Harmonic Sums, Polylogarithms, Special Numbers, and Their Generalizations

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Abstract In these introductory lectures we discuss classes of presently known nested sums, associated iterated integrals, and special constants which hierarchically appear in the evaluation of massless and massive Feynman diagrams at higher loops. These quantities are elements of stuffle and shuffle algebras implying algebraic relations being widely independent of the special quantities considered. They are supplemented by structural relations. The generalizations are given in terms of generalized harmonic sums, (generalized) cyclotomic sums, and sums containing in addition binomial and inverse-binomial weights. To all these quantities iterated integrals and special numbers are associated. We also discuss the analytic continuation of nested sums of different kind to complex values of the external summation bound N.

1 Introduction

In the solution of physical problems very often new classes of special functions have been created during the last three centuries, cf. [1–5]. This applies especially also to the analytic calculation of Feynman-parameter integrals [6] for massless and massive two- and more-point functions, also containing local operator insertions and corresponding quantities, cf. [7, 8]. In case of zero mass-scale quantities the associated integrals map to special numbers, lately having been called periods [9], see also [10]. In case of single-scale quantities, expressed as a ratio $x \in [0, 1]$ to

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the defining mass scale, the integrals are Poincaré iterated integrals [11, 12] or they emerge as a Mellin-transform at $N \in \mathbb{N}$ [13] in terms of multiply nested sums. A systematic way to these structures has been described in [14, 15]. Here an essential tool consists in representations by Mellin–Barnes [16] integrals. They are applicable also for integrals of multi-scale more-loop and multi-leg Feynman integrals [17], which are, however, less explored at present.

In the practical calculations dimensional regularization in $D = 4 + \varepsilon$ space-time dimensions [18] is used, which is essential to maintain conservation laws due to the Noether theorem and probability. It provides the singularities of the problem in terms of poles in ε. However, the Feynman parameter integrals are not performed over rational integrands but hyperexponential ones. Thus one passes through higher transcendental functions [4, 5] from the beginning. The renormalization is carried out in the $\overline{\text{MS}}$-scheme, chosen as the standard. In new calculations various ingredients as anomalous dimensions and expansion coefficients of the β-functions needed in the renormalization can thus be used referring to results given in the literature. At higher orders the calculation of these quantities requests a major investment and is not easily repeated at present within other schemes in a short time.

With growing complexity of the perturbative calculations in Quantum Field Theories the functions emerging in integration and summation had to be systematized. While a series of massless two-loop calculations, cf. [19], during the 1980s and 1990s initially still could be performed referring to the classical polylogarithms [12, 20–23] and Nielsen-integrals [24], the structure of the results became readily involved. In 1998 a first general standard was introduced [25, 26] by the nested harmonic sums, and shortly after the harmonic polylogarithms [27]. Further extensions are given by the generalized harmonic sums, the so-called S-sums [28, 29] and the (generalized) cyclotomic sums [30], see Fig. 1. Considering problems at even higher loops and a growing number of legs, also associated with more mass scales, one expects various new levels of generalization to emerge. In particular, also elliptic integrals will contribute [31]. These structures can be found systematically by applying symbolic summation, cf. [32], and integration formalisms, cf. [33, 34], which also allow to proof the relative transcendence of the basis elements found and are therefore applied in the calculation of Feynman diagrams.

In this survey we present an introduction to a series of well-studied structures which have been unraveled during the last years. The paper is organized as follows. In Sect. 2 a survey is given on polylogarithms, Nielsen integrals and harmonic polylogarithms. In Sect. 3 harmonic sums are discussed. Both harmonic polylogarithms and harmonic sums obey algebraic and structural relations on which a survey is given in Sect. 4. In Sect. 5 we discuss properties of the multiple zeta values which emerge as special constants in the context of harmonic sums and polylogarithms. The S-sums, associated iterated integrals, and special numbers are considered in Sect. 6. The generalization of harmonic sums and S-sums to (generalized) cyclotomic sums, polylogarithms and numbers is given in Sect. 7. A further generalization, which appears in massive multi-loop calculations, to nested binomial and inverse-binomial harmonic sums and polylogarithms is outlined in
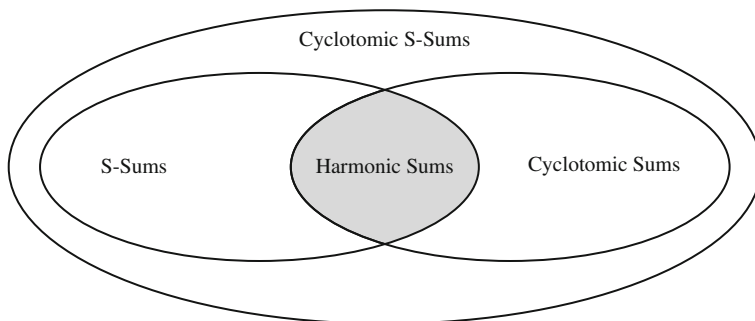
Fig. 1 Relations between the different extensions of harmonic sums

Sect. 8. Finally, we discuss in Sect. 9 the analytic continuation of the different kind of nested sums in the argument N to complex numbers, which is needed in various physical applications. Section 10 contains the conclusions. The various mathematical relations between the different quantities being discussed in the present article are implemented in the Mathematica package `HarmonicSums.m` [29, 35].

2 Polylogarithms, Nielsen Integrals, Harmonic Polylogarithms

Different particle propagators $1/A_k(p_i, m_i)$ can be linked using Feynman's integral representation [36]

$$\frac{1}{A_1^{\nu_1} \dots A_n^{\nu_n}} = \frac{\Gamma(\sum_{k=1}^n \nu_k)}{\prod_{k=1}^n \Gamma(\nu_k)} \int_0^1 \prod_{k=1}^n dx_k \frac{\prod_{k=1}^n x^{\nu_k - 1}}{\left(\sum_{k=1}^n x_k A_k\right)^{\sum_{k=1}^n \nu_k}} \delta\left(1 - \sum_{k=1}^n x_k\right), \ \nu_i \in \mathbb{R}. \quad (1)$$

While the momentum integrals over p_i can be easily performed, the problem consists in integrating the Feynman parameters x_k. In the simplest cases the associated integrand is a multi-rational function. In the first integrals one obtains multi-rational functions, but also logarithms [33]. The logarithms [37] have to be introduced as new functions being transcendental to the rational functions

$$\int_0^x \frac{dz}{1-z} = -\ln(1-x), \ \text{etc.} \quad (2)$$

Iterating this integral by

$$\int_0^x \frac{dz_1}{z_1} \int_0^{z_1} \frac{dz_2}{1-z_2} = \text{Li}_2(x) \quad (3)$$

one obtains the dilogarithm or Spence-function [20, 21], which may be extended to the classical polylogarithms [12, 21–23]

$$\int_0^x \frac{dz}{z} \text{Li}_{n-1}(z) = \text{Li}_n(x), n \in \mathbb{N} . \tag{4}$$

All these functions are transcendental to the former ones. For an early occurrence of the dilogarithm in Quantum Field Theory see [38].

The above iterations are special cases in iterating differential forms in $\{dz/z, dz/(1-z)\}$. The general case is described as Nielsen integrals [24].

$$\mathsf{S}_{n,p}(x) = \frac{(-1)^{n+p-1}}{(n-1)!p!} \int_0^1 \frac{dz}{z} \ln^{n-1}(z) \ln^p(1-xz) . \tag{5}$$

Likewise, one might also consider the set $\{dz/z, dz/(1+z)\}$. Nielsen integrals obey the relation

$$\mathsf{S}_{n-1,p}(x) = \frac{d}{dx}\mathsf{S}_{n,p}(x) . \tag{6}$$

One may derive serial representations around $x = 0$, as e.g.:

$$\text{Li}_n(x) = \sum_{k=1}^\infty \frac{x^k}{k^n}, \quad \mathsf{S}_{1,2}(x) = \sum_{k=2}^\infty \frac{x^k}{k^2}S_1(k-1), \quad \mathsf{S}_{2,2}(x) = \sum_{k=2}^\infty \frac{x^k}{k^3}S_1(k-1) , \tag{7}$$

see also [39]. Here $S_1(n) = \sum_{k=1}^n (1/k)$ denotes the harmonic sum. The Nielsen integrals obey various relations [12, 20–24]. A few examples are:

$$\text{Li}_2(1-x) = -\text{Li}_2(x) - \ln(x)\ln(1-x) + \zeta_2 \tag{8}$$

$$\text{Li}_2\left(-\frac{1}{x}\right) = -\text{Li}_2(-x) - \frac{1}{2}\ln^2(x) - \zeta_2 \tag{9}$$

$$\text{Li}_3(1-x) = -\mathsf{S}_{1,2}(x) - \ln(1-x)\text{Li}_2(x) - \frac{1}{2}\ln(x)\ln^2(1-x) + \zeta_2\ln(1-x) + \zeta_3 \tag{10}$$

$$\text{Li}_4\left(-\frac{x}{1-x}\right) = \ln(1-x)[\text{Li}_3(x) - \mathsf{S}_{1,2}(x)] + \mathsf{S}_{2,2}(x) - \text{Li}_4(x) - \mathsf{S}_{1,3}(x)$$
$$-\frac{1}{2}\ln^2(1-x)\text{Li}_2(x) - \frac{1}{24}\ln^4(1-x) \tag{11}$$

$$\text{Li}_n(x^2) = 2^{n-1}[\text{Li}_n(x) + \text{Li}_n(-x)] \tag{12}$$

$$\text{Li}_2(z) = \frac{1}{n}\sum_{x^n=z}\text{Li}_2(x), n \in \mathbb{N}\backslash\{0\} \tag{13}$$

$$S_{2,2}(1-x) = -S_{2,2}(x) + \ln(x)S_{1,2}(x) - [\text{Li}_3(x) - \ln(x)\text{Li}_2(x) - \zeta_3]\ln(1-x)$$
$$+\frac{1}{4}\ln^2(x)\ln^2(1-x) + \frac{\zeta_4}{4} . \tag{14}$$

Here $\zeta_n = \sum_{k=1}^{\infty}(1/k^n), \ \ n \geq 2, n \in \mathbb{N}$ are values of Riemann's ζ-function.

Going to higher orders in perturbation theory it turns out that the Nielsen integrals are sufficient for massless and some massive two-loop problems, cf. [26, 40], and as well for the three-loop anomalous dimensions [41], allowing for some extended arguments as $-x, x^2$. At a given level of complexity, however, one has to refer to a more general alphabet, namely

$$\mathfrak{A} = \{\omega_0, \omega_1, \omega_{-1}\} \equiv \{dz/z, dz/(1-z), dz/(1+z)\} . \tag{15}$$

The corresponding iterated integrals are called harmonic polylogarithms (HPLs) [27]. Possibly the first new integral is

$$H_{-1,0,0,1}(x) = \int_0^x \frac{dz}{z} \frac{\text{Li}_3(z)}{1+z} . \tag{16}$$

Here we use a systematic notion defining the Poincaré iterated integrals [11, 12], unlike the case in (5). The weight $w = 1$ HPLs are

$$H_0(x) = \ln(x), \quad H_1(x) = -\ln(1-x), \quad H_{-1}(x) = \ln(1+x), \tag{17}$$

with the definition of $H_{0,\dots,0}(x) = \ln^n(x)/n!$ for all x indices equal to zero. The above functions have the following representation

$$\text{Li}_n(x) = \int_0^x \omega_0^{n-1}\omega_1, \quad S_{p,n}(x) = \int_0^x \omega_0^p \omega_1^n, \quad H_{\mathbf{m}_w}(x) = \int_0^x \prod_{l=1}^k \omega_{m_l}, \tag{18}$$

where the corresponding products are non-commutative, $\mathbf{m}_w$ is of length k and $x \geq z_1 \geq \dots \geq z_m$.

Harmonic polylogarithms obey algebraic and structural relations, which will be discussed in Sect. 4. Numerical representations of HPLs were given in [42, 43].

3 Harmonic Sums

The harmonic sums are recursively defined by

$$S_{b,\mathbf{a}}(N) = \sum_{k=1}^N \frac{(\text{sign}(b))^k}{k^{|b|}} S_{\mathbf{a}}(k) , \quad S_{\emptyset}(N) = 1 , \quad b, a_i \in \mathbb{Z}\backslash\{0\}. \tag{19}$$

In physics applications they appeared early in [44, 45]. Their systematic use dates back to Refs. [25, 26]. They can be represented as a Mellin transform

$$S_{\mathbf{a}}(N) = \mathbf{M}\left[f(x)\right](N) = \int_0^1 dx\, x^{N-1}\, f(x), \quad N \in \mathbb{N}\backslash\{0\}, \tag{20}$$

where $f(x)$ denotes a linear combination of HPLs. For example,

$$S_{-2,1,1}(N) = (-1)^{N+1} \int_0^1 dx \frac{H_{0,1,1}(x) - \zeta_3}{x+1} - \text{Li}_4\left(\frac{1}{2}\right) - \frac{\ln^4(2)}{24} + \frac{\ln^2(2)\zeta_2}{4}$$
$$-\frac{7\ln(2)\zeta_3}{8} + \frac{\zeta_2^2}{8} \tag{21}$$

holds. Harmonic sums possess algebraic and structural relations, cf. Sect. 4. In the limit $N \to \infty$ they define the multiple zeta values, cf. Sect. 5. They are originally defined at integer argument N. In physical applications they emerge in the context of the light–cone expansion [46]. The corresponding operator matrix elements are analytically continued to complex values of N either from the even *or* the odd integers, cf. Sect. 9.

4 Algebraic and Structural Relations

4.1 Algebraic Relations

Algebraic relations of harmonic polylogarithms and harmonic sums, respectively, are implied by their products and depend on their index structure only, i.e. they are a consequence of the associated shuffle or quasi–shuffle (stuffle) algebras [47]. These properties are widely independent of the specific realization of these algebras. To one of us (JB) it appeared as a striking surprise, when finding the determinant-formula for harmonic sums of equal argument [26] Eqs. (157,158)

$$S_{\underbrace{a,\ldots,a}_{k}}(N) = \frac{1}{k} \sum_{l=0}^{k} S_{\underbrace{a,\ldots,a}_{l}}(N) S_{\wedge_{m=1}^{k-l}a}(N), \quad a \wedge b = \text{sign}(ab)(|a| + |b|) \tag{22}$$

also in Ramanujan's notebook [48], but for *integer sums*, which clearly differ in value from the former ones. Related relations to again different quantities were given by Faá die Bruno [49].

Iterated integrals with the same argument x obey shuffle relations w.r.t. their product,

$$H_{a_1,\ldots,a_k}(x) \cdot H_{b_1,\ldots,b_l}(x) = \sum_{\mathbf{c} \in \mathbf{a} \sqcup\!\sqcup \mathbf{b}} H_{c_1,\ldots c_{k+l}}(x). \tag{23}$$

The shuffle-operation runs over all combinations of the sets **a** and **b** leaving the order of these sets unchanged. Likewise, the (generalized) harmonic sums obey quasi-shuffle or stuffle-relations, which are found recursively using [28, 29]

$$
\begin{aligned}
\mathrm{S}_{a_1,\ldots,a_k}(x_1,\ldots,x_k;n)\,\mathrm{S}_{b_1,\ldots,b_l}(y_1,\ldots,y_l;n) = \\
\sum_{i=1}^{n} \frac{x_1^i}{i^{a_1}} \mathrm{S}_{a_2,\ldots,a_k}(x_2,\ldots,x_k;i)\,\mathrm{S}_{b_1,\ldots,b_l}(y_1,\ldots,y_l,i) \\
+\sum_{i=1}^{n} \frac{y_1^i}{i^{b_1}} \mathrm{S}_{a_1,\ldots,a_k}(x_1,\ldots,x_k,i)\,\mathrm{S}_{b_2,\ldots,b_l}(y_2,\ldots,y_l;i) \\
-\sum_{i=1}^{n} \frac{(x_1\cdot y_1)^i}{i^{a_1+b_1}} \mathrm{S}_{a_2,\ldots,a_k}(x_2,\ldots,x_k,i)\,\mathrm{S}_{b_2,\ldots,b_l}(y_2,\ldots,y_l;i)\,, \\
x_i,y_i \in \mathbb{C},a_i,b_i \in \mathbb{N}\backslash\{0\}\,.
\end{aligned}
\tag{24}
$$

The presence of trace terms in form of lower weight products in addition to the shuffled terms, cf. [50], leads to the name stuffle relations. In case the corresponding values exist, both (23,24) can be applied to the multiple zeta values or other special numbers applying the integral and sum-representations at $x = 1$ and $N \to \infty$, cf. [51]. The basis elements applying the (quasi) shuffle relations in case of the harmonic sums and polylogarithms at a given weight w can be identified by the Lyndon words [52,53]. Let $\mathfrak{A} = \{a,b,c,d,\ldots\}$ be an *ordered* alphabet and $\mathfrak{A}^*(\mathfrak{A})$ the set of words w given as concatenation products. Under the ordering of $\mathfrak{A}$ a Lyndon word is smaller than any of its suffixes. For example, the set $\{a,a,a,b,b,b\}$, $a < b$ is associated to the Lyndon words $\{aaabbb,aababb,aabbab\}$. Radford showed [54] that a shuffle algebra is freely generated by the Lyndon words. The number of Lyndon words can be counted using Witt formulae [55]. Let $\mathfrak{M}$ be a set of letters q in which the letter a_k emerges n_k times, and $n = \sum_{k=1}^{q} n_k$. The number of Lyndon words associated to this set is given by

$$
l_n(n_1,\ldots,n_q) = \frac{1}{n} \sum_{d|n_k} \mu(d) \frac{(n/d)!}{(n_1/d)!\ldots(n_q/d)!}\,.
\tag{25}
$$

Similarly one may count the basis elements occurring for all combinations at a given weight, if the alphabet has m letters:

$$
N_A(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) m^d\,,
\tag{26}
$$

where μ denotes Möbius' function [56]. In case of the harmonic sums and polylogarithms one has $m = 3$. The original number of harmonic polylogarithms is 3^w and in case of the harmonic sums $2\cdot 3^{w-1}$. Algebraic relations for the harmonic

polylogarithms and harmonic sums are implemented in the FORM-codes `summer` [25] and `harmpol` [27], HPL [57], and also `HarmonicSums.m` [29, 35].

4.2   Structural Relations

Structural relations of harmonic polylogarithms and harmonic sums are implied by operations on their arguments x and N, respectively.

4.2.1   Harmonic Polylogarithms

Harmonic polylogarithms satisfy argument-relations, as has been illustrated in (8–14) for some examples in case of the Nielsen integrals. Not all argument relations map inside the harmonic polylogarithms, however, cf. [27]. Some of them are valid only for the sub-alphabet $\{\omega_0, \omega_1\}$. While the transformation $x \to -x$ is general

$$H_{\mathbf{a}}(-x) = (-1)^p H_{-\mathbf{a}}(x), \tag{27}$$

with the last letter in $\mathbf{a}$ different from 0 and p the number of non-zero letters in $\mathbf{a}$. The transformations

$$x \to 1 - x, \quad x \to x^2 \tag{28}$$

apply to subsets only. Examples are:

$$H_{1,0,1}(1 - x) = -H_0(x)H_{0,1}(x) + 2H_{0,0,1}(x) - \zeta_2 H_0(x) - 2\zeta_3 \tag{29}$$

$$H_{1,0,0,1}\left(x^2\right) = 4\left[H_{1,0,0,1}(x) - H_{1,0,0,-1}(x) - H_{-1,0,0,1}(x) + H_{-1,0,0,-1}(x)\right]. \tag{30}$$

One may transform arguments by $x \to 1/y + i\varepsilon$,

$$H_{1,0,1}\left(\frac{1}{x}\right) = H_0(x)\left[H_{0,1}(x) + i\pi H_1(x) - 4\zeta_2 + \pi^2\right] - 2[H_{0,0,1}(x) - H_{0,1,1}(x)]$$

$$+\zeta_3] + [-H_1(x) - i\pi]H_{0,1}(x) + 2\zeta_2 H_1(x) - \frac{1}{6}H_0^3(x)$$

$$+\frac{1}{2}i\left[\pi + iH_1(x)\right]H_0^2(x). \tag{31}$$

An important general transformation is

$$x \to \frac{1 - t}{1 + t} \tag{32}$$

which acts on the HPLs but not on the subset of Nielsen-integrals. An example is:

$$
H_{1,-1,0}\left(\frac{1-x}{1+x}\right) = \frac{1}{6}H_{-1}^3(x) + H_{-1,-1,1}(x) - H_{0,-1,-1}(x) - H_{0,-1,1}(x) + \frac{15\zeta_3}{8}
$$

$$
- \frac{1}{2}\zeta_2\left[H_{-1}(x) - H_0(x)\right] - 2\left[\frac{\zeta_3}{8} - \frac{\ln(2)\zeta_2}{2}\right] - 2\ln(2)\zeta_2 .
$$

(33)

In most of these relations also HPLs at argument $x = 1$ contribute, cf. Sect. 5. Structural relations of HPLs are implemented in the packages `harmpol` [27], `HPL` [57], and `HarmonicSums.m` [29, 35].

4.2.2 Harmonic Sums

Harmonic sums obey the duplication relation

$$
S_{i_1,\dots,i_n}(N) = 2^{i_1+\dots+i_n-n}\sum_{\pm} S_{\pm i_1,\dots,\pm i_n}(2N), \;\; i_k \in \mathbb{N}\backslash\{0\} .
$$

(34)

This allows to define harmonic sums at half-integer, i.e. rational, values. Ultimately, one would like to derive expressions for $N \in \mathbb{C}$, cf. Sect. 9. Another extension is to $N \in \mathbb{R}$ [14, 26]. The representation of harmonic sums through Mellin-transforms (20) implies analyticity for a finite range around a given value of N. The Mellin-transform of a harmonic polylogarithm can thus be differentiated for N

$$
\frac{d}{dN}\int_0^1 dx\, x^{N-1}H_{\mathbf{a}}(x) = \int_0^1 dx\, x^{N-1}H_0(x)H_{\mathbf{a}}(x) .
$$

(35)

In turn, the shuffling relation (23) allows to represent the r.h.s. in (35) as the Mellin-transform of other HPLs. It turns out that differentiation of harmonic sums for N is closed under additional association of the multiple zeta values [14]. The number of basis elements by applying the duplication relation (H), resp. its combination with the algebraic relations is [58]

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

(36)

Differentiation in combination with the other relation yields

$$
N_D(w) = 4\cdot 3^{w-1}, N_{DH}(w) = 4\cdot 3^{w-2} - 2^{w-2}, N_{ADH}(w) = N_{AH}(w) - N_{AH}(w-1).
$$

(37)

Let us close with a remark on observables or related quantities in physics which are calculated to a certain loop level and can be thoroughly expressed in terms of harmonic sums. As a detailed investigation of massless and single mass two-loop quantities showed [40] seven basic functions of up to weight $w = 4$, cf. [14], are sufficient to express all quantities. The three-loop anomalous dimensions [41] contributing to the $1/\varepsilon$ poles of the corresponding matrix elements require 15 functions of up to weight $w = 5$ and further 20 basic functions are needed to also express the massless Wilson coefficients [7] in deep-inelastic scattering [59], cf. Ref. [60]. Despite of the complexity of these calculations finally a rather compact structure is obtained for the representation of the results. Structural relations of harmonic sums are implemented in the package `HarmonicSums.m` [29, 35].

5   Multiple Zeta Values

The multiple zeta values (MZVs) [61, 62][1] are obtained by the limit $N \to \infty$ of the harmonic sums

$$\lim_{N \to \infty} S_{\mathbf{a}}(N) = \sigma_{\mathbf{a}} \tag{38}$$

and may also be represented in terms of linear combinations of harmonic poly-logarithms $H_{\mathbf{b}}(1)$ over the alphabet $\{\omega_0, \omega_1, \omega_{-1}\}$.[2] In the former case one usually includes the divergent harmonic sums since all divergent contributions are uniquely represented in terms of polynomials in $\sigma_1(\infty) \equiv \sigma_0$ due to the algebraic relations. Likewise, not all harmonic polylogarithms can be calculated at $x = 1$, requiring their re-definition in terms of distributions. Some examples for MZVs, which already appear in case of Nielsen integrals, are:

$$\mathrm{Li}_n(1) = \zeta_n \tag{39}$$

$$\mathrm{Li}_n(-1) = -\left(1 - \frac{1}{2^{n-1}}\right)\zeta_n \tag{40}$$

$$\mathsf{S}_{1,p}(1) = \zeta_{p+1} \tag{41}$$

$$\mathsf{S}_{1,2}(-1) = \frac{1}{8}\zeta_3 \tag{42}$$

$$\mathrm{Li}_2\left(\frac{1}{2}\right) = \frac{1}{2}\left[\zeta_2 - \ln^2(2)\right] \tag{43}$$

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[1]For a detailed account on the literature on MZVs see [63, 64] and the surveys Ref. [65].

[2]The numbers associated with this alphabet are sometimes also called Euler-Zagier values and those of the sub-alphabet $\{\omega_0, \omega_1\}$ multiple zeta values.

$$\text{Li}_3\left(\frac{1}{2}\right) = \frac{7}{8}\zeta_3 - \frac{1}{2}\zeta_2 \ln(2) + \frac{1}{6}\ln^3(2) \tag{44}$$

$$\mathsf{S}_{2,2}(1) = \frac{1}{10}\zeta_2^2 \tag{45}$$

$$\mathsf{S}_{2,2}(-1) = -\frac{3}{4}\zeta_2^2 + 2\text{Li}_4\left(\frac{1}{2}\right) + \frac{7}{4}\zeta_3 \ln(2) - \frac{1}{2}\zeta_2 \ln^2(2) + \frac{1}{12}\ln^4(2) \tag{46}$$

$$\mathsf{S}_{1,3}(-1) = -\frac{2}{5}\zeta_2^2 + \text{Li}_4\left(\frac{1}{2}\right) + \frac{7}{8}\zeta_3 \ln(2) - \frac{1}{4}\zeta_2 \ln^2(2) + \frac{1}{24}\ln^4(2) . \tag{47}$$

In case of physics applications, MZVs played a role in loop calculations rather early, cf. [66]. Since for $\text{Li}_m(1/2)$ for $m = 2, 3$ these numbers are not elementary, (46, 47) seem to fail to provide a corresponding relation for $m = 4$. Similarly, for larger values of m also no reduction has been observed.

A central question concerns the representation of harmonic sums in terms of polynomial bases. This has been analyzed systematically in [63, 67].[3] For MZVs over $\{0, 1\}$ a proof on the maximum of basis elements at fixed weight w has been given in Refs. [68]. At the lowest weights the shuffle and stuffle relations imply all relations for the MZVs. Starting with weight $w = 8$ one also needs the duplication relation (34), and from weight $w = 12$ also the generalized duplication relations Sect. 4.1 in [63]. The latter are closely related to the conformal transformation relations of the HPLs at $x = 1$, see (32). Let us give one example for the combined use of the shuffle and stuffle relation for illustration, [51][4]:

$$\text{shuffle} : \quad \zeta_{2,1}\zeta_2 = 6\zeta_{3,1,1} + 2\zeta_{2,2,1} + \zeta_{2,1,2}$$

$$\text{stuffle} : \quad \zeta_{2,1}\zeta_2 = 2\zeta_{2,2,1} + \zeta_{41} + \zeta_{2,3} + \zeta_{2,1,2}$$

$$\implies \quad \zeta_{3,1,1} = \frac{1}{6}\left[\zeta_{4,1} + \zeta_{2,3} - \zeta_{2,2,1}\right] . \tag{48}$$

Finally one derives a basis for the MZVs using the above relations. Up to weight $w = 7$ reads, cf. [25],

$$\left\{ (\sigma_1(\infty), \ln(2)) ; \zeta_2 ; \zeta_3 ; \text{Li}_4\left(\tfrac{1}{2}\right) ; \left(\zeta_5, \text{Li}_5\left(\tfrac{1}{2}\right)\right) ; \left(\text{Li}_6\left(\tfrac{1}{2}\right), \sigma_{-5,-1}\right) ; \right.$$

$$\left. \left(\zeta_7, \text{Li}_7\left(\tfrac{1}{2}\right), \sigma_{-5,1,1}, \sigma_{-5,1,1}\right) ; \right\} \tag{49}$$

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[3]For some aspects of the earlier development including results by the Leuven-group, Zagier, Broadhurst, Vermaseren and the Lille-group, see [63].

[4]Here the $\zeta_{\mathbf{a}}$-values are defined $\zeta_{a_1,\dots,a_m} = \sum_{n_1 > n_2 > \dots > n_m}^{\infty} \prod_{k=1}^{m} n_k^{-a_1}$.

In [63] bases were calculated up to $w = 12$ for the alphabet $\{0, 1, -1\}$ and to $w = 22$ for the alphabet $\{0, 1\}$ in explicit form resp. for $w = 24$ restricting to basis elements only. In the latter case the conjecture by Zagier [62] that the shuffle, stuffle and duplication relations were the only ones was confirmed up to the weights quoted. For these cases counting relations were conjectured in Refs. [69, 70]. One may represent the basis for the MZVs over the alphabets $\{0, 1\}$ resp. $\{0, 1, -1\}$ by polynomial bases or count just the factors appearing in these polynomials of special numbers occurring newly in the corresponding weight, which is called Lyndon-basis [63]. In the first case the basis for the MZVs[$\{0, 1\}$] is conjectured to be counted by the Padovan numbers $\hat{P}_k$ [71] generated by

$$\frac{1 + x}{1 - x^2 - x^3} = \sum_{k=0}^{\infty} x^k \hat{P}_k, \quad \hat{P}_1 = \hat{P}_2 = \hat{P}_3 = 1. \tag{50}$$

In case of the Lyndon basis the Perrin numbers P_k appear [72]

$$\frac{3 - x^2}{1 - x^2 - x^3} = \sum_{k=0}^{\infty} x^k \hat{P}_k, \quad P_1 = 0, P_2 = 2, P_3, = 3. \tag{51}$$

Both the above sequences obey the Fibonacci-recurrence [73]

$$P_d = P_{d-2} + P_{d-3}, \quad d \geq 3. \tag{52}$$

The length of the Lyndon basis at weight w is given by

$$l(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) P_d. \tag{53}$$

Hoffman [74] conjectured that all MZVs over the alphabet $\{0, 1\}$ can be represented over a basis of MZVs carrying 2 and 3 as indices only. This has been confirmed up to $w = 24$. An explicit proof has been given in [75].

The polynomial basis of the MZVs[$\{0, 1, -1\}$] is conjectured to be counted by the Fibonacci numbers [76]

$$f_d = \frac{1}{\sqrt{5}} \left[\left(\frac{1 + \sqrt{5}}{2}\right)^d - \left(\frac{1 - \sqrt{5}}{2}\right)^d \right] \tag{54}$$

which obey

$$\frac{x}{1 - x - x^2} = \sum_{k=0}^{\infty} x^k f_k. \tag{55}$$

For the corresponding Lyndon basis the counting relation

$$l(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) L_d \tag{56}$$

is conjectured [69, 70], where L_d are the Lucas numbers [77],

$$L_d = \left(\frac{1+\sqrt{5}}{2}\right)^d + \left(\frac{1-\sqrt{5}}{2}\right)^d \tag{57}$$

$$\frac{2-x}{1-x-x^2} = \sum_{k=0}^{\infty} x^k L_k, \tag{58}$$

$$L_d = L_{d-1} + L_{d-2}, d \geq 4, \quad L_1 = 1, L_2 = 3, L_3 = 4. \tag{59}$$

There is a series of Theorems proven on the MZVs, see also [63], which can be verified using the data base [63]. The duality theorem [62] in case of the alphabet $\{\omega_0, \omega_1\}$ states

$$H_{\mathbf{a}}(1) = H_{\mathbf{a}^\dagger}(1), \quad \mathbf{a}^\dagger = \mathbf{a}_{0 \longleftrightarrow 1}^T. \tag{60}$$

In case of the alphabet $\{\omega_0, \omega_1, \omega_{-1}\}$ it is implied by the transformation (32), see [63]. Another relation is the sum theorem, Refs. [78, 79],

$$\sum_{i_1+\ldots+i_k=n, i_1>1} \zeta_{i_1,\ldots,i_k} = \zeta_n. \tag{61}$$

The sum-theorem was conjectured in [80], cf. [81]. For its derivation using the Euler connection formula for polylogarithms, cf. [82].

Further identities are given by the derivation theorem, [80, 83]. Let $I = (i_1, \ldots, i_k)$ any sequence of positive integers with $i_1 > 1$. Its derivation $D(I)$ is given by

$$D(I) = (i_1+1, i_2, \ldots, i_k) + (i_1, i_2+1, \ldots, i_k) + \ldots (i_1, i_2, \ldots, i_k+1)$$

$$\zeta_{D(I)} = \zeta_{(i_1+1, i_2, \ldots, i_k)} + \ldots + \zeta_{(i_1, i_2, \ldots, i_k+1)}. \tag{62}$$

The derivation theorem states

$$\zeta_{D(I)} = \zeta_{\tau(D(\tau(I)))}, \tag{63}$$

where τ denotes the duality-operation, cf. (60). An index-word w is called admissible, if its first letter is not 1. The words form the set $\mathfrak{H}^0$. $|w| = \mathsf{w}$ is the weight and $d(w)$ the depth of w. For the MZVs the words w are build in terms of concatenation products $x_0^{i_1-1} x_1 x_0^{i_2-1} x_0 \ldots x_0^{i_k-1} x_1$. The height of a word, $\mathrm{ht}(w)$, counts the number

of (non-commutative) factors $x_0^a x_1^b$ of w. The operator D and its dual $\overline{D}$ act as follows [84],

$$D x_0 = 0, \quad D x_1 = x_0 x_1, \quad \overline{D} x_0 = x_0 x_1, \quad \overline{D} x_1 = 0 \, .$$

Define an anti-symmetric derivation

$$\partial_n x_0 = x_0 (x_0 + x_1)^{n-1} x_1 \, .$$

A generalization of the derivation theorem was given in [83, 85]. The identity

$$\zeta(\partial_n w) = 0 \tag{64}$$

holds for any $n \geq 1$ and any word $w \in \mathfrak{H}^0$. Further theorems are the Le–Murakami theorem, [86], the Ohno theorem, [87], which generalizes the sum- and duality theorem, the Ohno–Zagier theorem, [88], which covers the Le–Murakami theorem and the sum theorem, which generalizes a theorem by Hoffman [80, 81], and the cyclic sum theorem, [89].

There are also relations for MZVs at repeated arguments, cf. [51, 84, 90], on which examples are:

$$\zeta(\{2\}_n) = \frac{2(2\pi)^{2n}}{(2n+1)!} \frac{1}{2} \tag{65}$$

$$\zeta(2, \{1\}_n) = \zeta(n+2) \tag{66}$$

$$\zeta(\{3, 1\}_n) = \frac{1}{4^n} \zeta(\{4\}_n) = \frac{2\pi^{4n}}{(4n+2)!} \tag{67}$$

$$\zeta(\{10\}_n) = \frac{10(2\pi)^{2n}}{(10n+5)!} \left[1 + \left(\frac{1 + \sqrt{5}}{2} \right)^{10n+5} + \left(\frac{1 - \sqrt{5}}{2} \right)^{10n+5} \right] \, . \tag{68}$$

Finally, we mention a main conjecture for the MZVs over $\{0, 1\}$. Consider tuples $\mathbf{k} = (k_1, \ldots, k_r) \in \mathbb{N}^r, k_1 \geq 1$. One defines

$$\mathscr{Z}_0 := \mathbb{Q}$$

$$\mathscr{Z}_1 := \{0\}$$

$$\mathscr{Z}_w := \sum_{|\mathbf{k}| = w} \mathbb{Q} \cdot \zeta(\mathbf{k}) \subset \mathbb{R} \, . \tag{69}$$

If further

$$\mathscr{Z}^{\text{Go}} := \sum_{w=0}^{\infty} \mathscr{Z}_w \subset \mathbb{R} \quad \text{(Goncharov)} \tag{70}$$

$$\mathscr{Z}^{\mathrm{Ca}} := \bigoplus_{w=0}^{\infty} \mathscr{Z}_w \qquad \text{(Cartier)} \tag{71}$$

the conjecture states

(a) $\mathscr{Z}^{\mathrm{Go}} \cong \mathscr{Z}^{\mathrm{Ca}}$. There are no relations over $\mathbb{Q}$ between the MZVs of different weight w.
(b) $\dim \mathscr{Z}_w = d_w$, with $d_0 = 1, d_1 = 0, d_2 = 1, d_w = d_{w-2} + d_{w-3}$.
(c) All algebraic relations between MZVs are given by the extended double-shuffle relations [91], cf. also [92]. If this conjecture turns out to be true all MZVs are irrational numbers.

Let us also mention a few interesting relations for $\mathrm{Li}_2(z)$ for special arguments found by Ramanujan [93], which are of use e.g. in massive calculations at three-loops [94]. These numbers relate to constants beyond the MZVs, which occur for generalized sums and their extension allowing for binomial and inverse binomial weights:

$$\mathrm{Li}_2\left(\frac{1}{3}\right) - \mathrm{Li}_2\left(\frac{1}{9}\right) = \frac{\pi^2}{18} - \frac{1}{6}\ln^2(3) \tag{72}$$

$$\mathrm{Li}_2\left(-\frac{1}{2}\right) + \frac{1}{6}\mathrm{Li}_2\left(\frac{1}{9}\right) = -\frac{\pi^2}{18} + \ln(2)\ln(3) - \frac{1}{2}\ln^2(2) - \frac{1}{3}\ln^2(3) \tag{73}$$

$$\mathrm{Li}_2\left(\frac{1}{4}\right) + \frac{1}{3}\mathrm{Li}_2\left(\frac{1}{9}\right) = \frac{\pi^2}{18} + 2\ln(2)\ln(3) - 2\ln^2(2) - \frac{2}{3}\ln^2(3) \tag{74}$$

$$\mathrm{Li}_2\left(-\frac{1}{3}\right) - \frac{1}{3}\mathrm{Li}_2\left(\frac{1}{9}\right) = -\frac{\pi^2}{18} + \frac{1}{6}\ln^2(3) \tag{75}$$

$$\mathrm{Li}_2\left(-\frac{1}{8}\right) + \frac{1}{3}\mathrm{Li}_2\left(\frac{1}{9}\right) = -\frac{1}{2}\ln^2\left(\frac{9}{8}\right) . \tag{76}$$

For further specific numbers, which occur in the context of Quantum Field Theory calculations see also Sects. 6.3, 7, and 9.

6 Generalized Harmonic Sums and Polylogarithms

6.1 Generalized Harmonic Sums

Generalized harmonic sums, also called S-sums, are defined by [28, 29, 95]

$$S_{a_1,\ldots,a_k}(x_1,\ldots,x_k;N) = \sum_{i_1=1}^{N} \frac{x_1^{i_1}}{i_1^{a_1}} S_{a_2,\ldots,a_k}(x_2,\ldots,x_k;i_1),$$

$$S_{\emptyset} = 1 , \quad x_i \in \mathbb{R}\backslash\{0\}, \quad a_i \in \mathbb{N}\backslash\{0\} \tag{77}$$

and form a quasi-shuffle and a Hopf algebra [96] under the multiplication (24) [28]. The multiplication relation in general leads outside the weight sets $\{a_i\}$, $\{b_i\}$. The S-sums cover (together with the limit $N \to \infty$) the classical polylogarithms, the Nielsen functions, the harmonic polylogarithms, the multiple polylogarithms [97], the two-dimensional HPLs [98], and the MZVs [28]. In Ref. [28] four algorithms were presented allowing to perform the ε-expansion of classes of sums in terms of S-sums, which were coded in two packages [99, 100]. In this way the ε-expansion can be performed using convergent serial representations for the generalized hypergeometric functions $_P F_Q$, The Appell-functions $F_{1,2}$, and the Kampé de Fériet function [101].

They can be represented in terms of a Mellin transformation over $x \in [0, x_1 \ldots x_k]$ [29]. E.g. the single sums are given by

$$S_m(b; N) = \int_0^b \frac{dx_m}{x_m} \ldots \int_0^{x_3} \frac{dx_2}{x_2} \int_0^{x_2} dx_1 \frac{x_1^N - 1}{x_1 - 1} . \tag{78}$$

Generalized harmonic sums obey the duplication relation

$$\sum S_{a_m,\ldots,a_1}(\pm b_m, \ldots, \pm b_1; 2N) = \frac{1}{2^{\sum_{i=1}^m a_i - m}} S_{a_m,\ldots,a_1}(b_m^2, \ldots, b_1^2; N) , \tag{79}$$

where the sum on the left hand side is over the 2^m possible combinations concerning $\pm$ and $a_i \in \mathbb{N}$, $b_i \in \mathbb{R} \backslash \{0\}$ and $n \in \mathbb{N}$. They also obey differential relations w.r.t. N, supplementing their set with the generalized harmonic sums at infinity, resp. of the generalized harmonic polylogarithms at $x = 1$. The mapping will usually also require objects with different weights x_i. Examples are [29]:

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

$$\frac{\partial}{\partial N} S_3\left(\tfrac{1}{4}; N\right) = 12 \left[-S_{3,1}\left(\tfrac{1}{2}, \tfrac{1}{2}; N\right) - \frac{1}{2} \frac{\partial}{\partial N} S_{2,1}\left(\tfrac{1}{2}, \tfrac{1}{2}; N\right) - \frac{1}{2} H_{1,0}\left(\tfrac{1}{2}\right) S_2\left(\tfrac{1}{2}; N\right) \right.$$

$$+ H_0\left(\tfrac{1}{2}\right) S_{2,1}\left(\tfrac{1}{2}, \tfrac{1}{2}; N\right) - \frac{1}{2} H_{\frac{1}{2}}\left(\tfrac{1}{4}\right) H_{0,1,0}\left(\tfrac{1}{2}\right) + \frac{1}{12} H_{0,0,1,0}\left(\tfrac{1}{4}\right)$$

$$\left. + \frac{1}{2} H_{\frac{1}{2},0,1,0}\left(\tfrac{1}{4}\right) - \frac{1}{12} H_0\left(\tfrac{1}{4}\right) S_3\left(\tfrac{1}{4}; N\right) - \frac{1}{4} S_2\left(\tfrac{1}{2}; N\right)^2 \right] . \tag{80}$$

The counting relations for the basis elements are

$$N_D(w) = N_S(w) - N_S(w - 1), \qquad N_{A,D}(w) = N_A(w) - N_A(w - 1), \tag{81}$$

where $N_S = (n - 1) \cdot n^{w-1}$ denotes the number of sums, given n letters in the alphabet, and N_A the basis elements after applying the algebraic equations. Explicit bases for a series of alphabets have been calculated in [29].

6.2 Generalized Harmonic Polylogarithms

Generalized harmonic polylogarithms are defined as the Poincaré-iterated integrals [11, 12]

$$H_{\mathbf{a}}(x) = \int_0^x \prod_{j=1}^m \frac{dz_j}{|a_j| - \text{sign}(a_j) z_j}, \quad a_j \in \mathbb{C}, \quad z_j \geq z_{j+1}. \tag{82}$$

For $a_j \in \mathbb{R}, 0 < a_j < 1, x > 1$ (82) is defined as Cauchy principal value only. Already A. Jonquière [12] has studied integrals of this type. Sometimes they are also called Chen-iterated integrals, cf. [11], or Goncharov polylogarithms [97].

The Mellin transforms of generalized harmonic polylogarithms map onto generalized harmonic sums [29]. Furthermore, the generalized harmonic polylogarithms obey various argument relations similar to the case if the HPLs, cf. Sect. 4.2.1, as

$$x + b \to x \tag{83}$$

$$b - x \to x \tag{84}$$

$$\frac{1-x}{1+x} \to x \tag{85}$$

$$kx \to x \tag{86}$$

$$\frac{1}{x} \to x. \tag{87}$$

6.3 Relations Between S-Sums at Infinity

S-sums at infinity exhibit a more divergent behaviour than harmonic sums if $a_1 > 1$. The degree of divergence is then at least $\propto a_1^N$, cf. Sect. 9. In the following we will discuss only convergent S-sums at infinity. They obey stuffle and shuffle relations, the duplication relation $N \to 2N$, and the duality relations for the generalized polylogarithms [29]

$$1 - x \to x \tag{88}$$

$$\frac{1-x}{1+x} \to x \tag{89}$$

$$\frac{c-x}{d+x} \to x, \quad c, d \in \mathbb{R}, d \neq 1. \tag{90}$$

Equation (88) implies

$$H_{a_1,\dots,a_k}(1) = H_{1-a_1,\dots,1-a_k}(1), \quad a_k \neq 0. \tag{91}$$

Examples for ([89](#), [90](#)) are:

$$S_1 \left(\tfrac{1}{2}; \infty \right) = -S_{-1}(\infty) \equiv \ln(2) \tag{92}$$

$$S_1 \left(\tfrac{1}{8}; \infty \right) = -S_{-1}(\infty) + S_1 \left(-\tfrac{1}{2}; \infty \right) . \tag{93}$$

In various cases S-sums at infinity reduce to MZVs, cf. also [102],

$$S_{1,1,1} \left(\tfrac{1}{2}, 2, 1; \infty \right) = \frac{3}{2} \zeta_2 \ln(2) + \frac{7}{4} \zeta_3 \tag{94}$$

$$S_{2,1} \left(\tfrac{1}{2}, 1; \infty \right) = -\frac{1}{2} \ln(2) \zeta_2 + \zeta_3 \tag{95}$$

$$S_m \left(\tfrac{1}{2}; \infty \right) = \mathrm{Li}_m \left(\tfrac{1}{2} \right) . \tag{96}$$

Otherwise, new basis elements occur which have both representations in infinite sums and iterated integrals. Using the above relations bases for different sets of S-sums at infinity were calculated in [102].

7 Cyclotomic Harmonic Sums and Polylogarithms and Their Generalization

The alphabet of the harmonic polylogarithms ([15](#)) contains two differential forms with denominators, which form the first two cyclotomic polynomials: $(1 - x)$ and $(1 + x)$. It turns out that quantum field theoretic calculations are also related to cyclotomic harmonic polylogarithms and sums [103]. Cyclotomic polynomials are defined by

$$\Phi_n(x) = \frac{x^n - 1}{\displaystyle\prod_{d|n, d<n} \Phi_d(x)} , \quad d, n \in \mathbb{N}_+ \tag{97}$$

and the generating alphabet reads

$$\mathfrak{A} = \left\{ \frac{dx}{x} \right\} \cup \left\{ \frac{x^l dx}{\Phi_k(x)} \,\middle|\, k \in \mathbb{N}_+, 0 \le l < \varphi(k) \right\} , \tag{98}$$

where $\Phi_k(x)$ denotes the kth cyclotomic polynomial [104], and $\varphi(k)$ denotes Euler's totient function [105]. The Poincaré iterated integrals over the alphabet ([98](#)) are called cyclotomic harmonic polylogarithms, cf. [30]. Due to the regularity of $1/\Phi_n(x)$ for $x \in [0, 1]$, except for $\Phi_1(x)$, no more singularities appear beyond those known in the case of the usual harmonic polylogarithms (or Nielsen integrals). Cyclotomic harmonic polylogarithms obey shuffle relations, cf. Sect. [4](#).

The cyclotomic harmonic sums [30] are related to the cyclotomic harmonic polylogarithms via a Mellin transform (20). The generalized cyclotomic harmonic sums are given by

$$S_{\{a_1,b_1,c_1\},\dots,\{a_l,b_l,c_l\}}(s_1,\dots,s_l;N) =$$

$$\sum_{k_1=1}^{N} \frac{s_1^k}{(a_1 k_1 + b_1)^{c_1}} S_{\{a_2,b_2,c_2\},\dots,\{a_l,b_l,c_l\}}(s_2,\dots,s_l;k_1), \quad S_\emptyset = 1, \qquad (99)$$

where $a_i, c_i \in \mathbb{N}_+, b_i \in \mathbb{N}, \ \ s_i \in \mathbb{R}\backslash\{0\}, a_i > b_i$; the weight of this sum is defined by $c_1 + \cdots + c_l$ and $\{a_i, b_i, c_i\}$ denote lists, not sets. If $s_i = \pm 1$ these are the usual cyclotomic harmonic sums. The simplest cyclotomic sums are the single sums

$$S_{\{a_1,b_1,c_1\}}(\pm 1; N) = \sum_{k=1}^{N} \frac{(\pm 1)^k}{(a_1 k + b_1)^{c_1}} , \qquad (100)$$

i.e. harmonic sums with cyclic gaps in the summation. The cyclotomic harmonic sums obey quasi-shuffle relations (A).

Beyond this the cyclotomic harmonic sums obey structural relations implied by differentiation for the upper summation bound N, (D), which require to also consider their values at $N \rightarrow \infty$. There are, furthermore, multiple argument relations, cf. [30], decomposing $S_{a_i,b_i,c_i}(k \cdot N)$, called synchronization (M), and two duplication relations (H_1, H_2). Let us consider the cyclotomic harmonic sums implied by the letters

$$\frac{1}{k^{l_1}}, \quad \frac{(-1)^k}{k^{l_2}}, \quad \frac{1}{(2k+1)^{l_3}}, \quad \frac{(-1)^k}{(2k+1)^{l_4}} . \qquad (101)$$

The length of the basis can be calculated by

$$N_S(w) = 4 \cdot 5^{w-1} \qquad (102)$$

$$N_A(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 5^d \qquad (103)$$

$$N_D(w) = N_S(w) - N_S(w-1) \qquad (104)$$

$$N_{A,D}(w) = N_A(w) - N_A(w-1) \qquad (105)$$

$$N_{A,D,M,H_1,H_2}(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) (5^2 - 3 \cdot 2^d) - \frac{1}{w-1} \sum_{d|w-1} \mu\left(\frac{w-1}{d}\right)(5^2 - 3 \cdot 2^d),$$

$$(106)$$

where $N_S(w)$ denotes the number of all sums. One may calculate the asymptotic representation of the cyclotomic harmonic sums analytically. Here also the values of cyclotomic sums at $N \to \infty$ occur. The singularities of the cyclotomic harmonic sums with $s_k = \pm 1$ are situated at the non-positive integers.

The cyclotomic sums for $N \to \infty$ are denoted by $\sigma_{\{a_1,b_1,c_1\},...,\{a_l,b_l,c_l\}}(s_1,\dots,s_l)$. For $\forall \, |s_k| \leq 1$ divergent series do only occur if $a_1 = b_1$ and $c_1 = 1$, where the degree of divergence is given by σ_0 as in the case of the harmonic sums and can be represented algebraically. They are related to the values of the cyclotomic harmonic polylogarithms at $x = 1$. At $w = 1$ the regularized sums may be given in terms of $\psi(k/l)$ and for higher weights in terms of $\psi^{(m)}(k/l), m \geq 1$. If l is an integer for which the l-polygon is constructable one obtains representations in terms of algebraic numbers and logarithms of algebraic numbers, as well as π [30]. In this way, ζ_2 being a basis element in case of the MZVs, looses its role. At depth $w = 2$ Catalan's constant [106] with

$$\sigma_{2,1,-2} = -1 + \mathbf{C} \tag{107}$$

contributes. At higher depth new numbers emerge, which partly can be given integral representations involving polylogarithms and roots of the integration variable x. The cyclotomic sums at infinity, as real representations, are closely related to the infinite generalized harmonic sums at weights s_k which are roots of unity, cf. also [107]. In [30] basis representations were worked out for $w = 1, 2$ for the lth roots, $l \in [1, 20]$, cf. also [108]. Counting relations for bases of the cyclotomic sums at infinity have also been derived in Ref. [30].

8 Nested Binomial and Inverse-Binomial Harmonic Sums and Associated Polylogarithms

In massive calculations further extensions to the nested sums and iterated integrals being discussed in the previous sections occur. Here summation terms of the kind $S_{\mathbf{a},\mathbf{b},\mathbf{c}}(\mathbf{x}; k)$, or their linear combinations are modulated by

$$S_{\mathbf{a},\mathbf{b},\mathbf{c}}(\mathbf{x}; k) \to \binom{2k}{k} S_{\mathbf{a},\mathbf{b},\mathbf{c}}(\mathbf{x}; k)$$

$$S_{\mathbf{a},\mathbf{b},\mathbf{c}}(\mathbf{x}; k) \to \frac{1}{\binom{2k}{k}} S_{\mathbf{a},\mathbf{b},\mathbf{c}}(\mathbf{x}; k) , \tag{108}$$

building iterated sums [94]. Sums of this kind occur in case of V-type three-loop graphs for massive operator matrix elements. Simpler sums are obtained in case of three-loop graphs with two fermionic lines of equal mass. Single sums of this kind

have been considered earlier, see e.g. [109]. One may envisage generalizations of (108) in choosing for the binomial a general hypergeometric term, i.e. a function, the ratio of which by all shifts of arguments being rational. The association of the corresponding iterated integrals in the foregoing cases has been found easily. Here the situation is more difficult and the functions representing these iterated sums are found in establishing differential equations [110]. It is found in the cases occurring in Ref. [94] that the corresponding differential equations finally factorize and one obtains iterated integrals over alphabets which also contain root-valued letters

$$\frac{1}{\sqrt{(x+a)(x+b)}}, \quad \frac{1}{\sqrt{(x+a)(x+b)}}\frac{1}{x+c}, \quad a,b,c \in \mathbb{Q} \qquad (109)$$

beyond those occurring in case of the generalized (cyclotomic) polylogarithms. A few examples of this type have been considered in [111]. The relative transcendence of the nested sums and iterated integrals has been proven. The V-type three-loop graphs require alphabets of about 30 root-valued letters. The corresponding nested sums do partly diverge $\propto a^N, a \in \mathbb{N}, a \geq 2$. A typical example for a nested binomial sums is given by:

$$\sum_{i=1}^{N}\binom{2i}{i}(-2)^i \sum_{j=1}^{i}\frac{1}{j\binom{2j}{j}}S_{1,2}\left(\tfrac{1}{2},-1;j\right) \qquad (110)$$

$$= \int_0^1 dx \frac{x^N - 1}{x-1}\sqrt{\frac{x}{8+x}}\left[\mathrm{H}^*_{w_{17},-1,0}(x) - 2\mathrm{H}^*_{w_{18},-1,0}(x)\right]$$

$$+ \frac{\zeta_2}{2}\int_0^1 dx \frac{(-x)^N - 1}{x+1}\sqrt{\frac{x}{8+x}}\left[\mathrm{H}^*_{12}(x) - 2\mathrm{H}^*_{13}(x)\right] + c_3\int_0^1 dx \frac{(-8x)^N - 1}{x+\tfrac{1}{8}}\sqrt{\frac{x}{1-x}},$$

with $c_3 = \sum_{j=0}^{\infty} S_{1,2}\left(\tfrac{1}{2},-1;j\right)(j!)^2/j/(2j)!/\pi$ one of the specific constants emerging in case of these sums. Here the iterated integrals H^* extend to $x = 1$ as firm bound, contrary to the cases discussed before where $x = 0$ is chosen. Here the new letters w_k are

$$w_{12} = \frac{1}{\sqrt{x(8-x)}}, \quad w_{13} = \frac{1}{(2-x)\sqrt{x(8-x)}},$$

$$w_{17} = \frac{1}{\sqrt{x(8+x)}}, \quad w_{18} = \frac{1}{(2+x)\sqrt{x(8+x)}}. \qquad (111)$$

The representations over the letters (109) are needed to eliminate the power growth $\propto a^N$ of these sums and can be used to derive the asymptotic representation at large values of N. While the terms $\propto 8^N$ and $\propto 4^N$ cancel, it may occur that individual scalar diagrams exhibit contributions $\propto 2^N$, cf. [94]. This behaviour is expected to cancel in the complete physics result.

Fig. 2 Path of the contour integral (112)
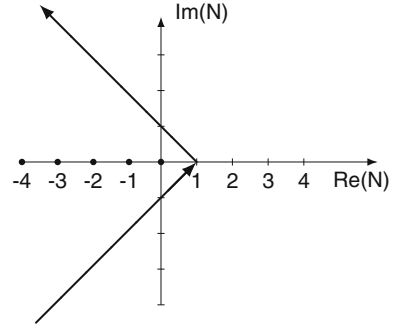
9 Analytic Continuation of Harmonic Sums

The loop-corrections to various physical quantities take a particular simple form in Mellin-space being expressed in terms of harmonic sums and their generalizations. Moreover, in this representation the renormalization group equations can be solved analytically, cf. [59,112]. For a wide variety of non-perturbative parton distributions Mellin-space representations can be given as well, see e.g. [113].

Thus one obtains complete representations for observables in N-space. In case of the perturbative part, the singularities are situated at the integers $N \leq N_0$, with usually $N_0 = 1$, see e.g. [114]. The harmonic sums possess a unique polynomial representation in terms of the sum $S_1(N)$ and harmonic sums which can be represented as Mellin transforms having a representation by factorial series [115, 116]. They are transformed to x-space by a single precise numerical contour integral around the singularities of the problem to compare with the data measured in experiment. The analytic continuation of the perturbative evolution kernels and Wilson coefficients from even or odd integers to complex values of N is unique [117].[5] To perform this integral a representation of the harmonic sums for $N \in \mathbb{C}$ is required. Accurate numeric representations up to $w = 5$ have been given in [118], see also [119]. Arbitrary precise representations can be obtained using the analytic expressions for the asymptotic representation [14, 60] together with the recursion relations given in Sect. 3. These are given up to $w = 8$ in [58]. A path to perform the inverse Mellin transform

$$f(x) = \frac{1}{\pi} \int_0^\infty dz \, \mathsf{Im} \left[e^{i\phi} \, x^{-C} \mathbf{M}[f](N = C) \right], \quad C = c + z e^{i\phi} \qquad (112)$$

is shown in Fig. 2. The asymptotic representations can also be obtained in analytic form for the S-sums [29], cyclotomic (S)-sums [30], as well as for the nested binomial cyclotomic S-sums [94, 110].

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[5]For a detailed proof also in case of generalized harmonic sums see [29].

In case the expressions in N-space result from Mellin transforms of functions $f(x) \sim x^\alpha, \alpha \in\ ]0, 1[$ the singularities are shifted by α. This is usually the case for the non-perturbative parton distribution functions, but also in case of some root-valued harmonic polylogarithms considered in Sect. 8.

The inverse Mellin-transform cannot be performed in the above way for integrands which do not vanish sufficiently fast enough as $|N| \to \infty$. Contributions of this kind are those leading to distribution-valued terms in x-space as to $\delta(1 - x)$, $[\ln^k(1 - x)/(1 - x)]_+$ the Dirac δ-distribution and the $+$-distribution defined by

$$\int_0^1 dx\ [f(x)]_+\ g(x) = \int_0^1 dx\ [g(x) - g(1)]\ f(x)\ . \tag{113}$$

Also for terms which grow like $a^N, a \in \mathbb{R}, a > 1$ in N-space, the Mellin transform cannot be performed numerically in general. They are not supposed to emerge in physical observables. The physical quantities in hadronic scattering contain the parton distribution functions, which, however, damp according contributions occurring in the evolution kernels sufficiently. On the other hand, the inverse Mellin transform can always be performed analytically changing form nested sum-representations in N-space to iterated integral representations in x-space as has been outlined before.

10 Conclusions

Feynman integrals in Quantum Field Theories generate a hierarchic series of special functions, which allow their unique representation. They emerge in terms of special nested sums, iterated integrals and numbers. Their variety gradually extends enlarging the number of loops and legs, as well as the associated mass scales. The systematic exploration of these structures has been started about 15 years ago and several levels of complexity have been unraveled since. The relations of the various associated sums and integrals are schematically illustrated in Fig. 3 and are widely explored. Many relations are implied by the shuffle resp. stuffle algebras, others are structural relations. The number of relations grows with the number of admissible operations.

A large amount of transformations and relations between the different quantities being discussed in this article are encoded in the package `HarmonicSums` [29, 35] for public use. For newly emerging structures the algebraic relations are easily generalized but they will usually apply structural relations of a new kind. With the present programme revealing their strict (atomic) structure, they are fully explored analytically and Feynman's original approach to completely organize the calculation of observables in Quantum Field Theory is currently extended to massive calculations at the three-loop level in Quantum Electrodynamics and Quantum Chromodynamics at the perturbative side. For these quantities efficient numerical
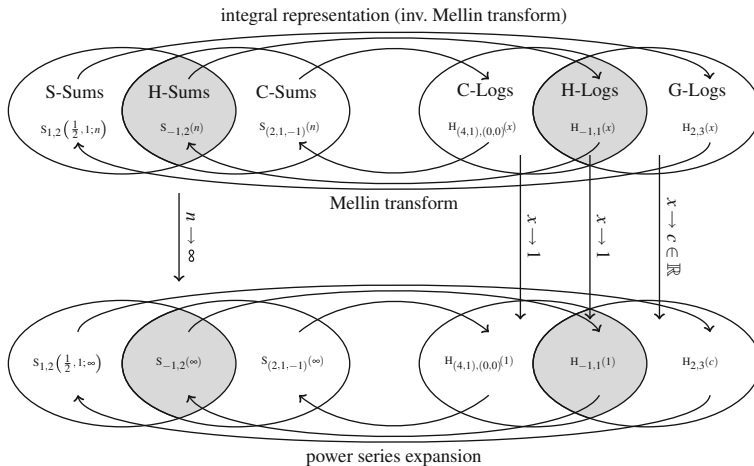
integral representation (inv. Mellin transform)

Fig. 3 Connection between harmonic sums (H-Sums), S-sums (S-Sums) and cyclotomic harmonic sums (C-Sums), their values at infinity and harmonic polylogarithms (H-Logs), generalized harmonic polylogarithms (G-Logs) and cyclotomic harmonic polylogarithms (C-Logs) and their values at special constants

representations have to be derived. Working in Mellin space the treatment may even remain *completely analytic*, in a very elegant way, up to a single final numerical contour integral around the singularities of the problem, cf. Sect. 9.

Despite of the achievements being obtained many more physical classes still await their systematic exploration in the future. It is clear, however, that the various concrete structures are realized as combinations of words over certain alphabets, which may be called the *genetic code of the microcosm* [120].

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