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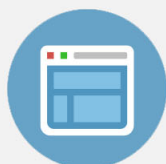
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Analytic and algorithmic aspects of generalized harmonic sums and polylogarithms

Jakob Ablinger,¹ Johannes Blümlein,² and Carsten Schneider¹

¹Research Institute for Symbolic Computation (RISC), Johannes Kepler University, Altenbergerstraße 69, A-4040, Linz, Austria

²Deutsches Elektronen-Synchrotron, DESY, Platanenallee 6, D-15738 Zeuthen, Germany

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In recent three-loop calculations of massive Feynman integrals within Quantum Chromodynamics (QCD) and, e.g., in recent combinatorial problems the so-called generalized harmonic sums (in short S -sums) arise. They are characterized by rational (or real) numerator weights also different from ± 1 . In this article we explore the algorithmic and analytic properties of these sums systematically. We work out the Mellin and inverse Mellin transform which connects the sums under consideration with the associated Poincaré iterated integrals, also called generalized harmonic polylogarithms. In this regard, we obtain explicit analytic continuations by means of asymptotic expansions of the S -sums which started to occur frequently in current QCD calculations. In addition, we derive algebraic and structural relations, like differentiation with respect to the external summation index and different multi-argument relations, for the compactification of S -sum expressions. Finally, we calculate algebraic relations for infinite S -sums, or equivalently for generalized harmonic polylogarithms evaluated at special values. The corresponding algorithms and relations are encoded in the computer algebra package `HarmonicSums`. © 2013 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4811117>]

I. INTRODUCTION

In loop calculations of Feynman diagrams in quantum field theories special classes of multiply nested sums and iterated integrals appear both in intermediate steps and in the final results. For example, this applies both to the massless case and diagrams characterized by a single mass scale, or in cases two sufficiently different mass scales appear and one may consider precise power expansions in their ratio. We will focus in the following on single differential quantities. They can be characterized either by a dimensional variable x with $x \in \mathbb{R}$, $0 \leq x \leq 1$ with exponential growth, or an integer variable N . Both representations are equivalent and are related by a Mellin transform (Here $f : \mathbb{R} \rightarrow \mathbb{R}$ can be a distribution valued function, cf. Ref. 138.)

$$M[f(x)](n) := \int_0^1 x^n f(x) dx. \quad (1.1)$$

The n -dependence may occur generically for Feynman diagrams with local operator insertions which appear, e.g., within the light-cone expansion^{133,142,36,63,18} in deep-inelastic scattering. As has been shown in Refs. 27, 29, and 131 these Feynman integrals can always be represented by multiply nested sums. However, in general the specific type of these sums is not easily predicted. It is assumed that the classes of sums do steadily extend going to higher loops and/or allowing for more masses and external off-shellness for a growing number of legs.

Systematic analyses for a large class of single-scale processes at the 2-loop level in the massless case revealed^{22,24} that the results for all processes could be expressed in terms of six basic functions in Mellin-space only. Here one allows as well to use argument-duplication and differential relations. The corresponding functions are multiple harmonic sums. (In the physics literature their use dates back to Ref. 67, see also Refs. 62 and 87.)

For a non-negative integer n and nonzero integers a_i ($1 \leq i \leq k$) the harmonic sums^{19,123} are defined as

$$S_{a_1, \dots, a_k}(n) = \sum_{n \geq i_1 \geq i_2 \geq \dots \geq i_k \geq 1} \frac{\text{sign}(a_1)^{i_1}}{i_1^{|a_1|}} \dots \frac{\text{sign}(a_k)^{i_k}}{i_k^{|a_k|}}. \quad (1.2)$$

If $a_1 \neq 1$, the limit $n \rightarrow \infty$ exists and the values can be expressed in terms of multiple zeta values, resp. Euler-Zagier values;^{56,139} for further properties and an extensive list of literature we refer to Ref. 28. Likewise, more general classes of sums also result into new classes of special numbers.

In physics applications harmonic sums emerge for the first time in case of the fermion-fermion anomalous dimension (the Mellin transform of the corresponding splitting function)⁶⁰ as the classical harmonic sum $S_1(n)$ (also called harmonic numbers). A first non-trivial nested harmonic sum appears at the 2-loop level with $S_{-2,1}(n)$.⁶⁷

Harmonic sums satisfy a quasi-shuffle algebra⁷¹ and can be formulated in terms of indefinite nested integrals. The Mellin transform (1.1) enables one to map harmonic sums to their integral representation in terms of weighted harmonic polylogarithms, and the inverse transform allows one to transform these integral representations back to harmonic sums.¹⁰⁵ These properties give rise to the analytic continuation^{20,13,23,81,25-27} of harmonic sums. In particular, one can calculate the asymptotic expansion of harmonic sums;^{26,27} for the special case $a_i \geq 1$, see also Ref. 47. Moreover, various relations between harmonic sums are derived which allows to compactify harmonic sum expressions coming from Quantum Chromodynamics (QCD) calculations. Here in particular the algebraic relations^{90,21,123} induced by the quasi-shuffle algebra and the structural relations^{27,26} based on the differentiation of harmonic sums contribute substantially.

Harmonic sums play a prominent role, e.g., in the field of combinatorics or number theory. Here the summation package `Sigma`¹¹³ based on difference field theory^{77,110,112,111,115} contributed to discover and prove identities such as Refs. 99, 109, 50, 114, and 101; as a special case these algorithms contain hypergeometric summation.¹⁰² Meanwhile these algorithms are combined with the `HarmonicSums` package⁶ (containing the analytic and algebraic properties summarized above) and lead to new packages^{1,29,31,8} dealing with definite multi-sums.

In recent calculations based on these packages new classes of functions have been arising not only in intermediate results but also in the final result of given Feynman integrals. Not only during such calculation but also for further considerations of the given result, it is crucial that the knowledge of these new function classes is explored to a similar advanced level as the harmonic sums. For instance, the new class of cyclotomic harmonic sums has been analyzed in detail in Ref. 5.

In particular, the generalized harmonic sums or so-called S -sums⁹⁰ occur in higher order calculations.^{125,2,3,7,9,11}

These sums may also emerge in connection with cyclotomic index alphabets⁵ and nested binomial and inverse binomial weights, cf. Refs. 11 and 12. In the context of statistics or number theory typical calculations can be found, e.g., in Refs. 99, 100, and 98. In case of pure harmonic weights they are defined by

$$S_{a_1, \dots, a_k}(x_1, \dots, x_k; n) = \sum_{n \geq i_1 \geq i_2 \geq \dots \geq i_k \geq 1} \frac{x_1^{i_1}}{i_1^{a_1}} \dots \frac{x_k^{i_k}}{i_k^{a_k}}, \quad (1.3)$$

with positive integers a_i and (usually) real numbers $x_i \neq 0$ ($1 \leq i \leq k$). Note that restricting $x_i = \pm 1$ gives back the class of harmonic sums (1.2), or in case that $x_i \in \{u \in \mathbb{C} | u^n = 1, n \in \mathbb{N}\}$ the complex representations of the cyclotomic sums.⁵ There are mutual applications of these functions in loop calculations, for a survey, see, e.g., Ref. 130. Special cases of the S -sums are, cf. Ref. 90: the harmonic sums^{123,19} and the multiple zeta values resp. Euler-Zagier values, cf., e.g., Ref. 28, the multiple polylogarithms,^{66,35} two-dimensional harmonic polylogarithms including the letters $\{0, 1, -1, 1-z, -z\}$,^{64,65} the harmonic polylogarithms over the alphabet $\{0, 1, -1\}$,¹⁰⁵ the Nielsen integrals over the alphabets $\{0, 1\}$, resp. $\{0, -1\}$,^{96,79,48,80} and the classical polylogarithms.^{84,85,48,140} Furthermore,⁹⁰ the generalized hypergeometric functions

${}_{P+1}F_P$ ^{78, 16, 120, 53, 57, 58} the Appell-functions $F_{1,2}$ and the Kampé De Fériet functions^{14–16, 120, 53, 57, 58} can be represented in terms of S -sums. Code-implementations of four general algorithms being described in Ref. 90 are given in Refs. 128, 92, and 127. In field theoretic calculations the ε -expansion in the dimensional parameter is of importance and needs to be solved for the S -sums and the analytic continuation in their parameters. For special classes the ε -expansion has been studied in Refs. 90, 129, 75, 76, 73, 74, 3, 29, and 41.

In Ref. 90 it is heavily exploited that these sums satisfy a quasi-shuffle algebra. S -sums form a Hopf algebra,^{72, 88, 121, 82, 46, 43} as has been shown in Ref. 90, see also Ref. 52. The quasi-shuffle property leads to new techniques to expand certain definite nested sums over hypergeometric terms in terms of S -sums. In addition, it has been worked out in Ref. 35 that the S -sums at infinity can be expressed in terms of Goncharov's multiple polylogarithms;⁶⁶ see also Ref. 35. Moreover, relations of infinite S -sums with x_i being roots of unity have been explored in Ref. 5.

In this article we aim at extending these results further to important technologies that are currently available for harmonic sums. First we observe that S -sums can be expressed in terms of a variant of multiple polylogarithms involving also the parameter n ; sending n to infinity gives back the standard generalized polylogarithms. As a consequence, S -sums can be analytically continued up to countable many poles. This gives rise to introduce Poincaré iterated integrals^{103, 83, 45} which we call generalized harmonic polylogarithms and which extend the harmonic polylogarithms from Ref. 105. It will turn out that an extended version of the Mellin transform applied to weighted generalized polylogarithms can be expressed in terms of S -sums. Conversely, the inverse Mellin transform enables one to express a certain class of S -sums in terms of weighted generalized polylogarithms. In addition, we extend the ideas of Ref. 105 to calculate the series expansion of generalized polylogarithms where the coefficients of the expansion are given in terms of S -sums. This enables one to transform and back-transform generalized polylogarithms evaluated at constants in terms of infinite S -sums. In addition, we obtain algorithms to calculate the differentiation of S -sums and calculate the asymptotic expansion of such sums. In general, we obtain complete algorithms for S -sums (1.3) with $x_i \in [-1, 1]$ and $x_i \neq 0$. For arising calculations in QCD we succeeded in extending the algorithms for larger ranges of x_i by using, e.g., the integral representation of S -sums. Finally, we calculate algebraic, structural, and duplication relations for S -sums, e.g., for the alphabet $x_i \in \{-\frac{1}{2}, \frac{1}{2}, 1, -2, 2\}$ to assist the compactification of S -sum expression. This alphabet is of special importance in case of heavy flavor corrections to deep-inelastic scattering at the 3-loop level. Results for related alphabets are obtained analogously. In addition, inspired by the work in Ref. 28 for multiple zeta values we deal with new relations for infinite S -sums coming from the relations of finite sums, shuffle relations from the generalized polylogarithms, and duality relations based on the argument transformations of the generalized polylogarithms.

All the underlying algorithms have been implemented in Ablinger's Mathematica package `HarmonicSums`. For the available commands illustrated by examples we refer to Appendix, see also Ref. 6.

The outline of this article is as follows. In Sec. II we define the basic properties of S -sums with their integral representation and the closely connected generalized polylogarithms. In Sec. III we state important argument transformations of generalized polylogarithms that will be used throughout this article. In Sec. IV we show how one can calculate the coefficients of the series expansion of generalized polylogarithms, and in Sec. V we use this result to derive an algorithm that transforms in both directions generalized polylogarithms evaluated at constants and S -sums at infinity. In Sec. VI we elaborate new aspects on the analytic continuation of S -sums and the special case of harmonic sums. In Sec. VII we define an appropriate Mellin transform for generalized polylogarithms and derive algorithms that calculate the Mellin transform in terms of S -sums and that perform the inverse Mellin transform in terms of generalized polylogarithms. In Sec. VIII we show how one can differentiate S -sums with the (inverse) Mellin transform or with the integral representation. In Sec. IX we explore the algebraic relations induced by the quasi-shuffle algebra, the structural relations based on the differentiation of S -sums and duplication relations. In Sec. X we consider relations of infinite S -sums. Finally, we present techniques to calculate the asymptotic expansion of S -sums in Sec. XI. In conclusion we discuss in Sec. XII examples of generalized harmonic sums emerging in massless and massive 3-loop calculations and their representation in the

complex n -plane. In the Appendix we summarize the available commands of the `HarmonicSums` package which supplement the presented algorithms.

II. BASIC PROPERTIES OF S -SUMS AND GENERALIZED POLYLOGARITHMS

Throughout this article let \mathbb{K} be a field containing the rational numbers \mathbb{Q} , let \mathbb{R}^+ be the positive real numbers, and let $\mathbb{N} = \{1, 2, \dots\}$ be the positive integers. For $a_i \in \mathbb{N}$ and (For a set A we define $A^* := A \setminus \{0\}$.) $x_i \in \mathbb{K}^*$ we define the class of *generalized harmonic sums*,⁹⁰ in short they are called *S-sums*, by

$$S_{a_1, \dots, a_k}(x_1, \dots, x_k; n) = \sum_{i_1=1}^n \frac{x_1^{i_1}}{i_1^{a_1}} \sum_{i_2=1}^{i_1} \frac{x_2^{i_2}}{i_2^{a_2}} \cdots \sum_{i_k=1}^{i_{k-1}} \frac{x_k^{i_k}}{i_k^{a_k}}; \quad (2.1)$$

for a different writing see (1.3). k is called the depth and $w = \sum_{i=0}^k a_i$ is called the weight of the S -sum $S_{a_1, \dots, a_k}(x_1, \dots, x_k; n)$.

Restricting the S -sums to the situation $x_i = \pm 1$ yields to the well understood class of harmonic sums.^{19,123} For harmonic sums the limit $n \rightarrow \infty$ of (2.1) exists if and only if $a_1 \neq 1$ or $x_1 = -1$; see Ref. 139. For S -sums this result extends as follows; for a detailed proof see Ref. 6.

Theorem 2.1. *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. $a_1 = 1 \wedge x_1 = -1 \wedge |x_2| \leq 1 \wedge \dots \wedge |x_2 \cdots x_k| \leq 1$.

If a S -sum is finite, i.e., the limit $n \rightarrow \infty$ exists, we define

$$S_{a_1, \dots, a_k}(x_1, \dots, x_k; \infty) := \lim_{n \rightarrow \infty} S_{a_1, \dots, a_k}(x_1, \dots, x_k; n).$$

Another crucial property is that for the product of two S -sums with the same upper summation limit the following quasi-shuffle relation holds (see Ref. 90): for $n \in \mathbb{N}$,

$$\begin{aligned} S_{a_1, \dots, a_k}(x_1, \dots, x_k; n) S_{b_1, \dots, b_l}(y_1, \dots, y_l; n) = \\ \sum_{i=1}^n \frac{x_1^i}{i^{a_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) S_{b_1, \dots, b_l}(y_1, \dots, y_l; i) \\ + \sum_{i=1}^n \frac{y_1^i}{i^{b_1}} S_{a_1, \dots, a_k}(x_1, \dots, x_k; i) S_{b_2, \dots, b_l}(y_2, \dots, y_l; i) \\ - \sum_{i=1}^n \frac{(x_1 \cdot y_1)^i}{i^{a_1+b_1}} S_{a_2, \dots, a_k}(x_2, \dots, x_k; i) S_{b_2, \dots, b_l}(y_2, \dots, y_l; i). \end{aligned} \quad (2.2)$$

Since the right hand-side consists of S -sums where at least one component of the product has smaller depth, this formula applied iteratively leads to a linear combination of S -sums with integer coefficients. The underlying quasi-shuffle algebra induced by this product property will be exploited further in Sec. IX.

Finally, we will exploit heavily the fact that each S -sum can be written as an indefinite nested integral. Namely, for $S_1(b; n)$ with $b \in \mathbb{R}^*$ we have

$$S_1(b; n) = \int_0^b \frac{x_1^n - 1}{x_1 - 1} dx_1$$

and by induction on $m \geq 1$ we obtain

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

Now consider, e.g., the sum $S_{2,1}(a, b; n)$ with $a, b \in \mathbb{R}^*$. Due to the integral representation for S -sums with depth 1 we obtain

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

Looking at this one arrives straightforwardly at the following theorem; the proof follows by induction on k and the integral representations of S -sums with depth $k = 1$.

Theorem 2.2. *Let $m_i \in \mathbb{N}$, $b_i \in \mathbb{R}^*$ and define*

$$\begin{aligned} I_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; z) &= \\ &\int_0^{b_1 \cdots b_k} \frac{dx_{k, m_k}}{x_{k, m_k}} \int_0^{x_{k, m_k}} \frac{dx_{k, m_k - 1}}{x_{k, m_k - 1}} \cdots \int_0^{x_{k, 3}} \frac{dx_{k, 2}}{x_{k, 2}} \int_0^{x_{k, 2}} \frac{dx_{k, 1}}{x_{k, 1} - b_1 \cdots b_{k-1}} \\ &\int_{b_1 \cdots b_{k-1}}^{x_{k, 1}} \frac{dx_{k-1, m_{k-1}}}{x_{k-1, m_{k-1}}} \int_0^{x_{k-1, m_{k-1}}} \frac{dx_{k-1, m_{k-1} - 1}}{x_{k-1, m_{k-1} - 1}} \cdots \int_0^{x_{k-1, 3}} \frac{dx_{k-1, 2}}{x_{k-1, 2}} \int_0^{x_{k-1, 2}} \frac{dx_{k-1, 1}}{x_{k-1, 1} - b_1 \cdots b_{k-2}} \\ &\int_{b_1 \cdots b_{k-2}}^{x_{k-1, 1}} \frac{dx_{k-2, m_{k-2}}}{x_{k-2, m_{k-2}}} \int_0^{x_{k-2, m_{k-2}}} \frac{dx_{k-2, m_{k-2} - 1}}{x_{k-2, m_{k-2} - 1}} \cdots \int_0^{x_{k-2, 3}} \frac{dx_{k-2, 2}}{x_{k-2, 2}} \int_0^{x_{k-2, 2}} \frac{dx_{k-2, 1}}{x_{k-2, 1} - b_1 \cdots b_{k-3}} \\ &\vdots \\ &\int_{b_1 b_2 b_3}^{x_{4, 1}} \frac{dx_{3, m_3}}{x_{3, m_3}} \int_0^{x_{3, m_3}} \frac{dx_{3, m_3 - 1}}{x_{3, m_3 - 1}} \cdots \int_0^{x_{3, 3}} \frac{dx_{3, 2}}{x_{3, 2}} \int_0^{x_{3, 2}} \frac{dx_{3, 1}}{x_{3, 1} - b_1 b_2} \\ &\int_{b_1 b_2}^{x_{3, 1}} \frac{dx_{2, m_2}}{x_{2, m_2}} \int_0^{x_{2, m_2}} \frac{dx_{2, m_2 - 1}}{x_{2, m_2 - 1}} \cdots \int_0^{x_{2, 3}} \frac{dx_{2, 2}}{x_{2, 2}} \int_0^{x_{2, 2}} \frac{dx_{2, 1}}{x_{2, 1} - b_1} \\ &\int_{b_1}^{x_{2, 1}} \frac{dx_{1, m_1}}{x_{1, m_1}} \int_0^{x_{1, m_1}} \frac{dx_{1, m_1 - 1}}{x_{1, m_1 - 1}} \cdots \int_0^{x_{1, 3}} \frac{dx_{1, 2}}{x_{1, 2}} \int_0^{x_{1, 2}} \frac{(x_{1, 1})^z - 1}{x_{1, 1} - 1} dx_{1, 1}. \end{aligned}$$

Then for all $n \in \mathbb{N}$,

$$S_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; n) = I_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; n).$$

Note that sending $n \rightarrow \infty$ we obtain back multiple polylogarithms stated, e.g., in Ref. 66, 35, and 90.

For later constructions based on analytic reasoning (see also Sec. VI), we will use the fact that one can transform S -sums to a particular form of integral representations, the so-called generalized harmonic polylogarithms using the inverse Mellin transform; see Sec. VII. Conversely, with the Mellin transform one can express a weighted generalized harmonic polylogarithm in terms of S -sums. In other words, the S -sums are strongly twisted with generalized harmonic polylogarithms which can be defined as follows.

For $a \in \mathbb{R}$ and

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

we introduce the auxiliary function $f_a : (0, q) \mapsto \mathbb{R}$ by

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

Then the *generalized harmonic polylogarithms* (in short generalized polylogarithm) H of the word m_1, \dots, m_w (resp. vector $\mathbf{m} = (m_1, \dots, m_w)$) with $m_i \in \mathbb{R}$ is defined as follows. For $x \in (0, q)$ with $q := \min_{m_i > 0} m_i$,

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

Generalized polylogarithms are also dealt with in Refs. 39, 40, 34, 7, and 10 as hyperlogarithms. The length w of the vector \mathbf{m} is called the weight of the generalized polylogarithm $H_{\mathbf{m}}(x)$.

Restricting $H_{m_1, m_2, \dots, m_w}(x)$ to $m_i \in \{-1, 0, 1\}$ gives the class of harmonic polylogarithms.¹⁰⁵ Typical examples are

$$H_1(x) = \int_0^x \frac{1}{1-x_1} dx_1 = -\log(1-x), \\ H_{-2}(x) = \int_0^x \frac{1}{2+x_1} dx_1 = \log(2+x) - \log(2), \\ H_{2,0,-\frac{1}{2}}(x) = \int_0^x \frac{1}{2-x_1} \int_0^{x_1} \frac{1}{x_2} \int_0^{x_2} \frac{1}{\frac{1}{2}+x_3} dx_3 dx_2 dx_1.$$

A generalized polylogarithm $H_{\mathbf{m}}(x) = H_{m_1, \dots, m_w}(x)$ with $q := \min_{m_i > 0} m_i$ is an analytic function for $x \in (0, q)$. For the limits $x \rightarrow 0$ and $x \rightarrow q$ the following holds. From the definition we have that $H_{\mathbf{m}}(0) = 0$ if and only if $\mathbf{m} \neq \mathbf{0}_w$. In addition, $H_{\mathbf{m}}(q)$ is finite if and only if one of the following cases holds

- $m_1 \neq q$
- $w \geq 2$, $q = m_1 = 1$, and $m_v = 0$ for all v with $1 < v \leq w$.

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

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

Summarizing, a generalized polylogarithm $H_{m_1, m_2, \dots, m_w}(x)$ with $q := \min_{m_i > 0} m_i$ is finite at $c \in \mathbb{R}$ for $c \geq 0$ if one of the following cases hold:

1. $c < q$
2. $c = q$ and $m_1 \neq q$
3. $(m_1, \dots, m_w) = (m_1, \dots, m_k, 1, 0, \dots, 0)$ with $q' := \min \{m_i | m_i > 0, i \leq k\}$ and $c < q'$.

Throughout this article, whenever we state that $H_{m_1, m_2, \dots, m_w}(c)$ is finite or well defined, we assume that one of the three conditions from above holds.

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

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

Besides that, the product of two generalized polylogarithms of the same argument can be expressed using the formula

$$H_p(x) H_q(x) = \sum_{r=p \sqcup\sqcup q} H_r(x); \tag{2.3}$$

here the shuffle operation $p \sqcup\sqcup q$ denotes all merges of p and q in which the relative orders of the elements of p and q are preserved. Thus, similar to \mathcal{S} -sums, one can write any product of generalized polylogarithms by a linear combination of generalized polylogarithms over the integers.

As utilized in Ref. 105 for harmonic polylogarithms, we use this shuffle product to remove trailing or leading constants in the vector of the arising generalized polylogarithms. For example, for $a \in \mathbb{R}$ the shuffle product gives

$$\begin{aligned} H_a(x) H_{m_1, \dots, m_w}(x) = & H_{a, m_1, \dots, m_w}(x) + H_{m_1, a, m_2, \dots, m_w}(x) \\ & + H_{m_1, m_2, a, m_3, \dots, m_w}(x) + \dots + H_{m_1, \dots, m_w, a}(x), \end{aligned}$$

or equivalently

$$\begin{aligned} H_{m_1, \dots, m_w, a}(x) = & H_a(x) H_{m_1, \dots, m_w}(x) - H_{a, m_1, \dots, m_w}(x) \\ & - H_{m_1, a, m_2, \dots, m_w}(x) - \dots - H_{m_1, \dots, a, m_w}(x). \end{aligned}$$

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

$$\begin{aligned} H_{m_1, \dots, m_w, a}(x) = & \frac{1}{2} (H_a(x) H_{m_1, \dots, m_{w-1}, a}(a) - H_{a, m_1, \dots, m_{w-1}, a}(x) \\ & - H_{m_1, a, m_2, \dots, m_{w-1}, a}(x) - \dots - H_{m_1, \dots, a, m_{w-1}}(x)). \end{aligned}$$

Applying this tactic iteratively leads to a polynomial representation in $H_a(x)$ with coefficients in terms of generalized polylogarithms with no trailing a 's. In particular, if a generalized polylogarithm is analytic for $(0, q)$ then also the occurring generalized polylogarithms of the linear combination are analytic for $(0, q)$. A typical example for $a = 0$ is, e.g.,

$$\begin{aligned} H_{2, -3, 0, 0}(x) = & \frac{1}{2} H_0(x)^2 H_{2, -3}(x) - H_0(x) H_{0, 2, -3}(x) - H_0(x) H_{2, 0, -3}(x) \\ & + H_{0, 0, 2, -3}(x) + H_{0, 2, 0, -3}(x) + H_{2, 0, 0, -3}(x). \end{aligned}$$

Note that there is one extra complication: given a generalized 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 $H_{2, 1, 0}(x)$ being analytic for $x \in (0, 2)$ 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. In later considerations these difficulties have to be handled separately.

Completely analogously, leading constants can be removed in generalized polylogarithms. In addition, using the quasi shuffle algebra (2.2) it is possible to extract leading (or trailing) indices of a \mathcal{S} -sum. For example, we have for $a \in \mathbb{N}$ and $b \in \mathbb{K}^*$

$$\begin{aligned} S_{a, 2, 1} \left(b, \frac{1}{2}, \frac{1}{3}; n \right) = & S_a(b; n) S_{2, 1} \left(\frac{1}{2}, \frac{1}{3}; n \right) + S_{2+a, 1} \left(\frac{b}{2}, \frac{1}{3}; n \right) + S_{2, 1+a} \left(\frac{1}{2}, \frac{b}{3}; n \right) \\ & - S_{2, a, 1} \left(\frac{1}{2}, b, \frac{1}{3}; n \right) - S_{2, 1, a} \left(\frac{1}{2}, \frac{1}{3}, b; n \right). \end{aligned}$$

For S -sums $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ with $a_i \in \mathbb{N}$ and $b_i \in [-1, 1] \setminus \{0\}$ this can be used to get a polynomial representation in $S_1(n)$ with coefficients in terms of convergent S -sums, such as,

$$\begin{aligned} S_{1,1,2}\left(1, 1, \frac{1}{2}; n\right) &= \frac{1}{2} S_1(n)^2 S_2\left(\frac{1}{2}; n\right) + S_1(n) \left(S_3\left(\frac{1}{2}; n\right) - S_{2,1}\left(\frac{1}{2}, 1; n\right)\right) \\ &\quad + \frac{1}{2} S_4\left(\frac{1}{2}; n\right) - \frac{1}{2} S_{2,2}\left(\frac{1}{2}, 1; n\right) + \frac{1}{2} S_{2,2}\left(1, \frac{1}{2}; n\right) \\ &\quad - S_{3,1}\left(\frac{1}{2}, 1; n\right) + S_{2,1,1}\left(\frac{1}{2}, 1, 1; n\right). \end{aligned}$$

For general S -sums this strategy usually fails to extract the divergency, e.g., in

$$\begin{aligned} S_{1,2,1}\left(5, \frac{1}{2}, \frac{1}{3}; n\right) &= S_1(5; n) S_{2,1}\left(\frac{1}{2}, \frac{1}{3}; n\right) + S_{2,2}\left(\frac{1}{2}, \frac{5}{3}; n\right) + S_{3,1}\left(\frac{5}{2}, \frac{1}{3}; n\right) \\ &\quad - S_{2,1,1}\left(\frac{1}{2}, \frac{1}{3}, 5; n\right) - S_{2,1,1}\left(\frac{1}{2}, 5, \frac{1}{3}; n\right), \end{aligned}$$

the sums $S_1(5; n)$, $S_{3,1}\left(\frac{5}{2}, \frac{1}{3}; n\right)$ and $S_{2,1,1}\left(\frac{1}{2}, 5, \frac{1}{3}; n\right)$ are divergent for $n \rightarrow \infty$.

III. IDENTITIES BETWEEN MULTIPLE POLYLOGARITHMS OF RELATED ARGUMENTS

In the following we want to look at several special transforms of the argument of generalized polylogarithms which will be useful for later considerations. In general, we start with a defined generalized polylogarithm $f(x) = H_{m_1, \dots, m_l}\left(\frac{ax+b}{cx+d}\right)$ with particular chosen integers a, b, c, d and $x \in \mathbb{R}$, and derive representations in terms of generalized polylogarithms in x . Since such a transformation holds not only for a point $x \in \mathbb{R}$, but in a region around x , all the transformations have the following additional property: if the input expression $f(x)$ is analytic in a certain region around x , then the arising generalized polylogarithms of the transformed representation are analytic in this region.

A. $x + b \rightarrow x$

Lemma 3.1. Let $m_i \in \mathbb{R} \setminus (0, 1)$ and $x > 0$ such that the generalized polylogarithm $H_{m_1, \dots, m_l}(x + 1)$ is defined. If $(m_1, \dots, m_l) \neq (1, 0, \dots, 0)$,

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

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

$$H_{m_1, \dots, m_l}(x + 1) = H_{1, 0, \dots, 0}(1) - H_{0, -1, \dots, -1}(x).$$

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

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

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

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

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

$$H_0(x + 1) = H_0(1) + \int_1^{x+1} \frac{1}{u} du = \int_0^x \frac{1}{1 + u} du = H_0(1) + H_{-1}(x).$$

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

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

If $m_1 = 0$ we get

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

□

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. 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 $j \in \{1, \dots, l\}$. If $H_{m_1, \dots, m_l}(x + b)$ is defined for $x > 0$,

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

Lemma 3.3. Let $(m_1, \dots, m_l) = (1, 0, \dots, 0)$ and let $x > 0$ such that $H_{m_1, \dots, m_l}(x + b)$ is defined. For $1 > b > 0$ and $1 - b > x > 0$,

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

For $x > 0$ and $b \geq 1$,

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

Lemma 3.4. 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 $(m_{k+1}, \dots, m_l) = (1, 0, \dots, 0)$. Let $x > 0$ such that $H_{m_1, \dots, m_l}(x + b)$ is defined. For $1 - b > x > 0$ and $1 > b > 0$,

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

For $b \geq 1$,

$$\begin{aligned} H_{m_1, \dots, m_l}(x + b) = & H_{m_1, m_2, \dots, m_l}(b) + H_{m_1-b}(x) H_{m_2, \dots, m_l}(b) + \dots + \\ & + H_{m_1-b, \dots, m_k-b}(x) H_{m_{k+1}, \dots, m_l}(b) - \left[H_{m_1-b, \dots, m_{k+1}-b}(x) H_{m_{k+2}, \dots, m_l}(b) + \right. \\ & \left. + \dots + H_{m_1-b, \dots, m_{l-1}-b}(x) H_{m_l}(b) - H_{m_1-b, \dots, m_l-b}(x) \right]. \end{aligned}$$

B. $b - x \rightarrow x$

In this subsection we assume that $b > 0$ and we consider indices $m_i \in \mathbb{R} \setminus (0, b)$. The following method transforms a defined generalized polylogarithm $H_{m_1, \dots, m_w}(b - x)$ for some $x \in \mathbb{R}$ in terms of generalized polylogarithm with argument x and evaluations at constants. Proceeding recursively on the weight w of the generalized polylogarithm we have

$$\begin{aligned} H_{m_1}(b - x) = & H_{m_1}(b) - H_{b-m_1}(x) \quad \text{for } m_1 \neq b, \\ H_b(b - x) = & H_0(x) - H_0(b). \end{aligned} \tag{3.1}$$

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 generalized polylogarithms of weight $< w$. If $m_1 = b$, we can remove leading b 's (see Sec. II) and end up with generalized polylogarithms without leading b 's and powers of $H_b(b - x)$. For the powers of $H_b(b - x)$ we can use (3.1); therefore, only the cases in which the first index $m_1 \neq b$ 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 $H_{m_2, \dots, m_w}(b - t)$. Linearizing the expression with the shuffle product using the definition of the generalized polylogarithm we finally obtain the required weight w identity. With the steps above one obtains, e.g.,

$$H_{3, -2, -1}(2 - x) = -H_{-1}(x)H_{-2, -1}(2) + H_{-1}(2)H_{-1, 4}(x) - H_{-1, 4, 3}(x) + H_{3, -2, -1}(2).$$

Remark 3.5. Analyzing the underlying algorithm we see that in the transform of $H_{m_1, m_2, \dots, m_w}(b - x)$ we find only one generalized polylogarithm of weight w and argument x , namely $H_{-(m_1-b), -(m_2-b), \dots, -(m_w-b)}(x)$. All other polylogarithms at argument x that appear have

lower weights. In general the indices of the generalized polylogarithms at argument x that appear in the transformed expression are in the set $\{-(m_1 - b), -(m_2 - b), \dots, -(m_w - b)\}$. Note that if we look at the reverse transform, i.e., $x \rightarrow b - x$ we can derive a similar property.

C. $\frac{1-x}{1+x} \rightarrow x$

Next, we present an algorithm that performs the transformation $\frac{1-x}{1+x} \rightarrow x$, such as,

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

Here we consider indices with $m_i \in \mathbb{R} \setminus (0, 1)$. Proceeding recursively on the weight w of the generalized polylogarithm we have for $0 < \frac{1-x}{1+x} < 1$, $y_1 < -1$, $-1 < y_2 < 0$ and $y_3 > 1$:

$$\begin{aligned} H_{y_1}\left(\frac{1-x}{1+x}\right) &= -H_0(-y_1) - H_{-1}(x) + H_0(1 - y_1) + H_{\frac{1-y_1}{1+y_1}}(x), \\ H_{-1}\left(\frac{1-x}{1+x}\right) &= H_{-1}(1) - H_{-1}(x), \\ H_{y_2}\left(\frac{1-x}{1+x}\right) &= -H_0(-y_2) - H_{-1}(x) + H_0(1 - y_2) - H_{\frac{1-y_2}{1+y_2}}(x), \\ H_0\left(\frac{1-x}{1+x}\right) &= -H_1(x) + H_{-1}(x), \end{aligned} \tag{3.2}$$

$$H_1\left(\frac{1-x}{1+x}\right) = -H_{-1}(1) - H_0(x) + H_{-1}(x), \tag{3.3}$$

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

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 generalized polylogarithms of weight $< w$. If $m_1 = 1$, we can remove leading ones and end up with generalized 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 (3.3); 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 $y_2 > 1$ we get

$$\begin{aligned} H_{y_1, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= H_{y_1, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ &\quad + \int_0^x \frac{1}{\frac{1-y_1}{1+y_1} + t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt, \\ H_{-1, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= H_{-1, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1+t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt, \\ H_{0, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= H_{0, m_2, \dots, m_w}(1) - \int_0^x \frac{1}{1-t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ &\quad - \int_0^x \frac{1}{1+t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt, \end{aligned} \tag{3.4}$$

$$\begin{aligned} H_{y_2, m_2, \dots, m_w}\left(\frac{1-x}{1+x}\right) &= H_{y_2, m_2, \dots, m_w}(1) + \int_0^x \frac{1}{1+t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt \\ &\quad - \int_0^x \frac{1}{\frac{1-y_2}{1+y_2} + t} H_{m_2, \dots, m_w}\left(\frac{1-t}{1+t}\right) dt. \end{aligned} \tag{3.5}$$

Note that the transformation (3.4) can be only applied if (m_2, \dots, m_w) is not the zero vector. However, by definition the arising special case $H_{0,\dots,0}(\frac{1-x}{1+x})$ reduces to $H_0(\frac{1-x}{1+x})$ which we handled in (3.2).

Since we know the transform for weights $< w$, we can apply it to $H_{m_2,\dots,m_w}(\frac{1-t}{1+t})$. Linearizing the arising products of generalized polylogarithms with the shuffle product and using the definition of the generalized polylogarithms we obtain the required weight w identity.

D. $kx \rightarrow x$

Lemma 3.6. If $m_i \in \mathbb{R}, m_l \neq 0, x \in \mathbb{R}^+$ and $k \in \mathbb{R}^+$ such that the generalized polylogarithm $H_{m_1,\dots,m_l}(k \cdot x)$ is defined then we have

$$H_{m_1,\dots,m_l}(k \cdot x) = H_{\frac{m_1}{k},\dots,\frac{m_l}{k}}(x). \tag{3.6}$$

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

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

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

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

For $m_1 = 0$ we get

$$\begin{aligned} H_{0,m_2,\dots,m_{l+1}}(k \cdot x) &= \int_0^{kx} \frac{H_{m_2,\dots,m_{l+1}}(u)}{u} du = \int_0^x \frac{H_{m_2,\dots,m_{l+1}}(ku)}{ku} kdu \\ &= \int_0^x \frac{H_{\frac{m_2}{k},\dots,\frac{m_{l+1}}{k}}(u)}{u} du = H_{\frac{0}{k},\frac{m_2}{k},\dots,\frac{m_{l+1}}{k}}(x). \end{aligned}$$

□

The proof of the following lemma is straightforward (compare Ref. 105, where it is stated for harmonic polylogarithms).

Lemma 3.7. If $m_i \in \mathbb{R}, m_l \neq 0$ and $x \in \mathbb{R}^-$ such that the generalized polylogarithm $H_{m_1,\dots,m_l}(-x)$ is defined then we have

$$H_{m_1,\dots,m_l}(-x) = (-1)^{l-k} H_{-m_1,\dots,-m_l}(x), \tag{3.7}$$

here k denotes the number of m_i which equals to zero.

E. $\frac{1}{x} \rightarrow x$

Here we assume that $0 < x < 1$. First, we consider only indices with $m_i \leq 0$. Proceeding recursively on the weight w of the generalized polylogarithm we have for $y < 0$ that

$$H_y\left(\frac{1}{x}\right) = H_{\frac{1}{y}}(x) - H_0(x) - H_0(-y) \quad \text{and} \quad H_0\left(\frac{1}{x}\right) = -H_0(x).$$

Now let us look at higher weights $w > 1$. We consider $H_{m_1,m_2,\dots,m_w}(\frac{1}{x})$ with $m_i \leq 0$ and suppose that we can already apply the transformation for generalized polylogarithms of weight $< w$. For $m_1 < 0$

we get (compare Ref. 105):

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

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

We can extend this transformation by the following observations. 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 $x \in (m, \infty)$. (For a definition of single-valued polylogarithms see Refs. 38, 51, 49, and 44.) 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

$$H_m \left(\frac{1}{x} \right) = H_{\frac{1}{m}}(x) + H_0(m) + H_0(x) - i\pi, \quad (3.8)$$

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 generalized polylogarithm has leading m 's, we remove them and end up with generalized polylogarithms without leading m 's and powers of $H_m \left(\frac{1}{x} \right)$. To deal with the generalized polylogarithms without leading m , we can slightly modify the previous part of this section and for the powers of $H_m \left(\frac{1}{x} \right)$ we can use (3.8). Following this tactic, we arrive, e.g., at the identity

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

IV. POWER SERIES EXPANSION OF MULTIPLE POLYLOGARITHMS

An algorithm to calculate series expansions for harmonic polylogarithms $H_{m_1, m_2, \dots, m_w}(x)$ with $m_i \in \{-1, 0, 1\}$ has been presented in Ref. 105. Subsequently, we generalize these steps for generalized polylogarithms, i.e., $m_i \in \mathbb{R}$. In general, $H_{m_1, m_2, \dots, m_w}(x)$ does not have a Taylor series expansion if trailing zeroes occur, i.e., the expansion consists of a $\log(x)$ -part and a part free of $\log(x)$. The separation into these two parts can be easily accomplished by removing trailing zeroes as described in Sec. II. In other words, one gets a polynomial expression in $H_0(x) = \log(x)$ with coefficients in terms of generalized polylogarithms that have no trailing 0's. For each of these coefficients we are now in the position to calculate a Taylor series expansion as follows.

For polylogarithms of weight 1 with $j \in \mathbb{R}$ and $x \in (0, |j|)$ we have

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

Let $\mathbf{m} = (m_1, \dots, m_w)$ be a non-zero vector 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 $x \in (0, \min(j, q))$

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

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

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

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

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

□

Separating the $\log(x) = H_0(x)$ part from the log-free part and applying the formulas from above we get, e.g.,

$$H_{-2,0}(x) = \sum_{i=1}^{\infty} \frac{2^{-i}(-x)^i}{i^2} - H_0(x) \sum_{i=1}^{\infty} \frac{2^{-i}(-x)^i}{i}.$$

Summarizing, given $H_{m_1,m_2,\dots,m_w}(x)$ with $m_w \neq 0$ and $q = \min_{m_i \neq 0} |m_i|$, one can calculate a Taylor series expansion which holds for $x \in [0, q)$ and where the coefficients of the Taylor expansion are given explicitly in terms of S -sums.

A. Inverse construction

In addition, since the formulas from above can be reversed, also the other direction is possible: given a sum of the form $\sum_i^{\infty} (cx)^i \frac{S_n(b;i)}{i^k}$ with $k \in \mathbb{N} \cup \{0\}$ and $c \in \mathbb{R}^*$, one can compute a linear combination of (possibly weighted) generalized polylogarithms $h(x)$ such that for $x \in (0, j)$ with $j > 0$ small enough $\sum_i^{\infty} (cx)^i \frac{S_n(b;i)}{i^k} = h(x)$.

For example, for $x \in (0, \frac{1}{2})$ we have

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

B. Asymptotic behavior

Moreover, one can determine the asymptotic behavior of a generalized polylogarithms $H_m(x)$: Define $y := \frac{1}{x}$. Using Sec. III E on $H_m(\frac{1}{y}) = H_m(x)$ we can rewrite $H_m(x)$ in terms of generalized polylogarithms at argument y together with some constants. Now we obtain the power series expansion of the generalized 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 $H_m(x)$.

For example, performing these steps yields

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

V. VALUES OF MULTIPLE POLYLOGARITHMS EXPRESSED BY S-SUMS AT INFINITY

Consider the generalized polylogarithm $H_{m_1,m_2,\dots,m_w}(x)$ with $q := \min_{m_i > 0} m_i$ and $c \in \mathbb{R}, c \geq 0$ such that $H_{m_1,m_2,\dots,m_w}(c)$ is finite. To be more precise, one of the following cases holds:

1. $c < q$
2. $c = q$ and $m_1 \neq q$
3. $(m_1, \dots, m_w) = (m_1, \dots, m_k, 1, 0, \dots, 0)$ with $q' := \min \{m_i | m_i > 0, i \leq k\}$ and $c < q'$.

If the generalized polylogarithm $H_m(c)$ has trailing zeroes, we first extract them. If $0 < c \leq 1$, we end up in an expression of generalized polylogarithms without trailing zeroes and powers of $H_0(c)$. Otherwise, if $c > 1$, we cannot handle polylogarithms of the form $H_{m_1,m_2,\dots,m_k,1,0,\dots,0}(c)$ (see Sec. II) and keep them untouched. Note that by the shuffle product no extra indices are introduced and the first non-zero index is again m_1 . Thus the arising polylogarithms are again finite at the evaluation point c .

To rewrite powers of $H_0(c)$ for $c > 0$ we note that we have

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

To rewrite generalized polylogarithms of the form $H_{m_1, m_2, \dots, m_w}(c)$ where $m_w \neq 0$ and $\min_{m_i \neq 0} |m_i| > c$, we use the power series expansion of $H_{m_1, m_2, \dots, m_w}(x)$ and send $x \rightarrow c$. For example, for one of the arising sums we obtain

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

What remains open are the situations of the type $H_{m_1, m_2, \dots, m_k, 1, 0, \dots, 0}(c)$ with $c > 1$ and polylogarithms $H_{m_1, m_2, \dots, m_w}(c)$ with $m_w \neq 0$, $\max_{m_i < 0} m_i > -c$, $\min_{m_i > 0} m_i \geq c$ and $m_1 \neq c$.

As shortcut, one can rewrite $H_{m_1, m_2, \dots, m_w}(c)$ with $(m_1, m_2, \dots, m_w) = (1, 0, \dots, 0)$ and $c > 1$ by using the following lemma iteratively.

Lemma 5.1. For $c > 1$ and $(m_1, m_2, \dots, m_w) = (1, 0, \dots, 0)$ we have

$$H_{m_1, m_2, \dots, m_w}(c) = (-1)^{w+1} S_w(1; \infty) - H_{0, m_1-1, \dots, m_w-1}(c-1).$$

To rewrite generalized polylogarithms of the form $H_{m_1, m_2, \dots, m_w}(c)$ where $m_1 \in \mathbb{R} \setminus (0, c]$, $m_w \neq 0$, $\min_{m_i > 0} m_i \geq c$ and $s := \max_{m_i < 0} m_i > -c$ we use Lemma 3.2 and afterwards send $x \rightarrow c + s$, i.e., we get

$$\begin{aligned} H_{m_1, \dots, m_w}(c) &= H_{m_1, m_2, \dots, m_w}(-s) + H_{m_1+s}(c+s) H_{m_2, \dots, m_w}(-s) \\ &+ H_{m_1+s, m_2+s}(c+s) H_{m_3, \dots, m_w}(-s) + \dots + \\ &+ H_{m_1+s, \dots, m_{k-1}+s}(c+s) H_{m_k}(-s) + H_{m_1+s, \dots, m_w+s}(c+s). \end{aligned}$$

Note that $-s < c$ and $c + s < c$. To rewrite generalized polylogarithms of the form $H_{m_1, m_2, \dots, m_k, 1, 0, \dots, 0}(c)$ where $c > 1$ we can proceed similar to the previous case: we use Lemma 3.4 to rewrite $H_{m_1, m_2, \dots, m_w}(x+1)$ and afterwards send $x \rightarrow c-1$. Observe that both cases reduce the problem to a simpler situation: We can either handle all arising polylogarithms by the recipes given above. If not, observe that the remaining polylogarithms are of the form $H_{n_1, \dots, n_l}(u)$ with $q' := \min_{n_i \neq 0} |n_i|$ and $u < c$. Note that the evaluation point gets smaller. In addition, the index vector (n_1, \dots, n_l) is given by a subset of (m_1, \dots, m_w) up to the possible addition of $s < 0$ where s is the maximum of the arising negative indices of (m_1, \dots, m_w) . Thus applying this reduction iteratively (to the polylogarithms that cannot be handled by the cases from above) decreases step by step the positive evaluation point and in the same time decreases the negative indices and thus enlarges the absolute value of s superlinearly. Consequently, from a certain point on q' gets larger than q and the difference between these values increases in each iteration. This guarantees that eventually $u < q'$, i.e., the arising polylogarithms can be transformed to S -sums by using the series expansion representation and the evaluation at $x = u$ as described above.

Summarizing, we can rewrite all finite generalized polylogarithms $H_{m_1, m_2, \dots, m_w}(c)$ in terms of S -sums at infinity, such as,

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

Note that this process can be reversed: given a finite S -sum at infinity we can rewrite it, e.g., in terms of generalized polylogarithms at one:

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

For a complete algorithm for the reverse direction we refer to Algorithm 1 of Ref. 6.

We note that if we consider the generalized polylogarithm $H_{m_1,m_2,\dots,m_w}(x)$ and $c \in \mathbb{R}$, $c < 0$ such that $H_{m_1,m_2,\dots,m_w}(c)$ is finite then we can use Lemma 3.7 to transform $H_{m_1,m_2,\dots,m_w}(x)$ to an expression in terms of generalized polylogarithms at argument $-c$. Hence we can again use the strategy presented above to rewrite this generalized polylogarithm in terms of S -sums at infinity.

VI. ANALYTIC CONTINUATION OF S-SUMS

It has been remarked in Ref. 137 that Carlson’s theorem^{42,122}(The original theorem needs to be extended to be even applicable in case of the harmonic sums.) can be used to perform the analytic continuation of harmonic sums: the evaluation of the harmonic sums at integer points determines uniquely (among a certain class of analytic functions with exponential growth) the analytic continuation in the complex plane. We will elaborate this property in further details for harmonic sums and more generally for S -sums.

A function $f : M \rightarrow \mathbb{C}$ for a region $M \subset \mathbb{C}$ is of Carlson-type (C-type) if

- it is analytic in the right half plane,
- it is of exponential type in the half plane, i.e., there exist $c, C \in \mathbb{R}^+$ such that for all $z \in \mathbb{C}$ with $\text{Im}(z) \geq 0$ we have that

$$|f(z)| \leq C e^{c|z|},$$

- and there exist $c, C \in \mathbb{R}^+$ with $c < \pi$ such that for all $y \in \mathbb{R}$ we have that

$$|f(iy)| \leq C e^{c|y|}.$$

For such functions the following theorem holds; for a detailed proof (together with even more general statements) we refer to Sec. 9.2 of Ref. 33.

Theorem 6.1 (Carlson). *Let $h(z)$ be a function of C-type. If $h(n) = 0$ for all $n \in \mathbb{N}$ then $h = 0$.*

Throughout the remaining article we rely on the following consequence: Let $f(z)$ and $g(z)$ be functions of C-type. If $f(n) = g(n)$ for all $n \in \mathbb{N}$, then $f = g$ in the domain where both functions are defined.

The following simple closure properties will be used later. The proofs are immediate.

Lemma 6.2. *Let $f(z)$ and $g(z)$ be functions of C-type and let $a \in \mathbb{R}^+$. Then $f(z) + g(z)$, $a^z = e^{z \ln(a)}$ and $a^z f(z)$ are of C-type.*

Proposition 6.3. *For $m_i \in \mathbb{N}$, $b_i \in \mathbb{R}^+$ and $z \in \mathbb{C}$ consider the integral $f(z) = I_{m_1,m_2,\dots,m_k}(b_1, b_2, \dots, b_k; z)$ from Theorem 2.2. Then $f(z)$ is of C-type.*

Proof. We note that $f(z)$ is analytic for $\text{Re}(z) \geq 0$. Next we show that $f(z)$ is of exponential type. For $1 \geq |z| \geq 0$ with $\text{Im}(z) \geq 0$ we can bound $|f(z)|$ by a constant. For $|z| > 1$ and $d := \max(b_1, b_1 b_2, \dots, b_1 b_2 \dots b_k) \geq 0$ we have

$$|f(z)| = \left| \int_0^{b_1 \dots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \dots \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_1 \dots b_{k-1}} \dots \int_{b_1}^{x_1^2} \frac{dx_1^{m_1}}{x_1^{m_1}} \dots \int_0^{x_1^2} \frac{x^z - 1}{x - 1} dx \right| \tag{6.1}$$

$$\leq \int_0^{b_1 \dots b_k} \frac{dx_k^{m_k}}{|x_k^{m_k}|} \dots \int_0^{x_k^2} \frac{dx_k^1}{|x_k^1 - b_1 \dots b_{k-1}|} \dots \int_{b_1}^{x_1^2} \frac{dx_1^{m_1}}{|x_1^{m_1}|} \dots \int_0^{x_1^2} \left| \frac{x^z - 1}{x - 1} \right| dx.$$

Now we show that there is a $c \in \mathbb{R}^+$ such that $\left| \frac{x^z-1}{x-1} \right| \leq c(d+1)^{|z|}$ for $0 \leq x \leq d$ and all $z = a + bi$ for $a \in \mathbb{R}^+, b \in \mathbb{R}$. If $d < 1$, we have

$$\left| \frac{x^z-1}{x-1} \right| \leq \frac{x^a+1}{1-d} \leq \frac{1}{1-d}(d+1)^{|z|}.$$

Finally, let $d \geq 1$. Since $\lim_{x \rightarrow 1} \left| \frac{x^z-1}{x-1} \right| = |z| \leq (d+1)^{|z|}$, there are $\epsilon > 0$ and $c > 0$ such that $\left| \frac{x^z-1}{x-1} \right| \leq c(d+1)^{|z|}$ for $1 - \epsilon \leq x \leq 1 + \epsilon$. It remains to show that $\left| \frac{x^z-1}{x-1} \right| \leq c(d+1)^{|z|}$ for $x \in (0, 1 - \epsilon) \cup (1 + \epsilon, d)$:

$$\left| \frac{x^z-1}{x-1} \right| \leq \frac{x^a+1}{\epsilon} \leq \frac{1}{\epsilon}(d+1)^{|z|}.$$

In summary, we can choose $c \in \mathbb{R}^+$ (independent of the choice of z) with $\left| \frac{x^z-1}{x-1} \right| \leq c(d+1)^{|z|}$ for $0 \leq x \leq d$ and using (6.1) it follows that

$$\begin{aligned} |f(z)| &\leq c \cdot e^{\log(d+1)|z|} \underbrace{\int_0^{b_1 \dots b_k} \left| \frac{dx_k^{m_k}}{x_k^{m_k}} \right| \dots \int_0^{x_k^2} \left| \frac{dx_k^1}{x_k^1 - b_1 \dots b_{k-1}} \right| \dots \int_{b_1}^{x_2^1} \left| \frac{dx_1^{m_1}}{x_1^{m_1}} \right| \dots \int_0^{x_1^2} 1 dx}_{\in \mathbb{R}^+, \text{ constant}} \\ &\leq \bar{c} \cdot e^{\log(d+1)|z|} \end{aligned}$$

for some $\bar{c} \in \mathbb{R}^+$ (again independent of the choice of z). To conclude that $f(z)$ is of C-type, we have to show that we can choose a $\bar{c} \in \mathbb{R}^+$ such that for all $b \in \mathbb{R}$ we have

$$\begin{aligned} |f(bi)| &= \\ &\left| \int_0^{b_1 \dots b_k} \frac{dx_k^{m_k}}{x_k^{m_k}} \dots \int_0^{x_k^2} \frac{dx_k^1}{x_k^1 - b_1 \dots b_{k-1}} \dots \int_{b_1}^{x_2^1} \frac{dx_1^{m_1}}{x_1^{m_1}} \dots \int_0^{x_1^2} \frac{x^{bi} - 1}{x - 1} dx \right| \leq \bar{c} \cdot e^{|b|}. \end{aligned}$$

We show that there is a $c \in \mathbb{R}^+$ such that $\left| \frac{x^{bi}-1}{x-1} \right| \leq c \cdot e^{|b|}$ for $0 \leq x \leq d$ and all $b \in \mathbb{R}^+$: If $d < 1$ we have $\left| \frac{x^{bi}-1}{x-1} \right| \leq \frac{2}{1-d} \leq \frac{2}{1-d} \cdot e^{|b|}$. Finally let $d \geq 1$. Since $\lim_{x \rightarrow 1} \left| \frac{x^{bi}-1}{x-1} \right| = |b| \leq e^{|b|}$ there are $\epsilon > 0$ and $c > 0$ such that $\left| \frac{x^{bi}-1}{x-1} \right| \leq c e^{|b|}$ for $1 - \epsilon \leq x \leq 1 + \epsilon$. It remains to show that $\left| \frac{x^{bi}-1}{x-1} \right| \leq c e^{|b|}$ for $x \in (0, 1 - \epsilon) \cup (1 + \epsilon, d)$: $\left| \frac{x^{bi}-1}{x-1} \right| \leq \frac{2}{\epsilon} \leq \frac{2}{\epsilon} e^{|b|}$. As for the proof part concerning the exponential growth the integral can be bounded as desired. \square

As a consequence the analytic continuation of S -sums $S_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; n)$ with $m_i \in \mathbb{N}$ and $b_i \in \mathbb{R}^+$ within the class of C-type functions is uniquely determined by the integral $I_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; z)$.

If not all $b_i \in \mathbb{R}^+$, we can split the integral at 0 whenever the integration interval contains 0. For example, let us consider the integral representation of $S_{1,2,2}(-1, 2, -\frac{1}{3}; n)$:

$$S_{1,2,2}\left(-1, 2, -\frac{1}{3}; n\right) = \int_0^{\frac{2}{3}} \int_0^{x_5} \int_{-2}^{x_4} \int_0^{x_3} \int_{-1}^{x_2} \frac{-1 + x_1^n}{x_5(2+x_4)x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 dx_4 dx_5.$$

Splitting at zero yields

$$\begin{aligned} &\left(\int_0^{\frac{2}{3}} \int_0^{x_5} \frac{1}{x_5(2+x_4)} dx_4 dx_5 \right) \int_{-2}^0 \int_{x_3}^0 \int_{-1}^{x_2} \frac{-1 + (-1)^n (-x_1)^n}{x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 \\ &+ \left(\int_0^{\frac{2}{3}} \int_0^{x_5} \int_0^{x_4} \int_0^{x_3} \frac{1}{x_5(2+x_4)x_3(1+x_2)} dx_2 dx_3 dx_4 dx_5 \right) \int_{-1}^0 \frac{-1 + (-1)^n (-x_1)^n}{-1+x_1} dx_1 \\ &+ \int_0^{\frac{2}{3}} \int_0^{x_5} \int_0^{x_4} \int_0^{x_3} \int_0^{x_2} \frac{-1 + x_1^n}{x_5(2+x_4)x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 dx_4 dx_5. \end{aligned}$$

An analytic continuation of $(-1)^n$ does not exist (in particular, it is not of C-type), hence we cannot continue $S_{1,2,2}(-1, 2, -\frac{1}{3}; n)$ analytically. However, we can continue the functions

$$\begin{aligned}
 f_e(n) &:= S_{1,2,2}\left(-1, 2, -\frac{1}{3}; 2n\right) \\
 &= \left(\int_0^{\frac{2}{3}} \int_0^{x_5} \frac{1}{x_5(2+x_4)} dx_4 dx_5\right) \int_{-2}^0 \int_{x_3}^0 \int_{-1}^{x_2} \frac{-1 + (-x_1)^{2n}}{x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 \\
 &\quad + \left(\int_0^{\frac{2}{3}} \int_0^{x_5} \int_0^{x_4} \int_0^{x_3} \frac{1}{x_5(2+x_4)x_3(1+x_2)} dx_2 dx_3 dx_4 dx_5\right) \int_{-1}^0 \frac{-1 + (-x_1)^{2n}}{-1+x_1} dx_1 \\
 &\quad + \int_0^{\frac{2}{3}} \int_0^{x_5} \int_0^{x_4} \int_0^{x_3} \int_0^{x_2} \frac{-1 + x_1^{2n}}{x_5(2+x_4)x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 dx_4 dx_5
 \end{aligned}$$

and

$$\begin{aligned}
 f_o(n) &:= S_{1,2,2}\left(-1, 2, -\frac{1}{3}; 2n+1\right) \\
 &= \left(\int_0^{\frac{2}{3}} \int_0^{x_5} \frac{1}{x_5(2+x_4)} dx_4 dx_5\right) \int_{-2}^0 \int_{x_3}^0 \int_{-1}^{x_2} \frac{-1 - (-x_1)^{2n+1}}{x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 \\
 &\quad + \left(\int_0^{\frac{2}{3}} \int_0^{x_5} \int_0^{x_4} \int_0^{x_3} \frac{1}{x_5(2+x_4)x_3(1+x_2)} dx_2 dx_3 dx_4 dx_5\right) \int_{-1}^0 \frac{-1 - (-x_1)^{2n+1}}{-1+x_1} dx_1 \\
 &\quad + \int_0^{\frac{2}{3}} \int_0^{x_5} \int_0^{x_4} \int_0^{x_3} \int_0^{x_2} \frac{-1 + x_1^{2n+1}}{x_5(2+x_4)x_3(1+x_2)(-1+x_1)} dx_1 dx_2 dx_3 dx_4 dx_5
 \end{aligned}$$

analytically since $(-1)^n = 1$ for n even and $(-1)^n = -1$ for n odd. For a graphical illustration we refer to Figure 1. More generally, there is the following result.

Proposition 6.4. For $m_i \in \mathbb{N}$, $b_i \in \mathbb{R}^*$ and $z \in \mathbb{C}$ consider the integral $f(z) = I_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; z)$ from Theorem 2.2. Then $f(2z)$ and $f(2z + 1)$ are of C-type.

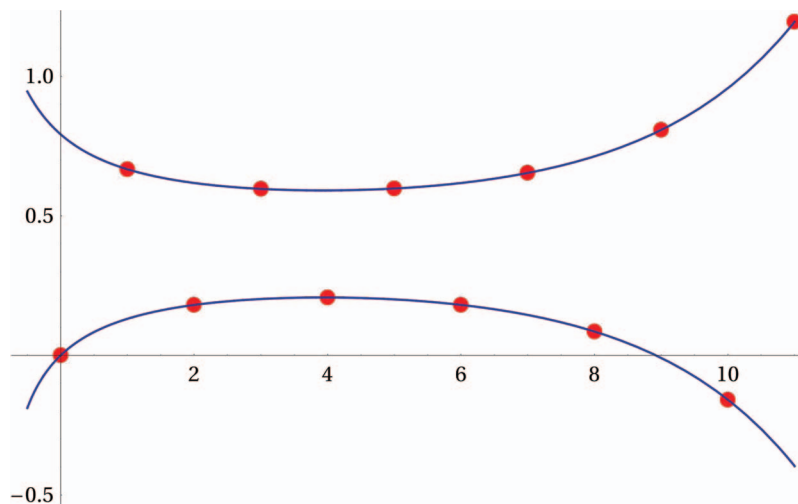


FIG. 1. $S_{1,2,2}(-1, 2, -\frac{1}{3}; n)$ for $n \in \{0, 1, \dots, 11\}$, and $f_e(\frac{n}{2})$, $f_o(\frac{n-1}{2})$ for $n \in (-\frac{1}{2}, 11)$.

The proof is analogous to Proposition 6.3. Consequently, the analytic continuation of even and odd S -sums $S_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; 2n)$ and $S_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; 2n + 1)$ with $m_i \in \mathbb{N}$ and $b_i \in \mathbb{R}^*$ within the class of C -type functions is uniquely determined with the integral representations $I_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; 2z)$ and $I_{m_1, m_2, \dots, m_k}(b_1, b_2, \dots, b_k; 2z + 1)$, respectively.

We remark that in physics applications due to the definiteness of the crossing relations in case of the respective process using the light-cone expansion^{133,142,36,63,18} n is either even or odd and the analytic continuation is carried out from the respective subset.

VII. THE MELLIN TRANSFORM AND INVERSE MELLIN TRANSFORM BETWEEN MULTIPLE POLYLOGARITHMS AND S -SUMS

For a harmonic polylogarithm $h(x)$, i.e., a generalized polylogarithm with the index set $\{-1, 0, 1\}$, the Mellin transform (1.1) can be expressed in terms harmonic sums and constants (written in terms of harmonic polylogarithms at 1 or equivalently in terms of generalized zeta values). Extending the Mellin transform to

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

gives a 1–1 correspondence between the harmonic polylogarithms and the harmonic sums via the extended Mellin transform and its inverse transform.

In this section we generalize this construction and look at the Mellin-transform of generalized 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 (containing the harmonic sums) together with constants (written in terms of generalized polylogarithms evaluated at certain points or equivalently in terms of infinite S -sums; see Sec. V). In particular, using the inverse Mellin transform, the S -sums can be expressed in terms of the Mellin transform of generalized polylogarithms.

In order to establish this connection, we have to deal with functions such as $f(x) = 1/(a - x)$ with $a \in (0, 1)$. However, already for this simple case, the Mellin transform is not defined since the integral $\int_0^1 \frac{x^n}{a-x}$ does not converge. Hence we modify the definition of the Mellin transform to include these cases, such as $1/(a - x)$, as follows.

Let $h(x)$ be a generalized 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:

$$\begin{aligned} M^+(h(x), n) &:= M(h(x), n) = \int_0^1 x^n h(x) dx, \\ M^+\left(\frac{h(x)}{a+x}, n\right) &:= M\left(\frac{h(x)}{a+x}, n\right) = \int_0^1 \frac{x^n h(x)}{a+x} dx, \\ M^+\left(\frac{h(x)}{a_1-x}, n\right) &:= M\left(\frac{h(x)}{a_1-x}, n\right) = \int_0^1 \frac{x^n h(x)}{a_1-x} dx, \\ M^+\left(\frac{h(x)}{a_2-x}, n\right) &:= \int_0^{1/a_2} \frac{(x^n - 1)h(a_2 x)}{1-x} dx = \int_0^1 \frac{\left(\left(\frac{x}{a_2}\right)^n - 1\right)h(x)}{a_2 - x} dx. \end{aligned} \quad (7.1)$$

In (7.1) both extensions $\int_0^{1/a_2} \frac{x^n - 1}{1-x} h(a_2 x) dx$ and $\int_0^1 \frac{[(x/a_2)^n - 1]}{a_2 - x} h(x) dx$ 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. From now on we will call the extended and modified Mellin transform M^+ just Mellin transform and we will write M instead of M^+ .

For later considerations the following property (see Sec. VI) will be helpful.

Lemma 7.1. Let $m_i \in \mathbb{R} \setminus (0, 1)$, $a \in \mathbb{R}^*$ and $m \in \{0, 1\}$ and define $f(z) = M\left(\frac{H_{m_1, \dots, m_k}(x)}{(a \pm x)^m}, z\right)$. Then $f(z)$, $f(2z)$ and $f(2z + 1)$ are of C-type.

A. Calculating the Mellin transform in terms of S-sums

Subsequently, we solve the following problem:

Given $\mathbf{m} = (m_1, \dots, m_k)$ with $m_i \in \mathbb{R} \setminus (0, 1)$, $a \in \mathbb{R}^*$ and $m \in \{0, 1\}$.

Find an expression $F(n)$ given as a linear combination of S-sums such that for all $n \in \mathbb{N}$ we have

$$M\left(\frac{H_{\mathbf{m}}(x)}{(a \pm x)^m}, n\right) = F(n). \tag{7.2}$$

Note that this construction represents the Mellin transform of weighted generalized polylogarithms only for positive integer points. However, the uniquely determined analytic continuation (among all the C-type functions) for even and odd S-sums describes the Mellin transform in the complex plane; further details are given below of (7.5).

In order to solve the specified problem, we enhance the ideas of Ref. 105 for analytic aspects from the class of harmonic polylogarithms to the class of generalized polylogarithms.

Namely, due to the following lemma we are able to reduce the calculation of the Mellin transform of generalized 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 generalized polylogarithms with indices in $\mathbb{R} \setminus (0, 1)$ which are not weighted, i.e., to the calculation of expressions of the form $M(H_{\mathbf{m}}(x), n)$.

Lemma 7.2. For $n \in \mathbb{N}$, $\mathbf{m} = (m_1, \overline{\mathbf{m}}) = (m_1, m_2, \dots, m_k)$ 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

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

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

Proof. For $a > 0$ we get

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

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

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

And hence

$$M\left(\frac{H_m(x)}{1-x}, n+1\right) = -(n+1)M(H_{1,m}(x), n). \quad (7.3)$$

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

$$\begin{aligned} M\left(\frac{H_{m_1,m}(x)}{a_2-x}, n\right) &= \frac{1}{a_2^n} \int_0^1 \frac{(x^n - a_2^n) H_{m_1,m}(x)}{a_2 - x} dx \\ &= -H_{m_1,m}(x) \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} \Big|_0^1 + \int_0^1 \frac{H_m(x)}{|m_1|+x} \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} dx \\ &= -H_{m_1,m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^1 \frac{x^i H_m(x)}{|m_1|+x} dx \\ &= -H_{m_1,m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} M\left(\frac{H_m(x)}{|m_1|+x}, i\right), \\ M\left(\frac{H_{0,m}(x)}{a_2-x}, n\right) &= \frac{1}{a_2^n} \int_0^1 \frac{(x^n - a_2^n) H_{0,m}(x)}{a_2 - x} dx \\ &= -H_{0,m}(x) \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} \Big|_0^1 + \int_0^1 \frac{H_m(x)}{x} \sum_{i=1}^n \frac{\left(\frac{x}{a_2}\right)^i}{i} dx \\ &= -H_{0,m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} \int_0^1 \frac{x^i H_m(x)}{x} dx \\ &= -H_{0,m}(1) S_1\left(\frac{1}{a_2}; n\right) + \sum_{i=1}^n \frac{\left(\frac{1}{a_2}\right)^i}{i} M\left(\frac{H_m(x)}{x}, i\right), \end{aligned}$$

and

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

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

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

□

To calculate a non-weighted Mellin transform $M(H_m(x), n)$ we proceed by recursion. First, let us state the base cases, i.e., the Mellin transforms of generalized polylogarithms with depth 1.

Lemma 7.3. For $n \in \mathbb{N}$, $a \in \mathbb{R} \setminus (0, 1)$ we have

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

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

$$\begin{aligned} M(H_a(x), n) &= \int_0^1 x^n H_a(x) dx = \frac{x^{n+1}}{n+1} H_a(x) \Big|_0^1 - \int_0^1 \frac{x^{n+1}}{n+1} \frac{1}{|a|+x} dx \\ &= \frac{H_a(1)}{n+1} - \frac{1}{n+1} \left(\int_0^1 \frac{x^{n+1} - a^{n+1}}{|a|+x} dx + a^{n+1} \int_0^1 \frac{1}{|a|+x} dx \right) \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{1}{n+1} \int_0^1 a^n \sum_{i=0}^n \frac{x^i}{a^i} dx \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{a^n}{n+1} \sum_{i=0}^n \frac{1}{a^i (i+1)} \\ &= \frac{H_a(1)}{n+1} (1 - a^{n+1}) - \frac{a^{n+1}}{n+1} S_1\left(\frac{1}{a}; n+1\right) \\ &= \frac{-1}{(n+1)^2} \left(1 + a^{n+1}(n+1)S_1\left(\frac{1}{a}; n\right) + (a^{n+1} - 1)(n+1)H_a(1) \right). \end{aligned}$$

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

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

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 follow 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

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

□

Summarizing, using Lemma 7.2 together with Lemma 7.3 and Lemma 7.4 we are able to calculate the Mellin transform of generalized 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.

As an example we compute the Mellin transform of

$$\frac{\mathbf{H}_{0,-2}(x)}{x+2}.$$

Using Lemma 7.2 we can write

$$\mathbf{M}\left(\frac{\mathbf{H}_{0,-2}(x)}{x+2}, n\right) = -n \cdot \mathbf{M}(\mathbf{H}_{-2,0,-2}(x), n-1) + \mathbf{H}_{-2,0,-2}(1).$$

Now we apply Lemma 7.4 which leads to

$$\mathbf{M}(\mathbf{H}_{-2,0,-2}(x), n-1) = \frac{1 - (-2)^n}{n} \mathbf{H}_{-2,0,-2}(1) - \frac{(-2)^{n-1}}{n} \sum_{i=0}^{n-1} \frac{\mathbf{M}(\mathbf{H}_{0,-2}(x), i)}{(-2)^i}.$$

Again using Lemma 7.4 we find

$$\mathbf{M}(\mathbf{H}_{0,-2}(x), i) = \frac{1}{i+1} \mathbf{H}_{0,-2}(1) - \frac{1}{i+1} \sum_{i=0}^n \mathbf{M}(\mathbf{H}_{-2}(x), i).$$

Finally, applying Lemma 7.3 we get

$$\mathbf{M}(\mathbf{H}_{-2}(x), i) = -\frac{(1 + (-2)^{i+1}(i+1)\mathbf{S}_1(-\frac{1}{2}; i) - ((-2)^{i+1} - 1)(i+1)\mathbf{S}_1(-\frac{1}{2}; \infty))}{(i+1)^2}.$$

Putting this together yields

$$\begin{aligned} \mathbf{M}\left(\frac{\mathbf{H}_{0,-2}(x)}{x+2}, n\right) &= (-2)^n \mathbf{H}_{-2,0,-2}(1) \\ &+ (-2)^{n-1} \sum_{i=0}^{n-1} \frac{(-2)^{-i}}{i+1} \left(\mathbf{H}_{0,-2}(1) + \frac{1+(-2)^{i+1}(i+1)\mathbf{S}_1(-\frac{1}{2}; i) - (-1+(-2)^{i+1})(i+1)\mathbf{S}_1(-\frac{1}{2}; \infty)}{(i+1)^2} \right). \end{aligned}$$

To this end, transforming this expression to S -sums we arrive at

$$\begin{aligned} \mathbf{M}\left(\frac{\mathbf{H}_{0,-2}(x)}{x+2}, n\right) &= -(-1)^n (2)^n \left[\mathbf{H}_{-2,0,-2}(1) + \mathbf{H}_{0,-2}(1) \mathbf{S}_1\left(-\frac{1}{2}; n\right) - \mathbf{S}_2(n) \mathbf{S}_1\left(-\frac{1}{2}; \infty\right) \right. \\ &\quad \left. + \mathbf{S}_1\left(-\frac{1}{2}; \infty\right) \mathbf{S}_2\left(-\frac{1}{2}; n\right) + \mathbf{S}_{2,1}\left(1, -\frac{1}{2}; n\right) \right]. \end{aligned} \quad (7.4)$$

Looking at the presented algorithm the representation $F(n)$ in (7.2) will be of the form

$$F(n) = (-1)^n \left[r_0 a_0^n f_0(n) + \dots + r_d a_d^n f_d(n) \right] + \left[r_{d+1} a_{d+1}^n f_{d+1}(n) + \dots + r_e a_e^n f_e(n) \right] \quad (7.5)$$

with $d \leq e$, $r_i \in \mathbb{R}$, $a_i \in \mathbb{R}^+$ and where each $f_i(n)$ stands for a S -sum.

Consider the C-type function $f(z) := M\left(\frac{H_m(x)}{(a \pm x)^m}, z\right)$; see Lemma 7.1. We remark that the right-hand side of (7.2) for even and odd n has also an analytic continuation by replacing the S -sums with the integral representation of Theorem 2.2. In particular, the function is of C-type due to Proposition 6.4 and Lemma 6.2. Because of Carlson’s theorem it follows that the constructed function agrees with $f(z)$. In other words, the representation of the Mellin transform with S -sums for integer values gives the representation in the complex plane.

B. Calculating the inverse Mellin transform in terms of generalized polylogarithms

Subsequently, we consider a subset of the generalized harmonic polylogarithms, namely, the set

$$\bar{H} := \left\{ H_{m_1, m_2, \dots, m_k}(x) \mid m_i \in \mathbb{R}, \left| \frac{1}{m_{j_k}} \right| \leq 1 \text{ and } \left| \frac{m_{j_i}}{m_{j_{i-1}}} \right| \leq 1 \text{ for } 2 \leq i \leq k \text{ where } \{m_{j_1}, m_{j_2}, \dots, m_{j_k}\} \text{ is the set of nonzero indices, and } j_u < j_v \text{ if } u < v \right\}$$

and call the elements \bar{H} -polylogarithms; note that $m_i \in \mathbb{R} \setminus (-1, 1)$ with $m_i \neq 0$. For this subclass, it turns out that the Mellin transform of properly weighted generalized polylogarithms can be expressed using the S -sums from the set

$$\bar{S} := \left\{ S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n) \mid a_i \in \mathbb{Z}^* \text{ for } 1 \leq i \leq k; b_1 \in \mathbb{R}^*; b_i \in [-1, 1] \setminus \{0\} \text{ for } 2 \leq i \leq k \right\}; \quad (7.6)$$

the elements of this set are also called \bar{S} -sums.

Restricting to this class, we solve the following problem:

Given an \bar{S} -sum $S_m(\mathbf{b}; n)$.

Find a linear combination $F(n)$ of Mellin transforms of weighted generalized polylogarithms from \bar{H} such that for all $n \in \mathbb{N}$ we have

$$S_m(\mathbf{b}; n) = F(n). \quad (7.7)$$

In other words, there is a certain bijection between the set of properly weighted \bar{H} -polylogarithms and \bar{S} -sums via the Mellin-transform and its inverse Mellin transform.

In order to present the algorithm for the inverse Mellin transform, we define the following 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

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

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

Then the inverse Mellin transform from \bar{S} to \bar{H} relies on the following main properties:

Lemma 7.5.

1. In the Mellin transform of a generalized polylogarithm $H_m(x) \in \bar{H}$ with $\mathbf{m} = (m_1, m_2, \dots, m_k)$ weighted by $1/(c - x)$ or $1/(c + x)$ ($c \in \mathbb{R}^*$) there is only one most complicated S -sum $S_a(\mathbf{b}; n) \in \bar{S}$ with $\mathbf{a} = (a_1, \dots, a_l)$ and $\mathbf{b} = (b_1, \dots, b_l)$, i.e.,

$$M\left(\frac{H_m(x)}{c \pm x}, n\right) = p \cdot S_a(\mathbf{b}; n) + t, \quad (7.8)$$

where $p \in \mathbb{R}^*$ and t consists of a linear combination of \bar{S} -sums over \mathbb{R} that are smaller than $S_a(\mathbf{b}; n)$. Note that if $H_m(x)$ is of weight w , then $S_a(\mathbf{b}; n)$ is of weight $w + 1$. In particular, if $m_k \neq 1$ then $a_l \neq 1$ or $b_l \neq 1$; these properties will be used later in Sec. XI.

- Given $S_a(\mathbf{b}; n) \in \bar{S}$ with $\mathbf{a} = (a_1, \dots, a_l)$ and $\mathbf{b} = (b_1, \dots, b_l)$, there is an algorithm (see Algorithm 3 of Ref. 6) that computes a $H_m(x) \in \bar{H}$ with $\mathbf{m} = (m_1, m_2, \dots, m_k)$, $d \in \{-1, 1\}$, and $c \in \mathbb{R}^*$ such that $S_a(\mathbf{b}; n)$ is the most complicated S -sum that occurs in $M\left(\frac{H_m(x)}{c+d x}, n\right)$. Note that if $S_a(\mathbf{b}; n)$ is of weight w , then $H_m(x)$ is of weight $w - 1$. In particular, if $a_l \neq 1$ or $b_l \neq 1$ then $m_k \neq 1$. Moreover, if $b_i \in [-1, 1]$ with $b_i \neq 0$ for all i then $c > 1$; again these properties will be used later in Sec. XI.

Note that parts of these properties have been exploited already in Ref. 105 to construct the inverse Mellin transform between harmonic sums and harmonic polylogarithms. The rigorous proofs for this special case given in Ref. 4 carry over to this more general case and are omitted here.

The computation of the inverse Mellin transform of a linear combination of \bar{S} -sums now is straightforward (compare Refs. 4 and 105):

- Locate the most complicated \bar{S} -sum.
- Exploit property (2) from above and compute a \bar{H} -polylogarithm weighted by $1/(c - x)$ or $1/(c + x)$ such that the \bar{S} -sum is the most complicated \bar{S} -sum in the Mellin transform of this weighted generalized polylogarithm.
- Add it and subtract it with an appropriate factor (see the next step).
- Perform the Mellin transform to the subtracted version. This will cancel the original \bar{S} -sum (by choosing the appropriate factor).
- 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 $\delta(1 - x)$ where $\delta(x)$ stands for the Dirac- δ -distribution.¹³⁸

In the following we will illustrate the computation of the inverse Mellin transformation by means of an example. We consider the sum $S_{2,1}\left(1, -\frac{1}{2}; n\right)$. It is the most complicated \bar{S} -sum in the Mellin transformation of $\frac{H_{0,-2}(x)}{x+2}$ which can be computed by Algorithm 3 in Ref. 6. So in a first step we get

$$S_{2,1}\left(1, -\frac{1}{2}; n\right) = S_{2,1}\left(1, -\frac{1}{2}; n\right) - \left(-\frac{1}{2}\right)^n M\left(\frac{H_{0,-2}(x)}{x+2}, n\right) + \left(-\frac{1}{2}\right)^n M\left(\frac{H_{0,-2}(x)}{x+2}, n\right).$$

Calculating the first of the two Mellin transforms (see (7.4)) we get

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

In the right-hand side of this expression we find a linear combination of the three \bar{S} -sums $S_2\left(-\frac{1}{2}; n\right)$, $S_2(n)$, and $S_1\left(-\frac{1}{2}; n\right)$, which we want to express using the Mellin transformation of generalized polylogarithms. The most complicated \bar{S} -sums from these three is $S_2\left(-\frac{1}{2}; n\right)$. In particular, it is the most complicated \bar{S} -sum in the Mellin transformation of $\frac{H_0(x)}{x+2}$. Hence following the above method we rewrite $S_{2,1}\left(1, -\frac{1}{2}; n\right)$ to the expression

$$\begin{aligned} & - \left(S_2\left(-\frac{1}{2}; n\right) - \left(-\frac{1}{2}\right)^n M\left(\frac{H_0(x)}{x+2}, n\right) + \left(-\frac{1}{2}\right)^n M\left(\frac{H_0(x)}{x+2}, n\right) \right) S_1\left(-\frac{1}{2}; \infty\right) \\ & + \left(-\frac{1}{2}\right)^n M\left(\frac{H_{0,-2}(x)}{x+2}, n\right) + S_2(n)S_1\left(-\frac{1}{2}; \infty\right) + S_1\left(-\frac{1}{2}; n\right)S_2\left(-\frac{1}{2}; \infty\right) \\ & + S_3\left(-\frac{1}{2}; \infty\right) - S_{1,2}\left(-\frac{1}{2}, 1; \infty\right). \end{aligned}$$

Performing the first of these occurring Mellin transformations yields

$$\begin{aligned} & \left(-\frac{1}{2}\right)^n \mathcal{M}\left(\frac{H_{0,-2}(x)}{x+2}, n\right) + \left(-\frac{1}{2}\right)^n S_1\left(-\frac{1}{2}; \infty\right) \mathcal{M}\left(\frac{H_0(x)}{x+2}, n\right) + S_2(n) S_1\left(-\frac{1}{2}; \infty\right) \\ & - S_{1,2}\left(-\frac{1}{2}, 1; \infty\right) + S_1\left(-\frac{1}{2}; n\right) S_2\left(-\frac{1}{2}; \infty\right) - S_1\left(-\frac{1}{2}; \infty\right) S_2\left(-\frac{1}{2}; \infty\right) + S_3\left(-\frac{1}{2}; \infty\right). \end{aligned}$$

Continuing this process for the remaining \bar{S} -sums we arrive at

$$\begin{aligned} S_{2,1}\left(1, -\frac{1}{2}; n\right) &= S_1\left(-\frac{1}{2}; \infty\right) \mathcal{M}\left(\frac{H_0(x)}{1-x}, n\right) + S_3\left(-\frac{1}{2}; \infty\right) - S_{1,2}\left(-\frac{1}{2}, 1; \infty\right) \\ &+ (-1)^n \left(\frac{1}{2}\right)^n \left[S_1\left(-\frac{1}{2}; \infty\right) \mathcal{M}\left(\frac{H_0(x)}{x+2}, n\right) + S_2\left(-\frac{1}{2}; \infty\right) \mathcal{M}\left(\frac{1}{x+2}, n\right) + \mathcal{M}\left(\frac{H_{0,-2}(x)}{x+2}, n\right) \right]. \end{aligned} \quad (7.9)$$

We remark that there is a second way to compute the inverse Mellin transform of a \bar{S} -sum by using the integral representation of Theorem 2.2: Repeated suitable integration by parts of the given integral representation provides the inverse Mellin transform in terms of integrals that can be expressed in terms of generalized polylogarithms.

Looking at the presented algorithm the representation $F(n)$ in (7.7) will be of the form

$$F(n) = (-1)^n \left[r_0 a_0^n f_0(n) + \dots + r_d a_d^n f_d(n) \right] + \left[r_{d+1} a_{d+1}^n f_{d+1}(n) + \dots + r_e a_e^n f_e(n) \right] \quad (7.10)$$

with $d \leq e$, $r_i \in \mathbb{R}$, $a_i \in \mathbb{R}^+$ and where each $f_i(n)$ stands for a Mellin transform of weighted harmonic polylogarithm from \bar{H} .

We remark that the right-hand side of (7.7) for even and odd n gives rise to an analytic continuation. In particular the function is of C-type due to Lemmas 7.1 and 6.2. Because of the generalized Carlson theorem it follows that the obtained function agrees with the integral representation of the even, resp., odd S -sum given in Theorem 2.2.

In many QCD applications one starts with a complicated function $f(x)$ in x -space where one knows that it can be expressed in terms of a linear combination of weighted generalized polylogarithms (or related classes of them) over real numbers. It is possible to choose either n as an even or odd positive integer, depending on the physics problem. In some cases the corresponding other choice may even yield a vanishing result due to a symmetry inherent in the process. Then one tactic is to perform the simplification on $\mathcal{M}(f(x), n)$ (e.g., with the symbolic summation packages^{1,29,31,8}) and to express it in terms of S -sums. Note that by Lemma 7.1 $\mathcal{M}(f(x), n)$ is of C-type. Finally, applying the inverse Mellin transform to each of these S -sums and combining these calculations, one obtains an expression $F(n)$ in the format (7.7). Usually, the alternating sign and the powers a_i^n vanish. Since also the output function $F(n)$ can be analytically continued, the continuation is of C-type and $\mathcal{M}(f(x), n) = F(n)$ for almost all integer n , their analytic continuations agree by Carlson's theorem. Now drop the Mellin operator from $F(n)$ which gives a linear combination $h(x)$ of generalized polylogarithms such that $\mathcal{M}(h(x), n) = F(n)$. This finally yields that $f(x) = h(x)$.

VIII. DIFFERENTIATION OF S -SUMS

As worked out in Sec. VI the even and odd S -sums can be uniquely analytically continued within the class of C-type functions. This allows one to consider differentiation with respect to n . As it turns out the obtained expressions are again integral representations of S -sum expressions. This will make it possible to define the differentiation of S -sums in an analytically consistent way.

We present two strategies to compute the differentiation of S -sums. The first approach follows the ideas from Refs. 27 and 26 for harmonic sums: compute the Mellin transform, differentiate the arising integrals (which can be analytically continued in n), and apply afterwards the inverse Mellin transform to bring these expressions back to S -sums. This method is restricted to \bar{S} -sums (for a definition see (7.6)) using our current technologies. Finally, we will present a second approach using directly the integral representation of S -sums that will work in general.

In both approaches one can start with an even S -sum $S_a(\mathbf{b}; 2n)$ or odd S -sum $S_a(\mathbf{b}; 2n + 1)$ (where the uniqueness property of the analytic continuation is given). For convenience, one can also work with the usual S -sum and obtains an output of the form

$$S_a(\mathbf{b}; n) = (-1)^n F(n) + G(n),$$

which encodes both cases: Setting $n \rightarrow 2n$, resp. $n \rightarrow 2n + 1$, yields the differentiation (uniquely determined among the C-type functions) for the even resp. odd case.

A. Differentiation by means of the Mellin transform and its inverse

Using the inverse Mellin transform we express an \bar{S} -sum to the form (7.10) where the $f_i(n)$ stands for an expression of the form $M\left(\frac{H_m(x)}{k \pm x}, n\right)$ with $H_m(x) \in \bar{H}$. Note that from now on the possibly occurring $(-1)^n$ in (7.10) remains untouched and we deal only with the remaining objects which can be analytically continued. Next we 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

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

Finally, for “-” and $k \in (0, 1]$ this leads to

$$\begin{aligned} \frac{d}{dn} M\left(\frac{H_m(x)}{k-x}, n\right) &= \frac{d}{dn} \int_0^1 \frac{\left(\frac{x^n}{k^n} - 1\right) H_m(x)}{k-x} dx = \int_0^1 \frac{\frac{x^n}{k^n} (H_0(x) - H_0(k)) H_m(x)}{k-x} dx \\ &= \int_0^1 \frac{\left(\frac{x^n}{k^n} - 1\right) H_0(x) H_m(x)}{k-x} dx - H_0(k) \int_0^1 \frac{\left(\frac{x^n}{k^n} - 1\right) H_m(x)}{k-x} dx \\ &\quad + \int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_m(x)}{k-x} dx. \end{aligned} \tag{8.1}$$

In the following lemmas we will see that $\int_0^1 \frac{H_0\left(\frac{x}{k}\right) H_m(x)}{k-x} dx$ is finite and in other words, the last integral in (8.1) is well defined. Moreover, we will see how we can evaluate this constant in terms of generalized polylogarithms. Hence in all three cases we eventually arrive at Mellin transforms of generalized polylogarithms. To this end, we perform the Mellin transform of these expressions and arrive at a final expression in terms of \bar{S} -sums together with infinite \bar{S} -sums.

Lemma 8.1. For a generalized polylogarithm $H_m(x)$ 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

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

exists and can be expressed in terms of generalized polylogarithms.

Proof. Using integration by parts we get

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

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

Lemma 8.2. 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 generalized polylogarithms.

Proof. If $H_{\mathbf{a}}(x)$ 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 generalized 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 3.1 and applying the integral we end up in generalized polylogarithms at one and at $\frac{1}{k} - 1$ which are all finite. Hence C is finite. Summarizing

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

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

We demonstrate this strategy by differentiating $S_2(2; n)$. After calculating

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

we differentiate with respect to n and obtain

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

B. Differentiation based on the nested integral representation

Using the integral representation from Theorem 2.2 the differentiation can be extended from \bar{S} -sums to S -sums. We demonstrate the underlying ideas by the differentiation of $S_{1,2,1}(\frac{1}{2}, 2, \frac{1}{3}; n)$. We start with the iterated integral representation

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

given by Theorem 2.2. Differentiation 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 generalized 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

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

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

$$\begin{aligned} C &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{1}{y} \int_0^y \frac{1}{z-\frac{1}{2}} \int_z^{\frac{1}{2}} -\frac{H_0(w)}{w-1} dw dz dy dx + \\ &\int_0^{\frac{1}{3}} \frac{1}{x-1} \int_{\frac{1}{2}}^1 -\frac{1}{y} \int_0^{\frac{1}{2}} \frac{1}{z-\frac{1}{2}} \int_z^{\frac{1}{2}} -\frac{H_0(w)}{w-1} dw dz dy dx + \\ &\int_0^{\frac{1}{3}} \frac{1}{x-1} \int_{\frac{1}{2}}^1 -\frac{1}{y} \int_{\frac{1}{2}}^y \frac{1}{z-\frac{1}{2}} \int_{\frac{1}{2}}^z \frac{H_0(w)}{w-1} dw dz dy dx \\ &= C_1 + C_2 + C_3. \end{aligned}$$

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

$$\begin{aligned}
 C_1 &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{1}{y} \int_0^y \frac{H_{1,0}(\frac{1}{2}) - H_{1,0}(z)}{z - \frac{1}{2}} dz dy dx \\
 &= \int_0^{\frac{1}{3}} \frac{1}{x-1} \int_x^{\frac{1}{2}} -\frac{H_{\frac{1}{2}}(y)H_{1,0}(\frac{1}{2}) + H_{\frac{1}{2},1,0}(y)}{y} dy dx \\
 &= \int_0^{\frac{1}{3}} \frac{H_{1,0}(\frac{1}{2}) \left(H_{0,\frac{1}{2}}(\frac{1}{2}) - H_{0,\frac{1}{2}}(x) \right) - H_{0,\frac{1}{2},1,0}(\frac{1}{2}) + H_{0,\frac{1}{2},1,0}(x)}{x-1} dx \\
 &= H_0(2)H_2(1)H_3(1)H_{0,1}(1) + H_3(1)H_{0,2}(1)H_{0,1}(1) - H_0(2)H_3(1)H_{0,1,2}(1) \\
 &\quad - H_0(2)H_2(1)H_{3,0,\frac{3}{2}}(1) - H_{0,2}(1)H_{3,0,\frac{3}{2}}(1) - 2H_3(1)H_{0,0,1,2}(1) - H_3(1)H_{0,1,0,2}(1) \\
 &\quad + H_0(3)H_{3,0,\frac{3}{2},3}(1) + H_{0,3,0,\frac{3}{2},3}(1) + 2H_{3,0,0,\frac{3}{2},3}(1) + H_{3,0,\frac{3}{2},0,3}(1).
 \end{aligned}$$

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:

$$\begin{aligned}
 \frac{\partial S_{1,2,1}(\frac{1}{2}, 2, \frac{1}{3}; n)}{\partial n} &= \\
 &H_0(2)H_{3,0,\frac{3}{2}}(1)S_1(\frac{1}{2}; n) - H_3(1)H_{0,1,0}(2)S_1(\frac{1}{2}; n) - H_0(3)H_{3,0,\frac{3}{2}}(1)S_1(\frac{1}{2}; n) \\
 &\quad - H_{0,3,0,\frac{3}{2}}(1)S_1(\frac{1}{2}; n) - 2H_{3,0,0,\frac{3}{2}}(1)S_1(\frac{1}{2}; n) + H_0(3)H_3(1)S_{1,2}(\frac{1}{2}, 2; n) \\
 &\quad + H_{0,3}(1)S_{1,2}(\frac{1}{2}, 2; n) - H_0(3)S_{1,2,1}(\frac{1}{2}, 2, \frac{1}{3}; n) - S_{1,2,2}(\frac{1}{2}, 2, \frac{1}{3}; n) \\
 &\quad - 2S_{1,3,1}(\frac{1}{2}, 2, \frac{1}{3}; n) - S_{2,2,1}(\frac{1}{2}, 2, \frac{1}{3}; n) + H_3(1)H_0(2)^2H_{0,-1}(1) \\
 &\quad + H_2(1)H_3(1)H_0(2)H_{0,1}(1) + H_3(1)H_0(2)H_{-1,0,1}(1) + H_3(1)H_0(2)H_{0,-1,1}(1) \\
 &\quad - H_3(1)H_0(2)H_{0,1,2}(1) - H_2(1)H_0(2)H_{3,0,\frac{3}{2}}(1) + H_3(1)H_{0,1}(1)H_{0,1}(1) - H_{0,2}(1)H_{3,0,\frac{3}{2}}(1) \\
 &\quad - H_3(1)H_{-1,0,1,-1}(1) - 2H_3(1)H_{0,0,1,2}(1) - H_3(1)H_{0,1,0,2}(1) \\
 &\quad + H_0(3)H_{3,0,\frac{3}{2},3}(1) + H_{0,3,0,\frac{3}{2},3}(1) + 2H_{3,0,0,\frac{3}{2},3}(1) + H_{3,0,\frac{3}{2},0,3}(1).
 \end{aligned} \tag{8.2}$$

As worked out in Ref. 6 the proposed strategy works in general for S -sums.

IX. RELATIONS BETWEEN S-SUMS

S -sums obey stuffle relations due to their quasi-shuffle algebra, differentiation relations, and generalized argument relations. Subsequently, the available ideas for harmonic sums^{21,27,26} and cyclotomic harmonic sums⁵ are extended and explored for S -sums.

A. Quasi-shuffle or stuffle relations

Based on Ref. 71 it has been worked out in Ref. 90 that Z -sums

$$Z_{a_1, \dots, a_k}(x_1, \dots, x_k; n) = \sum_{n \geq i_1 > i_2 > \dots > i_k \geq 1} \frac{x_1^{i_1}}{i_1^{a_1}} \cdots \frac{x_k^{i_k}}{i_k^{a_k}} \quad (9.1)$$

with their quasi-shuffle product form a quasi-shuffle algebra. Since S -sums and Z -sums can be transformed into each other, a quasi-shuffle algebra can be carried over to S -sums.

We remark that the quasi-shuffle algebra can be derived directly (without using the notion of Z -sums) as follows. 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

$$S_{m_1, m_2, \dots, m_k}(x_1, x_2, \dots, x_k; n)$$

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 shown analogously as in Ref. 4 (compare Ref. 71) that the S -sums form a quasi shuffle algebra which is the free polynomial algebra on the *Lyndon* words with alphabet A , see also Ref. 104.

As a consequence 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.^{135,136,106} The number of *Lyndon* words of length d over an alphabet of length n is given by

$$N_A(d) = \frac{1}{d} \sum_{q|d} \mu\left(\frac{d}{q}\right) n^q,$$

where

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

is the Möbius function.^{93,69} In the following we call the relations from the quasi-shuffle algebra also stuffle relations; cf. Ref. 28.

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 Refs. 21 and 4 for harmonic sums to find the basis S -sums together with the relations for the dependent S -sums.

For example, 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

$$\begin{aligned} S_{1,3}(\tfrac{1}{2}, \tfrac{1}{2}; n) &= -S_{3,1}(\tfrac{1}{2}, \tfrac{1}{2}; n) + S_1(\tfrac{1}{2}; n) S_3(\tfrac{1}{2}; n) + S_4(\tfrac{1}{4}; n), \\ S_{1,3}(-\tfrac{1}{2}, -\tfrac{1}{2}; n) &= -S_{3,1}(-\tfrac{1}{2}, -\tfrac{1}{2}; n) + S_1(-\tfrac{1}{2}; n) S_3(-\tfrac{1}{2}; n) + S_4(\tfrac{1}{4}; n), \\ S_{1,3}(\tfrac{1}{2}, -\tfrac{1}{2}; n) &= -S_{3,1}(-\tfrac{1}{2}, \tfrac{1}{2}; n) + S_1(\tfrac{1}{2}; n) S_3(-\tfrac{1}{2}; n) + S_4(-\tfrac{1}{4}; n), \\ S_{1,3}(-\tfrac{1}{2}, \tfrac{1}{2}; n) &= -S_{3,1}(\tfrac{1}{2}, -\tfrac{1}{2}; n) + S_1(-\tfrac{1}{2}; n) S_3(\tfrac{1}{2}; n) + S_4(-\tfrac{1}{4}; n), \\ S_{1,1}(-\tfrac{1}{2}, -\tfrac{1}{2}; n) &= \tfrac{1}{2} S_1(-\tfrac{1}{2}; n)^2 + \tfrac{1}{2} S_2(\tfrac{1}{4}; n), \\ S_{1,1}(\tfrac{1}{2}, \tfrac{1}{2}; n) &= \tfrac{1}{2} S_1(\tfrac{1}{2}; n)^2 + \tfrac{1}{2} S_2(\tfrac{1}{4}; n), \\ S_{1,1}(\tfrac{1}{2}, -\tfrac{1}{2}; n) &= -S_{1,1}(-\tfrac{1}{2}, \tfrac{1}{2}; n) + S_1(-\tfrac{1}{2}; n) S_1(\tfrac{1}{2}; n) + S_2(-\tfrac{1}{4}; n), \\ S_{3,3}(-\tfrac{1}{2}, -\tfrac{1}{2}; n) &= \tfrac{1}{2} S_3(-\tfrac{1}{2}; n)^2 + \tfrac{1}{2} S_6(\tfrac{1}{4}; n), \\ S_{3,3}(\tfrac{1}{2}, \tfrac{1}{2}; n) &= \tfrac{1}{2} S_3(\tfrac{1}{2}; n)^2 + \tfrac{1}{2} S_6(\tfrac{1}{4}; n), \\ S_{3,3}(\tfrac{1}{2}, -\tfrac{1}{2}; n) &= -S_{3,3}(-\tfrac{1}{2}, \tfrac{1}{2}; n) + S_3(-\tfrac{1}{2}; n) S_3(\tfrac{1}{2}; n) + S_6(-\tfrac{1}{4}; n), \end{aligned}$$

we find the 6 basis sums

$$\begin{aligned} S_{3,1}(\tfrac{1}{2}, \tfrac{1}{2}; n), S_{3,1}(-\tfrac{1}{2}, \tfrac{1}{2}; n), S_{3,1}(\tfrac{1}{2}, -\tfrac{1}{2}; n), S_{3,1}(-\tfrac{1}{2}, -\tfrac{1}{2}; n), \\ S_{1,1}(-\tfrac{1}{2}, \tfrac{1}{2}; n), S_{3,3}(-\tfrac{1}{2}, \tfrac{1}{2}; n), \end{aligned}$$

in which all the other 10 sums of depth 2 can be expressed.

B. Differential relations

In Sec. VIII we described the differentiation of S -sums with respect to the upper summation limit. Similar to the application of differentiation to harmonic sums, cf. Refs. 27 and 26, and cyclotomic sums, cf. Ref. 5, the differentiation leads to new relations in the class of S -sums. For instance we find

$$\frac{d}{dn} S_2(2; n) = -S_3(2; n) + H_0(2) S_2(2; n) + H_{0,0,-1}(1) + 2H_{0,0,1}(1) + H_{0,1,-1}(1).$$

Subsequently, we collect the derivatives with respect to n :

$$S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)^{(D)} = \left\{ \frac{\partial^N}{\partial n^N} S_{a_1, \dots, a_k}(b_1, \dots, b_k; n); N \in \mathbb{N} \right\}. \quad (9.2)$$

Continuing the example from above 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) \\
 &\quad - 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) \\
 &\quad + \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_0\left(\frac{1}{2}\right) H_{\frac{3}{4}}\left(\frac{1}{4}\right) S_2\left(\frac{1}{2}; n\right) \\
 &\quad - \frac{1}{2} H_{\frac{1}{2},0,-1,0}\left(\frac{1}{4}\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 sums are

$$S_{3,1}\left(\frac{1}{2}, -\frac{1}{2}; n\right), S_{1,1}\left(-\frac{1}{2}, \frac{1}{2}; n\right), S_{3,3}\left(-\frac{1}{2}, \frac{1}{2}; n\right). \quad (9.3)$$

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.

C. Duplication relations

As for harmonic sums and cyclotomic sums, cf. Refs. 123, 27, 26, 28, and 5 we have a duplication relation, see also Ref. 129:

Theorem 9.1 (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

$$\begin{aligned} S_a(-b, 2n) &= \sum_{i=1}^{2n} \frac{(-b)^i}{i^a} = \sum_{i=1}^n \left(\frac{b^{2i}}{(2i)^a} - \frac{b^{2i-1}}{(2i-1)^a} \right) = \frac{1}{2^a} S_a(b^2; n) - \sum_{i=1}^n \frac{b^{2i-1}}{(2i-1)^a} \\ &= \frac{1}{2^a} S_a(b^2; n) - \sum_{i=1}^n \left(\frac{b^{2i}}{(2i)^a} + \frac{b^{2i-1}}{(2i-1)^a} - \frac{b^{2i}}{(2i)^a} \right) \\ &= \frac{1}{2^a} S_a(b^2; n) - S_a(b; 2n) + \frac{1}{2^a} S_a(b^2; n) \\ &= \frac{1}{2^{a-1}} S_a(b^2, n) - S_a(b; 2n). \end{aligned}$$

Supposing that the theorem holds for $m \geq 1$, we obtain

$$\begin{aligned} \sum S_{a_{m+1}, \dots, a_1}(\pm b_{m+1}, \dots, \pm b_1; 2n) &= \\ &= \sum_{i=1}^n \left(\frac{(\pm b_{m+1}^{2i})}{(2i)^{a_{m+1}}} \sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2i) \right. \\ &\quad \left. + \frac{\pm b_{m+1}^{2i-1}}{(2i-1)^{a_{m+1}}} \sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2i+1) \right) \\ &= 2 \sum_{i=1}^n \frac{(b^2)^i}{(2i)^{a_{m+1}}} \sum S_{a_m, \dots, a_1}(\pm b_m, \dots, \pm b_1; 2i) \\ &= 2 \sum_{i=1}^n \frac{(b^2)^i}{(2i)^{a_{m+1}}} \frac{1}{2^{\sum_{i=1}^m a_i - m}} S_{a_m, \dots, a_1}(b_m^2, \dots, b_1^2; i) \\ &= \frac{1}{2^{\sum_{i=1}^{m+1} a_i - (m+1)}} S_{a_{m+1}, a_m, \dots, a_1}(\pm b_{m+1}, \pm b_m, \dots, \pm b_1; n). \end{aligned}$$

□

Considering again the example from above, the duplication relations are

$$\begin{aligned} S_{3,3}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= \frac{1}{16} S_{3,3}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{3,3}\left(\frac{-1}{2}, \frac{-1}{2}; 2n\right) - S_{3,3}\left(\frac{-1}{2}, \frac{1}{2}; 2n\right) - S_{3,3}\left(\frac{1}{2}, \frac{-1}{2}; 2n\right), \\ S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= S_{1,1}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{1,1}\left(\frac{-1}{2}, \frac{-1}{2}; 2n\right) - S_{1,1}\left(\frac{-1}{2}, \frac{1}{2}; 2n\right) - S_{1,1}\left(\frac{1}{2}, \frac{-1}{2}; 2n\right), \\ S_{3,1}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= \frac{1}{4} S_{3,1}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{3,1}\left(\frac{-1}{2}, \frac{-1}{2}; 2n\right) - S_{3,1}\left(\frac{-1}{2}, \frac{1}{2}; 2n\right) - S_{3,1}\left(\frac{1}{2}, \frac{-1}{2}; 2n\right), \\ S_{1,3}\left(\frac{1}{2}, \frac{1}{2}; 2n\right) &= \frac{1}{4} S_{1,3}\left(\frac{1}{4}, \frac{1}{4}; n\right) - S_{1,3}\left(\frac{-1}{2}, \frac{-1}{2}; 2n\right) - S_{1,3}\left(\frac{-1}{2}, \frac{1}{2}; 2n\right) - S_{1,3}\left(\frac{1}{2}, \frac{-1}{2}; 2n\right). \end{aligned}$$

Note that from duplication we do not get a further reduction in this particular example. We would have to introduce new sums of the same depth and weight to express the basis sums (9.3).

D. 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 I–III 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 sets $\{a_1, a_1, a_2\}$ and $\{x_1, x_2, x_3\}$; these sets stand for multi-sets and each element is allowed to be taken once to build all the possible

TABLE I. Number of basis sums for different index sets at depth 2.

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 II. Number of basis sums for different index sets at depth 3.

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 III. Number of basis sums for different index sets at depth 4.

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

S -sums. There we obtain the 18 sums:

$$\begin{aligned} &S_{a_1,a_1,a_2}(x_1, x_2, x_3; n), S_{a_1,a_1,a_2}(x_1, x_3, x_2; n), S_{a_1,a_1,a_2}(x_2, x_1, x_3; n), \\ &S_{a_1,a_1,a_2}(x_2, x_3, x_1; n), S_{a_1,a_1,a_2}(x_3, x_1, x_2; n), S_{a_1,a_1,a_2}(x_3, x_2, x_1; n), \\ &S_{a_1,a_2,a_1}(x_1, x_2, x_3; n), S_{a_1,a_2,a_1}(x_1, x_3, x_2; n), S_{a_1,a_2,a_1}(x_2, x_1, x_3; n), \\ &S_{a_1,a_2,a_1}(x_2, x_3, x_1; n), S_{a_1,a_2,a_1}(x_3, x_1, x_2; n), S_{a_1,a_2,a_1}(x_3, x_2, x_1; n), \\ &S_{a_2,a_1,a_1}(x_1, x_2, x_3; n), S_{a_2,a_1,a_1}(x_1, x_3, x_2; n), S_{a_2,a_1,a_1}(x_2, x_1, x_3; n), \\ &S_{a_2,a_1,a_1}(x_2, x_3, x_1; n), S_{a_2,a_1,a_1}(x_3, x_1, x_2; n), S_{a_2,a_1,a_1}(x_3, x_2, x_1; n). \end{aligned}$$

Using all applicable algebraic relations (provided by the quasi-shuffle algebra) such as,

$$\begin{aligned} S_{a_1,a_1,a_2}(x_1, x_2, x_3; n) &= S_{a_2}(x_3; n) S_{a_1,a_1}(x_1, x_2; n) + S_{a_1,a_1+a_2}(x_1, x_2x_3; n) \\ &\quad - S_{a_1}(x_1; n) S_{a_2,a_1}(x_3, x_2; n) - S_{a_2,2a_1}(x_3, x_1x_2; n) + S_{a_2,a_1,a_1}(x_3, x_2, x_1; n), \end{aligned}$$

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 IV we summarize the number of algebraic basis sums at specified weights for arbitrary indices in the x_i , while in Table V we summarize the number of algebraic and differential bases sums

TABLE IV. Number of basis sums for different index sets up to weight 6.

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
6	$\{x_1, x_2, x_3, x_4, x_5\}$	2101	625	1476
	$\{x_1, x_1, x_1, x_1, x_1, x_1\}$	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
	$\{x_1, x_1, x_2, x_2, x_3, x_4\}$	10 251	2646	7605
	$\{x_1, x_1, x_2, x_3, x_4, x_5\}$	17 841	4536	13 305
	$\{x_1, x_2, x_3, x_4, x_5, x_6\}$	31 031	7776	23 255

TABLE V. 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.

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	29 718	18 280	23 568	14 744

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. The corresponding numbers of basis elements at $w = 4$ are given in Table VI. The explicit representations of these sums in terms of basis elements are voluminous, and can be provided in electronic form on request. 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:

$$\begin{aligned}
& S_3(x_1 x_2 x_3; n), S_{1,2}(x_1, x_2 x_3; n), S_{1,2}(x_2, x_1 x_3; n), S_{1,2}(x_1 x_2, x_3; n), S_{1,2}(x_3, x_1 x_2; n), \\
& S_{1,2}(x_1 x_3, x_2; n), S_{1,2}(x_2 x_3, x_1; n), S_{2,1}(x_1, x_2 x_3; n), S_{2,1}(x_2, x_1 x_3; n), S_{2,1}(x_1 x_2, x_3; n), \\
& S_{2,1}(x_3, x_1 x_2; n), S_{2,1}(x_1 x_3, x_2; n), S_{2,1}(x_2 x_3, x_1; n), S_{1,1,1}(x_1, x_2, x_3; n), S_{1,1,1}(x_1, x_3, x_2; n), \\
& S_{1,1,1}(x_2, x_1, x_3; n), S_{1,1,1}(x_2, x_3, x_1; n), S_{1,1,1}(x_3, x_1, x_2; n), S_{1,1,1}(x_3, x_2, x_1; n).
\end{aligned}$$

TABLE VI. Number of basis constants (convergent infinite S -sums) for different alphabets up to weight 4.

Alphabet	Weight	Finite sums	Dependent sums	Basis sums
$\{1, -1\}$	1	1	0	1
	2	4	3	1
	3	12	11	1
	4	36	35	1
$\{1, \frac{1}{2}\}$	1	1	0	1
	2	4	2	2
	3	12	8	4
	4	36	24	12
$\{1, \frac{1}{2}, 2\}$	1	1	0	1
	2	5	3	2
	3	18	14	4
	4	66	53	13
$\{1, -1, \frac{1}{2}\}$	1	2	1	1
	2	9	7	2
	3	36	29	7
	4	144	113	31
$\{1, -1, \frac{1}{2}, -\frac{1}{2}\}$	1	3	1	2
	2	16	12	4
	3	80	63	17
	4	400	301	99
$\{1, -1, \frac{1}{2}, -\frac{1}{2}, 2, -2\}$	1	3	1	2
	2	20	16	4
	3	124	107	17
	4	788	678	110

Using all applicable algebraic relations (provided by the quasi-shuffle algebra) such as,

$$\begin{aligned} S_{1,2}(x_2x_3, x_1; n) &= S_1(x_2x_3; n) S_2(x_1; n) + S_3(x_1x_2x_3; n) - S_{2,1}(x_1, x_2x_3; n), \\ S_{1,1,1}(x_1, x_2, x_3; n) &= -S_1(x_3; n) S_{1,1}(x_2, x_1; n) + S_1(x_1; n) S_{1,1}(x_2, x_3; n) \\ &\quad + S_{2,1}(x_1x_2, x_3; n) - S_{2,1}(x_2x_3, x_1; n) + S_{1,1,1}(x_3, x_2, x_1; n), \end{aligned}$$

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 $w = 2$ where each of the indices from the index set $\{1/2, -1/2, 2, -2\}$ is allowed to appear just once, we consider the 38 sums:

$$\begin{aligned} &S_{-2}(n), S_2(n), S_{-1,-1}(n), S_{-1,1}(n), S_{1,-1}(n), S_{1,1}(n), S_2(-2; n), S_2(-\tfrac{1}{2}; n), \\ &S_2(\tfrac{1}{2}; n), S_2(2; n), S_{1,1}(-2, -1; n), S_{1,1}(-2, -\tfrac{1}{2}; n), S_{1,1}(-2, \tfrac{1}{2}; n), S_{1,1}(-2, 1; n), \\ &S_{1,1}(-2, 2; n), S_{1,1}(-1, -2; n), S_{1,1}(-1, -\tfrac{1}{2}; n), S_{1,1}(-1, \tfrac{1}{2}; n), S_{1,1}(-1, 2; n), \\ &S_{1,1}(-\tfrac{1}{2}, -2; n), S_{1,1}(-\tfrac{1}{2}, -1; n), S_{1,1}(-\tfrac{1}{2}, \tfrac{1}{2}; n), S_{1,1}(-\tfrac{1}{2}, 1; n), S_{1,1}(-\tfrac{1}{2}, 2; n), \\ &S_{1,1}(\tfrac{1}{2}, -2; n), S_{1,1}(\tfrac{1}{2}, -1; n), S_{1,1}(\tfrac{1}{2}, -\tfrac{1}{2}; n), S_{1,1}(\tfrac{1}{2}, 1; n), S_{1,1}(\tfrac{1}{2}, 2; n), \\ &S_{1,1}(1, -2; n), S_{1,1}(1, -\tfrac{1}{2}; n), S_{1,1}(1, \tfrac{1}{2}; n), S_{1,1}(1, 2; n), S_{1,1}(2, -2; n), S_{1,1}(2, -1; n), \\ &S_{1,1}(2, -\tfrac{1}{2}; n), S_{1,1}(2, \tfrac{1}{2}; n), S_{1,1}(2, 1; n). \end{aligned}$$

Using all algebraic and differential relations such as,

$$\begin{aligned} S_{1,1}(-\tfrac{1}{2}, 2; n) &= -\frac{\partial}{\partial n} S_{-1}(n) + H_{-1,0}(1) + S_1(-\tfrac{1}{2}; n) S_1(2; n) - S_{1,1}(2, -\tfrac{1}{2}; n), \\ S_{1,1}(-\tfrac{1}{2}, -2; n) &= -\frac{\partial}{\partial n} S_1(n) - H_{1,0}(1) + S_1(-2; n) S_1(-\tfrac{1}{2}; n) - S_{1,1}(-2, -\tfrac{1}{2}; n), \end{aligned}$$

we can express all these 38 sums using the following 17 basis sums:

$$\begin{aligned} &S_{1,-1}(n), S_{1,1}(-2, -\tfrac{1}{2}; n), S_{1,1}(-2, \tfrac{1}{2}; n), S_{1,1}(-2, 2; n), S_{1,1}(-1, -2; n), \\ &S_{1,1}(-1, -\tfrac{1}{2}; n), S_{1,1}(-1, \tfrac{1}{2}; n), S_{1,1}(-1, 2; n), S_{1,1}(-\tfrac{1}{2}, \tfrac{1}{2}; n), S_{1,1}(\tfrac{1}{2}, -\tfrac{1}{2}; n), \\ &S_{1,1}(1, -2; n), S_{1,1}(1, -\tfrac{1}{2}; n), S_{1,1}(1, \tfrac{1}{2}; n), S_{1,1}(1, 2; n), S_{1,1}(2, -2; n), \\ &S_{1,1}(2, -\tfrac{1}{2}; n), S_{1,1}(2, \tfrac{1}{2}; n). \end{aligned}$$

We remark that the found relations are induced by the quasi-shuffle algebra. Using the summation package `Sigma`¹¹³ and the underlying difference field theory^{77,118,116,117} we could verify that the found basis sums are also algebraic independent in the ring as sequences; for related work see also Ref. 68. To be more precise, the given S -sums evaluated as sequences form a polynomial ring which is a subring of the ring of sequences.

In general, we obtain the following relations

$$\begin{aligned} N_D(w) &= N_S(w) - N_S(w-1), \\ N_{AD}(w) &= N_A(w) - N_A(w-1), \end{aligned}$$

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.

X. RELATIONS BETWEEN S-SUMS AT INFINITY

In this section we will state several types of relations between the values of S -sums at infinity

$$S_{m_1, \dots, m_p}(x_1, \dots, x_p; \infty) \quad (10.1)$$

(or equivalently between the values of generalized polylogarithms) that extend various relations for infinite harmonic sums given in Ref. 28. This enables one to reduce the expressions that arise during the calculations of, e.g., the (inverse) Mellin transform, of the differentiation of S -sums, or of asymptotic expansions given below. We remark that the relations of S -sums with x_i being roots of unity have been considered in Refs. 141 and 5 already.

Stuffle relations: The first type of relations originates from the algebraic relations of S -sums, see Sec. IX A. Those relations which contain only convergent S -sums remain valid when we consider them at infinity.¹⁴³ We will refer to these relations as the quasi shuffle or stuffle relations.

Duplication relations: The duplication relations from Sec. IX C remain valid if we consider sums which are finite at infinity, since the limits n resp. $2n \rightarrow \infty$ agree.

Shuffle relations: We can generalize the shuffle relations form¹²³ 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

$$\begin{aligned} \lim_{n \rightarrow \infty} \sum_{i=1}^n \frac{y_1^i S_{m_1, \dots, m_p}(x_1, \dots, x_p; n-i) S_{k_2, \dots, k_q}(y_2, \dots, y_p; i)}{i^{k_1}} = \\ \sum_{a=1}^{k_1} \binom{k_1 + m_1 - 1 - a}{m_1 - 1} \sum_{i=1}^n \frac{x_1^i}{i^{m_1 + k_1 - a}} \\ \sum_{j=1}^i \frac{\left(\frac{y_1}{x_1}\right)^j S_{m_2, \dots, m_p}(x_2, \dots, x_p; i-j) S_{k_2, \dots, k_q}(y_2, \dots, y_p; j)}{j^a} \\ + \sum_{a=1}^{m_1} \binom{k_1 + m_1 - 1 - a}{m_1 - 1} \sum_{i=1}^n \frac{y_1^i}{i^{m_1 + k_1 - a}} \\ \sum_{j=1}^i \frac{\left(\frac{x_1}{y_1}\right)^j S_{k_2, \dots, k_q}(y_2, \dots, y_p; i-j) S_{m_2, \dots, m_p}(x_2, \dots, x_p; j)}{j^a}, \end{aligned}$$

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 generalized polylogarithms.

Duality relations: We can use duality relations of generalized polylogarithms; compare Ref. 28 where these relations are considered for harmonic sums.

$1 - x \rightarrow x$: For a generalized polylogarithm $H_{a_1, a_2, \dots, a_{k-1}, a_k}(1)$ with $a_k \neq 0$ this leads to the relation:

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

For example, we get $H_2(1) = H_{-1}(1)$ which gives in S -sum notation the new relation

$$S_1\left(\frac{1}{2}; \infty\right) = -S_{-1}(\infty).$$

$\frac{1-x}{1+x} \rightarrow x$: This transform leads, e.g., to the relation $H_2(1) = -H_{-1}(1) + H_{-\frac{1}{3}}(1)$ which gives in S -sum notation again the relation

$$S_1\left(\frac{1}{2}; \infty\right) = -S_{-1}(\infty).$$

$\frac{c-x}{d+x} \rightarrow x$: For $c, d \in \mathbb{R}$, $d \neq -1$ this transform can be calculated similarly as described in Sec. III C. The transform $\frac{2-x}{1+x} \rightarrow x$ produces, e.g., the relation $H_{-2}(1) = \frac{1}{2}(H_{-8}(1) + H_{-\frac{1}{2}}(1))$ which gives in S -sum notation the new relation

$$S_1\left(-\frac{1}{8}; \infty\right) = -S_{-1}(\infty) + S_1\left(-\frac{1}{2}; \infty\right).$$

If one considers a certain class of infinite S -sums (10.1) (with finite values) with given weight and a finite index set from which the x_i can be chosen, one can try to determine all relations from above that stay within the specified class. In general, we first have to extend the alphabet generated by the relations used. Then one exploits all relevant relations that lead back (after several applications) to the original alphabet.

In Subsections X A–X E we apply this tactic to a series of alphabets. We summarize in Table III how all the so far calculated relations for the particular alphabets contribute in reducing the number of infinite S -sums to a smaller set of sums. For the found constants we searched for new relations using PSLQ⁵⁹ using representations of up to 2000 digits. No further relations were found. These constants, which we also call *basis constants*, enlarge the number of constants generated by the multiple zeta values.²⁸ They are further extended by other special numbers related to cyclotomic harmonic sums and their generalization at infinity, cf., e.g., Refs. 37 and 5.

Subsequently, the found basis constants for the concrete alphabets are given. In the simpler cases also the relations between the dependent sums are printed explicitly.¹⁴⁴ Given an expression with the corresponding weight and alphabet and given these relations, one can bring the expression to its reduced form, i.e., in terms of the basis constants. Here one needs to replace the S -sum on the left-hand side of a given relation by its right-hand side.

A. Alphabet $\{1, \frac{1}{2}\}$

w = 1: Basis constant: $S_1\left(\frac{1}{2}; \infty\right) = \log(2)$
Relation: —

w = 2: Basis constants: $S_2(\infty) = \zeta_2$, $S_{1,1}(\frac{1}{2}, \frac{1}{2}; \infty)$
Relations:

$$S_{1,1}\left(\frac{1}{2}, 1; \infty\right) = \frac{\zeta_2}{2},$$

$$S_2\left(\frac{1}{2}; \infty\right) = -\frac{1}{2} \log^2(2) + \frac{\zeta_2}{2}.$$

w = 3: Basis constants: $S_3(\infty) = \zeta_3$, $S_{1,2}(\frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1,1}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1,1}(\frac{1}{2}, \frac{1}{2}, 1; \infty)$
Relations:

$$S_3\left(\frac{1}{2}; \infty\right) = \frac{\log^3(2)}{6} - \frac{1}{2} \log(2)\zeta_2 + \frac{7\zeta_3}{8},$$

$$S_{2,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) = \frac{\log^3(2)}{6} + \frac{1}{2} \log(2)\zeta_2 - \frac{7\zeta_3}{6} + 3S_{1,2}\left(\frac{1}{2}, \frac{1}{2}; \infty\right),$$

$$S_{2,1}\left(\frac{1}{2}, 1; \infty\right) = -\frac{1}{2}(\log(2)\zeta_2) + \zeta_3,$$

$$S_{2,1}\left(1, \frac{1}{2}; \infty\right) = \frac{\log^3(2)}{6} + \frac{1}{2} \log(2)\zeta_2 + \frac{\zeta_3}{4},$$

$$S_{2,1}(\infty) = 2\zeta_3,$$

$$S_{1,2}\left(\frac{1}{2}, 1; \infty\right) = \frac{5\zeta_3}{8},$$

$$S_{1,1,1}\left(\frac{1}{2}, 1, \frac{1}{2}; \infty\right) = \frac{1}{2} \log(2)\zeta_2 - \frac{5\zeta(3)}{12} + S_{1,2}\left(\frac{1}{2}, \frac{1}{2}; \infty\right),$$

$$S_{1,1,1}\left(\frac{1}{2}, 1, 1; \infty\right) = \frac{3\zeta_3}{4}.$$

B. Alphabet $\{1, \frac{1}{2}, 2\}$

w = 1: Basis constant: $S_1(\frac{1}{2}; \infty) = \log(2)$
Relation: —

w = 2: Basis constants: $S_2(\infty) = \zeta_2$, $S_{1,1}(\frac{1}{2}, \frac{1}{2}; \infty)$
Relations:

$$S_2\left(\frac{1}{2}; \infty\right) = -\frac{1}{2} \log^2(2) + \frac{\zeta_2}{2},$$

$$S_{1,1}\left(\frac{1}{2}, 1; \infty\right) = \frac{\zeta_2}{2},$$

$$S_{1,1}\left(\frac{1}{2}, 2; \infty\right) = \frac{3\zeta_2}{2}.$$

w = 3: Basis constants: $S_3(\infty) = \zeta_3$, $S_{1,2}(\frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1,1}(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1,1}(\frac{1}{2}, \frac{1}{2}, 1; \infty)$

Relations:

$$\begin{aligned}
 S_3\left(\frac{1}{2}; \infty\right) &= -\frac{1}{2}\zeta_2 \log(2) + \frac{\log^3(2)}{6} + \frac{7\zeta_3}{8}, \\
 S_{2,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) &= \frac{1}{2}\zeta_2 \log(2) + \frac{\log^3(2)}{6} + 3S_{1,2}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) - \frac{7\zeta_3}{6}, \\
 S_{2,1}\left(\frac{1}{2}, 1; \infty\right) &= -\frac{1}{2}\zeta_2 \log(2) + \zeta_3, \\
 S_{2,1}\left(\frac{1}{2}, 2; \infty\right) &= \frac{1}{2}(-3)\zeta_2 \log(2) + \frac{21\zeta(3)}{8}, \\
 S_{2,1}\left(1, \frac{1}{2}; \infty\right) &= \frac{1}{2}\zeta_2 \log(2) + \frac{\log^3(2)}{6} + \frac{\zeta_3}{4}, \\
 S_{2,1}(\infty) &= 2\zeta_3, \\
 S_{1,2}\left(\frac{1}{2}, 1; \infty\right) &= \frac{5\zeta(3)}{8}, \\
 S_{1,2}\left(\frac{1}{2}, 2; \infty\right) &= \frac{3}{2}\zeta_2 \log(2), \\
 S_{1,1,1}\left(\frac{1}{2}, \frac{1}{2}, 2; \infty\right) &= -\frac{1}{2}\zeta_2 \log(2) + \frac{\log^3(2)}{6} + \log(2)S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) \\
 &\quad + 2S_{1,2}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) + \frac{7\zeta_3}{24}, \\
 S_{1,1,1}\left(\frac{1}{2}, 1, \frac{1}{2}; \infty\right) &= \frac{1}{2}\zeta_2 \log(2) + S_{1,2}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) - \frac{5\zeta_3}{12}, \\
 S_{1,1,1}\left(\frac{1}{2}, 1, 1; \infty\right) &= \frac{3\zeta_3}{4}, \\
 S_{1,1,1}\left(\frac{1}{2}, 1, 2; \infty\right) &= \frac{7\zeta(3)}{4}, \\
 S_{1,1,1}\left(\frac{1}{2}, 2, \frac{1}{2}; \infty\right) &= \frac{3}{2}\zeta_2 \log(2) - \frac{\zeta_3}{4}, \\
 S_{1,1,1}\left(\frac{1}{2}, 2, 1; \infty\right) &= \frac{3}{2}\zeta_2 \log(2) + \frac{7\zeta_3}{4}.
 \end{aligned}$$

C. Alphabet $\{1, -1, \frac{1}{2}\}$

w = 1: Basis constant: $S_{-1}(\infty) = -\log(2)$

Relation:

$$S_1\left(\frac{1}{2}; \infty\right) = -S_{-1}(\infty).$$

w = 2: Basis constants: $S_2(\infty) = \zeta_2$, $S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right)$

Relations:

$$\begin{aligned}
 S_{-2}(\infty) &= -\frac{\zeta_2}{2}, \\
 S_2\left(\frac{1}{2}; \infty\right) &= \frac{\zeta_2}{2} - \frac{\log^2(2)}{2}, \\
 S_{-1,-1}(\infty) &= \frac{\zeta_2}{2} + \frac{\log^2(2)}{2}, \\
 S_{1,1}\left(-1, \frac{1}{2}; \infty\right) &= -\frac{\zeta_2}{2} - \frac{\log^2(2)}{2} + 2S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right), \\
 S_{-1,1}(\infty) &= -\frac{\zeta_2}{2} + \frac{\log^2(2)}{2}, \\
 S_{1,1}\left(\frac{1}{2}, -1; \infty\right) &= -\frac{1}{2}\log^2(2) - S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right), \\
 S_{1,1}\left(\frac{1}{2}, 1; \infty\right) &= \frac{\zeta_2}{2}, \\
 S_{1,1}\left(\frac{1}{2}, 2; \infty\right) &= \frac{3\zeta_2}{2}.
 \end{aligned}$$

w = 3: Basis constants: $S_3(\infty) = \zeta_3$, $S_{1,2}\left(-1, \frac{1}{2}; \infty\right)$, $S_{1,1,1}\left(-1, \frac{1}{2}, \frac{1}{2}; \infty\right)$, $S_{1,1,1}\left(-1, \frac{1}{2}, 1; \infty\right)$, $S_{1,1,1}\left(\frac{1}{2}, -1, \frac{1}{2}; \infty\right)$, $S_{1,1,1}\left(\frac{1}{2}, \frac{1}{2}, -1; \infty\right)$, $S_{1,1,1}\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \infty\right)$

Relations:

$$\begin{aligned}
 S_{-3}(\infty) &= -\frac{1}{4}(3\zeta_3), \\
 S_3\left(\frac{1}{2}; \infty\right) &= \frac{\log(2)^3}{6} - \frac{\log(2)\zeta_2}{2} + \frac{7\zeta_3}{8}, \\
 S_{-2,-1}(\infty) &= \frac{3\log(2)\zeta_2}{2} - \frac{5\zeta_3}{8}, \\
 S_{2,1}\left(-1, \frac{1}{2}; \infty\right) &= -\frac{\log(2)^3}{18} - \frac{\log(2)\zeta_2}{3} + \frac{7\zeta_3}{72} + \frac{1}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
 S_{-2,1}(\infty) &= -\frac{1}{8}(5\zeta_3), \\
 S_{2,1}\left(\frac{1}{2}, -1; \infty\right) &= \frac{4\log(2)^3}{9} - \frac{\log(2)\zeta_2}{3} - \frac{4\zeta_3}{9} - \frac{2}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
 S_{2,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) &= -\frac{1}{2}(\log(2)\zeta_2) + \zeta_3 + S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
 S_{2,1}\left(\frac{1}{2}, 1; \infty\right) &= -\frac{1}{2}(\log(2)\zeta_2) + \zeta_3, \\
 S_{2,-1}(\infty) &= -\frac{1}{2}(3\log(2)\zeta_2) + \frac{\zeta_3}{4}, \\
 S_{2,1}\left(1, \frac{1}{2}; \infty\right) &= \frac{\log(2)^3}{6} + \frac{\log(2)\zeta_2}{2} + \frac{\zeta_3}{4}, \\
 S_{2,1}(\infty) &= 2\zeta_3, \\
 S_{-1,-2}(\infty) &= -\log(2)\zeta_2 + \frac{13\zeta_3}{8}, \\
 S_{-1,2}(\infty) &= \frac{\log(2)\zeta_2}{2} - \zeta_3,
 \end{aligned}$$

$$\begin{aligned}
S_{1,2}\left(\frac{1}{2}, -1; \infty\right) &= -\frac{1}{24}(13\zeta_3), \\
S_{1,2}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) &= -\frac{\log(2)^3}{18} - \frac{\log(2)\zeta_2}{3} + \frac{13\zeta_3}{18} + \frac{1}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{1,2}\left(\frac{1}{2}, 1; \infty\right) &= \frac{5\zeta_3}{8}, \\
S_{-1,-1,-1}(\infty) &= -\frac{\log(2)^3}{6} - \frac{\log(2)\zeta_2}{2} - \frac{\zeta_3}{4}, \\
S_{1,1,1}\left(-1, -1, \frac{1}{2}; \infty\right) &= \frac{17\log(2)^3}{18} + \frac{13\log(2)\zeta_2}{6} - \frac{61\zeta_3}{36} - 4\log(2)S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) \\
&\quad - \frac{8}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{-1,-1,1}(\infty) &= -\frac{\log(2)^3}{6} - \frac{\log(2)\zeta_2}{2} + \frac{7\zeta_3}{4}, \\
S_{1,1,1}\left(-1, \frac{1}{2}, -1; \infty\right) &= -\frac{1}{3}(2\log(2)^3) - 3\log(2)\zeta_2 + \frac{85\zeta_3}{24} + 4\log(2)S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) \\
&\quad + 4S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{-1,1,-1}(\infty) &= -\frac{\log(2)^3}{6} + \frac{\log(2)\zeta_2}{2} + \frac{\zeta_3}{8}, \\
S_{1,1,1}\left(-1, 1, \frac{1}{2}; \infty\right) &= \frac{5\log(2)^3}{18} - \frac{5\log(2)\zeta_2}{6} + \frac{61\zeta_3}{72} + \frac{4}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{-1,1,1}(\infty) &= -\frac{\log(2)^3}{6} + \frac{\log(2)\zeta_2}{2} - \frac{7\zeta_3}{8}, \\
S_{1,1,1}\left(\frac{1}{2}, -1, -1; \infty\right) &= \frac{7\log(2)^3}{18} + \frac{4\log(2)\zeta_2}{3} - \frac{35\zeta_3}{36} - \log(2)S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) \\
&\quad - \frac{4}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{1,1,1}\left(\frac{1}{2}, -1, 1; \infty\right) &= \frac{2\log(2)^3}{9} + \frac{\log(2)\zeta_2}{3} - \frac{155\zeta_3}{144} - \frac{1}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right) \\
&\quad - \frac{1}{2}S_{1,1,1}\left(-1, \frac{1}{2}, 1; \infty\right), \\
S_{1,1,1}\left(\frac{1}{2}, \frac{1}{2}, 1; \infty\right) &= \frac{\log(2)^3}{18} - \frac{7\log(2)\zeta_2}{6} + \frac{217\zeta_3}{144} + \log(2)S_{1,1}\left(\frac{1}{2}, \frac{1}{2}; \infty\right) \\
&\quad + \frac{2}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right) + \frac{1}{2}S_{1,1,1}\left(-1, \frac{1}{2}, 1; \infty\right), \\
S_{1,1,1}\left(\frac{1}{2}, 1, -1; \infty\right) &= -\frac{1}{9}(2\log(2)^3) - \frac{5\log(2)\zeta_2}{6} + \frac{11\zeta_3}{36} + \frac{1}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{1,1,1}\left(\frac{1}{2}, 1, \frac{1}{2}; \infty\right) &= -\frac{\log(2)^3}{18} + \frac{\log(2)\zeta_2}{6} + \frac{11\zeta_3}{36} + \frac{1}{3}S_{1,2}\left(-1, \frac{1}{2}; \infty\right), \\
S_{1,1,1}\left(\frac{1}{2}, 1, 1; \infty\right) &= \frac{3\zeta_3}{4}.
\end{aligned}$$

D. Alphabet $\{1, -1, \frac{1}{2}, -\frac{1}{2}\}$ **w = 1:** Basis constant: $S_{-1}(\infty) = -\log(2)$, $S_1(-\frac{1}{2}; \infty)$ **w = 2:** Basis constants: $S_2(\infty) = \zeta_2$, $S_{1,1}(-\frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1}(\frac{1}{2}, -\frac{1}{2}; \infty)$, $S_{1,1}(\frac{1}{2}, \frac{1}{2}; \infty)$ **w = 3:** Basis constants:

$$\begin{aligned}
& S_3(\infty) = \zeta_3, S_3\left(-\frac{1}{2}; \infty\right), S_{1,2}\left(-\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,2}\left(-\frac{1}{2}, \frac{1}{2}; \infty\right), \\
& S_{1,2}\left(\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{2,1}\left(-\frac{1}{2}, \frac{1}{2}; \infty\right), S_{1,1,1}\left(-1, -\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-1, -\frac{1}{2}, \frac{1}{2}; \infty\right), \\
& S_{1,1,1}\left(-1, \frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, -1, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}; \infty\right), \\
& S_{1,1,1}\left(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, \frac{1}{2}, 1; \infty\right), \\
& S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}; \infty\right), S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, 1; \infty\right).
\end{aligned}$$

E. Alphabet $\{1, -1, \frac{1}{2}, -\frac{1}{2}, 2, -2\}$ **w = 1:** Basis constant: $S_{-1}(\infty) = -\log(2)$, $S_1(-\frac{1}{2}; \infty)$ **w = 2:** Basis constants: $S_2(\infty) = \zeta_2$, $S_{1,1}(\frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1}(-\frac{1}{2}, \frac{1}{2}; \infty)$, $S_{1,1}(\frac{1}{2}, -\frac{1}{2}; \infty)$ **w = 3:** Basis constants:

$$\begin{aligned}
& S_3(\infty) = \zeta_3, S_3\left(-\frac{1}{2}; \infty\right), S_{1,2}\left(-\frac{1}{2}, -2; \infty\right), S_{1,2}\left(-\frac{1}{2}, \frac{1}{2}; \infty\right), \\
& S_{1,2}\left(\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{2,1}\left(-\frac{1}{2}, \frac{1}{2}; \infty\right), S_{1,1,1}\left(-1, -\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-1, -\frac{1}{2}, \frac{1}{2}; \infty\right), \\
& S_{1,1,1}\left(-1, \frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, -1, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}; \infty\right), \\
& S_{1,1,1}\left(-\frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \infty\right), S_{1,1,1}\left(-\frac{1}{2}, \frac{1}{2}, 1; \infty\right), \\
& S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, -\frac{1}{2}; \infty\right), S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, \frac{1}{2}; \infty\right), S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, 1; \infty\right).
\end{aligned}$$

XI. ASYMPTOTIC EXPANSION OF S-SUMS

In this section we seek expansions of S -sums generalizing ideas for harmonic sums given in Ref. 26 [for further computer algebra aspects concerning the calculation of expansions we refer, e.g., to Refs. 61, 70, 108, and 134 and references therein]. We say that a function $f : \mathbb{R} \rightarrow \mathbb{R}$ is expanded in an asymptotic series¹³²

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

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 that for a function $g(x)$ we use the notion $g(x) \in o(G(x)) \Leftrightarrow \lim_{x \rightarrow \infty} \left| \frac{g(x)}{G(x)} \right| = 0$. When only the first coefficients of such an expansion are given (calculated), we often write $f(x) \sim a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n$ and cut off the remainder term.

We remark that Secs. XI A–XID provide algorithms to expand S -sums which come close to the class of \bar{S} -sums (for a definition see (7.6)). For the general class of S -sums the expansion problem is not handled completely. However, for current calculations in QCD (see, e.g., Sec. XII) the presented methods are completely sufficient.

A. Asymptotic expansions of harmonic sums $S_1(c; n)$ with $c \geq 1$

Version 1: The asymptotic representation of the harmonic numbers $S_1(n)$ is given by⁹⁴

$$S_1(n) \sim \gamma + \log(n) + \frac{1}{2n} - \sum_{k=1}^{\infty} \frac{B_{2k}}{2k n^{2k}}, \quad (11.1)$$

where γ is the Euler-Mascheroni constant and B_n are the Bernoulli numbers,^{17,107,97}

$$B_n = \sum_{k=0}^n \binom{n}{k} B_k, \quad B_0 = 1.$$

To compute the asymptotic expansion of $S_1(c; n)$ with $c > 1$ one may represent it using the Euler-Maclaurin formula:^{54,86}

$$S_1(c; n) = \bar{S}_1(c; n) + S_1(n),$$

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,^{55,95}

$$\int_0^x \frac{c^t - 1}{t} dt = \text{Ei}(x \log(c)) - \gamma - \log(x) - \log(\log(c))$$

and $R_k(c, n)$ stand for the rest term. The derivatives are given in closed form by

$$\begin{aligned} \frac{d^j}{di^j} \left(\frac{c^i - 1}{i} \right) &= \frac{c^i}{i} \sum_{k=0}^j \frac{\log^{j-k}(c)}{i^k} (-1)^k \frac{\Gamma(j+1)}{\Gamma(j+1-k)} - (-1)^j \frac{\Gamma(j+1)}{i^{j+1}} \\ \lim_{i \rightarrow 0} \frac{d^j}{di^j} \left(\frac{c^i - 1}{i} \right) &= \frac{\log^{j+1}(c)}{j+1}. \end{aligned}$$

The asymptotic representation for $S_1(c; n)$ with $c > 1$ can now be derived using

$$\text{Ei}(t) \sim \exp(t) \sum_{k=1}^{\infty} \frac{\Gamma(k)}{t^k}.$$

Version 2: A more suitable approach to compute the expansion of $S_1(c; n)$ with $c > 1$, and which is implemented in the `HarmonicSums` package, is as follows. Differentiating the integral

representation

$$\frac{S_1(c; n)}{c^n} = \sum_{i=1}^n \frac{\frac{1}{c^{n-i}}}{i} = \int_0^1 \frac{x^n - \frac{1}{c^n}}{x - \frac{1}{c}} dx$$

with respect to n we get

$$\begin{aligned} \frac{\partial}{\partial n} \frac{S_1(c; n)}{c^n} &= \int_0^1 \frac{x^n H_0(x) + \frac{1}{c^n} H_0(c)}{x - \frac{1}{c}} dx \\ &= \int_0^1 \frac{x^n (H_0(x) + H_0(c))}{x - \frac{1}{c}} dx - H_0(c) \int_0^1 \frac{x^n - \frac{1}{c^n}}{x - \frac{1}{c}} dx. \end{aligned}$$

Hence

$$\int_0^1 \frac{x^n (H_0(x) + H_0(c))}{x - \frac{1}{c}} dx = \frac{\partial}{\partial n} \frac{S_1(c; n)}{c^n} + H_0(c) \frac{S_1(c; n)}{c^n}. \quad (11.2)$$

We can now compute the asymptotic expansion of the integral using integration by parts. Let

$$\int_0^1 \frac{x^n (H_0(x) + H_0(c))}{x - \frac{1}{c}} dx \sim \sum_{i=0}^{\infty} \frac{a_i}{n^i}$$

with $a_i \in \mathbb{R}$ be this expansion and let $\sum_{i=0}^{\infty} \frac{b_i}{n^i}$ with $b_i \in \mathbb{R}$ be the asymptotic expansion of $\frac{S_1(c; n)}{c^n}$. We note that the differentiation of this expansion yields $\sum_{i=2}^{\infty} \frac{-(i-1)b_{i-1}}{n^i}$, i.e.,

$$\frac{\partial}{\partial n} \frac{S_1(c; n)}{c^n} \sim \sum_{i=2}^{\infty} \frac{-(i-1)b_{i-1}}{n^i}.$$

Plugging these expansions into Eq. (11.2) and comparing coefficients yields the recurrence relation

$$b_n = \frac{a_n}{H_0(c)} + \frac{(n-1)}{H_0(c)} b_{n-1} \text{ for } n \geq 2$$

with the initial values $b_0 = \frac{a_0}{H_0(c)}$ and $b_1 = \frac{a_1}{H_0(c)}$. Hence we get, for example,

$$\begin{aligned} S_1(2; n) &\sim 2^n \left(\frac{14174522}{n^{10}} + \frac{1091670}{n^9} + \frac{94586}{n^8} + \frac{9366}{n^7} + \frac{1082}{n^6} + \frac{150}{n^5} + \frac{26}{n^4} + \frac{6}{n^3} + \frac{2}{n^2} + \frac{2}{n} \right), \\ S_1(3; n) &\sim 3^n \left(\frac{566733}{4n^{10}} + \frac{17295}{n^9} + \frac{38001}{16n^8} + \frac{1491}{4n^7} + \frac{273}{4n^6} + \frac{15}{n^5} + \frac{33}{8n^4} + \frac{3}{2n^3} + \frac{3}{4n^2} + \frac{3}{2n} \right). \end{aligned}$$

B. Computation of asymptotic expansions by repeated partial integration

Next, we deal with generalized polylogarithms of the form

$$\mathbf{M} \left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c \pm x}, n \right) \text{ and } \mathbf{M} \left(\frac{H_{b_1, b_2, \dots, b_k}(1-x)}{c \pm x}, n \right) \quad (11.3)$$

with $|c| \geq 1$ where $m_i \in \mathbb{R} \setminus (0, 1]$ or $b_i \in \mathbb{R} \setminus (-1, 0) \cup (0, 1)$ with $b_i \neq 0$ using repeated integration by parts. The first two lemmas show that the arguments of the Mellin transform under consideration are analytic. Thus iterated integration by parts is possible for $c > 1$ using the already known integral

representation. The third lemma gives an integral representation for the special case $c = 1$ such that the method of repeated partial integration is also possible. The proofs are omitted here.

Lemma 11.1. Let $H_{m_1, m_2, \dots, m_k}(x)$ be a generalized polylogarithm with $m_i \in \mathbb{R} \setminus (0, 1]$ for $1 \leq i \leq k$. Then

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

are analytic for $|c| \geq 1$ and $x \in (0, 1]$.

Lemma 11.2. Let $H_{m_1, m_2, \dots, m_k}(x)$ be a generalized 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

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

are analytic for $|c| \geq 1$ and $x \in (0, 1]$.

For $c > 1$, we obtain a suitable integral representation for partial integration. For example, we get

$$\begin{aligned} M\left(\frac{H_{-2}(x)}{x+2}, n\right) &= \int_0^1 x^n \frac{H_{-2}(x)}{x+2} dx = \int_0^1 x^{n-1} \frac{x \cdot H_{-2}(x)}{x+2} dx \\ &= \frac{x^n}{n} \frac{x \cdot H_{-2}(x)}{x+2} \Big|_0^1 - \int_0^1 \frac{x^n}{n} \frac{2H_{-2}(x) + x}{(x+2)^2} dx \\ &= H_{-2}(1) \frac{3}{n} - \frac{1}{n} \int_0^1 x^{n-1} \frac{x(2H_{-2}(x) + x)}{(x+2)^2} dx \\ &= H_{-2}(1) \frac{3}{n} - \frac{1}{n} \left(\frac{x^n}{n} \frac{x(2H_{-2}(x) + x)}{(x+2)^2} \Big|_0^1 - \int_0^1 \frac{x^n}{n} \frac{6x - 2(x-2)H_{-2}(x)}{(x+2)^3} dx \right) \\ &= H_{-2}(1) \left(\frac{3}{n} - \frac{2}{9n^2} \right) - \frac{1}{9n^2} + \frac{1}{n^2} \int_0^1 x^{n-1} \frac{x(6x - 2(x-2)H_{-2}(x))}{(x+2)^3} dx \\ &= \dots = H_{-2}(1) \left(\frac{3}{n} - \frac{2}{9n^2} + \frac{2}{27n^3} + \frac{2}{27n^4} \right) - \frac{1}{9n^2} + \frac{2}{9n^3} - \frac{20}{81n^4} + O\left(\frac{1}{n^5}\right). \end{aligned}$$

For the special case $c = 1$ one can use the integral representation of the following lemma to calculate the expansion with partial integration as demonstrated above.

Lemma 11.3. 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 generalized 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

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

are finite constants.

Summarizing, we are able to calculate the asymptotic expansion of (11.3) using the method of repeated integration by parts.

C. Computation of asymptotic expansions of S-sums

Subsequently, we derive an algorithm that calculates the asymptotic expansion of S-sums $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ with $b_i \in [-1, 1]$ and $b_i \neq 0$ using the technologies of Subsections XI A and XI B.

Since these sums fall into the class of \bar{S} -sums, it follows by Sec. VII B that they can be represented using Mellin transforms of the form $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c \pm sx}, n\right)$ with $m_i \in \mathbb{R} \setminus ((-1, 0) \cup (0, 1))$ and $|c| \geq 1$. Conversely, given such a Mellin transform, it can be expressed in terms of S-sums of the above type with $b_i \in [-1, 1]$ and $b_i \neq 0$.

In addition, it is straightforward to see that this subclass is closed under the quasi shuffle product (2.2), i.e., the product can be expressed again as a linear combination of S-sums of this subclass over the rational numbers.

We are now ready to present 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 $b_i \neq 0$. The algorithm tries to attack the sums directly using Secs. XI A and XI B. If it fails one uses the transformation $x \rightarrow 1 - x$ from Sec. III B twice and reduces the problems to S-sums that are less complicated than the input sum. Recursive application will finally produce the expansion of the original S-sum. To be more precise, the algorithm can be described 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. Expand the powers of $S_1(n)$ using (11.1). Now apply the following items to each of the S-sums without trailing ones:
- Let $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ with $a_k \neq 1 \neq b_k$, and compute $\frac{H_{m_1, m_2, \dots, m_k}(x)}{c + sx}$ such that in the inverse Mellin transform the most complicated S-sum is $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$, i.e., express $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ as

$$S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n) = M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c + sx}, n\right) + T, \tag{11.4}$$

where T is an expression in 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 $b'_i \neq 0$ (which are less complicated than $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$) and constants. Note that $s = \pm 1$, $c \geq 1$ and $m_i \in \mathbb{R} \setminus ((-1, 0) \cup (0, 1))$ and that $m_i \neq 1$ (see the beginning of this subsection and Lemma 7.5).

- We proceed by expanding $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c + sx}, n\right)$ in (11.4):

all $m_i \neq 1$: Expand $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c + sx}, n\right)$ directly; see Section XI B.

not all $m_i \neq 1$:

- Transform $x \rightarrow 1 - x$ in $H_m(x)$ as described in Sec. III B and expand all products, i.e., we obtain

$$M\left(\frac{H_m(x)}{c + sx}, n\right) = \sum_{i=1}^p d_i M\left(\frac{H_{b_i}(1-x)}{c + sx}, n\right) + d \text{ with } d, d_i \in \mathbb{R}. \tag{11.5}$$

Note that due to Remark 3.5 the components of the b_i are in $\mathbb{R} \setminus (0, 1)$.

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

$b_j \neq 0$: Expand $\int_0^1 \frac{x^n H_b(1-x)}{c + sx}$; see Sec. XI B.

$b_j = 0$: As described in Sec. III B transform back $1 - x \rightarrow x$ in $H_b(1 - x)$ and expand all products, i.e., we obtain

$$M\left(\frac{H_b(1-x)}{c+sx}, n\right) = \sum_{i=1}^p e_i M\left(\frac{H_{g_i}(x)}{c+sx}, n\right) + e \quad (11.6)$$

with $e, e_i \in \mathbb{R}$. Finally, perform the Mellin transforms $M\left(\frac{H_{g_i}(x)}{c+sx}, n\right)$, i.e., express it in terms of S -sums and constants in terms of infinite S -sums. Note that these harmonic sums are less complicated (see below).

- Replace $M\left(\frac{H_{m_1, m_2, \dots, m_l}(x)}{c+sx}, n\right)$ in (11.4) by the result of this process.
- For all harmonic sums that remain in (11.4) apply the above points. Since these harmonic sums are less complicated (see below) this process will terminate.

Concerning termination the following remarks are in place. Since $a_k \neq 1$ in (11.4), we know due to Lemma 7.5 that $m_l \neq 1$ in (11.4). If not all $m_i \neq 1$ in (11.4), we have to transform $x \rightarrow 1 - x$ in $H_{m_1, m_2, \dots, m_l}(x)$ as described in Sec. III B. Due to Remark 3.5 we see that the single generalized polylogarithm at argument x with weight l , which will emerge, will not have trailing zeroes since $m_l \neq 1$. Hence we can compute the asymptotic expansion of the Mellin transform containing this generalized polylogarithm using repeated integration by parts. We might be able to compute the asymptotic expansion of some (or all) of the other Mellin transforms by repeated integration by parts as well, but if we fail we know at least that due to Remark 7.5 the S -sums which are appearing in (11.6) are less complicated (they are even of lower weight) than $S_{a_1, a_2, \dots, a_k}(b_1, b_2, \dots, b_k; n)$ of (11.4) and hence this algorithm will eventually terminate.

Applying the described algorithm to $S_{2,1}\left(\frac{1}{3}, \frac{1}{2}; n\right)$ produces the following asymptotic expansion:

$$\begin{aligned} S_{2,1}\left(\frac{1}{3}, \frac{1}{2}; n\right) &\sim -S_{1,2}\left(\frac{1}{6}, 3; \infty\right) + S_1\left(\frac{1}{2}; \infty\right) \left[-S_2\left(\frac{1}{6}; \infty\right) + S_2\left(\frac{1}{3}; \infty\right) + \frac{1}{6^n} \left(-\frac{1464}{625n^5} \right. \right. \\ &\quad \left. \left. + \frac{126}{125n^4} - \frac{12}{25n^3} + \frac{1}{5n^2} + 33\frac{2^{n-1}}{n^5} - 9\frac{2^{n-1}}{n^4} + 3\frac{2^{n-1}}{n^3} - \frac{2^{n-1}}{n^2} \right) \right] \\ &\quad + \frac{1}{6^n} \left(-\frac{4074}{3125n^5} + \frac{366}{625n^4} - \frac{42}{125n^3} + \frac{6}{25n^2} - \frac{1}{5n} \right) S_2\left(\frac{1}{2}; \infty\right) \\ &\quad + S_1\left(\frac{1}{6}; \infty\right) S_2\left(\frac{1}{2}; \infty\right) + S_3\left(\frac{1}{2}; \infty\right) + \frac{1}{6^n} \left(\frac{642}{125n^5} - \frac{28}{25n^4} + \frac{1}{5n^3} \right) \\ &\quad + \frac{1}{6^n} \left(\frac{2037}{3125n^5} - \frac{183}{625n^4} + \frac{21}{125n^3} - \frac{3}{25n^2} + \frac{1}{10n} \right) \zeta_2 + \frac{1}{6^n} \left(-\frac{2037}{3125n^5} \right. \\ &\quad \left. + \frac{183}{625n^4} - \frac{21}{125n^3} + \frac{3}{25n^2} - \frac{1}{10n} \right) \log^2(2) + \frac{1}{6^n} \left(\frac{1464}{625n^5} - \frac{126}{125n^4} + \frac{12}{25n^3} \right. \\ &\quad \left. - \frac{1}{5n^2} \right) \log(2), \end{aligned}$$

with $S_m\left(\frac{1}{k}, \infty\right) = \text{Li}_m\left(\frac{1}{k}\right)$, $m, k \in \mathbb{N}_+$, $m \geq 2$.

D. Further extensions

The following lemma extends 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 $|b_i| \leq 1$ and if $b_i = 1$ then $a_i > 1$ for $2 \leq i \leq k$. In this case, we obtain the

required form given in (11.4) except that $0 < c < 1$ and that the occurring \bar{S} -sums in T satisfy again the constraints from above. Then the following lemma yields a suitable integral representation of $M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c+x}, n\right)$ and repeated integration by parts produces its asymptotic expansion. In addition, the occurring \bar{S} -sums in T can be handled by recursion of the extended method.

Lemma 11.4. Let $H_{m_1, m_2, \dots, m_k}(x)$ be a generalized 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

$$\begin{aligned} M\left(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c-x}, n\right) &= \int_0^1 \frac{(\frac{x}{c})^n - 1}{c-x} H_{m_1, m_2, \dots, m_k}(x) dx = \\ &= \int_0^1 \frac{(\frac{x}{c})^n (H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c))}{c-x} dx \\ &\quad + \int_0^1 \frac{(\frac{x}{c})^n H_{m_1, m_2, \dots, m_k}(c) - H_{m_1, m_2, \dots, m_k}(x)}{c-x} dx \\ &= \int_0^1 \frac{(\frac{x}{c})^n (H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c))}{c-x} dx \\ &\quad + \underbrace{H_{m_1, m_2, \dots, m_k}(c) \int_0^1 \frac{(\frac{x}{c})^n - 1}{c-x} dx}_{A:=} \\ &\quad - \underbrace{\int_0^1 \frac{H_{m_1, m_2, \dots, m_k}(x) - H_{m_1, m_2, \dots, m_k}(c)}{c-x} dx}_{B:=}. \end{aligned}$$

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

$$\begin{aligned}
 B_1 &= -H_{m_1, c, m_2, \dots, m_k}(c) - \dots - H_{m_1, m_2, \dots, m_k, c}(c) \\
 B_2 &= \int_0^{1-c} \frac{H_{m_1, m_2, \dots, m_k}(x+c) - H_{m_1, m_2, \dots, m_k}(c)}{-x} dx \\
 &= - \int_0^{1-c} \frac{H_{m_2, \dots, m_k}(c) H_{m_1-c}(x) + \dots + H_{m_1-c, \dots, m_k-c}(x)}{x} dx \\
 &= -H_{m_2, \dots, m_k}(c) H_{0, m_1-c}(1-c) - H_{m_3, \dots, m_k}(c) H_{0, m_1-c, m_2-c}(1-c) \\
 &\quad - \dots - H_{m_k}(c) H_{0, m_1-c, \dots, m_{k-1}-c}(1-c) - H_{0, m_1-c, \dots, m_k-c}(1-c);
 \end{aligned}$$

thus the lemma follows. \square

A typical example for this extension is, e.g.,

$$\begin{aligned}
 S_{1,1}(3, \frac{1}{3}; n) &\sim \frac{1331}{240n^5} - \frac{63}{32n^4} + \frac{23}{24n^3} - \frac{5}{8n^2} + \frac{1}{2n} + S_1(\frac{1}{3}; \infty) S_1(3; n) \\
 &\quad - \frac{1}{2} S_1(\frac{1}{3}; \infty)^2 - S_2(\frac{1}{3}; \infty),
 \end{aligned}$$

with $S_1(\frac{1}{m}, \infty) = \ln(m) - \ln(m-1)$, $m \in \mathbb{N} \setminus \{1\}$.

More generally, this lemma enables one to deal also with S -sums which are outside of the \bar{S} -sum case. To be more precise, our strategy works if the given S -sum $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ can be written in the form (11.4) where $M(\frac{H_{m_1, m_2, \dots, m_k}(x)}{c+sx}, n)$ can be expanded directly by Lemma 11.4. In addition, we need that T consists of S -sums which are less complicated than $S_{a_1, \dots, a_k}(b_1, \dots, b_k; n)$ and which can be handled by iterative application of our expansion strategy (and using Lemma 11.4 if needed).

For example, our expansion technique produces

$$\begin{aligned}
 S_{1,1,1}(-\frac{1}{2}, 2, \frac{1}{4}; n) &\sim S_{1,1,1}(-\frac{1}{2}, 2, \frac{1}{4}; \infty) + (-\frac{1}{27n^3} + \frac{1}{9n^2} - \frac{1}{6n}) (-\frac{1}{2})^n S_2(\frac{1}{4}; \infty) \\
 &+ \left(-\frac{1}{2}\right)^n \left[\left(\frac{2}{27n^3} - \frac{2}{9n^2} + \frac{1}{3n}\right) \log^2(2) + \left(-\frac{2}{27n^3} + \frac{2}{9n^2} - \frac{1}{3n}\right) \log(3) \right] S_1(2; n) \\
 &+ \frac{(-\frac{1}{4})^n}{15n^3} + \left(-\frac{2}{27n^3} + \frac{2}{9n^2} - \frac{1}{3n}\right) \left(-\frac{1}{2}\right)^n \log^3(2) \\
 &+ \left[(-1)^n \left(\frac{1}{3n^2} - \frac{2}{9n^3}\right) + \left(-\frac{1}{2}\right)^n \left(\frac{1}{27n^3} - \frac{1}{9n^2}\right) + \frac{(-1)^n (\frac{1}{2})^n}{6n} \right] \log^2(2) \\
 &+ \left(\frac{2}{27n^3} - \frac{2}{9n^2} + \frac{1}{3n}\right) \left(-\frac{1}{2}\right)^n \log(2) \log(3) + (-1)^n \left(\frac{2}{9n^3} - \frac{1}{3n^2}\right) \log(3).
 \end{aligned}$$

XII. APPLICATION FROM QUANTUM CHROMODYNAMICS

In the following we concentrate on the discussion of the emergence of generalized harmonic sums in calculations of massless and massive Wilson coefficients in deep-inelastic scattering in QCD. Up to the 2-loop level neither for the anomalous dimensions nor for the Wilson coefficients generalized harmonic sums occur, cf. Refs. 89, 22, 24, and 25. They are also absent in case of the 3-loop anomalous dimensions.^{91,126} In intermediate results of the calculation of the massless 3-loop Wilson coefficients they emerge, e.g., for a graph called LA₂₇box(N) in Ref. 125. The generalized sums (2.1) have numerator-weights over the alphabet $x_i \in \{1, -1, 2, -2\}$ up to weight $w = 6$. Examples are:

$$S_1(2; n), S_{1,1,1,1,2}(2, 1, 1, 1, 1; n), S_{2,1,3}(2, 1, -1; n), S_{3,2,1}(-2, -1, 1; n), \text{ etc.}$$

All of these sums contain besides the numerator weights $i_k \in \{-1, 1\}$ only either the weight 2 or -2 once. For these cases one always may represent the corresponding sums such that

$$S_{n_1, \dots, n_m}(\pm 2, i_1, \dots, i_{m-1}; n) = \int_0^1 dx \frac{(\pm 2x)^n - 1}{\pm 2x - 1} \sum_j c_j H_{\bar{a}_j}(x), \quad (12.1)$$

where $H_{\bar{a}_j}(x)$ are usual harmonic polylogarithms. Since the corresponding expressions are weighted by a factor 2^{-n} , the individual expressions are transformed by the non-singular kernels $((\pm 1)^n x^n - 1/2^n)/(\pm 2x - 1)$. It even turns out that all generalized sums cancel in the final result.¹²⁵ In this way, the massless Wilson coefficients up to 3-loop order do not depend on generalized harmonic sums.

In Ref. 3 the $O(n_f T_F^2 C_{A,F})$ contributions to the 3-loop massive Wilson coefficient contributing to the structure function $F_2(x, Q^2)$ at high virtualities $Q^2 \gg m^2$ were calculated. Here m denotes the heavy quark mass. In this calculation most of the generated nested sums were calculated directly using the package `Sigma`.^{110,112,111,113,115} In this way individual Feynman diagrams were split into many terms being summed individually. Here the contributing alphabet of numerator weights was $x_i \in \{1, -1, \frac{1}{2}, -\frac{1}{2}, 2, -2\}$. Examples of generalized sums are:

$$S_1\left(\frac{1}{2}; n\right), S_2(-2; n), S_{2,1}(-1, 2; n), S_{3,1}\left(-2, -\frac{1}{2}; n\right), S_{1,1,1,2}\left(-1, \frac{1}{2}, 2, -1; n\right), S_{2,3}\left(-2, -\frac{1}{2}; n\right), \\ S_{2,2,1}\left(-1, -\frac{1}{2}, 2; n\right), S_{1,1,1,1,1}\left(2, \frac{1}{2}, 1, 1, 1; n\right), \text{ etc.}$$

The highest contributing weight was $w = 5$. In the final result all generalized harmonic sums canceled for the $O(n_f T_F^2 C_{A,F})$ -terms, even on a diagram-by-diagram basis.

This brought up the idea to combine all sums contributing to each diagram leading to Schneider's package `SumProduction`.¹¹⁹ Through this a much smaller amount of nested sums, however, with very large summands, have to be calculated.^{30,31} We have applied this method for the gluonic $O(n_f T_F^2 C_{A,F})$ contributions in Ref. 8.

In case of the massive 3-loop operator matrix elements generalized harmonic sums do not vanish always. For a series of ladder diagrams with six massive propagators they contribute for scalar integrals up to weight $w = 4$.⁷ This is likewise also the case for a series of Benz-type diagrams.⁹ Examples are:

$$S_1(2; n), S_{1,2}\left(\frac{1}{2}, 1; n\right), S_{1,1,1}\left(\frac{1}{2}, 1, 1; n\right), S_{1,1,2}\left(\frac{1}{2}, 1, 1; n\right), S_{1,1,2}\left(2, \frac{1}{2}, 1; n\right), \\ S_{1,1,1,1}\left(2, \frac{1}{2}, 1, 1; n\right), \text{ etc.}$$

Representing results for individual Feynman diagrams containing also S -sums sometimes involves divergent S -sum expressions in individual terms as $n \rightarrow \infty$. On the other hand, combinations of different terms contributing to the corresponding diagram are always convergent, as also the whole diagram, see Refs. 7, 10, and 11. We, therefore, limit the consideration to convergent combinations of terms containing S -sums here. Let us consider an example of Ref. 7. Integral $\hat{I}_4(n)$, Eq. (3.18), contains the following terms growing like 2^n for $n \rightarrow \infty$:

$$T_1(n) = 2^n \frac{n^3 - 4n^2 - 25n - 28}{(n+1)^2(n+2)(n+3)^2} \left[2S_{1,2}\left(\frac{1}{2}, 1, n\right) + S_{1,2}\left(\frac{1}{2}, 1, 1; n\right) - 2\zeta_3 \right], \\ T_2(n) = -\frac{1}{2} \frac{n+5}{(n+1)(n+3)} \left[S_{1,1,1,1}\left(2, \frac{1}{2}, 1, 1; n\right) + 2S_{1,1,2}\left(2, \frac{1}{2}, 1; n\right) - 2\zeta_3 S_1(2; n) \right].$$

One may represent these sums in terms of Mellin transforms, cf. Eq. (3.36)–(3.40).⁷ There it turns out that each of the S -sums contributing to $T_1(n)$ can be expressed in the form

$$r_{1,i} \zeta_3 + \frac{1}{2^n} F_{1,i}(n),$$

where $r_{1,i} \in \mathbb{Q}$ and $F_{1,i}(n)$ are convergent integrals for $n \rightarrow \infty$. Replacing the S -sums with these alternative representations in $T_1(n)$ shows that the ζ_3 part vanishes. In addition, rewriting the introduced integral representations back to S -sums produces finite S -sums. Similarly, each of the S -sums in $T_2(n)$ may be expressed in the form

$$r_{2,i} \zeta_3 S_1(2; n) + F_{2,i}(n),$$

where $r_{2,i} \in \mathbb{Q}$ and $F_{2,i}(n)$ are convergent integrals. Again, replacing the S -sums with these representations in T_2 cancels the $S_1(2; n)\zeta_3$ part; in addition, the introduced integrals can be transformed to an expression in terms of absolutely convergent S -sums. The remainder terms of $\hat{I}_4(n)$ are even nested harmonic sums. Due to this only absolutely convergent S -sum contribute to $\hat{I}_4(n)$ via $T_1(n)$ and $T_1(n)$. A decomposition of this or a similar kind is expected in case of physical expressions in general. As the above example shows a suitable decomposition of the contributing S -sums may be necessary.

In Refs. 10 and 11 we also considered graphs with an internal 4-leg local operator insertion and five massive lines. Here generalized harmonic sums of up to weight $w = 5$ occur. Examples are:

$$S_{1,4}\left(\frac{1}{2}, -2; n\right), S_{1,2,2}\left(\frac{1}{2}, -2, -1; n\right), S_{1,2,2}\left(\frac{1}{2}, -2, 1; n\right), S_{1,2,2}\left(\frac{1}{2}, -2, -1; n\right), \text{ etc.}$$

For this diagram also generalized harmonic sums nested with binomial-and inverse-binomial expressions contribute.

Generalized harmonic sums are a necessary asset both in higher loop and multi-leg Feynman diagram calculations. They are connected to the generalized harmonic polylogarithms via a Mellin transform. We have worked out their various relations and considered special new numbers associated to these quantities in the limit $n \rightarrow \infty$ of the generalized harmonic sums and special arguments of the generalized harmonic polylogarithms, generalizing the multiple zeta values. The relations discussed generate basis representations in the respective algebras. Note also that special classes of higher transcendental functions are contained in the generalized harmonic sums for $n \rightarrow \infty$, such as the generalized hypergeometric functions ${}_P+1F_P$ ^{78,16,120,53,57,58} the Appell-functions $F_{1,2}$, the Kampé De Fériet functions,^{14–16,120,53,57,58,90} and others.

In cases that generalized harmonic sums occur in physical results an efficient way of implementation consists in working in Mellin space, as being the case for the nested harmonic sums (see also the comments in the last paragraph of Sec. VII). Having determined the singularity structure of the problem, and knowing the shift relations $n \rightarrow n + 1$ of the corresponding quantities in analytic form, the knowledge of the asymptotic expansion at $|n| \gg 1$, $n \in \mathbb{C}$ is sufficient for the analytic continuation of anomalous dimensions and Wilson coefficients, similar to the case of the nested harmonic sums. The asymptotic representation is requested to be free of exponential divergences. Logarithmic terms $\sim \ln^k(n)$ with k related to the number of loops may contribute, however. The structure of the singularities may become more general, however, and has to be determined for the respective problem under investigation. A single numerical contour integral around the singularities yields the inverse Mellin-transform from n - to x -space, cf. Ref. 32. The techniques outlined above also allow to perform the inverse Mellin-transform analytically for applications in x -space directly. For this purpose the corresponding basis-functions still need to be represented numerically at sufficient precision, unlike the case in n -space.

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APPENDIX: AVAILABLE COMMANDS OF THE PACKAGE `HarmonicSums.m`

In the following we list some of the main commands of the code `HarmonicSums`, a package implemented in Mathematica, and illustrate their use by examples, with emphasis on the case of S -sums. The `HarmonicSums.m` package and the conditions of use are found under www.risc.jku.at/research/combinat/software/HarmonicSums/.

`S[a1, ..., am; n]`: defines the harmonic sum $S_{a_1, \dots, a_m}(n)$ of depth m with upper summation limit n and $a_i \in \mathbb{N}$, while `CS[{{a1, b1, c1}, ..., {am, bm, cm}}, {s1, ..., sm}, n]` defines cyclotomic harmonic sums $S_{(a_1, b_1, c_1), \dots, (a_m, b_m, c_m)}(s_1, \dots, s_m; n)$ with $a_i, c_i \in \mathbb{N}$, $b_i \in \mathbb{N} \cup \{0\}$ and $s_i \in \{-1, 1\}$; see (2.1) of Ref. 5.

$S[a_1, \dots, a_m, \{x_1, \dots, x_m\}, n]$: defines the S -sum $S_{a_1, \dots, a_m}(x_1, \dots, x_m; n)$ of depth m with upper summation limit n and¹⁴⁵ $a_i \in \mathbb{N}$, $x_i \in \mathbb{R}^*$.

$Z[a_1, \dots, a_m, \{x_1, \dots, x_m\}, n]$: defines the Z -sum $Z_{a_1, \dots, a_m}(x_1, \dots, x_m; n)$ of depth m with upper summation limit n and $a_i \in \mathbb{N}$, $x_i \in \mathbb{R}^*$; see (9.1).

$H[m_1, \dots, m_n, x]$: defines the harmonic polylogarithm $H_{m_1, \dots, m_n}(x)$ ($m_i \in \{-1, 0, 1\}$) or a generalized polylogarithm $H_{m_1, \dots, m_n}(x)$ ($m_i \in \mathbb{R}$), while $H[\{a_1, b_1\}, \dots, \{a_n, b_n\}, x]$ defines a cyclotomic harmonic polylogarithm⁵ with $a_i, b_i \in \mathbb{N}$.

$SToZ[S[a_1, \dots, a_m, \{x_1, \dots, x_m\}, n]]$: converts the S -sum $S_{a_1, \dots, a_m}(x_1, \dots, x_m; n)$ to Z -sums.

Example:

$$SToZ[S[1, 1, \{1/2, -1/4\}, n]] = Z_2\left(-\frac{1}{8}, n\right) + Z_{1,1}\left(\frac{1}{2}, -\frac{1}{4}, n\right).$$

$ZToS[Z[a_1, \dots, a_m, \{x_1, \dots, x_m\}, n]]$: converts the Z -sum $Z_{a_1, \dots, a_m}(x_1, \dots, x_m; n)$ to S -sums.

Example:

$$ZToS[Z[1, 1, \{1/2, -1/4\}, n]] = -S_2\left(-\frac{1}{8}, n\right) + S_{1,1}\left(\frac{1}{2}, -\frac{1}{4}, n\right).$$

$ReduceToBasis[expr]$: reduces occurring harmonic sums, S -sums or cyclotomic sums to basis sums which are (in the setting of their quasi-shuffle algebra) algebraic independent over each other. In general, tables (available at the `HarmonicSums` homepage) are exploited for this reduction. If sums are not covered by the given tables, one can set the option `Dynamic` \rightarrow `Automatic`; then for such sums (outside of the tables) the reduction is calculated online. Using the setting `Dynamic` \rightarrow `True` the reduction for all sums is calculated online.

Example:

$ReduceToBasis[S[1, 2, 2, n], n, \text{Dynamic} \rightarrow \text{True}] =$

$$S_2(n) (S_3(n) - S_{2,1}(n)) - S_{2,3}(n) - S_{4,1}(n) + S_{2,2,1}(n) + \frac{1}{2} S_1(n) (S_2(n)^2 + S_4(n)) + S_5(n).$$

$ReduceToHBasis[expr]$: reduces occurring harmonic polylogarithms, generalized polylogarithms, or cyclotomic polylogarithms to basis polylogarithms which are algebraic independent over each other by using given tables. If the option `Dynamic` \rightarrow `True` is set, the reduction is calculated online; this will help if certain polylogarithms are not stored in the table.

Example:

$ReduceToHBasis[H[1, 0, -1, 1, x]] =$

$$\begin{aligned} & H_{-1,1}(x) (H_0(x)H_1(x) - H_{0,1}(x)) + H_{-1,1}(x)H_{0,1}(x) - H_1(x) (H_{-1}(x)H_{0,1}(x) - H_{0,-1,1}(x) \\ & - H_{0,1,-1}(x)) - H_1(x) (H_0(x)H_{-1,1}(x) - H_{-1}(x)H_{0,1}(x) + H_{0,1,-1}(x)) - 2H_{0,-1,1,1}(x) \\ & - H_{0,1,-1,1}(x). \end{aligned}$$

$TransformToSSums[expr]$: returns an expression which transforms indefinite nested sums to harmonic sums, S -sums or cyclotomic sums whenever possible.

Example:

$$\begin{aligned} \text{expr} &= (n-1)^2 \sum_{i=4}^n \frac{(-1/3)^i}{(i-3)^2} + 4\zeta_3(n-2)^2(n-1)^2 \sum_{i=1}^n \frac{(-1)^i}{i-2} + n^2(n+1)^2 \sum_{i=2}^n \frac{(-1)^i}{i-1} \\ &+ \sum_{i=1}^n \frac{1}{2+i} \sum_{j=1}^i \frac{(-3)^j}{(1+3j)^2} - \frac{3}{2}(n-2)^2(1+n)^3\zeta_3 \sum_{i=4}^n \frac{1}{i-1} \sum_{j=4}^i \frac{(-1)^j}{(j-3)^2} + \sum_{i=1}^n \frac{(-1)^i}{i^2} S_1(i) \\ &+ \sum_{i=1}^n \frac{(-3)^i}{(3i+1)^2} S_1(i). \end{aligned}$$

TransformToSSums[expr] =

$$\begin{aligned} &\frac{1}{2} S_{(1,0,1),(3,1,2)}(1, -3; n) + S_{(3,1,2),(1,0,1)}(-3, 1; n) + 2(n-2)^2(n+1)^3 S_{-3}(\infty) \times \\ &\left[-S_{1,-2}(n) - \frac{(-1)^n}{n^3} - \frac{(-1)^n}{n^2} + S_{-3}(n) + \frac{S_{-2}(n)}{n} + S_{-2}(n) - 2S_{-1}(n) + \frac{(-1)^{n-1}}{n-1} + \frac{2(-1)^n}{n} \right. \\ &\left. - \frac{(-1)^{n-1}}{(n-1)^2} - 1 \right] + S_{-2,1}(n) + (n-2)^2 \left[-\frac{1}{27} S_2\left(-\frac{1}{3}; n\right) + \frac{(-1)^n 3^{-n-3}}{n^2} + \frac{(-1)^{n-2} 3^{-n-1}}{(n-2)^2} \right. \\ &\left. + \frac{(-1)^{n-1} 3^{-n-2}}{(n-1)^2} \right] + n^2(n+1)^3 \left(\frac{(-1)^n}{n^3} - S_{-3}(n) \right) + 4(n-2)^2(n-1)^2 \left[S_{-1}(n) - \frac{(-1)^{n-1}}{n-1} \right. \\ &\left. - \frac{(-1)^n}{n} \right] S_3(\infty). \end{aligned}$$

Here $S_{(a_1,b_1,c_1),\dots,(a_m,b_m,c_m)}(x_1, \dots, x_m; n)$ are generalized cyclotomic sums, cf. Ref. 5.

ReduceSums[expr]: returns an expression which transforms indefinite nested sums to harmonic sums, S-sums or cyclotomic sums whenever possible and reduces occurring harmonic sums, S-sum or cyclotomic sums to basis sums which are algebraic independent over each other by using given tables. If the option Dynamic \rightarrow True is set, the reduction is calculated online; this will help if certain sums are not stored in the table.

Example:

ReduceSums[expr] =

$$\begin{aligned} &\frac{1}{2} \left\{ S_{(1,0,1),(3,1,2)}(1, -3; n) + 2S_{(3,1,2),(1,0,1)}(-3, 1; n) - 3(n-2)^2(n+1)^3 S_3(\infty) \left[S_{-2,1}(n) \right. \right. \\ &\left. - \frac{(-1)^n}{n^3} - \frac{(-1)^n}{n^2} - 2S_{-1}(n) + S_{-2}(n) \left(-S_1(n) + \frac{1}{n} + 1 \right) - \frac{(-1)^n}{n-1} + \frac{2(-1)^n}{n} + \frac{(-1)^n}{(n-1)^2} \right. \right. \\ &\left. \left. - 1 \right] + \frac{3^{-n-3} \left(2(-1)^n (7n^4 - 12n^3 + 10n^2 - 12n + 4) - 2 \cdot 3^n n^2 (n^2 - 3n + 2)^2 S_2\left(-\frac{1}{3}; n\right) \right)}{(n-1)^2 n^2} \right. \\ &\left. + 2n^2(n+1)^3 \left(\frac{(-1)^n}{n^3} - S_{-3}(n) \right) + \frac{8(n-2)^2(n-1)((n-1)nS_{-1}(n) + (-1)^n) S_3(\infty)}{n} \right. \\ &\left. + 2S_{-2,1}(n) \right\}. \end{aligned}$$

LinearHExpand[expr]: expands all the products of harmonic polylogarithms, generalized polylogarithms and cyclotomic polylogarithms at same arguments.

Example:

$$\begin{aligned} & \text{LinearHExpand}[H[0, 1, x] * H[-1, 0, -1/2, x]] = \\ & H_{-1,0,-\frac{1}{2},0,1}(x) + 2H_{-1,0,0,-\frac{1}{2},1}(x) + 2H_{-1,0,0,1,-\frac{1}{2}}(x) + H_{-1,0,1,0,-\frac{1}{2}}(x) + H_{0,-1,0,-\frac{1}{2},1}(x) \\ & + H_{0,-1,0,1,-\frac{1}{2}}(x) + H_{0,-1,1,0,-\frac{1}{2}}(x) + H_{0,1,-1,0,-\frac{1}{2}}(x). \end{aligned}$$

`LinearExpand[expr]`: expands all the products of harmonic sums, S -sums and cyclotomic sums at same arguments.

Example:

$$\begin{aligned} & \text{LinearExpand}[S[1, 2, n] * S[-1, 2, 1/2, 1/3, n]] = \\ & S_{0,4} \left(\frac{1}{2}, \frac{1}{3}; n \right) - S_{-1,1,4} \left(\frac{1}{2}, 1, \frac{1}{3}; n \right) - S_{-1,3,2} \left(\frac{1}{2}, \frac{1}{3}, 1; n \right) - S_{0,2,2} \left(\frac{1}{2}, \frac{1}{3}, 1; n \right) \\ & - S_{0,2,2} \left(\frac{1}{2}, 1, \frac{1}{3}; n \right) - S_{1,-1,4} \left(1, \frac{1}{2}, \frac{1}{3}; n \right) - S_{1,1,2} \left(1, \frac{1}{2}, \frac{1}{3}; n \right) + S_{-1,1,2,2} \left(\frac{1}{2}, 1, \frac{1}{3}, 1; n \right) \\ & + S_{-1,1,2,2} \left(\frac{1}{2}, 1, 1, \frac{1}{3}; n \right) + S_{-1,2,1,2} \left(\frac{1}{2}, \frac{1}{3}, 1, 1; n \right) + S_{1,-1,2,2} \left(1, \frac{1}{2}, \frac{1}{3}, 1; n \right) \\ & + S_{1,-1,2,2} \left(1, \frac{1}{2}, 1, \frac{1}{3}; n \right) + S_{1,2,-1,2} \left(1, 1, \frac{1}{2}, \frac{1}{3}; n \right). \end{aligned}$$

`InvMellin[expr, n, x]`: calculates the inverse Mellin-Transform of `expr`.

Example:

$$\begin{aligned} & \text{ReduceConstants}[\text{InvMellin}[S[2, 2, 1, \{1, 1, 1/2\}, n], n, x], \text{ToKnownConstants} \rightarrow \text{True}] = \\ & -\frac{2^{-n} S_{2,2} \left(\frac{1}{2}, 1; \infty \right)}{x-2} - \frac{2^{-n-1} (\zeta_2 - \ln(2)^2) H_{0,2}(x)}{x-2} - \frac{\ln(2) 2^{-n} H_{0,2,0}(x)}{x-2} + \frac{\ln(2) H_{0,1,0}(x)}{x-1} \\ & + \frac{2^{-n} H_{0,2,0,2}(x)}{x-2} + \frac{2^{-n} S_4 \left(\frac{1}{2}; \infty \right)}{x-2} + \frac{2^{-n} H_0(x) \left(\frac{\ln(2)^3}{6} - \frac{\ln(2)\zeta_2}{2} + \frac{7\zeta_3}{8} \right)}{x-2} + \frac{5\zeta_3 H_0(x)}{8(x-1)} \\ & - \frac{H_0(x) \left(\frac{\ln(2)^3}{6} - \frac{\ln(2)\zeta_2}{2} + \frac{7\zeta_3}{8} \right)}{x-1} - \frac{5 \cdot 2^{-n-3} \zeta_3 H_0(x)}{x-2} + \frac{\ln(2) 2^{1-n} \left(\frac{\ln(2)^3}{6} - \frac{\ln(2)\zeta_2}{2} + \frac{7\zeta_3}{8} \right)}{2-x} \\ & + \frac{2^{-n-2} (\zeta_2 - \ln(2)^2)^2}{x-2} + \frac{2 \ln(2) \zeta_3}{x-1} + \delta(1-x) \left[\ln(2) \left(\frac{1}{4} (\zeta_2 - \ln(2)^2)^2 - 2 \left(-S_{1,3} \left(\frac{1}{2}, 1; \infty \right) \right. \right. \right. \\ & \left. \left. \left. + S_4 \left(\frac{1}{2}; \infty \right) + \ln(2) \left(\frac{\ln(2)^3}{6} - \frac{\ln(2)\zeta_2}{2} + \frac{7\zeta_3}{8} \right) \right) \right) - S_{1,4} \left(\frac{1}{2}, 1; \infty \right) - S_{3,2} \left(\frac{1}{2}, 1; \infty \right) \right. \\ & \left. + S_{1,2,2} \left(\frac{1}{2}, 1, 1; \infty \right) + S_5 \left(\frac{1}{2}; \infty \right) \right]. \end{aligned}$$

For the command `ReduceConstants`, see below. Note that some of the constants may be further identified by

$$S_k(z, \infty) = \text{Li}_k(z), \quad |z| \leq 1.$$

`Mellin[expr, x, n]`: calculates the Mellin-Transform of `expr`.

Example:

$$\begin{aligned} & \text{Mellin}[H[2, 1, -3, x], x, n]/.S[1, \{-1/3\}, \text{Infinity}] \rightarrow -\text{Log}[4/3] = \\ & -\frac{2^{n+1} S_{1,2}(\frac{1}{2}, -\frac{2}{3}; \infty)}{n+1} + \frac{S_{1,2}(\frac{1}{2}, -\frac{2}{3}; \infty)}{n+1} - \frac{2^{n+1} S_{2,1}(1, -\frac{1}{3}; \infty)}{n+1} + \frac{S_{2,1}(1, -\frac{1}{3}; \infty)}{n+1} \\ & + \frac{2^{n+1} S_{1,1,1}(\frac{1}{2}, 2, -\frac{1}{3}; \infty)}{n+1} - \frac{S_{1,1,1}(\frac{1}{2}, 2, -\frac{1}{3}; \infty)}{n+1} - \frac{S_{1,1}(-3, -\frac{1}{3}; n)}{(n+1)^2} - \frac{S_3(-\frac{1}{3}; \infty)}{n+1} \\ & - \frac{2^{n+1} S_{1,1,1}(\frac{1}{2}, -3, -\frac{1}{3}; n)}{n+1} - \frac{2^{n+1} \log(\frac{4}{3}) S_{1,1}(\frac{1}{2}, -3; n)}{n+1} + \frac{2^{n+1} \log(\frac{4}{3}) S_{1,1}(\frac{1}{2}, 1; n)}{n+1} \\ & + \frac{2^{n+1} S_3(-\frac{1}{3}; \infty)}{n+1} + \frac{(-1)^n 3^{n+1} S_1(-\frac{1}{3}; n)}{(n+1)^3} - \frac{\log(\frac{4}{3}) S_1(-3; n)}{(n+1)^2} + \frac{\log(\frac{4}{3}) S_1(n)}{(n+1)^2} \\ & - \frac{1}{(n+1)^4} + \frac{(-1)^n 3^{n+1} \log(\frac{4}{3})}{(n+1)^3} + \frac{\log(\frac{4}{3})}{(n+1)^3}. \end{aligned}$$

DifferentiateSSum[expr, n]: differentiates expr with respect to n.

Example:

$$\begin{aligned} & \text{DifferentiateSSum}[S[4, 1, \{1, -1/2\}, n], n] \\ & = H_0\left(\frac{1}{2}\right) S_{4,1}\left(1, -\frac{1}{2}; n\right) - S_{4,2}\left(1, -\frac{1}{2}; n\right) - 4S_{5,1}\left(1, -\frac{1}{2}; n\right) + H_{-1,0}\left(\frac{1}{2}\right) S_4(n) \\ & + H_{\frac{3}{2}}\left(\frac{1}{2}\right) H_{0,0,0,1,0}(1) + H_{-1,0,0,0,-1,0}\left(\frac{1}{2}\right). \end{aligned}$$

The constants may be further reduced to known multiple zeta values and/or cyclotomic numbers applying the command ReduceConstants[expr], see below.

RemoveLeading1 [H[m₁,...,m_n,x]]: extracts leading ones of H_{m₁,...,m_n}(x).

Example:

$$\begin{aligned} & \text{RemoveLeading1}[H[1, 1, -1, 0, 1/2, x]] \\ & = \frac{1}{2} H_1(x)^2 H_{-1,0,\frac{1}{2}}(x) - H_1(x) H_{-1,0,\frac{1}{2},1}(x) - H_1(x) H_{-1,0,1,\frac{1}{2}}(x) - H_1(x) H_{-1,1,0,\frac{1}{2}}(x) \\ & + H_{-1,0,\frac{1}{2},1,1}(x) + H_{-1,0,1,\frac{1}{2},1}(x) + H_{-1,0,1,1,\frac{1}{2}}(x) + H_{-1,1,0,\frac{1}{2},1}(x) + H_{-1,1,0,1,\frac{1}{2}}(x) \\ & + H_{-1,1,1,0,\frac{1}{2}}(x). \end{aligned}$$

RemoveTrailing0 [H[m₁,...,m_n,x]]: extracts trailing zeroes of H_{m₁,...,m_n}(x).

Example:

$$\begin{aligned} & \text{RemoveTrailing0}[H[1/2, -1/3, -1, 0, 0, x]] \\ & = \frac{1}{2} H_0(x)^2 H_{\frac{1}{2},-\frac{1}{3},-1}(x) - H_0(x) H_{0,\frac{1}{2},-\frac{1}{3},-1}(x) - H_0(x) H_{\frac{1}{2},-\frac{1}{3},0,-1}(x) - H_0(x) H_{\frac{1}{2},0,-\frac{1}{3},-1}(x) \\ & + H_{0,0,\frac{1}{2},-\frac{1}{3},-1}(x) + H_{0,\frac{1}{2},-\frac{1}{3},0,-1}(x) + H_{0,\frac{1}{2},0,-\frac{1}{3},-1}(x) + H_{\frac{1}{2},-\frac{1}{3},0,0,-1}(x) + H_{\frac{1}{2},0,-\frac{1}{3},0,-1}(x) \\ & + H_{\frac{1}{2},0,0,-\frac{1}{3},-1}(x). \end{aligned}$$

RemoveLeadingIndex [H[m₁,...,m_n,x]]: extracts the leading index m₁ of H_{m₁,...,m_n}(x).

RemoveLeadingIndex[expr, b] removes the leading index b of all polylogarithms in expr.

Examples:

RemoveLeadingIndex[H[1/2, 1/2, -1, 1, 1/3, x]] =

$$\begin{aligned} & \frac{1}{2} H_{\frac{1}{2}}(x)^2 H_{-1,1,\frac{1}{3}}(x) - H_{\frac{1}{2}}(x) H_{-1,\frac{1}{2},\frac{1}{3}}(x) - H_{\frac{1}{2}}(x) H_{-1,1,\frac{1}{3},\frac{1}{2}}(x) - H_{\frac{1}{2}}(x) H_{-1,1,\frac{1}{2},\frac{1}{3}}(x) \\ & + H_{-1,\frac{1}{2},\frac{1}{2},\frac{1}{3}}(x) + H_{-1,\frac{1}{2},1,\frac{1}{3},\frac{1}{2}}(x) + H_{-1,\frac{1}{2},1,\frac{1}{2},\frac{1}{3}}(x) + H_{-1,1,\frac{1}{3},\frac{1}{2},\frac{1}{2}}(x) + H_{-1,1,\frac{1}{2},\frac{1}{3},\frac{1}{2}}(x) \\ & + H_{-1,1,\frac{1}{2},\frac{1}{2},\frac{1}{3}}(x). \end{aligned}$$

RemoveLeadingIndex[H[b, 1/2, -1, 1, -1/3, x], b] =

$$H_{\frac{1}{2},-1,1,-\frac{1}{3}}(x) H_b(x) - H_{\frac{1}{2},-1,1,-\frac{1}{3},b}(x) - H_{\frac{1}{2},-1,1,b,-\frac{1}{3}}(x) - H_{\frac{1}{2},-1,b,1,-\frac{1}{3}}(x) - H_{\frac{1}{2},b,-1,1,-\frac{1}{3}}(x).$$

RemoveTrailingIndex[H[m₁, ..., m_n, x]]: extracts the trailing index m_n of H_{m₁, ..., m_n}(x).

RemoveTrailingIndex[expr, b] removes the trailing index b of all polylogarithms in expr.

Examples:

RemoveTrailingIndex[H[-1, 1, 1/3, 1/2, 1/2, x]] =

$$\begin{aligned} & \frac{1}{2} H_{\frac{1}{2}}(x)^2 H_{-1,1,\frac{1}{3}}(x) - H_{\frac{1}{2}}(x) H_{-1,\frac{1}{2},\frac{1}{3}}(x) - H_{\frac{1}{2}}(x) H_{-1,1,\frac{1}{2},\frac{1}{3}}(x) - H_{\frac{1}{2}}(x) H_{\frac{1}{2},-1,1,\frac{1}{3}}(x) \\ & + H_{-1,\frac{1}{2},\frac{1}{2},\frac{1}{3}}(x) + H_{-1,\frac{1}{2},1,\frac{1}{2},\frac{1}{3}}(x) + H_{-1,1,\frac{1}{2},\frac{1}{2},\frac{1}{3}}(x) + H_{\frac{1}{2},-1,\frac{1}{2},\frac{1}{3}}(x) + H_{\frac{1}{2},-1,1,\frac{1}{2},\frac{1}{3}}(x) \\ & + H_{\frac{1}{2},\frac{1}{2},-1,1,\frac{1}{3}}(x). \end{aligned}$$

RemoveTrailingIndex[H[-1, 1, 1/3, 1/2, b, x], b] =

$$H_{-1,1,\frac{1}{3},\frac{1}{2}}(x) H_b(x) - H_{-1,1,\frac{1}{3},b,\frac{1}{2}}(x) - H_{-1,1,b,\frac{1}{3},\frac{1}{2}}(x) - H_{-1,b,1,\frac{1}{3},\frac{1}{2}}(x) - H_{b,-1,1,\frac{1}{3},\frac{1}{2}}(x).$$

SRemoveLeading1[S[a₁, ..., a_m, {x₁, ..., x_m}, n]]: extracts leading ones of S_{a₁, ..., a_m}(x₁, ..., x_m; n).

Example:

SRemoveLeading1[S[1, 1, 1, -2, 4, {1, 1/3, 1/2, 1/2, 1/2}, n]] =

$$\begin{aligned} & S_1(n) S_{1,1,-2,4} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; n \right) + S_{1,1,-2,5} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; n \right) + S_{1,1,-1,4} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; n \right) \\ & + S_{1,2,-2,4} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; n \right) + S_{2,1,-2,4} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; n \right) - S_{1,1,-2,1,4} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, 1, \frac{1}{2}; n \right) \\ & - S_{1,1,-2,4,1} \left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}, 1; n \right) - S_{1,1,1,-2,4} \left(\frac{1}{3}, \frac{1}{2}, 1, \frac{1}{2}, \frac{1}{2}; n \right) \\ & - S_{1,1,1,-2,4} \left(\frac{1}{3}, 1, \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; n \right). \end{aligned}$$

SRemoveTrailing1[S[a₁, ..., a_m, {x₁, ..., x_m}, n]]: extracts trailing ones of S_{a₁, ..., a_m}(x₁, ..., x_m; n).

Example:

$$\begin{aligned} & \text{SRemoveTrailing1}[S[-2, 4, 1, 1, 1, \{1/3, 1/2, 1/2, -1/2, 1\}, n]] = \\ & S_1(n)S_{-2,4,1,1,1}\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right) + S_{-2,4,1,2}\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right) + S_{-2,4,2,1}\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right) \\ & + S_{-2,5,1,1}\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right) + S_{-1,4,1,1}\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right) - S_{-2,1,4,1,1}\left(\frac{1}{3}, 1, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right) \\ & - S_{-2,4,1,1,1}\left(\frac{1}{3}, \frac{1}{2}, \frac{1}{2}, 1, -\frac{1}{2}; n\right) - S_{-2,4,1,1,1}\left(\frac{1}{3}, \frac{1}{2}, 1, \frac{1}{2}, -\frac{1}{2}; n\right) \\ & - S_{1,-2,4,1,1}\left(1, \frac{1}{3}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2}; n\right). \end{aligned}$$

$\text{SRemoveTrailingIndex}[S[a_1, \dots, a_m, \{x_1, \dots, x_m\}, n]]$: extracts the trailing index (a_m, x_m) of $S_{a_1, \dots, a_m}(x_1, \dots, x_m; n)$.

Examples:

$$\begin{aligned} & \text{SRemoveTrailingIndex}[S[a_1, \dots, a_m, \{x_1, \dots, x_m\}, n]] = \\ & S_{a_3}(x_3; n) S_{a_1, a_2}(x_1, x_2; n) + S_{a_1, a_2 + a_3}(x_1, x_2 x_3, n) + S_{a_1 + a_3, a_2}(x_1 x_3, x_2; n) \\ & - S_{a_1, a_3, a_2}(x_1, x_3, x_2; n) - S_{a_3, a_1, a_2}(x_3, x_1, x_2; n). \end{aligned}$$

$\text{TransformH}[H[m_1, \dots, m_n, y], x]$: performs several transforms on the argument of a generalized polylogarithm.

Examples:

$$\begin{aligned} & \text{TransformH}[H[-1, 2, 0, 1/x], x] = \\ & \left(H_{0, \frac{1}{2}}(1) + H_{0,2}(1)\right) (-H_{-1}(x) + H_0(x) + \ln(2)) - H_{-1,0,0}(x) - H_{-1, \frac{1}{2},0}(x) + H_{0,0,0}(x) \\ & + H_{0, \frac{1}{2},0}(x) + H_{-1, \frac{1}{2},0}(1) + H_{-1,2,0}(1) - H_{0, \frac{1}{2},0}(1) + \frac{3\zeta_3}{4}. \end{aligned}$$

$$\text{TransformH}[H[-1, 2, 0, 1-x], x] = -H_{2,0}(1)H_2(x) - H_{2,-1,1}(x) + H_{-1,2,0}(1).$$

$$\text{TransformH}[H[-1, 2, 0, (1-x)/(1+x)], x] =$$

$$H_{2,0}(1)(-H_{-1}(x)) + H_{-1,-1,-1}(x) + H_{-1,-1,1}(x) - H_{-1,-\frac{1}{3},-1}(x) - H_{-1,-\frac{1}{3},1}(x) + H_{-1,2,0}(1).$$

$\text{HarmonicSumsSeries}[expr, \{x, c, ord\}]$: tries to compute the series expansion of $expr$ with respect to x about $c \in \mathbb{R} \cup \infty$ up to order $ord \in \mathbb{N}$. $expr$ may contain harmonic sums, cyclotomic sums, and their generalizations as well as their associated polylogarithms.

Examples:

HarmonicSumsSeries[H[-2/5, 3/24, 0, 1/4, x], {x, 0, 10}] =

$$\frac{40x^3}{3} + 35x^4 + \frac{2026x^5}{9} + \frac{20081x^6}{18} + \frac{12632239x^7}{1890} + \frac{1205544979x^8}{30240} + \frac{119322150247x^9}{476280} + \frac{188972192341x^{10}}{117600}.$$

HarmonicSumsSeries[S[1, -2, 1, n], {n, 0, 4}] =

$$n \left(-\frac{\zeta_2 \zeta_3}{2} - \frac{5\zeta_5}{8} \right) + n^2 \left(\frac{41\zeta_2^3}{168} + \frac{\zeta_3^2}{4} \right) + n^3 \left(S_{-5,-2}(\infty) + S_{-4,-3}(\infty) - S_{-4,1,-2}(\infty) \right) + \frac{\zeta_2^2 \zeta_3}{32} - \frac{29\zeta_2 \zeta_5}{32} - \zeta_7 + n^4 \left(-S_{-6,-2}(\infty) - S_{-5,-3}(\infty) + S_{-5,1,-2}(\infty) - \frac{31 \ln(2) \zeta_2 \zeta_5}{16} \right) + S_8(\infty) + s_6 \zeta_2 + \frac{23\zeta_2^4}{70} - \frac{3\zeta_2 \zeta_3^2}{4} + \frac{155\zeta_3 \zeta_5}{128}.$$

HarmonicSumsSeries[S[1, -2, 1, n], {n, Infinity, 10}] =

$$\frac{1}{8} \left[(-1)^n \left(\frac{2}{n^3} - \frac{5}{n^4} + \frac{4}{n^5} + \frac{7}{n^6} - \frac{16}{n^7} - \frac{27}{n^8} + \frac{108}{n^9} + \frac{187}{n^{10}} \right) \bar{\ln}(n) \right] + \zeta_3 \left(-\frac{5}{2n} + \frac{5}{12n^2} - \frac{1}{24n^4} + \frac{5}{252n^6} - \frac{1}{48n^8} + \frac{5}{132n^{10}} \right) - \frac{3\zeta_2^2}{5} + (-1)^n \left(\frac{3}{n^4} - \frac{20}{3n^5} - \frac{19}{12n^6} + \frac{1511}{60n^7} + \frac{59}{8n^8} - \frac{118529}{630n^9} - \frac{130213}{2520n^{10}} \right) - 5\zeta_3 \bar{\ln}(n) \Big] + O\left(\frac{1}{n^{10}}\right).$$

HarmonicSumsSeries[S[1, -2, 1, {1/2, 1/3, -1}, n], {n, Infinity, 3}] =

$$\frac{3}{2} S_{1,1} \left(-\frac{1}{6}, 2; \infty \right) - \frac{3}{2} S_{1,1} \left(-\frac{1}{6}, 6; \infty \right) + \frac{3}{2} \ln(2) S_1 \left(-\frac{1}{3}; \infty \right) - \frac{3}{2} \ln(2) S_1 \left(-\frac{1}{6}; \infty \right) + \frac{3}{2} \ln(2) S_1 \left(\frac{1}{6}; \infty \right) - \frac{9 \cdot 2^{-n} S_1 \left(-\frac{1}{3}; \infty \right)}{n^3} + \frac{3 \cdot 2^{-n} S_1 \left(-\frac{1}{3}; \infty \right)}{n^2} - \frac{3 \cdot 2^{-n-1} S_1 \left(-\frac{1}{3}; \infty \right)}{n} - \frac{3}{2} S_1 \left(-\frac{1}{3}; \infty \right) S_1 \left(-\frac{1}{6}; \infty \right) - \frac{1011}{800} S_1 \left(-\frac{1}{6}; \infty \right) - \frac{3}{2} S_2 \left(-\frac{1}{3}; \infty \right) - \frac{7 \ln(2) 2^{-n} 3^{2-n}}{125n^3} + \frac{\ln(2) 2^{-n} 3^{2-n}}{25n^2} - \frac{7}{25} \ln(2) 2^{-n-1} 3^{1-n} - \frac{1}{5} \ln(2) 2^{-n-1} 3^{-n} - \frac{\ln(2) 2^{-n-1} 3^{1-n}}{5n} - \frac{21 \ln(2)}{32} + \frac{79 \left(-\frac{1}{3}\right)^n 2^{-n-5}}{343n^3} + \frac{63 \cdot 2^{-n-4}}{n^3} - \frac{21 \cdot 2^{-n-4}}{n^2} - \frac{(-1)^n 2^{-n-4} 3^{1-n}}{49n^2} + \frac{1}{7} \left(-\frac{1}{3}\right)^n 2^{-n-3} + \frac{\left(-\frac{1}{3}\right)^n 2^{-n-5}}{7n} + \frac{21 \cdot 2^{-n-5}}{n} - \frac{3\zeta_2}{4} + \frac{9}{280} + O\left(\frac{1}{n^4}\right),$$

with $\bar{\ln}(b) = \ln(n) + \gamma_E$.

`ComputeSSumBasis` [$w, \{x_1, x_2, \dots\}, n$] : computes a basis representation of S -sums with indices x_i at weight w using algebraic, differential and half integer relations.

Example:

$$\begin{aligned} & \text{ComputeSSumBasis}[2, \{1, 1/2, 1/3\}, n] = \\ & \left\{ \left\{ S_{-2}(n), S_2(n), S_{-1,1}(n), S_2\left(\frac{1}{3}; n\right), S_2\left(\frac{1}{2}; n\right), S_{1,1}\left(1, \frac{1}{3}; n\right), S_{1,1}\left(1, \frac{1}{2}; n\right) \right\}, \right. \\ & \left\{ S_{1,-1}(n) \rightarrow -S_{-1,1}(n) + S_{-2}(n) + S_{-1}(n)S_1(n), \right. \\ & S_{1,1}(n) \rightarrow \frac{1}{2}S_1(n)^2 + \frac{S_2(n)}{2}, \\ & S_{1,1}\left(\frac{1}{3}, 1; n\right) \rightarrow -S_{1,1}\left(1, \frac{1}{3}; n\right) + S_1(n)S_1\left(\frac{1}{3}; n\right) + S_2\left(\frac{1}{3}; n\right), \\ & S_{1,1}\left(\frac{1}{2}, 1; n\right) \rightarrow -S_{1,1}\left(1, \frac{1}{2}; n\right) + S_1(n)S_1\left(\frac{1}{2}; n\right) + S_2\left(\frac{1}{2}; n\right), \\ & \left. \left. S_{-1,-1}(n) \rightarrow \frac{1}{2}S_{-1}(n)^2 + \frac{S_2(n)}{2} \right\} \right\}. \end{aligned}$$

`ComputeHLogBasis` [$w, x, \text{Alphabet} \rightarrow \{a_1, \dots, a_k\}$] : computes a basis representation of generalized polylogarithms with indices a_i at weight w using algebraic relations.

Example:

$$\begin{aligned} & \text{ComputeHLogBasis}[2, x, \text{Alphabet} \rightarrow \{1/2, -1/3, 1\}] = \\ & \left\{ \left\{ H_{-1, -\frac{1}{3}}(x), H_{-1, \frac{1}{2}}(x), H_{-1, 1}(x), H_{-\frac{1}{3}, \frac{1}{2}}(x), H_{-\frac{1}{3}, 1}(x), H_{\frac{1}{2}, 1}(x) \right\}, \right. \\ & \left\{ H_{1, 1}(x) \rightarrow \frac{1}{2}H_1(x)^2, \right. \\ & H_{1, \frac{1}{2}}(x) \rightarrow H_{\frac{1}{2}}(x)H_1(x) - H_{\frac{1}{2}, 1}(x), \\ & H_{1, -\frac{1}{3}}(x) \rightarrow H_{-\frac{1}{3}}(x)H_1(x) - H_{-\frac{1}{3}, 1}(x), \\ & H_{1, -1}(x) \rightarrow H_{-1}(x)H_1(x) - H_{-1, 1}(x), \\ & H_{\frac{1}{2}, \frac{1}{2}}(x) \rightarrow \frac{1}{2}H_{\frac{1}{2}}(x)^2, \\ & H_{\frac{1}{2}, -\frac{1}{3}}(x) \rightarrow H_{-\frac{1}{3}}(x)H_{\frac{1}{2}}(x) - H_{-\frac{1}{3}, \frac{1}{2}}(x), \\ & H_{\frac{1}{2}, -1}(x) \rightarrow H_{-1}(x)H_{\frac{1}{2}}(x) - H_{-1, \frac{1}{2}}(x), \\ & H_{-\frac{1}{3}, -\frac{1}{3}}(x) \rightarrow \frac{1}{2}H_{-\frac{1}{3}}(x)^2, \\ & H_{-\frac{1}{3}, -1}(x) \rightarrow H_{-1}(x)H_{-\frac{1}{3}}(x) - H_{-1, -\frac{1}{3}}(x), \\ & \left. \left. H_{-1, -1}(x) \rightarrow \frac{1}{2}H_{-1}(x)^2 \right\} \right\}. \end{aligned}$$

`ComputeSSumInfBasis` [$w, \{x_1, \dots, x_k\}$] : computes relations of S -sums at infinity and weight w with indices in $\{x_1, \dots, x_k\}$.

Example:

$$\begin{aligned}
 & \text{ComputeSSumInfBasis}[2, \{1/2, -1, -1/3, 1\}] = \\
 & \left\{ \left\{ S_{-2}(\infty), S_2\left(-\frac{1}{3}; \infty\right) \right\}, \right. \\
 & \left\{ S_{1,1}\left(1, \frac{1}{2}; \infty\right) \rightarrow S_1(\infty)S_1\left(\frac{1}{2}; \infty\right) - \frac{1}{2}S_{-1}(\infty)^2, \right. \\
 & S_{1,1}\left(1, -\frac{1}{3}; \infty\right) \rightarrow S_1(\infty)S_1\left(-\frac{1}{3}; \infty\right) - \frac{1}{2}S_1\left(-\frac{1}{3}; \infty\right)^2, \\
 & S_{1,1}(\infty) \rightarrow \frac{1}{2}S_1(\infty)^2 - S_{-2}(\infty), \\
 & S_{1,-1}(\infty) \rightarrow S_{-1}(\infty)S_1(\infty) - \frac{1}{2}S_{-1}(\infty)^2, \\
 & S_{1,1}\left(\frac{1}{2}, 1; \infty\right) \rightarrow -S_{-2}(\infty), \\
 & S_{1,1}\left(-\frac{1}{3}, 1; \infty\right) \rightarrow \frac{1}{2}S_1\left(-\frac{1}{3}; \infty\right)^2 + S_2\left(-\frac{1}{3}; \infty\right), \\
 & S_{-1,1}(\infty) \rightarrow \frac{1}{2}S_{-1}(\infty)^2 + S_{-2}(\infty), \\
 & S_{-1,-1}(\infty) \rightarrow \frac{1}{2}S_{-1}(\infty)^2 - S_{-2}(\infty), \\
 & S_2\left(\frac{1}{2}; \infty\right) \rightarrow -\frac{1}{2}S_{-1}(\infty)^2 - S_{-2}(\infty), \\
 & \left. \left. S_2(\infty) \rightarrow -2S_{-2}(\infty) \right\} \right\}.
 \end{aligned}$$

`ReduceConstants[expr]`: reduces (as much as possible) occurring harmonic sums, S -sums or cyclotomic sums at infinity and harmonic polylogarithms, generalized polylogarithms and cyclotomic polylogarithms at constants to a set of basis constants using given tables. Via the option `ToKnownConstants` \rightarrow `True` a special set of basis constants is used, i.e., $\log(2)$, ζ_2 , ζ_3 , ... For the multiple zeta values we use the basis given before in Ref. 123 for weights up to $w = 6$. The relations were calculated newly and agree with those in Ref. 123. Extended tables (for higher weights) both on the harmonic sums at $N \rightarrow \infty$ and the the harmonic polylogarithms at $x = 1$ were given in association with Refs. 123, 105, and 28 and are available using FORM¹²⁴ codes. It is straightforwardly possible to generate more extensive tables for special numbers as harmonic sums, cyclotomic harmonic sums, and classes of generalized harmonic sums at infinity and likewise special values of the corresponding harmonic polylogarithms at a given argument over respective bases using `HarmonicSums`.

Example:

$$\text{ReduceConstants}[S[4, 1, -1, \text{Infinity}], \text{ToKnownConstants} \rightarrow \text{True}] =$$

$$\text{Li}_4\left(\frac{1}{2}\right)\zeta_2 + \frac{\ln(2)^4\zeta_2}{24} - \frac{5\ln(2)^2\zeta_2^2}{8} + \frac{3\ln(2)\zeta_2\zeta_3}{2} + \frac{93\ln(2)\zeta_5}{32} - \frac{5s_6}{2} - \frac{149\zeta_2^3}{168} + \frac{49\zeta_3^2}{64}.$$

Also tables of sums and polylogarithms at general argument are available. The harmonic sums and polylogarithms are tabulated up to $w = 6$, for the cyclotomic harmonic sums over the alphabet $\{\pm 1\}^i/i^k$, $(\pm 1)^i/(2i + 1)^k$ and the alphabet for the special generalized sums discussed in the present paper both to weight $w = 4$. Depending on the weight and length of the alphabet the corresponding calculations may become more demanding. The corresponding tables of relations

grow correspondingly. If the option `Dynamic` \rightarrow `True` is set, the reduction is calculated online. This will help if certain sums are not stored in the tables yet.

`HToSinf[expr]`: transforms generalized polylogarithms and cyclotomic polylogarithms at 1 to S -sums and cyclotomic sums at infinity.

Example:

$$\begin{aligned} & \text{HToSinf}[H[1, 2, -4, 3, 1]] = \\ & -S_{1,3}\left(1, \frac{1}{3}; \infty\right) - S_{2,2}\left(\frac{1}{2}, \frac{2}{3}; \infty\right) - S_{3,1}\left(-\frac{1}{4}, -\frac{4}{3}; \infty\right) + S_{1,1,2}\left(1, \frac{1}{2}, \frac{2}{3}; \infty\right) \\ & + S_{1,2,1}\left(1, -\frac{1}{4}, -\frac{4}{3}; \infty\right) + S_{2,1,1}\left(\frac{1}{2}, -\frac{1}{2}, -\frac{4}{3}; \infty\right) - S_{1,1,1,1}\left(1, \frac{1}{2}, -\frac{1}{2}, -\frac{4}{3}; \infty\right) + S_4\left(\frac{1}{3}; \infty\right). \end{aligned}$$

`SinfToH[expr]`: transforms S -sums and cyclotomic sums at infinity to generalized polylogarithms and cyclotomic polylogarithms at 1.

Example:

$$\begin{aligned} & \text{SinfToH}[S[1, 2, 3, \{1/2, -1/3, 1/4\}, \text{Infinity}]] = \\ & H_{0,0,-6,0,0,-24}(1) - H_{0,0,0,0,0,-24}(1) + H_{2,0,-6,0,0,-24}(1) - H_{2,0,0,0,0,-24}(1). \end{aligned}$$

`HToS[expr]`: computes the power series expansion of generalized polylogarithms and cyclotomic polylogarithms without trailing zeroes.

Example:

$$\begin{aligned} & \text{HToS}[H[1, 2, -4, 3, x]] = \\ & - \sum_{\tau_1=1}^{\infty} \frac{2^{-\tau_1} x^{\tau_1} S_2\left(\frac{2}{3}; \tau_1\right)}{\tau_1^2} + \sum_{\tau_1=1}^{\infty} \frac{2^{-\tau_1} x^{\tau_1} S_{1,1}\left(-\frac{1}{2}, -\frac{4}{3}; \tau_1\right)}{\tau_1^2} - \sum_{\tau_1=1}^{\infty} \frac{x^{\tau_1} S_3\left(\frac{1}{3}; \tau_1\right)}{\tau_1} \\ & + \sum_{\tau_1=1}^{\infty} \frac{x^{\tau_1} S_{1,2}\left(\frac{1}{2}, \frac{2}{3}; \tau_1\right)}{\tau_1} + \sum_{\tau_1=1}^{\infty} \frac{x^{\tau_1} S_{2,1}\left(-\frac{1}{4}, -\frac{4}{3}; \tau_1\right)}{\tau_1} - \sum_{\tau_1=1}^{\infty} \frac{x^{\tau_1} S_{1,1,1}\left(\frac{1}{2}, -\frac{1}{2}, -\frac{4}{3}; \tau_1\right)}{\tau_1} \\ & - \sum_{\tau_1=1}^{\infty} \frac{4^{-\tau_1} (-x)^{\tau_1} S_1\left(-\frac{4}{3}; \tau_1\right)}{\tau_1^3} + \sum_{\tau_1=1}^{\infty} \frac{3^{-\tau_1} x^{\tau_1}}{\tau_1^4}. \end{aligned}$$

`SToH[expr]`: takes (part of) a power series expansion of a (generalized/cyclotomic) polylogarithm and finds the (generalized/cyclotomic) polylogarithm(s) it originates from. It is the inverse of `HToS`.

Example:

$$\text{SToH}\left[\sum_{\tau_1=1}^{\infty} 4^{-\tau_1} (-x)^{\tau_1} S_1\left(-\frac{4}{3}; \tau_1\right) \frac{1}{\tau_1^3}\right] = -H[0, 0, -4, 3, x] + H[0, 0, 0, 3, x].$$

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