can handle the weight one case.

We will now assume that we are able to compute the asymptotic expansions of linear cyclotomic harmonic sums with weight $w < k$ and we will consider the weight $w = k$ case. Note that we can always relate a cyclotomic harmonic sum with an index $(a_i, 0, c_i)$ to a cyclotomic harmonic sum with index $(1, 0, c_i)$ since

$$S_{(a_1, b_1, c_1), \dots, (a_i, 0, c_i), \dots, (a_k, b_k, c_k)}(n) = \frac{1}{a_i c_i} S_{(a_1, b_1, c_1), \dots, (1, 0, c_i), \dots, (a_k, b_k, c_k)}(n);$$

hence in the following we can always assume that $a_i = 1$ if an index $(a_i, 0, c_i)$ is present. Let now $S_{m_1, \dots, m_k}(n) = S_{(a_1, b_1, 1), \dots, (a_k, b_k, 1)}(n)$ be a linear cyclotomic harmonic sum with $a_i = 1$ if $b_i = 0$ and let q be the number of indices m_i that are different from $(1, 0, 1)$. If $m_k = (1, 0, 1)$, we extract the trailing $(1, 0, 1)$ and end up with a polynomial in $S_1(n)$ with coefficients in cyclotomic harmonic sums (these sums do not have to be linear cyclotomic sums) without trailing $(1, 0, 1)$. From the nonlinear cyclotomic harmonic sums we extract possible trailing ones (see Remark 4.1.5). We can handle the powers of $S_1(n)$ and for the sums without trailing ones we can use the algorithm of the previous section. What remains are linear sums without trailing $(1, 0, 1)$ having at most q indices different from $(1, 0, 1)$.

Assume now that $S_{m_1, \dots, m_k}(n) = S_{(a_1, b_1, 1), \dots, (a_k, b_k, 1)}(n)$ is a linear cyclotomic harmonic sum with q indices m_i different from $(1, 0, 1)$, where $m_k \neq (1, 0, 1)$. Note that we have

$$S_{m_1, \dots, m_k}(n) = \overbrace{\sum_{i_1=1}^n \frac{1}{a_1 i_1 + b_1} \cdots \sum_{i_{k-1}=1}^{i_{k-2}} \frac{1}{a_{k-1} i_{k-1} + b_{k-1}} \sum_{i_k=1}^{i_{k-1}} \left(\frac{1}{a_k i_k + b_k} - \frac{1}{a_k i_k} \right)}{=:A} + \frac{1}{a_k} S_{m_1, \dots, m_{k-1}, (1, 0, 1)}(n).$$

We now look for an integral representation of A . For the inner sum we get as before

$$\begin{aligned} \sum_{i_k=1}^{i_{k-1}} \left(\frac{1}{a_k i_k + b_k} - \frac{1}{a_k i_k} \right) &= \int_0^1 \frac{x^{a_k-1} (x^{b_k} - 1) (x^{a_k i_{k-1}} - 1)}{x^{a_k} - 1} dx \\ &= \int_0^1 x^{a_k-1} (x^{a_k i_{k-1}} - 1) \frac{\Phi_{b_k} \prod_{d|a_k, d < a_k} \Phi_d}{\Phi_{a_k} \prod_{d|b_k, d < b_k} \Phi_d} dx \\ &= \int_0^1 x^{a_k-1} (x^{a_k i_{k-1}} - 1) \frac{\Phi_{b_k} \prod_{d|a_k, 1 < d < a_k} \Phi_d}{\Phi_{a_k} \prod_{d|b_k, 1 < d < b_k} \Phi_d} dx. \end{aligned}$$

At this point we may perform a partial fraction decomposition (note that there is no factor of $(1 - x)$ in the denominator), split the integrals and proceed to get an integral representation of A as described in Section 4.5. Finally we can use repeated integration by parts to get a Mellin type representation of A . The cyclotomic harmonic polylogarithms at highest weight will not have trailing $(1, 0)$ because of the absence of $(1 - x)$ in the denominator and hence we can compute the asymptotic expansions of the Mellin transform of these cyclotomic harmonic polylogarithms (see Remark 4.8.11). If there are cyclotomic harmonic polylogarithms of lower weights with trailing $(1, 0)$, we can perform the Mellin transform which will lead to sums of lower weight which we can already expand asymptotically.

The last step is to compute the expansion of $S_{m_1, \dots, m_{k-1}, (1, 0, 1)}(n)$. If $q = 1$, we have $S_{m_1, \dots, m_{k-1}, (1, 0, 1)}(n) = S_{1, \dots, 1}(n)$ and hence we already know the expansion. If $q > 1$, we reduced at least the number of indices different from $(1, 0, 1)$ by one, and we can now apply the described strategy to $S_{m_1, \dots, m_{k-1}, (1, 0, 1)}(n)$. Summarizing, we step by step reduce the number of indices different from $(1, 0, 1)$. Eventually we will arrive at a cyclotomic sum with all indices equal to $(1, 0, 1)$. This case we already handled.

Example 4.8.13. We consider the sum $S_{(3, 1, 1), (3, 2, 1)}(n)$. We have

$$S_{(3, 1, 1), (3, 2, 1)}(n) = \overbrace{\sum_{i=1}^n \frac{1}{3i+1} \sum_{j=1}^i \left(\frac{1}{3j+2} - \frac{1}{3j} \right)}{=:A} + \frac{1}{3} S_{(3, 1, 1), (1, 0, 1)}(n).$$

The integral representation of A yields

$$\frac{1}{6} (-2H_{(3, 0)}(1) + 2H_{(3, 1)}(1) - 1) \int_0^1 \frac{x^{3n} - 1}{x - 1} dx + \frac{1}{3} \int_0^1 \frac{(x^{3n} - 1) H_{(3, 0)}(x)}{x - 1} dx$$

$$\begin{aligned}
& + \int_0^1 x^{3n} H_{(3,0)}(x) dx + \frac{2}{3} (H_{(3,0)}(1) - H_{(3,1)}(1) - 1) \int_0^1 \frac{x^{3n} - 1}{x^2 + x + 1} dx \\
& + \frac{1}{6} (2H_{(3,0)}(1) - 2H_{(3,1)}(1) + 1) \int_0^1 \frac{x(x^{3n} - 1)}{x^2 + x + 1} dx - \frac{2}{3} \int_0^1 \frac{(x^{3n} - 1) H_{(3,0)}(x)}{x^2 + x + 1} dx \\
& - \frac{1}{3} \int_0^1 \frac{x(x^{3n} - 1) H_{(3,0)}(x)}{x^2 + x + 1} dx + \frac{-2H_{(3,0)}(1) + 2H_{(3,1)}(1) + 2n + 1}{2(3n + 1)} \\
& - \int_0^1 x^{3n+1} dx + \frac{1}{3} \int_0^1 (x^{3n} - 1) dx.
\end{aligned}$$

We can handle all these integrals and the asymptotic expansion of A up to order 3 is

$$\begin{aligned}
& H_{(3,1)}(1) \left(\frac{1}{3} H_{(2,0)}(2) + \frac{10}{243n^3} - \frac{11}{108n^2} + \frac{5}{18n} + \frac{1}{3} (\log(n) + \gamma) - \frac{1}{6} \right) - \frac{2}{3} H_{(3,0)}(1)^2 \\
& + \left(\frac{1}{3} H_{(3,1)}(1) + \frac{2}{3} \right) H_{(3,0)}(1) + \frac{1}{3} H_{(3,1)}(1)^2 - \frac{1}{6} H_{(2,0)}(2) + \frac{1}{3} H_{(3,0),(1,0)}(1) \\
& + \frac{2}{3} H_{(3,0),(3,0)}(1) + \frac{1}{3} H_{(3,1),(3,0)}(1) - \frac{445}{4374n^3} + \frac{85}{648n^2} - \frac{23}{108n} + \frac{1}{6} (-\log(n) - \gamma).
\end{aligned}$$

Now we have to consider $S_{(3,1,1),(1,0,1)}(n)$. Removing the trailing $(1, 0, 1)$ yields

$$S_{(3,1,1),(1,0,1)}(n) = S_{(3,1,1)}(n) S_{(1,0,1)}(n) + S_{(1,0,1)}(n) - 3S_{(3,1,1)}(n) - S_{(1,0,1),(3,1,1)}(n).$$

The depth one sums are easy to handle and it remains to expand $S_{(1,0,1),(3,1,1)}(n)$. We have

$$S_{(1,0,1),(3,1,1)}(n) = \overbrace{\sum_{i=1}^n \frac{1}{i} \sum_{j=1}^i \left(\frac{1}{3j+1} - \frac{1}{3j} \right)}{=:B} + \frac{1}{3} S_{1,1}(n).$$

We can handle B as we have already worked with A . The asymptotic expansion of B up to order 3 is

$$\begin{aligned}
& H_{(3,0)}(1) \left(H_{(2,0)}(2) - \frac{1}{12n^2} + \frac{1}{2n} + \log(n) + \gamma - 2 \right) + H_{(3,1)}(1) \left(H_{(2,0)}(2) - \frac{1}{12n^2} + \frac{1}{2n} \right. \\
& \left. + \log(n) + \gamma - 1 \right) - H_{(2,0)}(2) + H_{(3,0),(1,0)}(1) - H_{(3,0),(3,0)}(1) - H_{(3,0),(3,1)}(1) \\
& + H_{(3,1),(1,0)}(1) - 2H_{(3,1),(3,0)}(1) - 2H_{(3,1),(3,1)}(1) - \frac{101}{1458n^3} + \frac{19}{108n^2} - \frac{11}{18n} \\
& - \log(n) - \gamma + 3.
\end{aligned}$$

Since we know the expansion of $S_{1,1}(n)$ (see Section 2.8) we can combine all these expansions and end up at the asymptotic expansion of $S_{(3,1,1),(3,2,1)}(n)$ up to order 3:

$$\begin{aligned}
& \frac{\frac{29}{162} - \frac{1}{108} H_{(2,0)}(2)}{n^2} + H_{(3,0)}(1) \left(-\frac{1}{3} H_{(2,0)}(2) + \frac{1}{3} H_{(3,1)}(1) + \frac{1}{108n^2} - \frac{1}{18n} - \frac{1}{9} (\log(n) + \gamma) \right. \\
& \left. + \frac{2}{3} \right) + (\log(n) + \gamma) \left(\frac{1}{9} H_{(2,0)}(2) + \frac{10}{729n^3} - \frac{11}{324n^2} + \frac{5}{54n} - \frac{1}{6} \right) + H_{(3,1)}(1) \left(\frac{10}{243n^3} \right. \\
& \left. - \frac{1}{12n^2} + \frac{1}{6n} + \frac{1}{9} (\log(n) + \gamma) - \frac{1}{6} \right) + \frac{\frac{1}{18} H_{(2,0)}(2) - \frac{25}{108}}{n} - \frac{2}{3} H_{(3,0)}(1)^2 + \frac{1}{3} H_{(3,1)}(1)^2 \\
& - \frac{1}{6} H_{(2,0)}(2) + H_{(3,0),(3,0)}(1) + \frac{1}{3} H_{(3,0),(3,1)}(1) - \frac{1}{3} H_{(3,1),(1,0)}(1) + H_{(3,1),(3,0)}(1)
\end{aligned}$$

$$+\frac{2}{3}\mathbf{H}_{(3,1),(3,1)}(1) - \frac{2285}{17496n^3} + \frac{1}{18}(\log(n) + \gamma)^2 - \frac{\zeta_2}{18}.$$

Example 4.8.14 (Example 4.8.12 continued). *The asymptotic expansion of $S_{(3,1,2),(1,0,1)}(n)$ up to order 3 yields*

$$\begin{aligned} & -\frac{1}{3}\zeta_2\mathbf{H}_{(2,0)}(2) + \frac{2}{3}\mathbf{H}_{(2,0)}(2)\mathbf{H}_{(3,0),(0,0)}(1) + \frac{1}{3}\mathbf{H}_{(2,0)}(2)\mathbf{H}_{(3,1),(0,0)}(1) \\ & + \frac{2}{3}\mathbf{H}_{(3,0),(0,0),(1,0)}(1) + \mathbf{H}_{(3,0),(1,0),(0,0)}(1) - \frac{2}{3}\mathbf{H}_{(3,0),(3,0),(0,0)}(1) - \frac{1}{3}\mathbf{H}_{(3,0),(3,1),(0,0)}(1) \\ & + \frac{1}{3}\mathbf{H}_{(3,1),(0,0),(1,0)}(1) + \mathbf{H}_{(3,1),(1,0),(0,0)}(1) - \frac{4}{3}\mathbf{H}_{(3,1),(3,0),(0,0)}(1) - \frac{2}{3}\mathbf{H}_{(3,1),(3,1),(0,0)}(1) \\ & + \frac{47}{972n^3} - \frac{1}{108n^2} + \left(-\frac{11}{162n^3} + \frac{5}{54n^2} - \frac{1}{9n}\right)(\log(n) + \gamma) - \frac{1}{9n} + \frac{\zeta_3}{3}. \end{aligned}$$

Note that the arising constants in the final result are not yet reduced with respect to the relations given in Section 4.7.1.

Chapter 5

Cyclotomic S-Sums

In this chapter we will extend the definition of harmonic sums once more. We will consider *cyclotomic S-sums*, which will unify the two already treated extensions, i.e., S-sums and cyclotomic harmonic sums are subsets of the *cyclotomic S-sums* as indicated in Figure 5.1.

5.1 Definition and Structure of Cyclotomic S-Sums

Definition 5.1.1 (Cyclotomic S-Sums). *Let $a_i, c_i, n, k \in \mathbb{N}, b_i \in \mathbb{N}_0$, with $a_i > b_i$ and $x_i \in \mathbb{R}^*$ for $i \in \{1, 2, \dots, k\}$. We define*

$$\begin{aligned} S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n) &= \\ &= \sum_{i_1 \geq i_2, \dots, i_k \geq 1} \frac{x_1^{i_1}}{(a_1 i_1 + b_1)^{c_1}} \frac{x_2^{i_2}}{(a_2 i_2 + b_2)^{c_2}} \cdots \frac{x_k^{i_k}}{(a_k i_k + b_k)^{c_k}} \end{aligned}$$

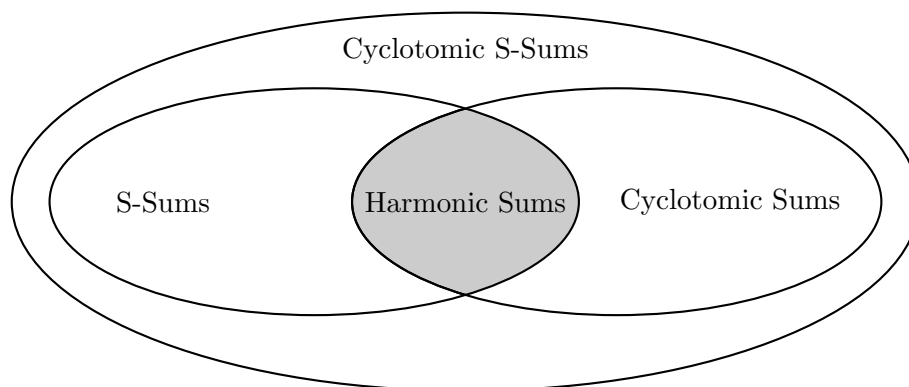


Figure 5.1: Relations between the different extensions of harmonic sums.

$$= \sum_{i_1=1}^n \frac{x_1^{i_1}}{(a_1 i_1 + b_1)^{c_1}} \sum_{i_2=1}^{i_1} \frac{x_2^{i_2}}{(a_2 i_2 + b_2)^{c_2}} \cdots \sum_{i_k=1}^{i_{k-1}} \frac{x_k^{i_k}}{(a_k i_k + b_k)^{c_k}}.$$

k is called the depth and $w = \sum_{i=0}^k c_i$ is called the weight of the cyclotomic S-sum $S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n)$.

For later use we define the following set

$$\mathcal{CS}(n) = \{q(s_1, \dots, s_r) \mid r \in \mathbb{N}; s_i \text{ a cyclotomic S-sum at } n; q \in \mathbb{R}[x_1, \dots, x_r]\};$$

note that $\mathcal{CS}(n) \supseteq \mathcal{C}(n) \supseteq \mathcal{S}(n)$ as introduced on pages 142 and 25.

5.1.1 Product

The product of harmonic sums can be generalized to *cyclotomic S-sums*. It turns out that they form again a quasi-shuffle algebra.

Theorem 5.1.2. *Let $a_i, c_i, d_i, f_i, k, l \in \mathbb{N}, b_i, e_i, n \in \mathbb{N}_0$ and $x_i, y_i \in \mathbb{R}^*$. If $a_1 e_1 \neq d_1 b_1$, we have*

$$\begin{aligned} & S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(y_1, y_2, \dots, y_l; n) = \\ & \sum_{i=1}^n \frac{x_1^i S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; i) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(y_1, \dots, y_l; i)}{(a_1 i + b_1)^{c_1}} \\ & + \sum_{i=1}^n \frac{y_1^i S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i)}{(d_1 i + e_1)^{f_1}} \\ & - \sum_{i=1}^n \left((-1)^{c_1} \sum_{j=1}^{c_1} (-1)^j \binom{c_1 + f_1 - j - 1}{f_1 - 1} \frac{a_1^{f_1} d_1^{c_1 - j}}{a_1 e_1 - d_1 b_1} \frac{1}{(a_1 i + b_1)^j} \right. \\ & \quad \left. + (-1)^{f_1} \sum_{j=1}^{f_1} (-1)^j \binom{c_1 + f_1 - j - 1}{f_1 - 1} \frac{a_1^{f_1 - j} d_1^{c_1}}{d_1 b_1 - a_1 e_1} \frac{1}{(d_1 i + e_1)^j} \right) \\ & S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i), \end{aligned}$$

and if $a_1 e_1 = d_1 b_1$ we have

$$\begin{aligned} & S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(y_1, y_2, \dots, y_l; n) = \\ & \sum_{i=1}^n \frac{x_1^i S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; i) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(y_1, \dots, y_l; i)}{(a_1 i + b_1)^{c_1}} \\ & + \sum_{i=1}^n \frac{y_1^i S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i)}{(d_1 i + e_1)^{f_1}} \\ & - \frac{a_1^{f_1}}{d_1^{f_1}} \sum_{i=1}^n \frac{x_1^i y_1^i S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i)}{(a_1 i + b_1)^{c_1 + f_1}}. \end{aligned}$$

Proof. From the identity

$$\sum_{i=1}^n \sum_{j=1}^n a_{ij} = \sum_{i=1}^n \sum_{j=1}^i a_{ij} + \sum_{j=1}^n \sum_{i=1}^j a_{ij} - \sum_{i=1}^n a_{ii}$$

we get immediately

$$\begin{aligned} & S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(y_1, y_2, \dots, y_l; n) = \\ & \sum_{i=1}^n \frac{x_1^i S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; i) S_{(d_1, e_1, f_1), \dots, (d_l, e_l, f_l)}(y_1, \dots, y_l; i)}{(a_1 i + b_1)^{c_1}} \\ & + \sum_{i=1}^n \frac{y_1^i S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i)}{(d_1 i + e_1)^{f_1}} \\ & - \sum_{i=1}^n \frac{(x_1 y_1)^i S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i)}{(a_1 i + b_1)^{c_1} (d_1 i + e_1)^{f_1}}. \end{aligned}$$

Using Lemma 4.1.2 we get the results. \square

5.1.2 Synchronization

In this subsection we consider cyclotomic S-sums with upper summation limit $n + c$, kn and $kn + c$ for $c \in \mathbb{Z}$ and $k \in \mathbb{N}$.

Lemma 5.1.3. *Let $a_i, c_i, n, k, c \in \mathbb{N}, b_i \in \mathbb{N}_0$ and $x_i \in \mathbb{R}^*$ for $i \in (1, 2, \dots, k)$. Then for $n \geq 0$*

$$\begin{aligned} & S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n + c) = S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; n) \\ & + \sum_{j=1}^c \frac{x_1^{j+n} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; n + j)}{(a_1(j + n) + b_1)^{c_1}}, \end{aligned}$$

and $n \geq c$,

$$\begin{aligned} & S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n - c) = S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; n) \\ & + \sum_{j=1}^c \frac{x_1^{j+n-c} S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; n - c + j)}{(a_1(j + n - c) + b_1)^{c_1}}. \end{aligned}$$

Given a cyclotomic S-sum of the form $S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; n + c)$ with $c \in \mathbb{Z}$, we can apply the previous lemma recursively in order to synchronize the upper summation limit of the arising cyclotomic S-sums to n .

Lemma 5.1.4. For $a, c, k \in \mathbb{N}, b \in \mathbb{N}_0, x \in \mathbb{R}^*, k \geq 2$:

$$S_{(a,b,c)}(x; k \cdot n) = \sum_{i=0}^{k-1} \frac{1}{x^i} S_{(k \cdot a, b - a \cdot i, c)}(x^k; n).$$

Proof.

$$\begin{aligned} S_{(a,b,c)}(x; k \cdot n) &= \sum_{j=1}^{k \cdot n} \frac{x^j}{(aj + b)^c} = \\ &= \sum_{j=1}^n \frac{x^{kj}}{(a(k \cdot j) + b)^c} + \sum_{j=1}^n \frac{x^{k(j-1)}}{(a(k \cdot j - 1) + b)^c} + \cdots + \sum_{j=1}^n \frac{x^{k(j-(k-1))}}{(a(k \cdot j - (k-1)) + b)^c} \\ &= \sum_{j=1}^n \frac{x^{kj}}{((ak)j + b)^c} + \sum_{j=1}^n \frac{x^{kj} x^{-1}}{((ak)j + (b-a))^c} + \cdots + \sum_{j=1}^n \frac{x^{kj} x^{-(k-1)}}{((ak)j + (b - (k-1)a))^c} \\ &= \sum_{i=0}^{k-1} \frac{1}{x^i} S_{(k \cdot a, b - a \cdot i, c)}(x^k; n). \end{aligned}$$

□

Theorem 5.1.5. For $a_i, c_i, m, k \in \mathbb{N}, b_i, n \in \mathbb{N}_0, x \in \mathbb{R}^*, k \geq 2$:

$$\begin{aligned} S_{(a_m, b_m, c_m), (a_{m-1}, b_{m-1}, c_{m-1}), \dots, (a_1, b_1, c_1)}(x_m, \dots, x_1; k \cdot n) = \\ \sum_{i=0}^{m-1} \sum_{j=1}^n \frac{S_{(a_{m-1}, b_{m-1}, c_{m-1}), \dots, (a_1, b_1, c_1)}(x_{m-1}, \dots, x_1; k \cdot j - i) x_m^{k \cdot j - i}}{(a_m(k \cdot j - i) + b_1)^{c_1}}. \end{aligned}$$

After applying Theorem 5.1.5 we can synchronize the cyclotomic S-sums in the inner sum with upper summation limit $k \cdot j - i$ to the upper summation limit $k \cdot j$. Now we can apply Theorem 5.1.5 to these sums. Repeated application of this procedure leads to cyclotomic S-sums with upper summation limit n .

Remark 5.1.6. Like for cyclotomic harmonic sums the synchronization of the upper summation limit leads again to multiple argument relations and as a special case to duplication relations, and since cyclotomic S-sums form a quasi shuffle algebra, there are again algebraic relations.

5.2 Integral Representation of Cyclotomic Harmonic S-Sums

Lemma 5.2.1. *Let $a, c \in \mathbb{N}$, $b \in \mathbb{N}_0$, $d \in \mathbb{R}^*$ and $n \in \mathbb{N}$; then*

$$\begin{aligned}
 S_{(a,b,1)}(d; n) &= \int_0^1 \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - \frac{1}{d}} dx_1 \\
 S_{(a,b,2)}(d; n) &= \int_0^1 \frac{1}{x_2} \int_0^{x_2} \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - \frac{1}{d}} dx_1 dx_2 \\
 S_{(a,b,c)}(d; n) &= \int_0^1 \frac{1}{x_c} \int_0^{x_c} \frac{1}{x_{c-1}} \dots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - \frac{1}{d}} dx_1 dx_2 \dots dx_c.
 \end{aligned}$$

Let us now look at the integral representation of cyclotomic S-sums of higher depths. We consider the sum $S_{(a_1,b_1,c_1),(a_2,b_2,c_2),\dots,(a_k,b_k,c_k)}(x_1, x_2, \dots, x_k; n)$ and apply Lemma 5.2.1 to the innermost sum ($a = a_k, b = b_k, c = c_k, d = x_k$). One now may perform the next sum in the same way, provided $a_{k-1} | a_k$. At this point we may need the fact:

$$\sum_{i=1}^n \frac{(dy^a)^i}{(ai + b)^c} = \frac{1}{y^b} \int_0^y \frac{1}{x_c} \int_0^{x_c} \frac{1}{x_{c-1}} \dots \int_0^{x_3} \frac{1}{x_2} \int_0^{x_2} \frac{x_1^{a+b-1} (d^n x_1^{an} - 1)}{x_1^a - \frac{1}{d}} dx_1 \dots dx_c$$

for $n, a, b, c, k \in \mathbb{N}$ and $d, y \in \mathbb{R}$. If $a_{k-1} \nmid a_k$, one transforms the integration variables such that the next denominator can be generated, etc. In this way, the sum $S_{(a_1,b_1,c_1),(a_2,b_2,c_2),\dots,(a_k,b_k,c_k)}(x_1, x_2, \dots, x_k; n)$ can be represented in terms of linear combinations of iterated integrals.

Let us illustrate the principle steps in case of the following example :

$$S_{(3,2,2),(2,1,1)}\left(\frac{1}{3}, 2; n\right) = \sum_{k=1}^n \frac{\frac{1}{3}^k}{(3k + 2)^2} \sum_{l=1}^k \frac{2^l}{(2l + 1)}.$$

The first sum yields

$$S_{(3,2,2),(2,1,1)}\left(\frac{1}{3}, 2; n\right) = \sum_{k=1}^n \int_0^1 \frac{\frac{1}{3}^k}{(3k + 2)^2} \frac{x^2((2x^2)^k - 1)}{x^2 - \frac{1}{2}} dx.$$

Setting $x = y^3$ one obtains

$$\begin{aligned}
 S_{(3,2,2),(2,1,1)}\left(\frac{1}{3}, 2; n\right) &= 12 \int_0^1 \frac{y^8}{y^6 - \frac{1}{2}} \sum_{k=1}^n \frac{\left(\frac{2y^6}{3}\right)^k - \left(\frac{1}{3}\right)^k}{(6k + 4)^2} dy \\
 &= 12 \int_0^1 \frac{y^4}{y^6 - \frac{1}{2}} \left\{ \int_0^y \frac{1}{z} \int_0^z t^9 \frac{\left(\frac{2t^6}{3}\right)^n - 1}{t^6 - \frac{3}{2}} dt dz \right.
 \end{aligned}$$

$$-y^4 \int_0^1 \frac{1}{z} \int_0^z t^9 \frac{\left(\frac{t^6}{3}\right)^n - 1}{t^6 - 3} dt dz \Bigg\} dy.$$

Due to the pole at $y^6 = \frac{1}{2}$ we cannot split the integral as we did in (4.11).

5.3 Cyclotomic S-Sums at Infinity

As in the case of S-sums we want to give conditions for convergence of cyclotomic harmonic S-sums. Of course, not all cyclotomic S-sums are finite at infinity, since for example $\lim_{n \rightarrow \infty} S_{(2,1,1)}(2; n)$ does not exist. In fact, we have the following theorem, compare Theorem 3.7.1 and Lemma 2.7.1:

Theorem 5.3.1. *Let $a_1, \dots, a_k, c_1, \dots, c_k \in \mathbb{N}, b_1, \dots, b_k \in \mathbb{N}_0$ and $x_1, x_2, \dots, x_k \in \mathbb{R} \setminus \{0\}$ for $k \in \mathbb{N}$. The cyclotomic S-sum $S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n)$ is absolutely convergent, when $n \rightarrow \infty$, if and only if one of the following conditions holds:*

1. $|x_1| < 1 \wedge |x_1 x_2| \leq 1 \wedge \dots \wedge |x_1 x_2 \cdots x_k| \leq 1,$
2. $c_1 > 1 \wedge |x_1| = 1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_k| \leq 1.$

In addition the cyclotomic S-sum is conditional convergent (convergent but not absolutely convergent) if and only if

3. $c_1 = 1 \wedge x_1 = -1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_k| \leq 1.$

The proof of this theorem is in principle analogue to the proof of Theorem 3.7.1.

Remark 5.3.2. *The relations for cyclotomic harmonic sums at infinity carry over to cyclotomic S-sums: we have algebraic relations, duplication and multiple argument relations (see Remark 5.1.6), and even the shuffle algebra relations carry over using Theorem 5.4.4.*

5.4 Summation of Cyclotomic S-Sums

With the summation techniques presented in [24], definite multi-sums (in particular certain Feynman integrals transformed to such sums [26]) can be simplified to indefinite nested sum expressions; similarly, such Feynman integrals can be simplified to such formats by using the techniques presented in Chapter 7. Then one of the crucial steps for further processing is the transformation of these sums to harmonic sums, S-sums, cyclotomic sums or most generally to cyclotomic S-sums.

This section follows the ideas of Chapter 5 of [1], however it is more general since it deals with cyclotomic S-sums instead of harmonic sums. With the package `Sigma` [79] we can simplify nested sums such that the nested depth is optimal and the degree of the denominator is minimal. This is possible due to a refined summation theory [82, 80] of $\Pi\Sigma$ -fields [51]. In the following we want to find sum representations of such simplified nested sums in terms of cyclotomic S-sums as much as it is possible. Inspired by [76] for harmonic numbers and [62, 85] we consider sums of the form

$$\sum_{i=1}^n s r(i) \quad (5.1)$$

where $s \in \mathcal{CS}(i)$ or $s \in \mathcal{CS}(i)[x_1^i, \dots, x_k^i]$ with $x_j \in \mathbb{R}$ and $r(i)$ is a rational function in i . We can use the quasi-shuffle algebra property of the cyclotomic S-sums to split such sums into sums of the form

$$\sum_{i=1}^n x^i r(i) S_a(\mathbf{b}; i) \quad (5.2)$$

where $r(i)$ is a rational function in i and $x \in \mathbb{R}$.

In this chapter we will present formulas to rewrite sums of the form (5.2) and we will show how we can use these formulas in combination with `Sigma`. In the following we consider the problem:

Given: a sum σ of the form (5.1).

Find: as much as possible a representation of σ in terms of cyclotomic S-sums.

5.4.1 Polynomials in the Summand

First we consider the case that $r(i)$ is a polynomial in $\mathbb{Z}[i]$, i.e., $r(i) = p_m i^m + \dots + p_1 i + p_0$ with $p_k \in \mathbb{Z}$. If we are able to work out the sum for any power of i times a cyclotomic S-sum (i.e., $\sum_{i=1}^n x^i i^m S_a(\mathbf{b}; i)$, $m \in \mathbb{N}$), we can work out the sum for each polynomial $r(i)$.

Theorem 5.4.1. *Let $k, n \in \mathbb{N}$ and $a_i, c_i \in \mathbb{N}, b_i \in \mathbb{N}_0$ with $a_i > b_i$ and $x, x_i \in \mathbb{R}^*$.*

Then

$$\begin{aligned} \sum_{i=1}^n x^i i^k S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots}(x_1, x_2, \dots; i) = \\ S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots}(x_1, x_2, \dots; n) \sum_{i=1}^n x^i i^k \\ - \sum_{j=1}^n \frac{x_1^j S_{(a_2, b_2, c_2), \dots}(x_2, \dots; i)}{(a_1 j + b_1)^{c_1}} \sum_{i=1}^{j-1} x^i i^k. \end{aligned}$$

Proof.

$$\begin{aligned}
\sum_{i=1}^n x^i i^k S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots}(x_1, x_2, \dots; i) &= \tag{5.3} \\
&= \sum_{i=1}^n x^i i^k \sum_{j=1}^i \frac{x_1^j S_{(a_2, b_2, c_2), \dots}(x_2, \dots; j)}{(a_1 j + b_1)^{c_1}} \\
&= \sum_{j=1}^n \frac{x_1^j S_{(a_2, b_2, c_2), \dots}(x_2, \dots; j)}{(a_1 j + b_1)^{c_1}} \sum_{i=j}^n x^i i^k \\
&= \sum_{j=1}^n \frac{x_1^j S_{(a_2, b_2, c_2), \dots}(x_2, \dots; j)}{(a_1 j + b_1)^{c_1}} \left(\sum_{i=1}^n x^i i^k - \sum_{i=1}^{j-1} x^i i^k \right) \\
&= S_{(a_1, b_1, c_1), (a_2, b_2, c_2), \dots}(x_1, x_2, \dots; n) \sum_{i=1}^n x^i i^k \\
&\quad - \sum_{j=1}^n \frac{x_1^j S_{(a_2, b_2, c_2), \dots}(x_2, \dots; j)}{(a_1 j + b_1)^{c_1}} \sum_{i=1}^{j-1} x^i i^k.
\end{aligned}$$

□

The sums $\sum_{i=1}^{j-1} x^i i^k$ can be expressed as a polynomial in j , together with a factor $(x)^j$. Hence we can apply partial fraction decomposition on

$$\frac{x_1^j S_{(a_2, b_2, c_2), \dots}(x_2, \dots; j)}{(a_1 j + b_1)^{c_1}} \sum_{i=1}^{j-1} x^i i^k$$

after applying Theorem 5.4.1. The result can be rewritten in cyclotomic S-sums easily. Summarizing, we can always work out the sums $\sum_{i=1}^n x^i r(i) S_{\mathbf{a}}(\mathbf{b}; i)$ where $r(i)$ is a polynomial in i and $x \in \mathbb{R}$; the result will be a combination of cyclotomic S-sums in the upper summation index n , rational functions in n and the factor x^n .

5.4.2 Rational Functions in the Summand

If we want to work out sums of the form (5.2) for a general rational function $r(n) = \frac{p(n)}{q(n)}$, where $p(n)$ and $q(n)$ are polynomials, we can proceed as follows:

If the degree of p is greater than the degree of q , we compute by polynomial division polynomials $\bar{r}(n)$ and $\bar{p}(n)$ such that $r(n) = \bar{r}(n) + \frac{\bar{p}(n)}{q(n)}$ and the degree of $\bar{p}(n)$ is smaller than the degree of q . We split the sum into two parts, *i.e.*, into

$$\sum_{i=1}^n x^i r(i) S_{\mathbf{a}}(\mathbf{b}; i) = \sum_{i=1}^n x^i \bar{r}(i) S_{\mathbf{a}}(\mathbf{b}; i) + \sum_{i=1}^n x^i \frac{\bar{p}(i)}{q(i)} S_{\mathbf{a}}(\mathbf{b}; i).$$

The first sum can be done using Theorems 5.4.1. For the second sum we proceed as follows:

1. Factorize the denominator $q(i)$ over \mathbb{Q} .
2. Let A be the product of all factors of the form $(ai + b)^c$ with $a, c \in \mathbb{N}$ and $b \in \mathbb{Z}$, and let B be the product of all remaining factors such that $A(i)B(i) = q(i)$.
3. For example with the extended Euclidean algorithm we compute polynomials $s(i)$ and $t(i)$ such that $s(i)A(i) + t(i)B(i) = \bar{p}(i)$. This is always possible since A and B are relatively prime. Hence we get

$$\frac{\bar{p}}{q} = \frac{t}{A} + \frac{s}{B}.$$

4. Split the sum into two sums, each sum over one fraction, *i.e.*,

$$\sum_{i=1}^n x^i \frac{\bar{p}(i)}{q(i)} S_a(\mathbf{b}; i) = \sum_{i=1}^n x^i \frac{t}{A} S_a(\mathbf{b}; i) + \sum_{i=1}^n x^i \frac{s}{B} S_a(\mathbf{b}; i).$$

5. The sum with the denominator B remains untouched (for details see Remark 5.4.2). We can now do a complete partial fraction decomposition to the first summand and split the sum such that we sum over each fraction separately.
6. Each of these new sums can be expressed in terms of cyclotomic S-sums following Subsection 5.4.1.
7. We end up in a combination of rational functions in n , cyclotomic S-sums with upper index n , the factor x^n and perhaps a sum over the fraction with denominator B .

Remark 5.4.2. *In our implementation the sum $\sum_{i=1}^n \frac{s}{B} S_a(i)$ is passed further to Schneider's *Sigma* package. The underlying difference field and difference ring algorithms [82, 81, 80] can simplify those sums further to sum expressions where the denominator has minimal degree. The result of *Sigma* is again passed to the package *HarmonicSums*. If possible, it finds a closed form in terms of cyclotomic S-sums.*

5.4.3 Two Cyclotomic S-sums in the Summand

Lemma 5.4.3. *Let $a_1, a_2, c_1, c_2, i \in \mathbb{N}, b_1, b_2 \in \mathbb{N}_0$. If $a_1 b_2 \neq a_2 b_1$, we have*

$$\frac{1}{(a_1(i_1 - i_2) + b_1)^{c_1} (a_2 i_2 + b_2)^{c_2}} =$$

$$\begin{aligned} & \sum_{j=1}^{c_1} \binom{c_1 + c_2 - j - 1}{c_2 - 1} \frac{a_1^{c_2} a_2^{c_1 - j}}{(a_1 b_2 + a_2 b_1 + i_1 a_1 a_2)^{c_1 + c_2 - j}} \frac{1}{(a_1(i_1 - i_2) + b_1)^j} \\ & + \sum_{j=1}^{c_2} \binom{c_1 + c_2 - j - 1}{c_1 - 1} \frac{a_1^{c_2 - j} a_2^{c_1}}{(a_1 b_2 + a_2 b_1 + i_1 a_1 a_2)^{c_1 + c_2 - j}} \frac{1}{(a_2 i_2 + b_2)^j}, \end{aligned}$$

and if $a_1 b_2 = a_2 b_1$ we have

$$\frac{1}{(a_1 i + b_1)^{c_1} (a_2 i + b_2)^{c_2}} = \left(\frac{a_1}{a_2}\right)^{c_2} \frac{1}{(a_1 i + b_1)^{c_1 + c_2}}.$$

Theorem 5.4.4. Let $a_i, c_i, d_i, f_i, k, l, n \in \mathbb{N}, b_i, e_i \in \mathbb{N}_0, a_i > b_i, d_i > e_i$, and $x_i, y_i \in \mathbb{R}^*$. Then

$$\begin{aligned} & \sum_{i=1}^n \frac{S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, \dots, x_k; n - i) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i) y_1^i}{(d_1 i + e_1)^{f_1}} = \\ & \sum_{k=1}^{f_1} \binom{c_1 + f_1 - k - 1}{c_1 - 1} a_1^{f_1 - k} d_1^{c_1} \sum_{i=1}^n \frac{x_1^i}{(d_1 b_1 + a_1 e_1 + i a_1 d_1)^{c_1 f_1 - k}} \\ & \sum_{j=1}^{i-1} \frac{S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; i - j) S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; j) \frac{y_1^j}{x_1^j}}{(d_1 j + e_1)^k} \\ & + \sum_{k=1}^{c_1} \binom{c_1 + f_1 - k - 1}{c_2 - 1} a_1^{f_1} d_1^{c_1 - k} \sum_{i=1}^n \frac{y_1^i}{(d_1 b_1 + a_1 e_1 + i a_1 d_1)^{c_1 f_1 - k}} \\ & \sum_{j=1}^{i-1} \frac{S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, \dots, y_l; i - j) S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, \dots, x_k; j) \frac{x_1^j}{y_1^j}}{(a_1 j + b_1)^k}. \end{aligned}$$

Proof. We use the following abbreviations:

$$\begin{aligned} S_1(n) &= S_{(a_1, b_1, c_1), \dots, (a_k, b_k, c_k)}(x_1, x_2, \dots, x_k; n) \\ \bar{S}_1(n) &= S_{(a_2, b_2, c_2), \dots, (a_k, b_k, c_k)}(x_2, x_3, \dots, x_k; n) \\ S_2(n) &= S_{(d_2, e_2, f_2), \dots, (d_l, e_l, f_l)}(y_2, y_3, \dots, y_l; n). \end{aligned}$$

We have

$$\begin{aligned} \sum_{i=1}^n \frac{S_1(n - i) S_2(i) y_1^i}{(d_1 i + e_1)^{f_1}} &= \sum_{i=1}^n \sum_{j=1}^{n-i} \frac{\bar{S}_1(j) S_2(i) y_1^i}{(a_1 j + b_1)^{c_1} (d_1 i + e_1)^{f_1}} \\ &= \sum_{i=1}^n \sum_{j=i+1}^n \frac{\bar{S}_1(j - i) S_2(i) y_1^i}{(a_1(j - i) + b_1)^{c_1} (d_1 i + e_1)^{f_1}} \\ &= \sum_{j=1}^n \sum_{i=1}^{j-1} \frac{\bar{S}_1(j - i) S_2(i) y_1^i}{(a_1(j - i) + b_1)^{c_1} (d_1 i + e_1)^{f_1}} \end{aligned}$$

$$= \sum_{i=1}^n \sum_{j=1}^{i-1} \frac{\bar{S}_1(i-j)S_2(i)y_1^j}{(a_1(i-j) + b_1)^{c_1}(d_1j + e_1)^{f_1}}.$$

Now we use Lemma 5.4.3 and complete the proof:

$$\begin{aligned} \sum_{i=1}^n \sum_{j=1}^{i-1} \frac{\bar{S}_1(i-j)S_2(i)y_1^j}{(a_1(i-j) + b_1)^{c_1}(d_1j + e_1)^{f_1}} = \\ \sum_{k=1}^{f_1} \binom{c_1 + f_1 - k - 1}{c_1 - 1} a_1^{f_1-k} d_1^{c_1} \sum_{i=1}^n \frac{x_1^i}{(d_1b_1 + a_1e_1 + ia_1d_1)^{c_1f_1-k}} \sum_{j=1}^{i-1} \frac{\bar{S}_1(i-j)S_2(j)\left(\frac{y_1}{x_1}\right)^j}{(d_1j + e_1)^k} \\ + \sum_{k=1}^{c_1} \binom{c_1 + f_1 - k - 1}{c_2 - 1} a_1^{f_1} d_1^{c_1-k} \sum_{i=1}^n \frac{y_1^i \sum_{j=1}^{i-1} \frac{S_2(i-j)\bar{S}_1(j)\left(\frac{x_1}{y_1}\right)^j}{(a_1j + b_1)^k}}{(d_1b_1 + a_1e_1 + ia_1d_1)^{c_1f_1-k}}. \end{aligned}$$

□

5.5 Reducing the Depth of Cyclotomic S-Sums

In this section we will define cyclotomic Euler-Sums (compare [41] for the depth 2 case). We will show that we can use cyclotomic Euler-Sums to express cyclotomic S-sums and thereby we are able to reduce the nested depth.

Definition 5.5.1 (Cyclotomic Euler-Sums). For $a, c, n, i, k \in \mathbb{N}; b \in \mathbb{N}_0$ and $x \in \mathbb{R}^*$ we define cyclotomic Euler-Sums of depth $d = 1$ as

$$E_{(a,b,c,x)}(n) = \sum_{i=1}^n \frac{x^i}{(ai + b)^c} = S_{(a,b,c)}(x, n)$$

and cyclotomic Euler-Sums of depth $d > 1$ as

$$E_{(a,b,c,x)}(e_1, e_2, \dots, e_k)(n) = \sum_{i=1}^n \frac{x^i e_1(i) e_2(i) \dots e_k(i)}{(ai + b)^c}$$

where $e_1(i), e_2(i), \dots, e_k(i)$ are cyclotomic Euler-Sums of depth less than d and at least one of the cyclotomic Euler-sums $e_1(i), e_2(i), \dots, e_k(i)$ has depth $d - 1$.

Example 5.5.2.

$$\begin{aligned} E_{(2,1,4,2)}(E_{(3,1,2,3)}, E_{(5,2,6,4)}(E_{(1,2,3,5)}))(n) &= \sum_{i=1}^n \frac{2^i \sum_{j=1}^i \frac{3^j}{(3j+1)^2} \sum_{j=1}^i \frac{4^j \sum_{k=1}^j \frac{5^k}{(k+2)^3}}{(5j+2)^6}}{(2i+1)^4} \\ E_{(2,1,4,2)}(E_{(3,1,2,3)}, (E_{(5,2,6,4)}), n) &= \sum_{i=1}^n \frac{2^i \sum_{j=1}^i \frac{3^j \sum_{k=1}^j \frac{4^k}{(5k+2)^6}}{(3j+1)^2}}{(2i+1)^4} \end{aligned}$$

$$= S_{(2,1,4),(3,1,2),(5,2,6)}(2, 3, 4; n).$$

Lemma 5.5.3. Consider the functions $I : \mathbb{N} \mapsto \mathbb{R}$ and $T : \mathbb{N} \mapsto \mathbb{R}$. Let $n, a_1, c_1, a_2, c_2 \in \mathbb{N}, b_1, b_2 \in \mathbb{N}_0$. Then we have:

$$\begin{aligned} \sum_{i=1}^n \frac{T(i) \sum_{j=1}^i \frac{I(j)}{(a_2j+b_2)^{c_2}}}{(a_1i+b_1)^{c_1}} &= \sum_{i=1}^n \frac{T(i)I(i)}{(a_1i+b_1)^{c_1}(a_2i+b_2)^{c_2}} - \sum_{i=1}^n \frac{I(i) \sum_{j=1}^i \frac{T(j)}{(a_1j+b_1)^{c_1}}}{(a_2i+b_2)^{c_2}} \\ &+ \sum_{i=1}^n \frac{I(i)}{(a_2i+b_2)^{c_2}} \sum_{i=1}^n \frac{T(i)}{(a_1i+b_1)^{c_1}}. \end{aligned}$$

Proof. This follows immediately from

$$\begin{aligned} \sum_{i=1}^n \frac{I(i)}{(a_2i+b_2)^{c_2}} \sum_{i=1}^n \frac{T(i)}{(a_1i+b_1)^{c_1}} &= \sum_{i=1}^n \sum_{j=1}^i \frac{I(i)T(j)}{(a_2i+b_2)^{c_2}(a_1j+b_1)^{c_1}} \\ &+ \sum_{j=1}^n \sum_{i=1}^j \frac{I(i)T(j)}{(a_2i+b_2)^{c_2}(a_1j+b_1)^{c_1}} \\ &- \sum_{i=1}^n \frac{I(i)T(i)}{(a_1i+b_1)^{c_1}(a_2i+b_2)^{c_2}}. \end{aligned}$$

□

Theorem 5.5.4. A cyclotomic S-sum of depth k can be expressed as a polynomial in $\mathbb{Q}[s_1, s_2, \dots, s_n]$ where the s_i are cyclotomic Euler-sums with depth less or equal $\log_2(k) + 1$.

Proof. For sake of simplicity and readability we will give the proof for harmonic sums only. The proof for cyclotomic S-sums would require Lemma 4.1.2 at some points, but in general the proof follows analogously. Consider the harmonic sum $S_{a_k, a_{k-1}, \dots, a_1}(n)$. We proceed by induction on the depth k .

$k = 1$: $S_{a_1}(n)$ has depth $1 \leq \log_2(1) + 1 = 1$.

$k = 2$: $S_{a_2, a_1}(n)$ has depth $2 \leq \log_2(2) + 1 = 2$.

Now let $k > 2$ and we assume that the theorem holds for all depths $\leq k$ (we will refer to this induction hypothesis by (IH1)). We want to show that the theorem holds for $k + 1$:

$$\begin{aligned} S_{a_{k+1}, a_k, \dots, a_1}(n) &= \sum_{i=1}^n \frac{S_{a_k, a_{k-1}, \dots, a_1}(i)}{i^{a_{k+1}}} \\ &\stackrel{\text{Lemma 5.5.3}}{=} \sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i)}{i^{a_{k+1}+a_k}} + \sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i)}{i^{a_k}} \sum_{i=1}^n \frac{1}{i^{a_{k+1}}} \end{aligned}$$

$$\begin{aligned}
& - \sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i) \sum_{j=1}^i \frac{1}{j^{a_{k+1}}}}{i^{a_k}} \\
= & S_{a_{k+1}+a_k, a_{k-1}, \dots, a_1}(n) + S_{a_k, a_{k-1}, \dots, a_1}(n) S_{a_{k+1}}(n) \\
& - \sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i) \sum_{j=1}^i \frac{1}{j^{a_{k+1}}}}{i^{a_k}}.
\end{aligned}$$

$S_{a_{k+1}}(n)$ has depth $1 < \log_2(k+1) + 1$. The depth of $S_{a_{k+1}+a_k, a_{k-1}, \dots, a_1}(n)$ and $S_{a_k, a_{k-1}, \dots, a_1}(n)$ is k . Using the induction hypothesis (IH1) we can express these sums by polynomials of sums with depth $\leq \log_2(k) + 1$. Since $\log_2(k) + 1 < \log_2(k+1) + 1$ it remains to show that we can express the sum

$$\sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i) \sum_{j=1}^i \frac{1}{j^{a_{k+1}}}}{i^{a_k}}$$

by polynomials of sums with depth $\leq \log_2(k+1) + 1$. Let therefore be $m \leq k$. We will show the more general statement that for $r \geq 1$, $s \geq 1$, $s \geq r$ and $r + s = m$ the sum

$$\sum_{i=1}^n \frac{S_{a_s, \dots, a_1}(i) S_{b_r, \dots, b_1}(i)}{i^c}$$

can be express by polynomials of sums with depth $\leq \log_2(m+1) + 1$. We proceed by induction on m .

$m = 2$: $\sum_{i=1}^n \frac{S_{a_1}(i) S_{b_1}(i)}{i^c}$ has depth $2 \leq \log_2(2+1) + 1$.

Now assume that the property holds for $m-1$ (we will refer to this induction hypothesis by (IH2)). We want to show that the property holds for m . We will distinguish three different cases:

s=r: Using (IH1) the sum

$$\sum_{i=1}^n \frac{S_{a_s, \dots, a_1}(i) S_{b_s, \dots, b_1}(i)}{i^c}$$

can be express by polynomials of sums with depth $\leq \log_2\left(\frac{m}{2}\right) + 1 + 1 = \log_2(m) + 1 \leq \log_2(m+1) + 1$. Hence the property holds.

s=r+1: Using (IH1) the sum

$$\sum_{i=1}^n \frac{S_{a_s, \dots, a_1}(i) S_{b_{s-1}, \dots, b_1}(i)}{i^c}$$

can be express by polynomials of sums with depth $\leq \log_2\left(\frac{m+1}{2}\right) + 1 + 1 = \log_2(m+1) + 1$. Hence the property holds.

s=r+d: For $d = 0$ and $d = 1$ see the previous cases. Suppose now the property holds for $d < \hat{d}$. We will show that the property holds for \hat{d} (we will refer to this induction hypothesis by (IH3)):

$$\begin{aligned} \sum_{i=1}^n \frac{S_{a_s, \dots, a_1}(i) S_{b_{s-\hat{d}}, \dots, b_1}(i)}{i^c} &\stackrel{\text{Lemma 5.5.3}}{=} \sum_{i=1}^n \frac{S_{a_{s-1}, \dots, a_1}(i) S_{b_{s-\hat{d}}, \dots, b_1}(i)}{i^{c+a_s}} \\ &\quad + S_{a_s, a_{s-1}, \dots, a_1}(n) S_{b_{c, s-\hat{d}}, \dots, b_1}(n) \\ &\quad - \sum_{i=1}^n \frac{S_{a_{s-1}, \dots, a_1}(i) S_{c, b_{s-\hat{d}}, \dots, b_1}(i)}{i^{a_s}}. \end{aligned}$$

Due to (IH2) the first sum can be express by polynomials of sums with depth $\leq \log_2(m - 1 + 1) + 1 \leq \log_2(m + 1) + 1$. Due to (IH1) the sum $S_{a_s, a_{s-1}, \dots, a_1}(n)$ can be express by polynomials of sums with depth $\leq \log_2(s + 1) + 1 \leq \log_2(m + 1) + 1$. Due to (IH1) the sum $S_{b_{c, s-\hat{d}}, \dots, b_1}(n)$ can be express by polynomials of sums with depth $\leq \log_2(s - \hat{d} + 1) + 1 \leq \log_2(m + 1) + 1$. Due to (IH3) the last sum can be express by polynomials of sums with depth $\leq \log_2(m + 1) + 1$. Hence the property hods for \hat{d} .

We proved that we can express the sum

$$\sum_{i=1}^n \frac{S_{a_s, \dots, a_1}(i) S_{b_r, \dots, b_1}(i)}{i^c}$$

by polynomials of sums with depth $\leq \log_2(m + 1) + 1$. Hence we can express the sum

$$\sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i) \sum_{j=1}^i \frac{1}{j^{a_k+1}}}{i^{a_k}} = \sum_{i=1}^n \frac{S_{a_{k-1}, \dots, a_1}(i) S_{a_k+1}(i)}{i^{a_k}}$$

by polynomials of sums with depth $\leq \log_2(k + 1) + 1$. This finishes the proof. □

Example 5.5.5.

$$\begin{aligned} S_{(2,1,4),(3,1,2),(5,2,6)}(2, 3, 4, n) &= 432 \sum_{i=1}^n \frac{6^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{2i+1} + 108 \sum_{i=1}^n \frac{6^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{(2i+1)^2} \\ &\quad + 24 \sum_{i=1}^n \frac{6^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{(2i+1)^3} + 4 \sum_{i=1}^n \frac{6^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{(2i+1)^4} - 648 \sum_{i=1}^n \frac{6^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{3i+1} \\ &\quad + \sum_{i=1}^n \frac{2^i}{(2i+1)^4} \sum_{i=1}^n \frac{3^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{(3i+1)^2} + 81 \sum_{i=1}^n \frac{6^i \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{(3i+1)^2} \\ &\quad - \sum_{i=1}^n \frac{3^i \sum_{j=1}^i \frac{2^j}{(2j+1)^4} \sum_{j=1}^i \frac{4^j}{(5j+2)^6}}{(3i+1)^2} \\ &= 432E_{(2,1,1,6)}(E_{(5,2,6,4)})(n) + 108E_{(2,1,2,6)}(E_{(5,2,6,4)})(n) \\ &\quad + 24E_{(2,1,3,6)}(E_{(5,2,6,4)})(n) + 4E_{(2,1,4,6)}(E_{(5,2,6,4)})(n) \end{aligned}$$

$$\begin{aligned}
& -648E_{(3,1,1,6)}(E_{(5,2,6,4)})(n) + E_{(2,1,4,2)}(n)E_{(3,1,2,3)}(E_{(5,2,6,4)})(n) \\
& +81E_{(3,1,2,6)}(E_{(5,2,6,4)})(n) - E_{(3,1,2,3)}(E_{(5,2,6,4)}, E_{(2,1,4,2)})(n).
\end{aligned}$$

Remark 5.5.6. In *Sigma* indefinite nested sums and products are represented in so-called depth-optimal $\Pi\Sigma^*$ -extensions [80], i.e., the sums are represented with respect to optimal nesting depth [82]. The underlying algorithm of Theorem 5.5.4 supports *Sigma* in this representation, and might lead for various instances to more sufficient algorithms.

Remark 5.5.7. We mention that the reversed direction, i.e., transforming Euler sums to cyclotomic S-sums can be achieved with the method presented in Section 5.4.

Chapter 6

The Package HarmonicSums

This chapter is dedicated to the presentation of the basic features of the package `HarmonicSums` which was developed [1] and which was extended and generalized in the frame of this thesis. All the algorithms for harmonic sums, S-sums, cyclotomic harmonic sums, cyclotomic S-sums, harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms which were presented in the previous chapters of this thesis have been implemented. This chapter contains a whole Mathematica session that runs throughout the sections. The inputs are given in the way how one has to type them into Mathematica and the outputs are displayed as Mathematica gives them back. We start the session by loading the package:

HarmonicSums session.

```
In[1]:= << HarmonicSums.m
```

```
HarmonicSums by Jakob Ablinger -RISC Linz- Version 1.0 (01/03/12)
```

Defintion of the Nested Sums

Harmonic sums, S-sums, cyclotomic harmonic sums and cyclotomic S-sums are denoted by the letter `S` as we can see in the following examples.

The command `ToHarmonicSumsSum` yields the definition of the sums.

HarmonicSums session.

```
In[2]:= S[1, 2, 3, 4, n]//ToHarmonicSumsSum
```

$$\text{Out[2]} = \sum_{\iota_1=1}^n \frac{\sum_{\iota_2=1}^{\iota_1} \frac{\sum_{\iota_3=1}^{\iota_2} \frac{\sum_{\iota_4=1}^{\iota_3} \frac{1}{\iota_4}}{\iota_3}}{\iota_2}}{\iota_1}$$

```
In[3]:= S[1, 2, 3, {2, 1/3, 4}, n]//ToHarmonicSumsSum
```

$$\text{Out[3]} = \sum_{\iota_1=1}^n \frac{2^{\iota_1} \sum_{\iota_2=1}^{\iota_1} \frac{3^{-\iota_2} \sum_{\iota_3=1}^{\iota_2} \frac{4^{\iota_3}}{\iota_3^2}}{\iota_2^2}}{\iota_1}$$

In[4]:= S[{{3, 2, 1}, {4, 1, 2}, {2, 0, -2}}, n]//ToHarmonicSumsSum

$$\text{Out[4]} = \sum_{\iota_1=1}^n \frac{\sum_{\iota_2=1}^{\iota_1} \frac{\sum_{\iota_3=1}^{\iota_2} \frac{(-1)^{\iota_3}}{4\iota_3^2}}{(4\iota_2+1)^2}}{3\iota_1+2}$$

In[5]:= S[{{3, 2, 1}, {4, 1, 2}, {2, 0, -2}}, {2, 1/3, 4}, n]//ToHarmonicSumsSum

$$\text{Out[5]} = \sum_{\iota_1=1}^n \frac{2^{\iota_1} \sum_{\iota_2=1}^{\iota_1} \frac{3^{-\iota_2} \sum_{\iota_3=1}^{\iota_2} 4^{\iota_3+1} \iota_3^2}{(4\iota_2+1)^2}}{3\iota_1+2}$$

Note that for internal reasons, sometimes the name **CS** is used to denote cyclotomic harmonic sums and cyclotomic S-sums.

HarmonicSums session.

In[6]:= CS[{{3, 2, 1}, {4, 1, 2}, {2, 0, -2}}, n]//ToHarmonicSumsSum

$$\text{Out[6]} = \sum_{\iota_1=1}^n \frac{\sum_{\iota_2=1}^{\iota_1} \frac{\sum_{\iota_3=1}^{\iota_2} \frac{(-1)^{\iota_3}}{4\iota_3^2}}{(4\iota_2+1)^2}}{3\iota_1+2}$$

In[7]:= CS[{{3, 2, 1}, {4, 1, 2}, {2, 0, -2}}, {2, 1/3, 4}, n]//ToHarmonicSumsSum

$$\text{Out[7]} = \sum_{\iota_1=1}^n \frac{2^{\iota_1} \sum_{\iota_2=1}^{\iota_1} \frac{3^{-\iota_2} \sum_{\iota_3=1}^{\iota_2} 4^{\iota_3+1} \iota_3^2}{(4\iota_2+1)^2}}{3\iota_1+2}$$

Transformation to Nested Sums

Using the command **TransformToSSums** the algorithm described in Section 5.4 is performed to rewrite nested sum expressions in terms of harmonic sums, S-sums, cyclotomic harmonic sums and cyclotomic S-sums.

HarmonicSums session.

$$\text{In[8]} = \sum_{\iota_1=2}^{n-1} \frac{(-5)^{\iota_1} \left(\sum_{\iota_2=1}^{\iota_1} \frac{2^{\iota_2}}{\iota_2^2} \right) \sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2+1}}{5\iota_1+3} // \text{TransformToSSums}$$

$$\text{Out[8]} = \frac{1}{40(3+5n)} (75 + 125n + 200nS[\{\{5, 3, 1\}, \{1, 0, 3\}, \{1, 0, 1\}\}, \{-5, 2, 1\}, n] + 300nS[\{\{5, 3, 1\}, \{1, 0, 3\}\}, \{-5, 2\}, n] - 120S[\{\{5, 3, 1\}, \{1, 0, 3\}, \{1, 0, 1\}\}, \{-5, 2, 1\}, n] - 200nS[\{\{5, 3, 1\}, \{1, 0, 4\}\}, \{-5, 2\}, n] + 120S[\{\{5, 3, 1\}, \{1, 0, 1\}, \{1, 0, 3\}\}, \{-5, 1, 2\}, n] +$$

$$\begin{aligned}
& 200nS[\{\{5, 3, 1\}, \{1, 0, 1\}, \{1, 0, 3\}\}, \{-5, 1, 2\}, n] + 120S[\{\{5, 3, 1\}, \{1, 0, 4\}\}, \{-5, 2\}, n] + \\
& 180S[\{\{5, 3, 1\}, \{1, 0, 3\}\}, \{-5, 2\}, n] - 12(-1)^n 5^{1+n} S[3, \{2\}, n] - 12S[4, \{-10\}, n] - \\
& 20nS[4, \{-10\}, n] + 8(-1)^n 5^{1+n} S[4, \{2\}, n] + 12S[1, 3, \{-5, 2\}, n] + 20nS[1, 3, \{-5, 2\}, n] - \\
& 8(-1)^n 5^{1+n} S[1, 3, \{1, 2\}, n] - 8(-1)^n 5^{1+n} S[3, 1, \{2, 1\}, n]
\end{aligned}$$

If in addition `Sigma` is loaded into Mathematica, sums can be handled whose denominators do not factor linearly over \mathbb{Q} see Remark 5.4.2.

Synchronization

After executing `AutoSync[True]` harmonic sums, S-sums, cyclotomic harmonic sums and cyclotomic S-sums at argument $a \cdot n + b$ for $a \in \mathbb{N}, b \in \mathbb{N}_0$ are synchronized automatically to argument n .

HarmonicSums session.

In[9]:= `S[1, 2, 2 n + 1]`

Out[9]= $1 + 2S[\{\{2, 1, 1\}\}, n] + S[\{\{2, 1, 2\}\}, n] + \frac{1}{2}S[\{\{1, 0, 1\}, \{2, 1, 2\}\}, n] + \frac{1}{4}S[\{\{2, 1, 1\}, \{1, 0, 2\}\}, n] + S[\{\{2, 1, 1\}, \{2, 1, 2\}\}, n] + \frac{1}{8}S[1, 2, n]$

In[10]:= `S[\{\{2, 1, 2\}, \{3, 1, 2\}\}, 2 n + 1]`

Out[10]= $\frac{1}{144} - \frac{18}{125}S[\{\{3, 2, 1\}\}, n] - \frac{9}{100}S[\{\{3, 2, 2\}\}, n] + \frac{24}{125}S[\{\{4, 1, 1\}\}, n] - \frac{39}{400}S[\{\{4, 1, 2\}\}, n] + \frac{1}{16}S[\{\{4, 3, 2\}\}, n] + \frac{1}{4}S[\{\{4, 1, 2\}, \{3, 2, 2\}\}, n] + S[\{\{4, 1, 2\}, \{6, 1, 2\}\}, n] + \frac{1}{4}S[\{\{4, 3, 2\}, \{3, 2, 2\}\}, n] + S[\{\{4, 3, 2\}, \{6, 1, 2\}\}, n]$

Definition of the Nested Integrals

Harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms are denoted by the letter `H` as we can see in the following examples. The command `ToHarmonicSumsIntegrate` yields the definition of the nested integrals.

HarmonicSums session.

In[11]:= `H[0, 1, 0, -1, x]//ToHarmonicSumsIntegrate`

$$\text{Out[11]} = \int_0^x \int_0^{a_1} \frac{\int_0^{a_2} \frac{\int_0^{a_3} \frac{1}{a_4+1} da_4 da_3}{a_3} da_2}{a_2-1} da_1 da_2$$

`In[12]:= H[1, 2, -3, 4, x]//ToHarmonicSumsIntegrate`

$$\text{Out[12]} = \int_0^x \int_0^{a_1} \frac{\int_0^{a_2} \frac{\int_0^{a_3} \frac{1}{a_4-4} da_4 da_3}{a_3+3} da_2}{a_2-2} da_1 da_2$$

`In[13]:= H[{3, 1}, {5, 1}, {2, 0}, x]//ToHarmonicSumsIntegrate`

$$\text{Out[13]} = \int_0^x \frac{a_1 \left(\int_0^{a_1} \frac{a_2 \left(\int_0^{a_2} \frac{1}{a_3+1} da_3 \right) da_2}{a_2^2+a_2^3+a_2^2+a_2+1} \right) da_1}{a_1^2+a_1+1}$$

Shuffle and Quasi-Shuffle Product

We can use the functions `LinearExpand` and `LinearHExpand` to expand products of harmonic sum, S-sums, cyclotomic harmonic sums and cyclotomic S-sums and products of harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms, respectively.

HarmonicSums session.

`In[14]:= S[1,-2, {1, 4}, n] S[1, {-3}, n]//LinearExpand`

`Out[14]=` $-S[1, -1, \{1, -12\}, n] - S[2, -2, \{-3, 4\}, n] + S[1, -2, 1, \{1, 4, -3\}, n] + S[1, 1, -2, \{-3, 1, 4\}, n] + S[1, 1, -2, \{1, -3, 4\}, n]$

`In[15]:= S[{{3, 2, 1}, {2, 0, -2}}, {1, 4}, n] S[{{3, 1, 1}}, {-3}, n]//LinearExpand`

`Out[15]=` $-S[{{3, 1, 1}, \{2, 0, -2\}}, \{-3, 4\}, n] + S[{{3, 2, 1}, \{2, 0, -2\}}, \{-3, 4\}, n] + S[{{3, 1, 1}, \{3, 2, 1\}, \{2, 0, -2\}}, \{-3, 1, 4\}, n] + S[{{3, 2, 1}, \{2, 0, -2\}, \{3, 1, 1\}}, \{1, 4, -3\}, n] + S[{{3, 2, 1}, \{3, 1, 1\}, \{2, 0, -2\}}, \{1, -3, 4\}, n]$

`In[16]:= H[1, 2, x] H[3, 4, x]//LinearHExpand`

`Out[16]=` $H[1, 2, 3, 4, x] + H[1, 3, 2, 4, x] + H[1, 3, 4, 2, x] + H[3, 1, 2, 4, x] + H[3, 1, 4, 2, x] + H[3, 4, 1, 2, x]$

`In[17]:= H[{3, 1}, {5, 1}, x] H[{5, 2}, {2, 0}, x]//LinearHExpand`

`Out[17]=` $H[\{3, 1\}, \{5, 1\}, \{5, 2\}, \{2, 0\}, x] + H[\{3, 1\}, \{5, 2\}, \{2, 0\}, \{5, 1\}, x] + H[\{3, 1\}, \{5, 2\}, \{5, 1\}, \{2, 0\}, x] + H[\{5, 2\}, \{2, 0\}, \{3, 1\}, \{5, 1\}, x] + H[\{5, 2\}, \{3, 1\}, \{2, 0\}, \{5, 1\}, x] + H[\{5, 2\}, \{3, 1\}, \{5, 1\}, \{2, 0\}, x]$

Transformation of the Argument of the Nested Integrals

The function `TransformH` is used to transform the argument of harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms as described in the Sections 2.3, 3.2 and 4.3. Some examples are:

HarmonicSums session.

In[18]:= `TransformH[H[-1, 0, (1 - x)/(1 + x)], x]`

Out[18]= $H[-1, -1, x] + H[-1, 0, 1] + H[-1, 1, x]$

In[19]:= `TransformH[H[-3, 0, -2, x + 2], x]`

Out[19]= $H[-2, 2]H[-5, -2, x] + H[-5, x]H[0, -2, 2] + H[-5, -2, -4, x] + H[-3, 0, -2, 2]$

In[20]:= `TransformH[H[-3, 0, -2, 2 x], x]`

Out[20]= $H[-3/2, 0, -1, x]$

In[21]:= `TransformH[H[1, -2, 1 - x], x]`

Out[21]= $-H[-2, 1]H[0, x] + H[-2, 0, 1] - H[-2, 1, 1] + H[0, -2, 1] + H[0, 3, x]$

In[22]:= `TransformH[H[2, 1, 2, 0, x], 1/x]`

Out[22]= $-H[\{0, -1\}, \{0, 0\}, 1] + H[\{0, -1\}, \{0, 0\}, 1/x] + H[\{0, -1\}, \{2, 0\}, 1] - H[\{0, -1\}, \{2, 0\}, 1/x] + H[\{0, 0\}, \{0, 0\}, 1] - H[\{0, 0\}, \{0, 0\}, 1/x] - H[\{0, 0\}, \{2, 0\}, 1] + H[\{0, 0\}, \{2, 0\}, 1/x] - H[\{2, 0\}, \{0, 0\}, 1] + H[\{2, 0\}, \{0, 0\}, 1/x] + H[\{2, 0\}, \{2, 0\}, 1] - H[\{2, 0\}, \{2, 0\}, 1/x] + H[\{2, 1\}, \{2, 0\}, 1]$

Power Series Expansions of the Nested Integrals

The function `HToS` can be used to compute the power series expansions of harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms about 0. `SToH` is used to perform the reverse direction.

HarmonicSums session.

In[23]:= `HToS[H[-1, 0, -1, x]]`

Out[23]= $\sum_{\iota_1=1}^{\infty} \frac{S[2, \iota_1](-x)^{\iota_1}}{\iota_1} - \sum_{\iota_1=1}^{\infty} \frac{(-x)^{\iota_1}}{\iota_1^3}$

In[24]:= `SToH[\sum_{\iota_1=1}^{\infty} \frac{(-x)^{\iota_1} S[6, \iota_1]}{\iota_1}]`

$$\begin{aligned}
\text{Out[24]} &= \text{H}[-1, 0, -1, x] - \text{H}[0, 0, -1, x] \\
\text{In[25]} &:= \text{HToS}[\text{H}[-3, 0, -1/2, x]] \\
\text{Out[25]} &= \sum_{\ell_1=1}^{\infty} \frac{3^{-\ell_1} (-x)^{\ell_1} \text{S}[2, \{6\}, \ell_1]}{\ell_1} - \sum_{\ell_1=1}^{\infty} \frac{2^{\ell_1} (-x)^{\ell_1}}{\ell_1^3} \\
\text{In[26]} &:= \text{SToH}\left[\sum_{\ell_1=1}^{\infty} \frac{3^{-\ell_1} (-x)^{\ell_1} \text{S}[2, \{6\}, \ell_1]}{\ell_1}\right] \\
\text{Out[26]} &= \text{H}[-3, 0, -\frac{1}{2}, x] - \text{H}[0, 0, -\frac{1}{2}, x] \\
\text{In[27]} &:= \text{HToS}[\text{H}[3, 1, 1, 0, x]] \\
\text{Out[27]} &= \sum_{\ell_1=1}^{\infty} \frac{x^{3\ell_1+1} \text{S}[\{\{3, -2, 1\}\}, \ell_1]}{3\ell_1+1} - \sum_{\ell_1=1}^{\infty} \frac{x^{3\ell_1+1} \text{S}[\{\{3, -1, 1\}\}, \ell_1]}{3\ell_1+1} + \sum_{\ell_1=1}^{\infty} \frac{x^{3\ell_1+2} \text{S}[\{\{3, -1, 1\}\}, \ell_1]}{3\ell_1+2} - \\
&\quad \sum_{\ell_1=1}^{\infty} \frac{x^{3\ell_1+2} \text{S}[\{\{3, 0, 1\}\}, \ell_1]}{3\ell_1+2} + \sum_{\ell_1=1}^{\infty} \frac{x^{3\ell_1+3} \text{S}[\{\{3, 0, 1\}\}, \ell_1]}{3\ell_1+3} - \sum_{\ell_1=1}^{\infty} \frac{x^{3\ell_1} \text{S}[\{\{3, -2, 1\}\}, \ell_1]}{3\ell_1}
\end{aligned}$$

The function `HInfSeries` can be used to compute the asymptotic behavior of harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms for $x \rightarrow \infty$.

HarmonicSums session.

$$\begin{aligned}
\text{In[28]} &:= \text{HInfSeries}[\text{H}[-1, -2, x], x] \\
\text{Out[28]} &= \sum_{\ell_1=1}^{\infty} \frac{\left(-\frac{1}{x}\right)^{\ell_1} S_1(2; \ell_1)}{\ell_1} - \text{H}[0, x] \left(\sum_{\ell_1=1}^{\infty} \frac{\left(-\frac{1}{x}\right)^{\ell_1}}{\ell_1} \right) - \text{H}[0, 2] \left(- \sum_{\ell_1=1}^{\infty} \frac{\left(-\frac{1}{x}\right)^{\ell_1}}{\ell_1} + \text{H}[0, xx] - \text{H}[-1, 1] \right) - \\
&\quad \sum_{\ell_1=1}^{\infty} \frac{\left(-\frac{1}{x}\right)^{\ell_1}}{\ell_1^2} + \text{H}[-1, -2, 1] + \text{H}[-1, 0, 1] - \text{H}[-1, -\frac{1}{2}, 1] - \text{H}[0, 0, 1] + \text{H}[0, -\frac{1}{2}, 1] + \frac{1}{2} \text{H}[0, x]^2 \\
\text{In[29]} &:= \text{HInfSeries}[\text{H}[\{3, 1\}, x], x] \\
\text{Out[29]} &= - \sum_{\ell_1=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3\ell_1}}{3\ell_1} + \sum_{\ell_1=1}^{\infty} \frac{\left(\frac{1}{x}\right)^{3\ell_1-2}}{3\ell_1-2} - \text{H}[\{0, 0\}, \frac{1}{x}] + \text{H}[\{0, 0\}, 1] - \text{H}[\{3, 0\}, 1]
\end{aligned}$$

Note that the function `HarmonicSumsSeries` can be used to compute the power series expansion of expressions involving harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms up to a specified order. As well it can be used to determine the asymptotic behavior of expressions involving harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms up to a specified order.

HarmonicSums session.

In[30]:= **HarmonicSumsSeries**[$x^3 + H[-1, 0, -1, x]/x$, x , 0 , 5]

$$\text{Out[30]} = \left(\frac{49x^4}{1080} + \frac{x^3}{18} + \frac{x^2}{18} \right) H[0, x] - \frac{139x^4}{2400} + \frac{11x^3}{12} - \frac{11x^2}{108}$$

In[31]:= **HarmonicSumsSeries**[$1/x^3 + H[-1, -2, x]/x$, x , ∞ , 5]

$$\text{Out[31]} = -\frac{131x^4}{960} + \frac{x^3}{6} + \frac{1}{x^3} - \frac{5x^2}{24} + \frac{x}{4}$$

Transforming Nested Integrals at Special Values to Nested Sums at Infinity and Vice Versa

The function **HToSinf** expresses values given by finite harmonic polylogarithms and multiple polylogarithms at real arguments using harmonic sums and S-sums at infinity while **SinfToH** transforms harmonic sums and S-sums at infinity to harmonic polylogarithms and multiple polylogarithms at real arguments. In addition **HToSinf** can be used to express values given by finite cyclotomic harmonic polylogarithms at argument 1 using cyclotomic harmonic sums at infinity.

HarmonicSums session.

In[32]:= **HToSinf**[**H**[-2, -1, 1]]

$$\text{Out[32]} = -S[-2, \infty] + S[1, 1, \{-\frac{1}{2}, 2\}, \infty]$$

In[33]:= **SinfToH**[**S**[1, 1, $\{-\frac{1}{2}, 2\}$, ∞]]

$$\text{Out[33]} = H[-2, -1, 1] - H[0, -1, 1]$$

In[34]:= **HToSinf**[**H**[{2, 0}, {2, 1}, 1]]

$$\begin{aligned} \text{Out[34]} = & \frac{1}{2}S[\{1, 0, 1\}, \infty] + \frac{1}{4}S[\{1, 0, 2\}, \infty] - S[\{2, 1, 1\}, \infty] - S[\{2, 1, 2\}, \infty] \\ & - \frac{1}{4}S[\{1, 0, 1\}, \{1, 0, 1\}, \infty] - \frac{1}{2}S[\{1, 0, 1\}, \{2, 1, 1\}, \infty] + \frac{1}{2}S[\{2, 1, 1\}, \{1, 0, 1\}, \infty] + \\ & S[\{2, 1, 1\}, \{2, 1, 1\}, \infty] \end{aligned}$$

Mellin Transformation and Inverse Mellin Transformation

To compute the Mellin transform of possibly weighted harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms **hlog[x]** we can use the

command `Mellin[hlog[x], x, n]`. Using the option `PlusFunctionDefinition→2` the function `Mellin` computes the Mellin transform as it is defined in [1] and [73].

HarmonicSums session.

In[35]:= `Mellin[H[1, 0, x]/(1 + x), x, n]`

Out[35]= $(-1)^n(-S[-1, 2, n] - 2S[3, \infty] + S[-2, -1, \infty] + S[-1, -2, \infty])$

In[36]:= `Mellin[H[2, 3, x]/(2 + x), x, n]`

Out[36]= $(-2)^n \left(S[-1, n]S[2, \left\{\frac{1}{3}\right\}, \infty] - S[1, \left\{-\frac{1}{2}\right\}, n]S[2, \left\{\frac{1}{3}\right\}, \infty] + S[1, 1, \left\{-1, \frac{1}{2}\right\}, n]S[1, \left\{\frac{1}{3}\right\}, \infty] - S[1, 1, \left\{-1, \frac{3}{2}\right\}, n]S[1, \left\{\frac{1}{3}\right\}, \infty] - S[-1, n]S[1, 1, \left\{\frac{1}{2}, \frac{2}{3}\right\}, \infty] + S[1, \left\{-\frac{1}{2}\right\}, n]S[1, 1, \left\{\frac{1}{2}, \frac{2}{3}\right\}, \infty] + S[1, 1, 1, \left\{-1, \frac{3}{2}, \frac{1}{3}\right\}, n] - S[3, \left\{\frac{1}{3}\right\}, \infty] + S[1, 2, \left\{-\frac{1}{2}, -\frac{2}{3}\right\}, \infty] + S[2, 1, \left\{\frac{1}{2}, \frac{2}{3}\right\}, \infty] - S[1, 1, 1, \left\{-\frac{1}{2}, -1, \frac{2}{3}\right\}, \infty] \right)$

In[37]:= `Mellin[H[{3, 1}, {3, 0}, x], x, 3 n + 1]`

Out[37]= $\frac{n}{36n + 24} \left(-24S[\{\{3, 2, 1\}\}, n]S[\{\{3, 1, 1\}\}, \infty] + (4S[\{\{3, 1, 1\}\}, n] + 4S[\{\{3, 2, 1\}\}, n] + 6)S[\{\{1, 0, 1\}\}, \infty] + 6S[\{\{3, 1, 1\}\}, n](2S[\{\{3, 1, 1\}\}, \infty] - 4S[\{\{3, 2, 1\}\}, \infty] - 1) + 12S[\{\{3, 2, 1\}\}, n]S[\{\{3, 2, 1\}\}, \infty] + 6S[\{\{3, 2, 1\}\}, n] - 4S[\{\{3, 1, 1\}, \{1, 0, 1\}\}, n] + 12S[\{\{3, 1, 1\}, \{3, 2, 1\}\}, n] - 4S[\{\{3, 2, 1\}, \{1, 0, 1\}\}, n] + 12S[\{\{3, 2, 1\}, \{3, 1, 1\}\}, n] + 24S[\{\{3, 1, 1\}\}, \infty] + 12S[\{\{3, 1, 2\}\}, \infty] - 42S[\{\{3, 2, 1\}\}, \infty] - 12S[\{\{3, 2, 2\}\}, \infty] + 8S[\{\{1, 0, 1\}, \{3, 1, 1\}\}, \infty] + 4S[\{\{1, 0, 1\}, \{3, 2, 1\}\}, \infty] - 12S[\{\{3, 1, 1\}, \{3, 1, 1\}\}, \infty] - 24S[\{\{3, 1, 1\}, \{3, 2, 1\}\}, \infty] - 12S[\{\{3, 2, 1\}, \{3, 1, 1\}\}, \infty] + 12S[\{\{3, 2, 1\}, \{3, 2, 1\}\}, \infty] - 9) \right)$

To compute the inverse Mellin transform of a harmonic sum or a \bar{S} -sum denoted by `sum` we can use the command `InvMellin[sum, n, x]`. Note that `Delta1x` denotes the Dirac δ -distribution $\delta(1 - x) \in D'[0, 1]$. For cyclotomic harmonic sums and S-sums which are not \bar{S} -sums `InvMellin` yields an integral representation, where `Mellin[a[x, n]] := $\int_0^1 a(x, n) dx$` and `Mellin[a[x, n], {x, c, d}] := $\int_c^d a(x, n) dx$` .

HarmonicSums session.

In[38]:= `InvMellin[S[1, 2, n], n, x]`

Out[38]= $\frac{H[1, 0, x]}{1 - x}$

In[39]:= `InvMellin[S[1, 2, {1, 1/3}, n], n, x]`

Out[39]= $\text{Delta1x} \left(-S[1, \left\{\frac{1}{3}\right\}, \infty]S[2, \left\{\frac{1}{3}\right\}, \infty] - 2S[3, \left\{\frac{1}{3}\right\}, \infty] + S[1, 2, \left\{\frac{1}{3}, 1\right\}, \infty] + S[2, 1, \left\{\frac{1}{3}, 1\right\}, \infty] \right) + \frac{3^{-n}S[2, \left\{\frac{1}{3}\right\}, \infty]}{3 - x} - \frac{S[2, \left\{\frac{1}{3}\right\}, \infty]}{1 - x} - \frac{3^{-n}H[3, 0, x]}{x - 3}$

In[40]:= `InvMellin[S[\{\{3, 1, 2\}\}, n], n, x]`

$$\text{Out[40]} = -\text{Mellin}[x^{3n}H[0, x]] - \frac{1}{3}\text{Mellin}\left[\frac{(x^{3n}-1)H[0, x]}{x-1}\right] + \frac{1}{3}\left(2\text{Mellin}\left[\frac{(x^{3n}-1)H[0, x]}{x^2+x+1}\right] + \text{Mellin}\left[\frac{x(x^{3n}-1)H[0, x]}{x^2+x+1}\right]\right) - 1$$

$$\text{In[41]} := \text{InvMellin}[\mathbf{S}[1, 1, \{2, 3\}, n], n, x]$$

$$\text{Out[41]} = H[0, 4]\text{Mellin}\left[\frac{x^n-1}{x-1}, \{x, 2, 6\}\right] - \text{Mellin}\left[\frac{x^n H[0, x-2]}{x-1}, \{x, 2, 6\}\right] \\ + \text{Mellin}\left[\frac{(x^n-1)H[2, x]}{x-1}, \{x, 0, 2\}\right] + \text{Mellin}\left[\frac{H[0, x]}{x+1}, \{x, 0, 4\}\right]$$

Differentiation of the Nested Sums

In order to differentiate harmonic sums, S-sums or cyclotomic harmonic sums, we can use the function `DifferentiateSSum`. Note that `z2`, `z3`, ... denote the values of the Riemann zeta function $\zeta(s)$ at $s = 2, s = 3, \dots$ while `ln2` = $\log 2$.

HarmonicSums session.

$$\text{In[42]} := \text{DifferentiateSSum}[\mathbf{S}[3, 1, n], n]$$

$$\text{Out[42]} = -S[3, 2, n] - 3 S[4, 1, n] + z2 S[3, n] - z2 z3 + \frac{9 z5}{2}$$

$$\text{In[43]} := \text{DifferentiateSSum}[\mathbf{S}[3, 1, \{2, 3\}, n], n]$$

$$\text{Out[43]} = -H[1, 0, 3]S[3, \{2\}, n] + H[0, 2]S[3, 1, \{2, 3\}, n] + H[0, 3]S[3, 1, \{2, 3\}, n] - S[3, 2, \{2, 3\}, n] - \\ 3S[4, 1, \{2, 3\}, n] + H[1, 0, 2]H[0, -2, -2, -1] - H[1, 0, 2]H[0, -2, -2, 4] + H[0, -2, -1]H[0, 1, 0, 2] \\ - H[0, -2, 4]H[0, 1, 0, 2] - H[0, 2]H[0, -2, -2, -1, -1] + H[0, 2]H[0, -2, -2, -1, 4] \\ - H[2, 1]H[0, 0, 1, 0, 2] - H[0, -2, -2, -1, -2, -1] + H[0, -2, -2, -1, -2, 4] + H[2, 0, 0, 1, 0, 1]$$

$$\text{In[44]} := \text{DifferentiateSSum}[\mathbf{S}[\{\{2, 1, 1\}, \{2, 0, 1\}\}, n], n]$$

$$\text{Out[44]} = \frac{1}{24}\left(-96 \ln 2 S[\{\{2, 1, -1\}\}, \infty]^2 - 192 \ln 2 S[\{\{2, 1, -1\}\}, \infty] + \right. \\ 16S[\{\{2, 1, 1\}\}, n] S[\{\{2, 1, -1\}\}, \infty]^2 + 32 S[\{\{2, 1, 1\}\}, n]S[\{\{2, 1, -1\}\}, \infty] + 6(S[\{\{2, 1, 1\}\}, n] + \\ 1)S[\{\{1, 0, 2\}\}, \infty] + 12(S[\{\{2, 1, 2\}\}, n] + 1)S[\{\{1, 0, 1\}\}, \infty] - 12S[1, \infty] S[\{\{2, 1, 2\}\}, n] + \\ 4 S[\{\{2, 1, 1\}\}, n] - 12S[\{\{2, 1, 1\}, \{1, 0, 2\}\}, n] - 24S[\{\{2, 1, 2\}, \{1, 0, 1\}\}, n] + \\ \left. 16S[\{\{2, 1, -1\}\}, \infty]^2 + 32S[\{\{2, 1, -1\}\}, \infty] - 96\ln 2 - 12 S[1, \infty] + 21 z3 + 4\right)$$

Series Expansions of the Nested Sums

The function `TaylorSeries[sum,x,n,ord]` can be used to calculate the Taylor series expansion around `x` of a harmonic sum, \bar{S} -sum or cyclotomic harmonic sum `sum` at argument `n` up to order `ord`.

HarmonicSums session.

In[45]:= `TaylorSeries[S[2, 1, n], 0, n, 3]`

$$\text{Out[45]}= n^3 \left(\frac{74 z^2}{105} - z^3 \right) + n^2 \left(2 z^2 z^3 - \frac{11 z^5}{2} \right) + \frac{7 n z^2}{10}$$

In[46]:= `TaylorSeries[S[{{3, 1, 2}}, n], 0, n, 2]`

$$\text{Out[46]}= \frac{1}{2} n^2 \left(36 H[\{3, 0\}, 0, 0, 0, 1] + 18 H[\{3, 1\}, 0, 0, 0, 1] - \frac{36 z^2}{5} + 54 \right) + n(4 H[\{3, 0\}, 0, 0, 1] + 2 H[\{3, 1\}, 0, 0, 1] + 2 z^3 - 6)$$

The function `SExpansion[sum,n,ord]` can be used to calculate the asymptotic expansion of a harmonic sum, \bar{S} -sum or a cyclotomic harmonic sum `sum` at argument `n` up to order `ord`.

HarmonicSums session.

In[47]:= `SExpansion[S[3, 1, n], n, 3]`

$$\text{Out[47]}= \left(\frac{1}{2n^3} - \frac{1}{2n^2} \right) L[n] - \frac{1}{6n^3} - \frac{1}{4n^2} + \frac{z^2}{2}$$

In[48]:= `SExpansion[S[3, 1, {1/2, 1/3}, n], n, 3]`

$$\begin{aligned} \text{Out[48]}= & S[1, \left\{ \frac{1}{3} \right\}, \infty] \left(-S[3, \left\{ \frac{1}{6} \right\}, \infty] + S[3, \left\{ \frac{1}{2} \right\}, \infty] + 6^{-n} \left(\frac{1}{5n^3} - \frac{3^n}{n^3} \right) \right) + \\ & 6^{-n} \left(\frac{12}{25n^3} - \frac{1}{5n^2} \right) S[2, \left\{ \frac{1}{3} \right\}, \infty] + 6^{-n} \left(\frac{42}{125n^3} - \frac{6}{25n^2} + \frac{1}{5n} \right) S[3, \left\{ \frac{1}{3} \right\}, \infty] + \\ & S[2, \left\{ \frac{1}{6} \right\}, \infty] S[2, \left\{ \frac{1}{3} \right\}, \infty] - S[1, \left\{ \frac{1}{6} \right\}, \infty] S[3, \left\{ \frac{1}{3} \right\}, \infty] - S[4, \left\{ \frac{1}{3} \right\}, \infty] + S[1, 3, \left\{ \frac{1}{6}, 2 \right\}, \infty] + \\ & 6^{-n} \left(\frac{1}{5n^2} - \frac{12}{25n^3} \right) H[0, 3, 1] + 6^{-n} \left(-\frac{42}{125n^3} + \frac{6}{25n^2} - \frac{1}{5n} \right) H[0, 0, 3, 1] - \frac{H[3, 1] 6^{-n}}{5n^3} \end{aligned}$$

In[49]:= `SExpansion[S[{{3, 1, 1}, {2, 1, 1}}, n], n, 3]`

$$\begin{aligned} \text{Out[49]}= & H[\{6, 0\}, 1] \left(-\frac{1}{3} H[-1, 5] - \frac{L[n]}{3} + \ln 2 - \frac{10}{243n^3} + \frac{11}{108n^2} - \frac{5}{18n} + \frac{5}{3} \right) + \\ & H[\{6, 1\}, 1] \left(\frac{2}{3} (H[-1, 5] - 2) + \frac{2L[n]}{3} - \ln 2 + \frac{20}{243n^3} - \frac{11}{54n^2} + \frac{5}{9n} \right) + \\ & H[\{3, 1\}, 1] \left(-H[\{6, 0\}, 1] + H[\{6, 1\}, 1] - \frac{1}{2} H[-1, 2] - \frac{L[n]}{3} + \frac{1}{36n^2} - \frac{1}{6n} + \frac{8}{3} \right) + \\ & H[\{3, 0\}, 1] \left(H[\{6, 0\}, 1] - H[\{6, 1\}, 1] - \frac{1}{2} H[-1, 2] - \frac{L[n]}{6} + \frac{1}{72n^2} - \frac{1}{12n} + \frac{1}{3} \right) - H[\{6, 0\}, 1]^2 + \\ & H[\{6, 1\}, 1]^2 - \frac{2}{3} H[-1, \{6, 0\}, 1] + \frac{1}{3} H[-1, \{6, 1\}, 1] - \frac{1}{3} H[\{3, 0\}, -1, 1] + \frac{1}{2} H[\{3, 0\}, 1, 1] + \\ & \frac{1}{2} H[\{3, 0\}, \{3, 0\}, 1] + \frac{1}{2} H[\{3, 0\}, \{3, 1\}, 1] - \frac{2}{3} H[\{3, 0\}, \{6, 0\}, 1] + \frac{1}{3} H[\{3, 0\}, \{6, 1\}, 1] + \end{aligned}$$

$$\begin{aligned} & \frac{1}{3}H[\{3, 1\}, -1, 1] + \frac{1}{2}H[\{3, 1\}, 1, 1] + H[\{3, 1\}, \{3, 0\}, 1] + H[\{3, 1\}, \{3, 1\}, 1] + \frac{2}{3}H[\{3, 1\}, \{6, 0\}, 1] - \\ & \frac{1}{3}H[\{3, 1\}, \{6, 1\}, 1] + \frac{1}{3}H[\{6, 0\}, -1, 1] - \frac{2}{3}H[\{6, 0\}, 1, 1] + \frac{2}{3}H[\{6, 0\}, \{6, 0\}, 1] - \\ & \frac{1}{3}H[\{6, 0\}, \{6, 1\}, 1] + \frac{1}{3}H[\{6, 1\}, -1, 1] + \frac{1}{3}H[\{6, 1\}, 1, 1] + \frac{2}{3}H[\{6, 1\}, \{6, 0\}, 1] - \\ & \frac{1}{3}H[\{6, 1\}, \{6, 1\}, 1] + \ln 2 \left(\frac{1}{3}(H[-1, 5] - 5) + \frac{L[n]}{3} + \frac{10}{243n^3} - \frac{11}{108n^2} + \frac{5}{18n} \right) \\ & + L[n] \left(\frac{1}{6}(H[-1, 2] - 2) + \frac{5}{243n^3} - \frac{11}{216n^2} + \frac{5}{36n} \right) + \frac{\frac{25}{96} - \frac{1}{72}H[-1, 2]}{n^2} + \frac{\frac{1}{12}H[-1, 2] - \frac{7}{18}}{n} - \\ & \frac{1}{3}H[-1, 5] + \frac{L[n]^2}{12} - \frac{3905}{23328n^3} - \frac{z2}{4} \end{aligned}$$

Note that the function `HarmonicSumsSeries[expr, n, p, ord]` can be used to compute series expansions about the point $x=p$ of expressions `expr` involving harmonic sums, \bar{S} -sums, cyclotomic harmonic sums, harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms up to a specified order `ord`.

HarmonicSums session.

```
In[50]:= HarmonicSumsSeries[n*S[2, n] + n*H[-2, n], n, 0, 4] // ReduceConstants
```

$$\text{Out[50]= } n^4 \left(4z5 + \frac{1}{24} \right) + n^3 \left(-\frac{6z2^2}{5} - \frac{1}{8} \right) + n^2 \left(2z3 + \frac{1}{2} \right)$$

```
In[51]:= HarmonicSumsSeries[n*S[2, n] + n*H[-2, n], n, 1, 4]
```

$$\begin{aligned} \text{Out[51]= } & (n-1) \left(H[-2, 1] + 2z3 - \frac{2}{3} \right) + H[-2, 1] + (n-1)^4 \left(-\frac{8z2^3}{7} + 4z5 + \frac{109}{108} \right) \\ & + (n-1)^2 \left(-\frac{6z2^2}{5} + 2z3 + \frac{23}{18} \right) + (n-1)^3 \left(-\frac{6z2^2}{5} + 4z5 - \frac{169}{162} \right) + 1 \end{aligned}$$

```
In[52]:= HarmonicSumsSeries[n*S[2, n] + n*H[-2, n], n, ∞, 4] // ReduceConstants
```

$$\text{Out[52]= } -n H[0, 2] + n H[0, n] - \frac{4}{n^3} + \frac{5}{2n^2} + n z2 - \frac{3}{2n} + 1$$

Basis Representations

In order to look for basis representations of harmonic sums, S-sums, cyclotomic harmonic sums, harmonic polylogarithms and multiple polylogarithms, the functions `ComputeHSumBasis`, `ComputeSSumBasis`, `ComputeCSumBasis` and `ComputeHLogBasis` are provided.

- `ComputeHSumBasis[w, n]` computes a basis and the corresponding relations for harmonic sums at weight `w`. With the options `UseDifferentiation` and `UseHalfInteger` it can be specified whether relations due to differentiation and argument duplication should be used.

- `ComputeSSumBasis[w,x,n]` computes a basis and the corresponding relations for S-sums at weight `w` where the allowed “`x`”-indices are defined in the list `x`. With the options `UseDifferentiation` and `UseHalfInteger` it can be specified whether relations due to differentiation and argument duplication should be used.
- `ComputeCSumBasis[w,let,n]` computes a basis and the corresponding relations for cyclotomic harmonic sums at weight `w` with letters `let`. With the options `UseDifferentiation`, `UseMultipleInteger` and `UseHalfInteger` it can be specified whether relations due to differentiation and argument multiplication should be used.
- `ComputeHLogBasis[w,n]` computes a basis and the corresponding relations for multiple polylogarithms at weight `w`. The option `Alphabet->a` and `IndexStructure->ind` can be used to specify an alphabet or a special index structure respectively.

HarmonicSums session.

```
In[53]:= ComputeCSumBasis[2, {{2, 1}}, n, UseDifferentiation -> False,
      UseMultipleInteger -> False, UseHalfInteger -> False
```

```
Out[53]= { {S[{{2, 1, -2}}, n], S[{{2, 1, 2}}, n], S[{{2, 1, -1}, {2, 1, 1}}, n]},
      {S[{{2, 1, 1}, {2, 1, 1}}, n] -> 1/2 S[{{2, 1, 1}}, n]^2 + 1/2 S[{{2, 1, 2}}, n],
      S[{{2, 1, 1}, {2, 1, -1}}, n] -> S[{{2, 1, -2}}, n] + S[{{2, 1, -1}}, n] S[{{2, 1, 1}}, n]
      - S[{{2, 1, -1}, {2, 1, 1}}, n], S[{{2, 1, -1}, {2, 1, -1}}, n] -> 1/2 S[{{2, 1, -1}}, n]^2 +
      1/2 S[{{2, 1, 2}}, n] }
```

In order to look for relations for harmonic sums, S-sums and and cyclotomic harmonic sums at infinity we can use the functions `ComputeHSumInfBasis`, `ComputeSSumInfBasis` and `ComputeCSumInfBasis`.

HarmonicSums session.

```
In[54]:= ComputeCSumInfBasis[2, {{2, 1}}]
```

```
Out[54]= { {S[{{2, 1, -2}}, ∞], S[{{2, 1, 2}}, ∞], S[{{2, 1, -1}, {2, 1, 1}}, ∞]},
      {S[{{2, 1, 1}, {2, 1, 1}}, ∞] -> 1/2 S[{{2, 1, 1}}, ∞]^2 + 1/2 S[{{2, 1, 2}}, ∞],
      S[{{2, 1, 1}, {2, 1, -1}}, ∞] -> S[{{2, 1, -2}}, ∞] + S[{{2, 1, -1}}, ∞] S[{{2, 1, 1}}, ∞]
      - S[{{2, 1, -1}, {2, 1, 1}}, ∞], S[{{2, 1, -1}, {2, 1, -1}}, ∞] -> 1/2 S[{{2, 1, -1}}, ∞]^2 +
      1/2 S[{{2, 1, 2}}, ∞] }
```

For harmonic sums and cyclotomic harmonic sums tables with relations are provided. These tables can be applied using the command `ReduceToBasis`. With the options `UseDifferentiation` and `UseHalfInteger` it is possible to specify whether relations due to differentiation and argument duplication should be used. `ReduceToBasis[expr, n, Dynamic->True]` computes relations between harmonic sums, S-sums and cyclotomic harmonic sums in `expr` from scratch and applies them. `ReduceToHBasis` uses precomputed tables with relations between harmonic polylogarithms and applies them to expressions involving harmonic polylogarithms. `ReduceConstants` uses precomputed tables with relations between harmonic polylogarithms at argument 1 and harmonic sums at infinity to reduce the appearing constants as far as possible.

HarmonicSums session.

```
In[55]:= ReduceToBasis[S[2, 1, n] + S[1, 2, n], n]
```

```
Out[55]= S[1, n]S[2, n] + S[3, n]
```

```
In[56]:= ReduceToBasis[S[5, 5, 3, 3, n], n, Dynamic -> True]
```

```
Out[56]=  $\frac{1}{2} (S[5, \{3\}, n]^2 + S[10, \{9\}, n])$ 
```

```
In[57]:= ReduceToHBasis[H[1, 0, x] + H[0, 1, x]]
```

```
Out[57]= H[0, x]H[1, x]
```

```
In[58]:= ReduceConstants[S[2, ∞] + 2 H[1, 0, 1] + H[0, 1, -1, 1]]
```

```
Out[58]=  $-\frac{3}{2} S[-1, \infty] S[2, \infty] - S[2, \infty] - S[3, \infty]$ 
```

Depth Reduction

To reduce the depth of a harmonic sum, S-sum, cyclotomic harmonic sum or cyclotomic S-sum as described in the proof of Theorem 5.5.4 the function `ReduceDepth` is provided.

HarmonicSums session.

```
In[59]:= ReduceDepth[S[1, 2, 3, 4, n]] // ToHarmonicSumsSum
```

$$\begin{aligned}
\text{Out[59]} = & \sum_{\iota_1=1}^n \frac{\left(\sum_{\iota_2=1}^{\iota_1} \frac{\sum_{\iota_3=1}^{\iota_2} \frac{1}{\iota_3^4}}{\iota_3^3} \right) \sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2}}{\iota_1} - \left(\sum_{\iota_1=1}^n \frac{\left(\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2} \right) \sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2}}{\iota_1^3} \right) \sum_{\iota_1=1}^n \frac{1}{\iota_1} + \\
& \sum_{\iota_1=1}^n \frac{\left(\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2} \right) \left(\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2} \right) \sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2}}{\iota_1^3} - \sum_{\iota_1=1}^n \frac{\left(\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2} \right) \sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2}}{\iota_1^4} - \\
& \sum_{\iota_1=1}^n \frac{\left(\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2} \right) \sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2}}{\iota_1^5} + \left(\sum_{\iota_1=1}^n \frac{1}{\iota_1} \right) \sum_{\iota_1=1}^n \frac{\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2^4}}{\iota_1^5} + \sum_{\iota_1=1}^n \frac{\sum_{\iota_2=1}^{\iota_1} \frac{1}{\iota_2^4}}{\iota_1^6}
\end{aligned}$$

Chapter 7

Multi-Variable Almkvist Zeilberger Algorithm and Feynman Integrals

In [26] integrals emerging in renormalizable Quantum Field Theories, like Quantum Electrodynamics or Quantum Chromodynamics are transformed by means of symbolic computation to hypergeometric multi-sums. The very general class of Feynman integrals which are considered in [26] are of relevance for many physical processes at high energy colliders, such as the Large Hadron Collider, LHC, and others. The considered integrals are two-point Feynman integrals in D -dimensional Minkowski space with one time- and $(D - 1)$ Euclidean space dimensions, $\varepsilon = D - 4$ and $\varepsilon \in \mathbb{R}$ with $|\varepsilon| \ll 1$ of the following structure:

$$\mathcal{I}(\varepsilon, N, p) = \int \frac{d^D p_1}{(2\pi)^D} \cdots \int \frac{d^D p_k}{(2\pi)^D} \frac{\mathcal{N}(p_1, \dots, p_k; p; m_1 \dots m_k; \Delta, N)}{(-p_1^2 + m_1^2)^{l_1} \dots (-p_k^2 + m_k^2)^{l_k}} \prod_V \delta_V. \quad (7.1)$$

They can be shown to obey difference equations with respect to N , see, e.g., [25]. In (7.1) the external momentum p and the loop momenta p_i denote D -dimensional vectors, $m_i > 0, m_i \in \mathbb{R}$ are scalars (masses), $m_i \in \{0, M\}$, $k, l_i \in \mathbb{N}$, $k \geq 2, l_i \geq 1$, and Δ is a light-like D -vector, $\Delta \cdot \Delta = 0$. The numerator function \mathcal{N} is a polynomial in the scalar products $p \cdot p_i$, $p_i \cdot p_k$ and of monomials $(\Delta \cdot p_{(i)})^{n_i}$, $n_i \in \mathbb{N}, n_i \geq 0$. $N \in \mathbb{N}$ denotes the spin of a local operator stemming from the light cone expansion, see, e.g., [42] and references therein, which contributes to the numerator function \mathcal{N} with a polynomial in $\Delta \cdot p_i$ of maximal degree N , cf. [17]. Furthermore it is assumed for simplicity that only one of the loops is formed of massive lines. The δ_V occurring in (7.1) are shortcuts for Dirac delta distributions in D dimensions $\delta_V = \delta^{(D)} \left(\sum_{l=1}^k a_{V,l} p_l \right)$, $a_{V,l} \in \mathbb{Q}$. These integrals are mathematically well defined and in [26] it is showed how they can be mapped onto integrals on the m -dimensional unit cube with the following structure:

$$\mathcal{I}(\varepsilon, N) = C(\varepsilon, N, M) \int_0^1 dy_1 \dots \int_0^1 dy_m \frac{\sum_{i=1}^k \prod_{l=1}^{r_i} [P_{i,l}(y)]^{\alpha_{i,l}(\varepsilon, N)}}{[Q(y)]^{\beta(\varepsilon)}}, \quad (7.2)$$

with $k \in \mathbb{N}$, $r_1, \dots, r_k \in \mathbb{N}$ and where $\beta(\varepsilon)$ is given by a rational function in ε , i.e., $\beta(\varepsilon) \in \mathbb{R}(\varepsilon)$, and similarly $\alpha_{i,l}(\varepsilon, N) = n_{i,l}N + \bar{\alpha}_{i,l}$ for some $n_{i,l} \in \{0, 1\}$ and $\bar{\alpha}_{i,l} \in \mathbb{R}(\varepsilon)$, see also [29] in the case no local operator insertions are present. $C(\varepsilon, N, M)$ is a factor, which depends on the dimensional parameter ε , the integer parameter N and the mass M . $P_i(y), Q(y)$ are polynomials in the remaining Feynman parameters $y = (y_1, \dots, y_m)$ written in multi-index notation. In (7.2) all terms which stem from local operator insertions were geometrically resummed; see [17]. In [26] it was already mentioned that after splitting the integral (7.2), the integrands fit into the input class of the multivariate Almkvist-Zeilberger algorithm. Hence, if the split integrals are properly defined, they obey homogenous recurrence relations in N due to the theorems in [14]. In [26] the integrals of (7.2) are transformed further to a multi-sum representation, while in this chapter we want to tackle them directly by looking on integrals of the form

$$\mathcal{I}(\varepsilon, N) = \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d; \varepsilon) dx_1 \dots dx_d, \quad (7.3)$$

with $d, N \in \mathbb{N}$, $F(n; x_1, \dots, x_d; \varepsilon)$ a hyperexponential term, $\varepsilon > 0$ a real parameter and $u_i, o_i \in \mathbb{R} \cup \{-\infty, \infty\}$. Here we will use our package `MultiIntegrate` that can be considered as an enhanced implementation of the multivariate Almkvist Zeilberger algorithm to compute recurrences for the integrands and integrals we will subsequently take a closer look onto it. Subsequently, \mathbb{K} denotes a field with $\mathbb{Q} \subseteq \mathbb{K}$ (e.g., $\mathbb{K} = \mathbb{Q}(\varepsilon)$ forms a rational function field) in which the usual operations can be computed.

7.1 Finding a Recurrence for the Integrand

In order to find a recurrence for the integrand we will use the following theorem given in [14] which gives rise to the multi-variable Almkvist Zeilberger algorithm.

Theorem 7.1.1 (mAZ; see [14]). *Let*

$$F(n; x_1, \dots, x_d) = POL(n; x_1, \dots, x_d) \cdot H(n; x_1, \dots, x_d), \quad (7.4)$$

where $POL(n; x_1, \dots, x_d) \in \mathbb{K}[n, x_1, \dots, x_d]$, and

$$H(n; x_1, \dots, x_d) = e^{a(x_1, \dots, x_d)/b(x_1, \dots, x_d)} \cdot \left(\prod_{p=1}^P S_p(x_1, \dots, x_d)^{\alpha_p} \right) \cdot \left(\frac{s(x_1, \dots, x_d)}{t(x_1, \dots, x_d)} \right)^n,$$

where $a(x_1, \dots, x_d), b(x_1, \dots, x_d), s(x_1, \dots, x_d), t(x_1, \dots, x_d)$ and $S_p(x_1, \dots, x_d) \in \mathbb{K}[x_1, \dots, x_d]$ ($1 \leq p \leq P$), and $\alpha_p \in \mathbb{K}$. Note that such a sequence $F(n; x_1, \dots, x_d)$ is called hyperexponential. Then there exists a non-negative integer L and there ex-

ist $e_0(n), e_1(n), \dots, e_L(n) \in \mathbb{K}[n]$, not all zero, and there also exist $R_i(n; x_1, \dots, x_d) \in \mathbb{K}(n, x_1, \dots, x_d)$ ($i = 1, \dots, d$) such that

$$G_i(n; x_1, \dots, x_d) := R_i(n; x_1, \dots, x_d)F(n; x_1, \dots, x_d)$$

satisfy

$$\sum_{i=0}^L e_i(n)F(n+i; x_1, \dots, x_d) = \sum_{i=1}^d D_{x_i}G_i(n; x_1, \dots, x_d). \quad (7.5)$$

In the proof of the theorem given in [14] the following expression is defined for a non-negative integer L

$$\overline{H}(n; x_1, \dots, x_d) = e^{a(x_1, \dots, x_d)/b(x_1, \dots, x_d)} \cdot \left(\prod_{p=1}^P S_p(x_1, \dots, x_d)^{\alpha_p} \right) \cdot \frac{s(x_1, \dots, x_d)^n}{t(x_1, \dots, x_d)^{n+L}}.$$

From the logarithmic derivatives (for $i = 1, \dots, d$) of $\overline{H}(n; x_1, \dots, x_d)$

$$\frac{D_{x_i}\overline{H}(n; x_1, \dots, x_d)}{\overline{H}(n; x_1, \dots, x_d)} = \frac{q_i(x_1, \dots, x_d)}{r_i(x_1, \dots, x_d)}$$

the ansatz for $i = 1, \dots, d$,

$$G_i(n; x_1, \dots, x_d) = \overline{H}(n; x_1, \dots, x_d) \cdot r_i(x_1, \dots, x_d) \cdot X_i(x_1, \dots, x_d), \quad (7.6)$$

where $X_i(x_1, \dots, x_d) \in \mathbb{K}[x_1, \dots, x_d]$ to be determined, is built. With this ansatz (7.5) is equivalent to

$$\sum_{i=1}^d [D_{x_i}r_i(x_1, \dots, x_d) + q_i(x_1, \dots, x_d)] \cdot X_i(x_1, \dots, x_d) + r_i(x_1, \dots, x_d) \cdot D_{x_i}X_i(x_1, \dots, x_d) = h(x_1, \dots, x_d). \quad (7.7)$$

The general algorithm now is straightforward: Given an integrand of the form (7.4), we can set $L = 0$, look for degree bounds for $X_i(x_1, \dots, x_d)$ and try to find a solution of (7.7) by coefficient comparison. If we do not find a solution of (7.7) with not all $e_i(n)$'s equal to zero, we increase L by one, look for new degree bounds for $X_i(x_1, \dots, x_d)$ and try again to find a solution of (7.7). Again, if we do not find a solution with not all $e_i(n)$'s equal to zero, we increase L by one and repeat the process. Since according to [14] the existence of a solution of (7.7) with not all the $e_i(n)$'s equal to zero is guaranteed for sufficiently large L , this process will eventually terminate.

A crucial point in this algorithm is the determination of degree bounds for the $X_i(x_1, \dots, x_d)$, in `MultiIntegrate` we use similar considerations as in the proof of Theorem mZ of [14] to determine such bounds.

During the implementation of our package `MultiIntegrate` it turned out that setting up the system (7.7) can be done usually rather fast. However the bottle neck for complicated examples usually is the solving of (7.7) especially when there are several symbolic parameters around. Hence we put special emphasis on this step. In the following we want to describe a method using homomorphic images to speed up the solving of (7.7) and at the same time the whole algorithm: Note that parts of these speed ups have been exploited the first time in `MultiSum` [86, 57]. Similar techniques are used in `Sigma`.

- Replace all parameters (especially n and α_p) in (7.7) which pop up in (7.4) by primes q_j of a size which can be handled by hardware arithmetic and denote the resulting equation by Eq_h .
- Use coefficient comparison with respect to x_1, \dots, x_d in Eq_h ; this leads to a system of equations SEq_h and let A_h be the corresponding matrix
- Solve the system of equations SEq_h modulo a prime q distinct from the q_j , by computing the null space of A_h and denote the obtained basis by NS_h ; in our implementation we use `Nullspace` of Mathematica to accomplish this task.
 - If NS_h is the empty set, conclude, that there is no solution of (7.7) and hence increase L and compute a new ansatz
 - If NS_h is not empty, sort the elements of NS_h by the number of contained zeros (most zeroes on top) and denote them by l_1, \dots, l_k .
- Start with l_1 ; set the variables which correspond to zero entries in l_1 to zero; in this way Eq_h (and Eq) gets simpler (if there are zero entries in l_1) and coefficient comparison with respect to x_1, \dots, x_d leads to a smaller system of equations SEq_h ; let A_h now be the corresponding matrix; note that in comparison to the original A_h the new one has less columns; in the next step the number of rows is reduced (if possible).
- Compute the null space of the transpose of A_h modulo q ; read off the rows, which can be removed (these rows correspond to equations in SEq_h which can be removed); using `Nullspace` of Mathematica this means interpreting the output as a matrix and looking for the last non zero element in each row.
- Apply coefficient comparison in Eq and remove the equations which correspond to the row numbers which we found in the previous step.
- Solve the system of equations SEq (which is usually now much smaller as in the beginning). If there are solution with not all $e_i(n)$'s equal to zero, take them

and plug them into (7.7) to test whether it is a solution of (7.5); if none of these solutions is a solution of (7.7), try the next l_i ; if none of the l_i leads to a solution of (7.5), increase L and compute a new ansatz.

Remark 7.1.2. *By replacing the parameters by primes we might introduce fake solutions, however this is quite unlikely and it has so far never happened in all the examples we have calculated so far. If we would run into such a fake solution this will not harm at all since we can always check if our solution solves the original problem. Although we might introduce new fake solutions we will not lose solutions of the original problem, since we just add structure and do not remove it.*

Removing columns and rows might as well introduce fake solutions however in the end we will always have a certificate which guarantees the correctness of our result.

7.2 Finding a Recurrence for the Integral

From [14] we know that if $F(n; \pm\infty) = 0$ (and hence $G(n; \pm\infty) = 0$) in Theorem 7.1.1 then it follows, by integrating over $[-\infty, \infty]^d$, that

$$a(n) := \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} F(n; x_1, \dots, x_d) dx_1 \dots dx_d$$

satisfies a homogenous linear recurrence equation with polynomial coefficients of the form

$$\sum_{i=0}^L e_i(n) a(n+i) = 0. \quad (7.8)$$

We are interested in different integration limits and of course this can be generalized to other limits of integration: if $F(n; \dots, x_{i-1}, u_i, x_{i+1}, \dots) = 0$ and $F(n; \dots, x_{i-1}, o_i, x_{i+1}, \dots) = 0$ (and hence $G(n; \dots, x_{i-1}, u_i, x_{i+1}, \dots) = 0$ and $G(n; \dots, x_{i-1}, o_i, x_{i+1}, \dots) = 0$) in Theorem 7.1.1 then

$$a(n) := \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d) dx_1 \dots dx_d,$$

satisfies the homogenous linear recurrence equation with polynomial coefficients (7.8). However, in general the integrand in (7.3) does not necessarily vanish at the limits of integration. Therefore we have to extend the above sketched algorithm. Subsequently we are going to present two ways of extending the algorithm such that we can handle integrals where $F(n; x_1, \dots, x_d)$ (and hence $G(n; x_1, \dots, x_d)$) does not vanish at the integration limits.

The first extension consists in forcing the G_i to vanish at the integration bounds by modifying the ansatz (7.6). For $u_i, o_i \in \mathbb{R}$ we can for example use the ansatz (for multi-sums we refer, e.g., to [86])

$$G_i(n; x_1, \dots, x_d) = \overline{H}(n; x_1, \dots, x_d) \cdot r_i(x_1, \dots, x_d) \cdot X_i(x_1, \dots, x_d)(x_i - u_i)(x_i - o_i), \tag{7.9}$$

In principle, this new ansatz works, however the drawback is that it might increase the order of the recurrence that we find drastically. It might even happen that we would find a recurrence (suggested by homomorphic image testing) using ansatz (7.6), but due to time and space limitations we do not explicitly find a recurrence using ansatz (7.9).

Example 7.2.1. *As a straightforward example we consider the integral*

$$I(\varepsilon, n) = \int_0^1 \int_0^1 \frac{(1 + x_1 \cdot x_2)^n}{(1 + x_1)^\varepsilon} dx_1 dx_2.$$

Note that the integrand does not vanish at the integration bounds, hence we apply the algorithm using ansatz (7.9); this leads to the recurrence

$$\begin{aligned} &2(n + 1)(\varepsilon - n - 2)I(\varepsilon, n) - (n + 2)(5\varepsilon - 5n - 13)I(\varepsilon, n + 1) \\ &+ (n + 3)(4\varepsilon - 4n - 13)I(\varepsilon, n + 2) - (n + 4)(\varepsilon - n - 4)I(\varepsilon, n + 3) = 0. \end{aligned}$$

Using Sigma, the solution of the recurrence together with the initial values of the integral leads to the result

$$I(\varepsilon, n) = \frac{1}{n + 1} \left(\sum_{i=1}^n \frac{1}{-i + \varepsilon - 1} - 2^{1-\varepsilon} \sum_{i=1}^n \frac{2^i}{-i + \varepsilon - 1} + \frac{2^{-\varepsilon} (2^\varepsilon - 2)}{\varepsilon - 1} \right)$$

The second extension keeps the ansatz (7.6), however it deals with the inhomogeneous recurrence similar to [26]; this will give rise to a recursive method. We consider the integral

$$a(n) := \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d) dx_1 \dots dx_d.$$

Suppose that we found

$$\sum_{i=0}^L e_i(n) F(n + i; x_1, \dots, x_d) = \sum_{i=1}^d D_{x_i} G_i(n; x_1, \dots, x_d) \tag{7.10}$$

where at least one $G_i(n; x_1, \dots, x_d)$ does not vanish at the integration limits. By integration with respect to x_1, \dots, x_d we can deduce that $a(n)$ satisfies the inhomogeneous linear recurrence equation

$$\sum_{i=0}^L e_i(n) a(n + i) = \sum_{i=1}^d \int_{u_d}^{o_d} \dots \int_{u_{i-1}}^{o_{i-1}} \int_{u_{i+1}}^{o_{i+1}} \dots \int_{u_1}^{o_1} O_i(n) dx_1 \dots dx_{i-1} dx_{i+1} \dots dx_d$$

$$-\sum_{i=1}^d \int_{u_d}^{o_d} \cdots \int_{u_{i-1}}^{o_{i-1}} \int_{u_{i+1}}^{o_{i+1}} \cdots \int_{u_1}^{o_1} U_i(n) dx_1 \cdots dx_{i-1} dx_{i+1} \cdots dx_d$$

with

$$\begin{aligned} U_i(n) &:= G_i(n; x_1, \dots, x_{i-1}, o_i, x_{i+1}, \dots, x_d) \\ O_i(n) &:= G_i(n; x_1, \dots, x_{i-1}, u_i, x_{i+1}, \dots, x_d). \end{aligned}$$

Note that the inhomogeneous part of the above recurrence equation is a sum of $2 \cdot d$ integrals of dimension $d - 1$, which fit again into the input class of the Almkvist-Zeilberger algorithm. Hence we can apply the algorithms to the $2 \cdot d$ integrals recursively until we arrive at the base case of one-dimensional integrals for which we have to solve an inhomogeneous linear recurrence relation where the inhomogeneous part is free of integrals. Given the solutions for the one-dimensional integrals we can step by step find the solutions of higher dimensional integrals until we finally find the solution for $a(n)$ by solving again an inhomogeneous linear recurrence equation and combining it with the initial values. Note that we have to calculate initial values with respect to n for all the integrals arising in this process.

To compute the solutions of the arising recurrences we exploit algorithms from [70, 11, 78, 77] which can constructively decide if a solution with certain initial values is expressible in terms of indefinite nested products and sums. To be more precise, we use the summation package `Sigma` in which algorithms are implemented with which one can solve the following problem (see [26]).

Problem RS: Recurrence Solver for indefinite nested product-sum expressions.

Given $a_0(N), \dots, a_d(N) \in \mathbb{K}[N]$; given $\mu \in \mathbb{N}$ such that $a_d(k) \neq 0$ for all $k \in \mathbb{N}$ with $N \geq \mu$; given an expression $h(N)$ in terms of indefinite nested product-sum expressions which can be evaluated for all $N \in \mathbb{N}$ with $N \geq \mu$; given the initial values $(c_\mu, \dots, c_{\mu+d-1})$ which produces the sequence $(c_i)_{i \geq \mu} \in \mathbb{K}^{\mathbb{N}}$ by the defining recurrence relation

$$a_0(N)c_N + a_1(N)c_{N+1} + \cdots + a_d(N)c_{N+d} = h(N) \quad \forall N \geq \mu.$$

Find, if possible, $\lambda \in \mathbb{N}$ with $\lambda \geq \mu$ and an indefinite nested product-sum expression $g(N)$ such that $g(k) = c_k$ for all $k \geq \lambda$.

Summarizing, with these algorithms we use the following strategy (note that we assume that we are able to compute the initial values for the arising integrals); compare [26]:

Divide and conquer strategy

1. BASE CASE: If $\mathcal{I}(N)$ has no integration quantifiers, return $\mathcal{I}(N)$.

2. DIVIDE: As worked out in above, compute a recurrence relation

$$a_0(N)\mathcal{I}(N) + \cdots + a_d(N)\mathcal{I}(N + d) = h(N) \quad (7.11)$$

with polynomial coefficients $a_i(N) \in \mathbb{K}[N]$, $a_m(N) \neq 0$ and the right side $h(N)$ containing a linear combination of hyperexponential multi-integrals each with less than d summation quantifiers.

3. CONQUER: Apply the strategy recursively to the simpler integrals in $h(N)$. This results in an indefinite nested product-sum expressions $\tilde{h}(N)$ with

$$\tilde{h}(N) = h(N) \quad (7.12)$$

if the method fails to find the $\tilde{h}(N)$ in terms of indefinite nested product-sum expressions, STOP.

4. COMBINE: Given (7.11) with (7.12), compute, if possible, $\tilde{\mathcal{I}}(N)$ in terms of nested product-sum expressions such that

$$\tilde{\mathcal{I}}(N) = \mathcal{I}(N) \quad (7.13)$$

by solving problem RS.

Example 7.2.2. *Again we consider the integral*

$$I(\varepsilon, n) = \int_0^1 \int_0^1 \underbrace{\frac{(1 + x_1 \cdot x_2)^n}{(1 + x_1)^\varepsilon}}_{F(n; x_1, x_2) :=} dx_1 dx_2,$$

however now we will use the second proposed extension of the algorithm. Applying the algorithm using ansatz (7.6) and choosing $\mathbb{K} = \mathbb{Q}(\varepsilon)$ leads to

$$-(n + 1)F(n; x_1, x_2) + (n + 2)F(n + 1; x_1, x_2) = D_{x_1}0 + D_{x_2} \frac{x_2(x_1 \cdot x_2 + 1)^{n+1}}{(1 + x_1)^\varepsilon}$$

and hence it follows by integration

$$-(n + 1)I(\varepsilon, n) + (n + 2)I(\varepsilon, n + 1) = \underbrace{\int_0^1 (x_1 + 1)^{n+1-\varepsilon} dx_1}_{I_1(n)} - \int_0^1 0 dx_1. \quad (7.14)$$

In the next step apply the algorithm to $I_1(n)$; we find

$$I_1(\varepsilon, n) = \frac{4 \cdot 2^n - 2^\varepsilon}{2^\varepsilon(n + 2 - \varepsilon)}.$$

Plugging in this result into (7.14) yields

$$-(n+1)I(\varepsilon, n) + (n+2)I(\varepsilon, n+1) = \frac{4 \cdot 2^n - 2^\varepsilon}{2^\varepsilon(n+2-\varepsilon)}.$$

The solution of this recurrence together with the initial values of the integral yields again the result

$$I(\varepsilon, n) = \frac{1}{n+1} \left(\sum_{i=1}^n \frac{1}{-i+\varepsilon-1} - 2^{1-\varepsilon} \sum_{i=1}^n \frac{2^i}{-i+\varepsilon-1} + \frac{2^{-\varepsilon}(2^\varepsilon-2)}{\varepsilon-1} \right).$$

Remark 7.2.3. We can as well combine both extensions and thereby balance the size of the inhomogeneous part and the order of the recurrence. Although we could handle a much larger class of integrals using the second extension we again ran into integrals which we could not process due to time and space limitations. Note that another bottle neck might be the calculation of the initial values of all the integrals arising.

7.3 Finding ε -Expansions of the Integral

As already mentioned we ran into integrals which we could not process due to time and space limitations using the methods described in the previous section. Therefore, inspired by [26], we develop subsequently another method which computes ε -expansions of integrals of the form (7.3). In the following we assume that the integral $\mathcal{I}(\varepsilon, N)$ from (7.3) has a Laurent expansion in ε for each $N \in \mathbb{N}$ with $N \geq \lambda$ for some $\lambda \in \mathbb{N}$ and thus it is an analytic function in ε throughout an annular region centered by 0 where the pole at $\varepsilon = 0$ has some order L . Hence we can write it in the form

$$\mathcal{I}(\varepsilon, N) = \sum_{l=-L}^{\infty} \varepsilon^l I_l(N). \quad (7.15)$$

In the following we try to find the first coefficients $I_t(N), I_{t+1}(N), \dots, I_u(N)$ in terms of indefinite nested product-sum expressions of the expansion

$$\mathcal{I}(\varepsilon, N) = I_t(N)\varepsilon^t + I_{t+1}(N)\varepsilon^{t+1} + I_{t+2}(N)\varepsilon^{t+2} + \dots \quad (7.16)$$

with $t = -L$, ($t \in \mathbb{Z}$).

Restricting the \mathcal{O} -notation to formal Laurent series $f = \sum_{i=r}^{\infty} f_i \varepsilon^i$ and $g = \sum_{i=s}^{\infty} g_i \varepsilon^i$ the notation

$$f = g + O(\varepsilon^t)$$

for some $t \in \mathbb{Z}$ means that the order of $f - g$ is larger or equal to t , i.e., $f - g = \sum_{i=t}^{\infty} h_i \varepsilon^i$. We start by computing a recurrence for $\mathcal{I}(\varepsilon, N)$ in the form

$$a_0(\varepsilon, N)T(\varepsilon, N) + \dots + a_d(\varepsilon, N)T(\varepsilon, N+d) = h_0(N) + \dots + h_u(N)\varepsilon^u + O(\varepsilon^{u+1}); \quad (7.17)$$

in order to accomplish this task we can use the methods presented in the previous two sections. Given the recurrence we exploit an algorithm from [26] which can constructively decide if a formal Laurent series solution with certain initial values is expressible (up to a certain order) in terms of indefinite nested products and sums. To be more precise, with the algorithm FLSR presented in [26] and implemented in **Sigma** we can solve the following problem.

Problem FLSR: Formal Laurent Series solutions of linear Recurrences.

Given $\mu \in \mathbb{N}$; $a_0(\varepsilon, N), \dots, a_d(\varepsilon, N) \in \mathbb{K}[\varepsilon, N]$ such that $a_d(0, k) \neq 0$ for all $k \in \mathbb{N}$ with $k \geq \mu$; indefinite nested product-sum expressions $h_t(N), \dots, h_u(N)$ ($t, u \in \mathbb{Z}$ with $t \leq u$) which can be evaluated for all $N \in \mathbb{N}$ with $N \geq \mu$; $c_{i,j} \in \mathbb{K}$ with $t \leq i \leq u$ and $\mu \leq j < \mu + d$

Find, if possible, $(r, \lambda, \tilde{T}(N))$, where $r \in \{t-1, t, \dots, u\}$ is the maximal number such that for the unique solution $T(N) = \sum_{i=t}^u F_i(N)\varepsilon^i$ with $F_i(k) = c_{i,k}$ for all $\mu \leq k < \mu + d$ and with the relation (7.17) the following holds: there are indefinite nested product-sum expressions $\tilde{F}_t(N), \dots, \tilde{F}_r(N)$ that compute the $F_t(N), \dots, F_r(N)$ for all $N \geq \lambda$ for some $\lambda \geq \mu$; if $r \geq t$, $\tilde{T}(N) = \sum_{i=t}^r \tilde{F}_i(N)\varepsilon^i$.

Summarizing the considerations leads to the following theorem (compare [26]).

Theorem 7.3.1. *Let $\mathcal{I}(\varepsilon, N)$ be an integral of the form (7.3) which forms an analytic function in ε throughout an annular region centered by 0 with the Laurent expansion $\mathcal{I}(\varepsilon, N) = \sum_{i=t}^{\infty} f_i(N)\varepsilon^i$ for some $t \in \mathbb{Z}$ for each non-negative N ; let $u \in \mathbb{N}$. Then there is an algorithm (provided that we can compute initial values for the arising integrals) which finds the maximal $r \in \{t-1, 0, \dots, u\}$ such that the $f_t(N), \dots, f_r(N)$ are expressible in terms of indefinite nested product-sums; it outputs such expressions $F_t(N), \dots, F_r(N)$ and $\lambda \in \mathbb{N}$ s.t. $f_i(k) = F_i(k)$ for all $0 \leq i \leq r$ and all $k \in \mathbb{N}$ with $k \geq \lambda$.*

Let $\mathcal{I}(\varepsilon, N)$ be a multi-integral of the form (7.3) and assume that $\mathcal{I}(\varepsilon, N)$ has a series expansion (7.16) for all $N \geq \lambda$ for some $\lambda \in \mathbb{N}$. Combining the methods of the previous sections we obtain the following general method (compare [26]) to compute the first coefficients, say $F_t(N), \dots, F_u(N)$ of (7.16). Note that we assume that we can handle the initial values.

Divide and conquer strategy

1. BASE CASE: If $\mathcal{I}(\varepsilon, N)$ has no integration quantifiers, compute the expansion by standard methods.
2. DIVIDE: As worked out in Section 7.2, compute a recurrence relation

$$a_0(\varepsilon, N)\mathcal{I}(\varepsilon, N) + \cdots + a_d(\varepsilon, N)\mathcal{I}(\varepsilon, N + d) = h(\varepsilon, N) \quad (7.18)$$

with polynomial coefficients $a_i(\varepsilon, N) \in \mathbb{K}[\varepsilon, N]$, $a_m(\varepsilon, N) \neq 0$ and the right side $h(\varepsilon, N)$ containing a linear combination of hyperexponential multi-integrals each with less than d integration quantifiers.

3. CONQUER: Apply the strategy recursively to the simpler integrals in $h(\varepsilon, N)$. This results in an expansion of the form

$$h(\varepsilon, N) = h_t(N) + h_1(N)\varepsilon + \cdots + h_u(N)\varepsilon^u + O(\varepsilon^{u+1}); \quad (7.19)$$

if the method fails to find the $h_t(N), \dots, h_u(N)$ in terms of indefinite nested product-sum expressions, STOP.

4. COMBINE: Given (7.18) with (7.19), compute, if possible, the $F_t(N), \dots, F_u(N)$ of (7.16) in terms of nested product-sum expressions by executing Algorithm FLSR of Sigma.

Example 7.3.2. *Again we consider the integral*

$$I(\varepsilon, n) = \int_0^1 \int_0^1 \underbrace{\frac{(1 + x_1 \cdot x_2)^n}{(1 + x_1)^\varepsilon}}_{F(n; x_1, x_2) :=} dx_1 dx_2,$$

however now we will use the second proposed extension of the algorithm. Applying the algorithm using ansatz (7.6) leads to

$$-(n+1)F(n; x_1, x_2) + (n+2)F(n+1; x_1, x_2) = D_{x_1}0 + D_{x_2} \frac{x_2(x_1 \cdot x_2 + 1)^{n+1}}{(1+x_1)^\varepsilon}$$

and hence it follows by integration

$$-(n+1)I(\varepsilon, n) + (n+2)I(\varepsilon, n+1) = \underbrace{\int_0^1 (x_1 + 1)^{n+1-\varepsilon} dx_1}_{I_1(n)} - \int_0^1 0 dx_1. \quad (7.20)$$

In the next step apply the method to $I_1(n)$; we find

$$\begin{aligned} I_1(\varepsilon, n) &= \frac{2^{n+2} - 1}{n+2} + \frac{\varepsilon(-2^{n+2}(\mathbf{H}_{-1}(1)(n+2) - 1) - 1)}{(n+2)^2} \\ &\quad + \frac{\varepsilon^2(2^{n+1}(\mathbf{H}_{-1}(1)^2(n+2)^2 - 2\mathbf{H}_{-1}(1)(n+2) + 2) - 1)}{(n+2)^3} + O(\varepsilon^3). \end{aligned}$$

Plugging in this result into (7.14) and solving the resulting recurrence by means of FLSR and combining the solution with the initial values of the integral yields the result

$$\begin{aligned}
I(\varepsilon, n) &= \frac{S_1(2; n)}{n+1} - \frac{S_1(n)}{n+1} + \frac{2(n+1)^3 + 4(-n+2^n-1)(n+1)^2 + 2n(n+1)^2}{2(n+1)^4} \\
&+ \varepsilon \left(H_{-1}(1) \left(\frac{-2^{n+2}(n+1) - 2^{n+2}n(n+1)}{2(n+1)^4} - \frac{S_1(2; n)}{n+1} \right) \right. \\
&+ \frac{(2(n+1)n^2 + 4(n+1)n + 2(n+1)) S_2(2; n)}{2(n+1)^4} - \frac{S_2(n)}{n+1} \\
&+ \left. \frac{2^{n+2}(n+1) - 2(n+1)}{2(n+1)^4} \right) + \varepsilon^2 \left(H_{-1}(1)^2 \left(\frac{S_1(2; n)}{2(n+1)} + \frac{2^{n+1}(n^2 + 2n + 1)}{2(n+1)^4} \right) \right. \\
&+ H_{-1}(1) \left(\frac{-2^{n+2}n - 2^{n+2}}{2(n+1)^4} - \frac{S_2(2; n)}{n+1} \right) + \frac{S_3(2; n)}{n+1} - \frac{S_3(n)}{n+1} + \left. \frac{2^{n+2} - 2}{2(n+1)^4} \right) \\
&+ O(\varepsilon^3).
\end{aligned}$$

7.4 The Package MultiIntegrate

This section is dedicated to the presentation of the basic features of the package `MultiIntegrate`, which was developed in the frame of this thesis. In order to use the package `MultiIntegrate` C. Schneider's packages `Sigma` [79] and `EvaluateMultiSum` (see [24]) as well as the package `HarmonicSums` have to be loaded.

MultiIntegrate session.

```

ln[1]:= << Sigma.m
        << HarmonicSums.m
        << EvaluateMultiSums.m
        << MultiIntegrate.m

```

Sigma by Carsten Schneider -RISC Linz- Version 1.0
--

HarmonicSums by Jakob Ablinger -RISC Linz- Version 1.0 (01/03/12)

EvaluateMultiSums by Carsten Schneider -RISC Linz- Version 1.0
--

MultiIntegrate by Jakob Ablinger -RISC Linz- Version 1.0 (01/03/12)

The function `mAZ` which is provided by the package `MultiIntegrate` performs the multivariate Almkvist-Zeilberger and hence finds recurrences for hyperexponential integrands:

MultiIntegrate session.

```

ln[2]:= mAZ \left[ \frac{(1 + x_1 x_2)^n}{(1 + x_1)^\varepsilon}, n, \{x_1, x_2\}, f \right]

```

$$\text{Out[2]} = \left\{ \left\{ 1, \frac{(x_1 x_2 + 1)^n}{(x_1 + 1)^2} \right\}, \left\{ \frac{(x_1 x_2 + 1)^n}{(x_1 + 1)^2}, \{0, x_1\}, \{x_1 x_2^2 + x_2, x_2\}, (-n-1)f(n) + (n+2)f(n+1) \right\} \right\}$$

The 3 different integration methods discussed in Sections 7.2 and 7.3 are implemented in the package `MultiIntegrate`. Suppose we want to compute the integral

$$\int_{u_d}^{o_d} \cdots \int_{u_1}^{o_1} F[n; x_1, \dots, x_d] dx_1 \dots dx_d$$

where $F[n; x_1, \dots, x_d]$ is of the form (7.4) then the first method described in Section 7.2 corresponds to the function call

$$\text{mAZDirectIntegrate}[F[n; x_1, \dots, x_d], n, \{\{x_1, u_1, o_1\}, \dots, \{x_d, u_d, o_d\}\}]$$

whereas the second method corresponds to

$$\text{mAZIntegrate}[F[n; x_1, \dots, x_d], n, \{\{x_1, u_1, o_1\}, \dots, \{x_d, u_d, o_d\}\}].$$

MultiIntegrate session.

$$\text{In[3]} := \text{mAZDirectIntegrate}\left[\frac{(1 + x_1 x_2)^n}{(1 + x_1)^\epsilon}, n, \{\{x_1, 0, 1\}, \{x_2, 0, 1\}\}\right]$$

$$\text{Out[3]} = \frac{\sum_{\ell_1=1}^n \frac{1}{-\epsilon + \ell_1 + 1}}{-n - 1} - \frac{2^{1-\epsilon} \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\epsilon - \ell_1 - 1}}{n + 1} + \frac{2^{-\epsilon} (2^\epsilon - 2)}{(n + 1)(\epsilon - 1)}$$

$$\text{In[4]} := \text{mAZIntegrate}\left[\frac{(1 + x_1 x_2)^n}{(1 + x_1)^\epsilon}, n, \{\{x_1, 0, 1\}, \{x_2, 0, 1\}\}\right]$$

$$\text{Out[4]} = \frac{\sum_{\ell_1=1}^n \frac{1}{-\epsilon + \ell_1 + 1}}{-n - 1} - \frac{2^{1-\epsilon} \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\epsilon - \ell_1 - 1}}{n + 1} + \frac{2^{-\epsilon} (2^\epsilon - 2)}{(n + 1)(\epsilon - 1)}$$

If more discrete variables i.e., n_1, \dots, n_k are present one can use

$$\text{mAZDirectIntegrate}[F[n_1, \dots, n_k; x_1, \dots, x_d], \{n_1, \dots, n_k\}, \{\{x_1, u_1, o_1\}, \dots\}]$$

or

$$\text{mAZIntegrate}[F[n_1, \dots, n_k; x_1, \dots, x_d], \{n_1, \dots, n_k\}, \{\{x_1, u_1, o_1\}, \dots\}].$$

MultiIntegrate session.

$$\text{In[5]} := \text{mAZIntegrate}\left[\frac{(1 + x_1 x_2)^{n_1} x_2^{n_2}}{(1 + x_1)^\epsilon}, \{n_1, n_2\}, \{\{x_1, 0, 1\}, \{x_2, 0, 1\}\}\right]$$

$$\text{Out[5]} = \frac{2^{-\varepsilon} (n_2 2^\varepsilon - 2n_2 - 2\varepsilon + 2^\varepsilon) \left(\prod_{\ell_1=1}^{n_1} \frac{\ell_1}{n_2 + \ell_1 + 1} \right)}{(n_2 + 1)(\varepsilon - 1)(n_2 + \varepsilon)} + \frac{\left(\prod_{\ell_1=1}^{n_1} \frac{\ell_1}{n_2 + \ell_1 + 1} \right) \sum_{\ell_1=1}^{n_1} \frac{\prod_{\ell_2=1}^{\ell_1} \frac{n_2 + \ell_2 + 1}{-\varepsilon + \ell_1 + 1}}{-n_2 - \varepsilon}}{-n_2 - \varepsilon} -$$

$$\frac{2^{1-\varepsilon} \left(\prod_{\ell_1=1}^{n_1} \frac{\ell_1}{n_2 + \ell_1 + 1} \right)}{n_2 + \varepsilon} \left(\sum_{\ell_1=1}^{n_1} \frac{2^{\ell_1} \prod_{\ell_2=1}^{\ell_1} \frac{n_2 + \ell_2 + 1}{\ell_2}}{n_2 + \ell_1 + 1} + \sum_{\ell_1=1}^{n_1} \frac{2^{\ell_1} \prod_{\ell_2=1}^{\ell_1} \frac{n_2 + \ell_2 + 1}{\ell_2}}{\varepsilon - \ell_1 - 1} \right) + \frac{1}{(n_2 + 1)(n_2 + \varepsilon)}$$

In order to find ε -expansions of hyperexponential integrals (see Section 7.3) the function `mAZExpandedIntegrate` is provided. Suppose we want to compute the coefficients $\varepsilon^p, \varepsilon^{p+1}, \dots, \varepsilon^q$ of in the ε -expansion of the integral

$$\int_{u_d}^{o_d} \cdots \int_{u_1}^{o_1} F[\varepsilon; n; x_1, \dots, x_d] dx_1 \dots dx_d$$

we can use the function call

`mAZExpandedIntegrate[F[\varepsilon; n; x_1, \dots, x_d], n, {\varepsilon, p, q}, {{x_1, u_1, o_1}, \dots, {x_d, u_d, o_d}}]`.

MultiIntegrate session.

```
ln[6]:= mAZExpandedIntegrate[ $\left[ \frac{(1+x_1 x_2)^n}{(1+x_1)^\varepsilon}, n, \{\varepsilon, 0, 2\}, \{\{x_1, 0, 1\}, \{x_2, 0, 1\}\} \right]$ 
```

$$\text{Out[6]} = \left\{ \left\{ \frac{\sum_{\ell_1=1}^n \frac{1}{\ell_1+1}}{-n-1} + \frac{2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\ell_1+1}}{n+1} + \frac{1}{n+1}, -\frac{2 \ln 2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\ell_1+1}}{n+1} + \frac{\sum_{\ell_1=1}^n \frac{1}{(\ell_1+1)^2}}{-n-1} + \frac{2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{(\ell_1+1)^2}}{n+1} + \frac{1 - 2 \ln 2}{n+1}, \frac{\ln 2^2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\ell_1+1}}{n+1} - \frac{2 \ln 2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{(\ell_1+1)^2}}{n+1} + \frac{\sum_{\ell_1=1}^n \frac{1}{(\ell_1+1)^3}}{-n-1} + \frac{2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{(\ell_1+1)^3}}{n+1} + \frac{(\ln 2 - 1)^2}{n+1} \right\}, 0, 2 \right\}$$

```
ln[7]:= %[[1]].Table[ $\varepsilon^i, \{i, \%[[2]], \%[[3]]\}$ ]
```

$$\text{Out[7]} = \varepsilon^2 \left(\frac{\ln 2^2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\ell_1+1}}{n+1} - \frac{2 \ln 2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{(\ell_1+1)^2}}{n+1} + \frac{\sum_{\ell_1=1}^n \frac{1}{(\ell_1+1)^3}}{-n-1} + \frac{2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{(\ell_1+1)^3}}{n+1} + \frac{(\ln 2 - 1)^2}{n+1} \right) +$$

$$\varepsilon \left(-\frac{2 \ln 2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\ell_1+1}}{n+1} + \frac{\sum_{\ell_1=1}^n \frac{1}{(\ell_1+1)^2}}{-n-1} + \frac{2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{(\ell_1+1)^2}}{n+1} + \frac{1 - 2 \ln 2}{n+1} \right) + \frac{\sum_{\ell_1=1}^n \frac{1}{\ell_1+1}}{-n-1} +$$

$$\frac{2 \sum_{\ell_1=1}^n \frac{2^{\ell_1}}{\ell_1+1}}{n+1} + \frac{1}{n+1}$$

Note that we can use the package `HarmonicSums` to rewrite the occurring sums in terms of S-sums.

We conclude this chapter with the following integral that occurs in the direct computation of a 3-loop diagram of the ladder-type which emerges for local quarkonic twist-2 operator matrix elements [3].

$$\int_0^1 \int_0^1 \left(\frac{(s(x-1) + t(u-1) + 1)^n}{(w-1)(z-1)(sx-s+tu-t-u+1)(sx-s+tu-t-x+1)} \right. \\ + \frac{1}{(z-1)(sx-s+tu-t-x+1)} \\ \times \frac{(z(-s+tu-t+1) + x((s-1)z+1))^n}{-swx + sw + sxz - sz - tuw + tuz + tw - tz + uw - u - w - xz + x + z} \\ \left. + \frac{1}{(w-1)(sx-s+tu-t-u+1)} \right. \\ \times \frac{(u((t-1)w+1) - w(s(-x) + s+t-1))^n}{swx - sw - sxz + sz + tuw - tuz - tw + tz - uw + u + w + xz - x - z} \Big) dudx.$$

All three summands of the integrand are of the form

$$\frac{(a + bx + cu)^n}{(d + ex + fu)(g + hx + iu)}.$$

Therefore we solve the integral

$$\int_0^1 \int_0^1 \frac{(a + bx + cu)^n}{(d + ex + fu)(g + hx + iu)} dudx$$

for general $a, b, c, d, e, f, g, h, i$ using `mAZIntegrate`:

MultiIntegrate session.

```
In[8]:= mAZIntegrate  $\left[ \frac{(a + bx + cu)^n}{(d + ex + fu)(g + hx + iu)}, n, \{\{x, 0, 1\}, \{u, 0, 1\}\} \right]$ 

Out[8]:=  $\frac{(-aei+afh+bdi-bfg-cdh+ceg)^n}{fgh-ehi} \left( \log(d+e) \log\left(\frac{dfh-efg}{e(d+e)i-ef(g+h)}\right) - \log(d+e+f) \log\left(\frac{f((d+f)h-e(g+i))}{e(d+e)i-ef(g+h)}\right) + \right.$ 
 $\log(d+f) \log\left(\frac{f(e(g+i)-(d+f)h)}{e(fg-dh)}\right) - \log(g+i) \log\left(\frac{i(e(g+i)-(d+f)h)}{h(fg-dh)}\right) - \log(d) \log\left(\frac{efg-dfh}{efg-dhi}\right) +$ 
 $\log(g) \log\left(\frac{egh-dhi}{fgh-dhi}\right) - \log(g+h) \log\left(\frac{(eg-dh)i}{fh(g+h)-(d+e)hi}\right) + \log(g+h+i) \log\left(\frac{i(e(g+i)-(d+f)h)}{fh(g+h)-(d+e)hi}\right) +$ 
 $\text{Li}_2\left(\frac{(d+e)(ei-fh)}{e(d+e)i-ef(g+h)}\right) - \text{Li}_2\left(\frac{(d+e+f)(ei-fh)}{e(d+e)i-ef(g+h)}\right) + \text{Li}_2\left(\frac{(d+f)(fh-ei)}{e(fg-dh)}\right) - \text{Li}_2\left(\frac{(g+i)(fh-ei)}{h(fg-dh)}\right) -$ 
 $\text{Li}_2\left(\frac{dfh-dhi}{efg-dhi}\right) + \text{Li}_2\left(\frac{fgh-egi}{fgh-dhi}\right) - \text{Li}_2\left(\frac{(g+h)(fh-ei)}{fh(g+h)-(d+e)hi}\right) + \text{Li}_2\left(\frac{(g+h+i)(fh-ei)}{fh(g+h)-(d+e)hi}\right) + (\log(d+e) -$ 
 $\log(d)) \text{S}[1, \left\{ \frac{(a-bd)}{ceg-bfg-cdh+afh+bdi-aei} \right\}, n] + (\log(d) - \log(d+f)) \text{S}[1, \left\{ \frac{(a-cd)}{ceg-bfg-cdh+afh+bdi-aei} \right\}, n] + (\log(g) -$ 
 $\log(g+h)) \text{S}[1, \left\{ \frac{(a-bg)}{ceg-bfg-cdh+afh+bdi-aei} \right\}, n] + (\log(g+i) - \log(g)) \text{S}[1, \left\{ \frac{(a-cg)}{ceg-bfg-cdh+afh+bdi-aei} \right\}, n] +$ 
 $(\log(d+f) - \log(d+e+f)) \text{S}[1, \left\{ \frac{((a+c)e-b(d+f))(fh-ei)}{e(ceg-bfg-cdh+afh+bdi-aei)} \right\}, n] + (\log(d+e+f) - \log(d+e)) \text{S}[1, \left\{ \frac{((a+b)f-c(d+e))(fh-ei)}{f(ceg-bfg-cdh+afh+bdi-aei)} \right\}, n] + (\log(g+h+i) - \log(g+i)) \text{S}[1, \left\{ \frac{(fh-ei)((a+c)h-b(g+i))}{h(ceg-bfg-cdh+afh+bdi-aei)} \right\}, n] +$ 
 $(\log(g+h) - \log(g+h+i)) \text{S}[1, \left\{ \frac{((a+b)i-c(g+h))(fh-ei)}{i(ceg-bfg-cdh+afh+bdi-aei)} \right\}, n] - \text{S}[1, 1, \left\{ \frac{(a-bd)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{ae}{ae-bd} \right\}, n] +$ 
 $\text{S}[1, 1, \left\{ \frac{(a-bd)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{(a+b)e}{ae-bd} \right\}, n] - \text{S}[1, 1, \left\{ \frac{(a+c)e-b(d+f)}{e(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+b+c)e}{(a+c)e-b(d+f)} \right\}, n] -$ 
 $\text{S}[1, 1, \left\{ \frac{(a-cd)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{(a+c)f}{af-cd} \right\}, n] + \text{S}[1, 1, \left\{ \frac{((a+b)f-c(d+e))(fh-ei)}{f(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+b+c)f}{(a+b)f-c(d+e)} \right\}, n] -$ 
 $\text{S}[1, 1, \left\{ \frac{(a-bg)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{(a+b)h}{ah-bg} \right\}, n] + \text{S}[1, 1, \left\{ \frac{((a+b)i-c(g+h))(fh-ei)}{i(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+b)i}{(a+b)i-c(g+h)} \right\}, n] +$ 
 $\text{S}[1, 1, \left\{ \frac{(a-cg)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{(a+c)i}{ai-cg} \right\}, n] + \text{S}[1, 1, \left\{ \frac{((a+c)e-b(d+f))(fh-ei)}{e(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+c)e}{(a+c)e-b(d+f)} \right\}, n] +$ 
```

$$\begin{aligned}
& S[1,1, \left\{ \frac{(a-\frac{cg}{f})(fh-ei)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{af}{af-cd} \right\}, n] - S[1,1, \left\{ \frac{((a+b)f-c(d+e))(fh-ei)}{f(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+b)f}{(a+b)f-c(d+e)} \right\}, n] + \\
& S[1,1, \left\{ \frac{(a-\frac{bg}{h})(fh-ei)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{ah}{ah-bg} \right\}, n] - S[1,1, \left\{ \frac{(fh-ei)((a+c)h-b(g+i))}{h(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+c)h}{(a+c)h-b(g+i)} \right\}, n] + \\
& S[1,1, \left\{ \frac{(fh-ei)((a+c)h-b(g+i))}{h(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+b+c)h}{(a+c)h-b(g+i)} \right\}, n] - S[1,1, \left\{ \frac{(a-\frac{cg}{i})(fh-ei)}{ceg-bfg-cdh+afh+bdi-aei}, \frac{ai}{ai-cg} \right\}, n] - \\
& S[1,1, \left\{ \frac{((a+b)i-c(g+h))(fh-ei)}{i(ceg-bfg-cdh+afh+bdi-aei)}, \frac{(a+b+c)i}{(a+b)i-c(g+h)} \right\}, n] \Big)
\end{aligned}$$

Using this general solution we arrive after simplification at the following solution for the whole integral:

$$\begin{aligned}
& \frac{1}{(w-1)(z-1)(s+t-1)} \left(S_{1,1} \left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1}, \frac{sw-sz+z-1}{z-1}; n \right) \right. \\
& - S_{1,1} \left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1}, \frac{(t-1)(sw-sz+z-1)}{(s+t-1)(z-1)}; n \right) + S_{1,1} \left(\frac{s+t-1}{t-1}, (1-t)w; n \right) \\
& - S_{1,1} \left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1}, \frac{z(sw-sz+z-1)}{w(z-1)}; n \right) + S_{1,1} \left(\frac{s+t-1}{t-1}, -\frac{(s-1)(t-1)}{s+t-1}; n \right) \\
& + S_{1,1} \left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1}, \frac{(sw-sz+z-1)(tz-1)}{(s+t-1)w(z-1)}; n \right) - S_{1,1} \left(\frac{s+t-1}{t-1}, 1-t; n \right) \\
& + S_{1,1} \left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1}, \frac{-tw+w+tz-1}{w-1}; n \right) - S_{1,1} \left(\frac{s+t-1}{t-1}, -\frac{(t-1)(sw-1)}{s+t-1}; n \right) \\
& - S_{1,1} \left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1}, \frac{(s-1)(-tw+w+tz-1)}{(s+t-1)(w-1)}; n \right) - S_{1,1} \left(\frac{s+t-1}{s-1}, 1-s; n \right) \\
& - S_{1,1} \left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1}, -\frac{w((t-1)w-tz+1)}{(w-1)z}; n \right) - S_{1,1} \left(\frac{s+t-1}{s-1}, -\frac{(s-1)(tz-1)}{s+t-1}; n \right) \\
& + S_{1,1} \left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1}, -\frac{(sw-1)((t-1)w-tz+1)}{(s+t-1)(w-1)z}; n \right) + S_{1,1} \left(\frac{s+t-1}{s-1}, (1-s)z; n \right) \\
& + S_{1,1} \left(\frac{s+t-1}{s-1}, -\frac{(s-1)(t-1)}{s+t-1}; n \right) - S_{1,1}(1, (1-s)z; n) + S_{1,1}(1, z-sz; n) + S_2((1-s)z; n) \\
& - S_{1,1}(1, (1-t)w; n) + S_{1,1}(1, w-tw; n) - S_2((-s-t+1)w; n) - S_2((-s-t+1)z; n) \\
& \left. + 2S_2(-s-t+1; n) - S_2(1-s; n) + S_2((1-t)w; n) - S_2(1-t; n) \right).
\end{aligned}$$

Bibliography

- [1] J. Ablinger. A computer algebra toolbox for harmonic sums related to particle physics. Master's thesis, Johannes Kepler University, February 2009.
- [2] J. Ablinger, I. Bierenbaum, J. Blümlein, A. Hasselhuhn, S. Klein, C. Schneider, and F. Wissbrock. Heavy flavor DIS Wilson coefficients in the asymptotic regime. *Nucl. Phys. B (Proc. Suppl.)*, 205-206:242–249, 2010. arXiv:1007.0375 [hep-ph].
- [3] J. Ablinger, J. Blümlein, A. Hasselhuhn, S. Klein, and C. Schneider. In preparation. 2012.
- [4] J. Ablinger, J. Blümlein, A. Hasselhuhn, S. Klein, C. Schneider, and F. Wissbrock. New heavy flavor contributions to the DIS structure function $F_2(x, Q^2)$ at $O(\alpha_s^3)$. In *Proceedings of RADCOR 2011*, pages 1–8, 2012. arXiv:1202.2700 [hep-ph].
- [5] J. Ablinger, J. Blümlein, S. Klein, and C. Schneider. Modern summation methods and the computation of 2- and 3-loop Feynman diagrams. *Nucl. Phys. B (Proc. Suppl.)*, 205-206:110–115, 2010. arXiv:1006.4797 [math-ph].
- [6] J. Ablinger, J. Blümlein, S. Klein, C. Schneider, and F. Wissbrock. 3-Loop heavy flavor corrections to DIS with two massive fermion lines. In *19th International Workshop On Deep-Inelastic Scattering And Related Subjects (DIS 2011)*. American Institute of Physics (AIP), 2011. arXiv:1106.5937 [hep-ph].
- [7] J. Ablinger, J. Blümlein, S. Klein, C. Schneider, and F. Wissbrock. The $O(\alpha_s^3)$ massive operator matrix elements of $O(n_f)$ for the structure function $F_2(x, Q^2)$ and transversity. *Nucl. Phys. B*, 844:26–54, 2011. arXiv:1008.3347 [hep-ph].
- [8] J. Ablinger, J. Blümlein, and C. Schneider. Harmonic sums and polylogarithms generated by cyclotomic polynomials. *J. Math. Phys.*, 52(10):1–52, 2011. arXiv:1007.0375 [hep-ph].
- [9] J. Ablinger, J. Blümlein, and C. Schneider. In preparation. 2012.
- [10] J. Ablinger and C. Schneider. In preparation. 2012.

-
- [11] S. Abramov and M. Petkovšek. D'Alembertian solutions of linear differential and difference equations. In J. von zur Gathen, editor, *Proc. ISSAC'94*, pages 169–174. ACM Press, 1994.
- [12] S. Albino. Analytic continuation of harmonic sums. *Phys.Lett.*, B674:41–48, 2009. arXiv:0902.2148 [hep-ph].
- [13] G. Almkvist and D. Zeilberger. The method of differentiating under the integral sign. *J. Symb. Comp.*, 10:571–591, 1990.
- [14] M. Apagodu and D. Zeilberger. Multi-variable Zeilberger and Almkvist-Zeilberger algorithms and the sharpening of Wilf-Zeilberger theory. *Adv. Appl. Math. (Special Regev issue)*, 37:139–152, 2006.
- [15] B. Berndt. *Ramanujan's notebooks*. Springer, 1985.
- [16] J. Bernoulli. *Ars conjectandi, opus posthumum. Accedit tractus de seriebus infinitis, et epistola gallice scripta de ludo pilae reticularis*. Brüder Thurneysen, Basel, 1713.
- [17] I. Bierenbaum, J. Blümlein, and S. Klein. Mellin moments of the $o(\alpha_s^3)$ heavy flavor contributions to unpolarized deep-inelastic scattering at $q^2 \gg m^2$ and anomalous dimensions. *Nucl. Phys.*, pages 417–482, 2009. arXiv:0904.3563 [hep-ph].
- [18] J. Blümlein. Analytic continuation of Mellin transforms up to two-loop order. *Comput. Phys. Commun.*, 133:76, 2000. arXiv:hep-ph/0003100.
- [19] J. Blümlein. Algebraic relations between harmonic sums and associated quantities. *Comput. Phys. Commun.*, 159:19, 2004. arXiv:hep-ph/0311046v1.
- [20] J. Blümlein. Structural relations between nested harmonic sums. *Nuclear Physics B (Proc. Suppl.)*, 183:232–237, 2008.
- [21] J. Blümlein. Structural relations of harmonic sums and Mellin transforms up to weight $w=5$. *DESY 08-206 07-042*, 2009. arXiv:0901.3106 [hep-ph].
- [22] J. Blümlein. Structural relations of harmonic sums and Mellin transforms at weight $w=6$. In A. Carey, D. Ellwood, S. Paycha, and S. Rosenberg, editors, *Motives, Quantum Field Theory, and Pseudodifferential Operators*, volume 12 of *Clay Mathematics Proceedings*, pages 167–186, 2010. DESY 08–206, SFB-CPP/09-002, arXiv:0901.0837 [math-ph].
- [23] J. Blümlein, D.J. Broadhurst, and J.A.M. Vermaseren. The multiple zeta value data mine. *Computer Physics Communications*, 181(3):582 – 625, 2010.

- arXiv:0907.2557v2 [math-ph].
- [24] J. Blümlein, A. Hasselhuhn, and C. Schneider. Evaluation of multi-sums for large scale problems. In *Proceedings of RADCOR 2011*, 2012. arXiv:1202.2700 [math-ph].
- [25] J. Blümlein, M. Kauers, S. Klein, and C. Schneider. Determining the closed forms of the $O(a_s^3)$ anomalous dimensions and Wilson coefficients from Mellin moments by means of computer algebra. 2009. arXiv:0902.4091 [hep-ph].
- [26] J. Blümlein, S. Klein, C. Schneider, and F. Stan. A symbolic summation approach to Feynman integral calculus. *J. Symb. Comp.*, 2011. To appear.
- [27] J. Blümlein and S. Kurth. Harmonic sums and Mellin transforms up to two-loop order. *Phys. Rev.*, D60 014018, 1999. arXiv:hep-ph/9810241v2.
- [28] J. Blümlein and S. Moch. Analytic continuation of the harmonic sums for the 3-loop anomalous dimensions. *Phys. Lett. B*, 614:53, 2005. arXiv:hep-ph/0503188v1.
- [29] C. Bogner and S. Weinzierl. Feynman graph polynomials. *Int. J. Mod. Phys. A*, 25:2585–2618, 2010. arXiv:1002.3458v3 [hep-ph].
- [30] D. Borwein, J.M. Borwein, and R. Girgensohn. Explicit evaluation of Euler sums. In *Proceedings of the Edinburgh Mathematical Society*, volume 38, pages 277–294, 1995.
- [31] J.M. Borwein and R. Girgensohn. Evaluation of triple Euler sums. *Electron. J. Combin.*, 3:1–27, 1996.
- [32] D.J. Broadhurst. On the enumeration of irreducible k fold Euler sums and their roles in knot theory and field theory. arXiv:hep-th/9604128v1.
- [33] D.J. Broadhurst and D. Kreimer. Association of multiple zeta values with positive knots via Feynman diagrams up to 9 loops. *Phys. Lett.*, B393:403–412, 1997. arXiv:hep-th/9609128v3.
- [34] P. Deligne. Le groupe fondamental de $\mathbb{G}(m) - \mu_n$, pour $N=2,3,4,6$, ou 8. *Publications Mathématiques de l'Institut des Hautes Études Scientifiques*, 101, 2010.
- [35] P. Deligne and A.B. Gocharov. Groupes fondamentaux motivique de tate mixte. *IAS preprint*.
- [36] F. Faà di Bruno. *Einleitung in die Theorie der binären Formen*. Teubner, 1881.

-
- [37] K. Dilcher. Some q -series identities related to divisor functions. *Discr. Math.*, 145:83–93, 1995.
- [38] L. Euler. *Methodus generalis summandi progressionibus*. Comm. Acad. Sci. Imp., Petropoli, 1738.
- [39] L. Euler. Theoremata arithmetica nova methodo demonstrata. *Novi Commentarii academiae scientiarum imperialis Petropolitanae*, 8, 1760/1, 1763.
- [40] L. Euler. *Institutiones calculi integralis*, volume 20. Impensis Academiae Imperialis Scientiarum, Petropoli, 1768.
- [41] P. Flajolet and B. Salvy. Euler sums and contour integral representations. *Experiment. Math.*, 7:15–35, 1998.
- [42] Y. Frishman. Operator products at almost light like distances. *Annals Phys.*, 66:373–389, 1971.
- [43] A. B. Goncharov. Multiple polylogarithms, cyclotomy and modular complexes. *Mathematical Research Letters*, 5:497, 1998.
- [44] A. Gonzalez-Arroyo and C. Lopez. Second order contributions to the structure functions in deep inelastic scattering. 3. the singlet case. *Nucl. Phys. B*, 166:429, 1980.
- [45] A. Gonzalez-Arroyo, C. Lopez, and F. J. Yndurain. Second order contributions to the structure functions in deep inelastic scattering. 1. theoretical calculations. *Nucl. Phys. B*, 153:161, 1979.
- [46] G.W. Hardy and E.M. Wright. *An introduction to the theory of numbers*. Clarendon Press, Oxford, 1979.
- [47] M. Hoffman. Multiple harmonic series. *Pacific J. Math.*, 152:275–290, 1992.
- [48] M. Hoffman. The algebra of multiple harmonic series. *J. Algebra*, 194:477–495, 1997.
- [49] M. Hoffman. Quasi-shuffle products. *J. Algebraic Combin.*, 11:49–68, 2000.
- [50] D. J. Broadhurst, J. M. Borwein, D. M. Bradley and P. Lisonek. Special values of multiple polylogarithms. *Trans. Am. Math. Soc.*, 353:907, 2001. arXiv:math/9910045v1 [math.CA].

- [51] M. Karr. Summation in finite terms. *J. ACM*, 28:305–350, 1981.
- [52] P. Kirschenhofer. A note on alternating sums. *Electron. J. Combin*, 3, 1996.
- [53] E. Landau. *Über die Grundlagen der Theorie der Fakultätenreihen*. S.-Ber. math.-naturw. Kl. Bayerische Akad. Wiss. München, 1906.
- [54] S. Lang. *Algebra*. Springer, New York, 2002.
- [55] J.A. Lappo-Danielevsky. *Mémoires sur la théorie des systèmes différentielles linéaires*. Chelsea Publishing Company, 1953.
- [56] H. Lugowski and J. Weinert. *Grundzüge der Algebra*. Teubner, Leipzig, 1960.
- [57] R. Lyons, P. Paule, and A. Riese. A computer proof of a series evaluation in terms of harmonic numbers. *Appl. Algebra Engrg. Comm. Comput.*, 13:327–333, 2002.
- [58] C. MacLaurin. *Treatise of fluxions*, volume 20. T. W. and T. Ruddimans, Edinburgh, 1742.
- [59] R. Mertig and W. L. van Neerven. The calculation of the two-loop spin splitting functions $P_{ij}^{(1)}(x)$. *Z. Phys. C*, 70:637, 1996. arXiv:hep-ph/9506451v1.
- [60] Hoang Ngoc Minh and J. van der Hoeven M. Petitot. Structure and asymptotic expansion of multiple harmonic sums. *Discr. Math.*, page 100, 2000.
- [61] A.F. Möbius. Über eine besondere Art von Umkehrung der Reihen. *J. reine angew. Math.*, 9:105–123, 1832.
- [62] S. Moch, P. Uwer, and S. Weinzierl. Nested sums, expansion of transcendental functions, and multiscale multiloop integrals. *Journal of Math. Physics*, 43:3363, 2002. arXiv:hep-ph/0110083v2.
- [63] S. Moch, J.A.M. Vermaseren, and A. Vogt. The three-loop splitting functions in QCD: The non-singlet case. *Nucl. Phys. B*, 688:101, 2004. arXiv:hep-ph/0403192v1.
- [64] S. Moch, J.A.M. Vermaseren, and A. Vogt. The three-loop splitting functions in QCD: The singlet case. *Nucl. Phys. B*, 691:129, 2004. arXiv:hep-ph/0404111v1.
- [65] S. Moch, J.A.M. Vermaseren, and A. Vogt. The third-order QCD corrections to deep-inelastic scattering by photon exchange. *Nucl. Phys. B*, 724:3, 2005. arXiv:hep-ph/0504242v1.

- [66] N. Nielsen. *Traité élémentaire des nombre de Bernoulli*. Gauthier-Villars, Paris, 1923.
- [67] N. Nielsen. *Handbuch der Theorie der Gammafunktion*. (Teubner, Leipzig, 1906); reprinted by Chelsea Publishing Company, Bronx, NY, 1965.
- [68] N. Nielsen. *Theorie des Integrallogarithmus und verwandter Transzendenten*. (BG Teubner, Leipzig, 1906); reprinted by Chelsea Publishing Company, Bronx, NY, 1965.
- [69] R. B. Paris and D. Kaminski. *Asymptotics and Mellin-Barnes integrals*. Cambridge University Press, 2001.
- [70] M. Petkovšek. Hypergeometric solutions of linear recurrences with polynomial coefficients. *J. Symb. Comp.*, 14:243–264, 1992.
- [71] H. Poincaré. *Acta Math* 4, 4:201, 1884.
- [72] D. Radford. A natural ring basis for the shuffle algebra and an application to group schemes. *J. Algebra*, 58:432, 1979.
- [73] E. Remiddi and J.A.M. Vermaseren. Harmonic polylogarithms. *Int. J. Mod. Phys.*, A 15:725, 2000. arXiv:hep-ph/9905237v1.
- [74] C. Reutenauer. *Free Lie algebras*. Oxford University Press, 1969.
- [75] L. Saalschütz. *Vorlesungen über die Bernoullischen Zahlen*. Springer, Berlin, 1893.
- [76] D. Y. Savio, E. A. Lamagna, and Shing-Min Liu. Summation of harmonic numbers.
- [77] C. Schneider. Solving parameterized linear difference equations in terms of indefinite nested sums and products. *J. Differ. Equations Appl.*, 11(9):799–821, 1992.
- [78] C. Schneider. *Symbolic summation in difference fields*. PhD thesis, RISC, J. Kepler University Linz, May 2001. (published as Technical report no. 01-17 in RISC Report Series.).
- [79] C. Schneider. Symbolic summation assists combinatorics. *Sém. Lothar. Combin.*, 56:1–36, 2007.
- [80] C. Schneider. A refined difference field theory for symbolic summation. *J. Symb. Comp.*, 43(9):611–644, 2008.

-
- [81] C. Schneider. Parameterized telescoping proves algebraic independence of sums. *Ann. Comb.*, 14(4):533–552, 2010.
- [82] C. Schneider. A symbolic summation approach to find optimal nested sum representations. In A. Carey, D. Ellwood, S. Paycha, and S. Rosenberg, editors, *Motives, Quantum Field Theory, and Pseudodifferential Operators*, volume 12 of *Clay Mathematics Proceedings*, pages 285–308. Amer. Math. Soc, 2010. arXiv:0904.2323v1 [cs.SC].
- [83] C. Schneider and R. Pemantle. When is $0.999\dots$ equal to 1? *Amer. Math. Monthly*, 114(4):344–350, 2007.
- [84] M. Takase. Euler’s theory of numbers. In R. Baker, editor, *Euler reconsidered*, pages 377–421. Kedrick Press, Heber City, UT, 2007.
- [85] J.A.M. Vermaseren. Harmonic sums, Mellin transforms and integrals. *Int.J.Mod.Phys.*, A14:2037–2076, 1999. arXiv:hep-ph/9806280v1.
- [86] K. Wegschaider. Computer generated proofs of binomial multi-sum identities. Master’s thesis, RISC, J. Kepler University, May 1997.
- [87] E. Witt. Treue Darstellung Liescher Ringe. *J. Reine Angew. Math*, 177:152, 1937.
- [88] E. Witt. Die Unterringe der freien Lieschen Ringe. *Math. Z.*, 64:195, 1956.
- [89] K. Yoshida. *Functional analysis*. Springer, Berlin, 1978.
- [90] D. Zagier. *Values of zeta functions and their applications*, page 497. First European Congress of Mathematics, Vol II, 1994.

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