Generalized Harmonic, Cyclotomic, and Binomial Sums, their Polylogarithms and Special Numbers

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Abstract. A survey is given on mathematical structures which emerge in multi-loop Feynman diagrams. These are multiply nested sums, and, associated to them by an inverse Mellin transform, specific iterated integrals. Both classes lead to sets of special numbers. Starting with harmonic sums and polylogarithms we discuss recent extensions of these quantities as cyclotomic, generalized (cyclotomic), and binomially weighted sums, associated iterated integrals and special constants and their relations.

1. Introduction

During the late 1990ies several massless and massive two-loop calculations in Quantum Chromodynamics reached a complexity, see e.g. [1–5], which made it necessary to introduce new functions a systematic manner to represent the analytic results in an adequate form. Dilogarithms, polylogarithms [6–16] and Nielsen integrals [17–19] with complicated arguments did not allow to perform further calculations. Due to this harmonic sums, resp. specific types of Mellin transforms, were independently introduced in [20] and [21] as the basic building blocks. Shortly after the harmonic polylogarithms over the alphabet $\{1/x, 1/(1-x), 1/(1+x)\}$ were found [22]. These are iterated integrals of the Volterra-type having been studied by Poincaré [23–26] more than 100 years before.

Physics expressions, such as massless and massive Wilson coefficients in the asymptotic region to 2-loops, can be expressed in terms of harmonic sums only [27–31]. This also applies to the 3-loop anomalous dimensions [32–35]. However, in the calculation of the massless 3-loop Wilson coefficients in deep-inelastic scattering [36], resp. the massive case [34,35,37], generalized harmonic sums, also called S-sums [38,39], emerge at least in intermediate results. For massive 3-loop graphs $4th$ and $6th$ root of unity weights contribute. At the side of the nested sums they belong to the cyclotomic harmonic sums [40]. Furthermore, root-valued letters occur in the alphabets of iterated integrals [41]. They correspond to binomially-weighted generalized cyclotomic sums. Finally, also elliptic integrals emerge in the calculation of massive Feynman diagrams [42–47]. Special numbers are associated to the above nested sums in the limit $N \to \infty$

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and the iterated integrals for $x = 1$. In the simplest case these are the multiple zeta values (MZVs) [48]. It is obvious, that more structures are expected to contribute calculating Feynman diagrams at even higher loops and for more legs. In this article we give a brief survey on the structures having been found so far.[2] The *method* to unravel these structures consists in applying modern summation techniques to the multiply nested sums, through which the corresponding Feynman diagrams are represented, and to solve them in difference fields using the algorithms [50–58] being encoded in the `Mathematica`-package `Sigma` [59,60].

2. Harmonic Sums, Polylogarithms and Multiple Zeta Values

Let us consider the 2-point functions in Quantum Chromodynamics with local operator insertions. Already in case of the quark-quark anomalous dimension the most simple harmonic sum

$$S_1(N) = \sum_{k=1}^{N} \frac{1}{k}, \quad N \in \mathbb{N} \tag{1}$$

occurs, cf. e.g. [5]. At higher orders more general harmonic sums contribute. They are defined by [20,21]

$$S_{b,\vec{a}}(N) = \sum_{k=1}^{N} \frac{(\text{sign}(b))^k}{k^{|b|}} S_{\vec{a}}(k), \quad S_\emptyset = 1 \quad b, a_i \in \mathbb{Z}\backslash\{0\} . \tag{2}$$

The Mellin transformation [61,62]

$$\mathbf{M}[f(x)](N) = \int_0^1 dx \ x^N \ f(x) \tag{3}$$

relates harmonic sums to harmonic polylogarithms

$$S_{\vec{a}}(N) = \sum_c r_c \, \mathbf{M}[\mathrm{H}_{\vec{b}}(x)](N) + \sum_d r_d \sigma_{\vec{c}_d}, \quad r_c \in \mathbb{Q} , \tag{4}$$

with $\sigma_{\vec{c}_d}$ multiple zeta values. The harmonic polylogarithms [22] may be defined as iterated integrals

$$\mathrm{H}_{b,\vec{a}}(x) = \int_0^x \frac{dy}{y-b} \mathrm{H}_{\vec{a}}(y), \quad b \in \{0, 1, -1\}, \quad \mathrm{H}_\emptyset(x) = 1 \tag{5}$$

$$\mathrm{H}_{\underbrace{0, \ldots, 0}_{k}}(x) = \frac{1}{k!} \ln^k(x) . \tag{6}$$

An example for relation (4) is

$$\begin{aligned}
S_{-2,1,1}(N) &= -(-1)^N \, \mathbf{M}\left[\frac{\mathrm{H}_{0,1,1}(x)}{x+1}\right](N) + (-1)^N \zeta_3 \, \mathbf{M}\left[\frac{1}{x+1}\right](N) \\
&\quad - \mathrm{Li}_4\left(\frac{1}{2}\right) - \frac{\ln^4(2)}{24} + \frac{\ln^2(2)\zeta_2}{4} - \frac{7\ln(2)\zeta_3}{8} + \frac{\zeta_2^2}{8} .
\end{aligned} \tag{7}$$

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[2] For a recent review see [49].

Here also special constants occur, either as infinite nested harmonic sums or as values of the harmonic polylogarithms at $x = 1$ as long as these are defined,

$$\sigma_{\vec{a}} = \lim_{N \to \infty} S_{\vec{a}}(N) \ . \tag{8}$$

They are called multiple zeta values [48]. Since for $N \to \infty$ the Mellin transforms in (7) vanish one obtains

$$\sigma_{-2,1,1} \quad = \quad -\mathrm{Li}_4\left(\frac{1}{2}\right) - \frac{\ln^4(2)}{24} + \frac{\ln^2(2)\zeta_2}{4} - \frac{7\ln(2)\zeta_3}{8} + \frac{\zeta_2^2}{8} \ . \tag{9}$$

Here

$$\zeta_k = \sum_{l=1}^{\infty} \frac{1}{l^k}, \quad k \geq 2, \quad k \in \mathbb{N}, \qquad \mathrm{Li}_k(x) = \sum_{l=1}^{\infty} \frac{x^l}{l^k} \tag{10}$$

are the values of Riemann's ζ-function and Li_k denotes the polylogarithm. It is useful also to associate the symbol

$$\sigma_0 \equiv \sum_{k=1}^{\infty} \frac{1}{k} \tag{11}$$

to the multiple zeta values. All divergencies of the multiple zeta values can be expressed polynomially by σ_0.[3]

Harmonic sums obey quasi-shuffle algebras [63] as harmonic polylogarithms obey shuffle algebras. These are implied by their multiplication relations at equal argument N resp. x. The shuffle product is given by the sum of all permutations of indices of the two sets, which preserve the original ordering. In case of the quasi-shuffle (stuffle [64]) algebras additional terms occur, cf. [65]. The product of two harmonic polylogarithms is thus given by

$$\mathrm{H}_a(x) \cdot \mathrm{H}_{bcd}(x) = \mathrm{H}_a(x) \sqcup\!\sqcup \mathrm{H}_{bcd}(x) = \mathrm{H}_{abcd}(x) + \mathrm{H}_{bacd}(x) + \mathrm{H}_{bcad}(x) + \mathrm{H}_{bcda}(x) \ . \tag{12}$$

The stuffle and shuffle relations imply relations between the harmonic sums and harmonic polylogarithms, respectively, which do not depend on their arguments N and x and are called algebraic relations [65]. Both these algebras can also be applied to the multiple zeta values. Their action is not identical.

The algebraic relations are not the only relations of the harmonic sums or polylogarithms. Other relations concern the argument of these quantities and are sometimes only valid for sub-classes of indices. They are called structural relations. In case of harmonic sums they are implied by the duplication relation [48] and differentiation w.r.t. N referring to an analytic continuation [21, 66–68]. At a given weight $\mathsf{w} = \sum_i |a_i|$ there are

$$N_{\mathsf{all}}(\mathsf{w}) \quad = \quad 2 \cdot 3^{\mathsf{w}-1} \tag{13}$$

harmonic sums. The algebraic (A), differential (D) and duplication (H) relations lead to

$$N_A(\mathsf{w}) = \frac{1}{\mathsf{w}} \sum_{d|\mathsf{w}} \mu\left(\frac{\mathsf{w}}{d}\right) 3^d, \quad N_D(\mathsf{w}) = 4 \cdot 3^{\mathsf{w}-2}, \quad N_H(\mathsf{w}) = 2 \cdot 3^{\mathsf{w}-1} - 2^{\mathsf{w}-1}, \tag{14}$$

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[3] This also holds for the special numbers occurring in case of the cyclotomic harmonic sums.

independent sums individually. Here, $\mu(\xi)$ denotes the Möbius function [69]. Applying these relations one obtains

$$N_{ADH}(\mathsf{w}) \quad = \quad \frac{1}{\mathsf{w}} \sum_{d \mid \mathsf{w}} \mu\left(\frac{\mathsf{w}}{d}\right) \left[3^d - 2^d\right] - \frac{1}{\mathsf{w}-1} \sum_{d \mid \mathsf{w}-1} \mu\left(\frac{\mathsf{w}-1}{d}\right) \left[3^d - 2^d\right] \qquad (15)$$

independent sums. For $\mathsf{w} = 8$ the 4374 harmonic sums can thus be expressed by 486 basic sums. The harmonic polylogarithms obey a general argument relation under the transformation

$$x \to \frac{1-x}{1+x} \ . \qquad (16)$$

An example is

$$
\begin{aligned}
\mathrm{H}_{-1,0,1}\left[\frac{1-x}{1+x}\right] \quad = \quad & -\mathrm{H}_{-1,1}(x)\left(\mathrm{H}_0(x) + \ln(2)\right) + \mathrm{H}_{-1}(x)\left[\mathrm{H}_{-1,1}(x) + \mathrm{H}_{0,-1}(x)\right. \\
& +\mathrm{H}_{0,1}(x) - \zeta_2\big] - 2\,\mathrm{H}_{-1,-1,1}(x) - \mathrm{H}_{0,-1,-1}(x) - \mathrm{H}_{0,1,-1}(x) \\
& -\frac{1}{2}\,\mathrm{H}_{-1}^2(x)\left[\mathrm{H}_0(x) + \ln(2)\right] + \frac{1}{6}\,\mathrm{H}_{-1}^3(x) + \ln(2)\zeta_2 - \frac{5}{8}\zeta_3.
\end{aligned}
\qquad (17)
$$

There are other relations for $x \to \{1-x, 1/x, x^2\}$ which are valid for special index sets [22].

For the multiple zeta values over the alphabet $\{0, 1, -1\}$ the shuffle and stuffle relations imply all relations up to $\mathsf{w} = 7$. From $\mathsf{w} = 8$ the duplication and from $\mathsf{w} = 12$ the generalized duplication relation [48] leads to new relations. The number of newly contributing basis elements for the lowest weights are, [48],

w	1	2	3	4	5	6	7	8	9	10	11	12
# basis	2	1	1	1	2	2	4	5	8	11	18	25

I.e. up to $\mathsf{w} = 12$ 80 basis elements span the multiple zeta values. Up to $\mathsf{w} = 7$ one possible representation reads [20]

$$\left\{\sigma_0, \ln(2), \zeta_2, \zeta_3, \mathrm{Li}_4\left(\frac{1}{2}\right), \zeta_5, \mathrm{Li}_5\left(\frac{1}{2}\right), \mathrm{Li}_6\left(\frac{1}{2}\right), \sigma_{-5,-1}, \zeta_7, \mathrm{Li}_7\left(\frac{1}{2}\right), \sigma_{-5,1,1}, \sigma_{5,-1,-1}\right\}. \quad (18)$$

It is not proven at present, whether these are all relations. For special sequences of harmonic sums there are further relations, see e.g. [48]. A global property of the MZVs over the alphabet $\{0, 1\}$, stating that they can be expressed in terms of MZVs having only indices $a_i = 2, 3$, has been conjectured in [70] and recently proven in [71].

3. Cyclotomic Harmonic Sums, Polylogarithms, and Numbers

The denominators $(x - 1)$ and $(x + 1)$ appearing in the harmonic polylogarithms form the first two cyclotomic polynomials [72]. One may extend the alphabet in allowing all cyclotomic polynomials [40]. They are given by

$$\Phi_n(x) = \frac{x^n - 1}{\prod_{d \mid n, d < n} \Phi_d(x)}, \quad d, n \in \mathbb{N}\backslash\{0\}. \qquad (19)$$

We define the corresponding set of letters by

$$f_0^0(x) = \frac{1}{x}, \quad f_k^l(x) = \frac{x^l}{\Phi_k(x)}, k \in \mathbb{N}\backslash\{0\},\ l \in \mathbb{N},\ l < \varphi(k), \qquad (20)$$

with $\varphi(k)$ being Euler's totient function [72]. A few early examples of Mellin transforms of cyclotomic polylogarithms were given in [73].

Iterating these letters one forms the cyclotomic polylogarithms which obey a shuffle algebra. Applying the Mellin transform (3) one obtains combinations of the cyclotomic harmonic sums and the associated constants. As an extension of the normal harmonic sums, the single cyclotomic sums are given by

$$S_{l,m,n}(N) = \sum_{k=0}^{N} \frac{(\text{sign}(n))^k}{(lk+m)^{|n|}} , \qquad (21)$$

i.e. harmonic sums with periodic gaps in the terms accounted. By iteration of this structure the general cyclotomic sums are obtained. They occur in the calculation of massive Feynman diagrams. The cyclotomic sums obey algebraic and differentiation relations as well as three multiple argument relations [40], for which counting relations are available.

The special constants being associated to the cyclotomic sums and polylogarithms extend the multiple zeta values. The single sums at $\mathsf{w}= 1$ can be expressed by $\sigma_0, \ln(2)$ and π, which replaces $\zeta_2 = \pi^2/6$ as a more fundamental constant. At higher cyclotomy l also the logarithms $\ln(3), \ln(\sqrt{2}-1), \ln(\sqrt{3}-1), \ln(\sqrt{5}-1)$ and several algebraic numbers occur. For $l \leq 6$ and $\mathsf{w} \geq 2$ the basic constants $\zeta_{2k+1}, \psi^{(2k+1)}(1/3), \text{Ti}_{2k}(1), \psi^{(k)}(1/5), \psi^{(2k+1)}(2/5), \psi^{(k)}(1/8), \psi^{(2k)}(1/12)$ contribute. Here ψ denotes the di-gamma function and $\text{Ti}_l(1) = \sum_{k=0}^{\infty}(-1)^k/(2k+1)^l$, with $\text{Ti}_2(1) = \mathbf{C}$ being Catalan's constant [74]. These are the real representations of these constants. Likewise one may consider the infinite generalized harmonic sums with weights at the roots of unity

$$\lim_{N\to\infty} S_{k_1,...,k_m}(x_1,...,x_m;N) \equiv \sigma_{k_1,...,k_m}(x_1,...,x_m), \quad x_j \in \mathcal{C}_n, \ n \geq 1, \ k_1 \neq 1 \text{ for } x_1 = 1, \quad (22)$$

with $\mathcal{C}_n \in \{e_n | e_n^n = 1, e_n \in \mathbb{C}\}$. The real representations being discussed above are related to these complex representations. For lower weights they have been studied for cyclotomy $l \leq 20$ in [40].

4. Generalized Harmonic Sums, Polylogarithms, and Numbers

Generalized harmonic sums are defined by [38, 39]

$$S_{b,\vec{a}}(\zeta, \vec{\xi}; N) = \sum_{k=1}^{N} \frac{\zeta^k}{k^b} S_{\vec{a}}(\vec{\xi}; k), \quad b, a_i \in \mathbb{N}\backslash\{0\}; \quad \zeta, \xi_i \in \mathbb{R}\backslash\{0\}. \qquad (23)$$

The corresponding iterated integrals are built over the alphabet $\{0, \zeta, \vec{\xi}\}$. To also associate the constants, i.e. the sums in the limit $N \to \infty$, one has to restrict the range of weights ζ, ξ_i accordingly to obtain convergent expressions. In intermediate physics results, however, divergent sums for $|\xi_i| > 1$ do occur and have to be dealt with [41]. Known examples refer to alphabets $\xi_i \in \{1, -1, 1/2, -1/2, 2, -2, 1/3, -1/3, 3, -3, ...\}$. [4] In some applications the weights ξ_i are general real numbers. One may generalize the sums (23) introducing cyclotomic denominators [39]

$$S_{\{a_1,b_1,c_1\},...,\{a_l,b_l,c_l\}}(s_1, ..., s_l; N) = \sum_{k_1=1}^{N} \frac{s_1^k}{(a_1 k_1 + b_1)^{c_1}} S_{\{a_2,b_2,c_2\};...;\{a_l,b_l,c_l\}}(s_2, ..., s_l; k_1), \quad (24)$$

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[4] We would like to thank W. Bernreuther and O. Dekkers for a remark.

with $S_\emptyset = 1$, $a_i, c_i \in \mathbb{N}\backslash\{0\}$, $b_i \in \mathbb{N}$, $s_i \in \mathbb{R}\backslash\{0\}, a_i > b_i$. Also these sums are related to the corresponding polylogarithms by the inverse Mellin transform. The elements of both spaces obey (quasi)shuffle relations and a series of structural relations which were worked out in Ref. [39]. An even wider class of special numbers is associated to the generalized (cyclotomic) harmonic sums and polylogarithms. A convenient way to work with these and the more special functions being listed above is provided by the `Mathematica`-package `HarmonicSums` [39,75].

5. Nested Binomial Sums

In case of some Feynman diagrams [41] contributing to the massive Wilson coefficient for the structure function $F_2(x, Q^2)$ at higher scales of Q^2 at 3-loop order further extensions of weighted generalized cyclotomic sums occur :

$$\sum_{i=1}^{N} \binom{2i}{i}(-2)^i \sum_{j=1}^{i} \frac{1}{j\binom{2j}{j}} S_{1,2}\left(\tfrac{1}{2}, -1; j\right) \tag{25}$$

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

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

where

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

$$w_{17} = \frac{1}{\sqrt{x(8+x)}}, \qquad w_{18} = \frac{1}{(2+x)\sqrt{x(8+x)}} \,. \tag{26}$$

The iterated integrals H^* are defined here on the interval $[x, 1]$. The new element consists in binomial $\binom{2i}{i}$ terms emerging both in the numerators and denominators of the finite nested sums.[5] About 100 independent nested sums of similar type contribute. The associated iterated integrals request square-root valued alphabets with about 30 new letters, extending those in case of the generalized harmonic polylogarithms. Examples are given in Eqs. (26).

6. Elliptic Integrals

Nested binomial sums, weighting generalized cyclotomic sums, lead to square-root values letters. One may now imagine that Mellin convolutions of these quantities do also emerge, as it happens already for ordinary harmonic polylogarithms. Let us consider a simple case of this kind :

$$T(x) = \frac{1}{\sqrt{1-x}} \otimes \frac{1}{\sqrt{1-x}} = \int_x^1 \frac{dy}{y} \frac{1}{\sqrt{1-y}} \frac{1}{\sqrt{1-\frac{x}{y}}}$$

$$= 2i \left[\mathbf{F}\left(\arcsin\left(\frac{1}{\sqrt{x}}\right), x\right) - \mathbf{K}(x)\right] \tag{27}$$

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[5] Infinite single sums with binomial weights in the numerator and denominator over (generalized) harmonic sums were studied in [76,77].

It involves the elliptic integrals

$$F(x;k) = \int_0^x \frac{dt}{\sqrt{(1-t^2)(1-k^2t^2)}} \tag{28}$$

$$K(k) = F(1,k) = \frac{\pi}{2}{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;k^2\right). \tag{29}$$

On the other hand, the Mellin transform of $T(x)$ yields the following simple expression.

$$\mathbf{M}[T(x)](N) = \int_0^1 dx\, x^N T(x) = \frac{4^{2N}}{\binom{2N}{N}^2 (N+\frac{1}{2})^2}. \tag{30}$$

Higher powers of the binomial $\binom{2N}{N}$ emerge in Mellin space, which are seemingly one source of elliptic integrals in x-space. One has to contest, that the N-space expression is more simple here.

7. Analytic Continuations the various Sums

In Mellin space one may thoroughly perform the solution of the QCD evolution equations analytically, cf. e.g. [78]. The convolution of the Wilson coefficients with the evolved parton distribution functions is given by a simple product. This representation is therefore preferred in fitting the non-perturbative parton distribution functions. On the numerical side only one final contour integral around the singularities of the problem has to be performed. This requests the analytic continuation of the variable N in the nested sums to $N \in \mathbb{C}$. Observing the crossing relations of the respective process the analytic continuation proceeds either from the even *or* the odd values of N. First the singularities in the complex plane have to be determined. For the harmonic sums and cyclotomic harmonic sums the singularities are located at the non-positive integers and one obtains meromorphic functions. This is not necessarily the case for generalized sums since they may diverge in some cases exponentially as $N \to \infty$. Whenever an asymptotic expansion exists, it can be calculated analytically [39, 68, 75][6] and thus be given at arbitrary precision in principle. Starting with this representation, the shift-property of the nested sums for $N \to N+1$ allows to arrive at any non-singular point in the complex plane using a thoroughly analytic representation to be evaluated numerically. Physical quantities like the massless and the known massive Wilson coefficients and massive operator matrix elements [32–35, 81] possess regular asymptotic representations. For these quantities a corresponding representation is therefore possible. This also applies for the Wilson coefficients of the Drell-Yan process, hadronic Higgs-boson production [27] and time-like quantities [28]. Furthermore, precise representations can be derived also in case cross sections are given numerically only, cf. [82].

8. Conclusions

The mathematical functions expressing Feynman diagrams in N-space form a hierarchy starting with rational functions, harmonic sums, followed by generalized harmonic sums, cyclotomic sums, their generalization, binomially weighted generalized cyclotomic sums, etc. Accordingly, the corresponding iterated integrals and special numbers are organized. The relations of the different quantities can be illustrated by Figure 1 [49].

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[6] Precise numerical implementations for the analytic continuations of special Mellin-transforms up to those needed to express the 3-loop anomalous dimensions were given in [79, 80].
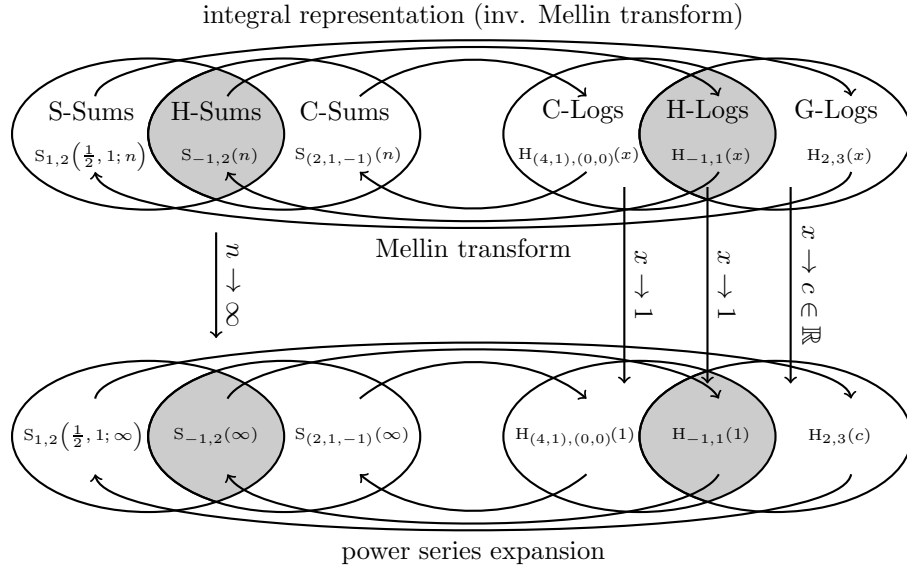
Figure 1. Connection between harmonic sums (H-Sums), S-sums (S-Sums) and cyclotomic harmonic sums (C-Sums), their values at infinity and harmonic polylogarithms (H-Logs), generalized harmonic polylogarithms (G-Logs) and cyclotomic harmonic polylogarithms (C-Logs) and their values at special constants.

The cyclotomic polynomials provide a natural extensions of the letters used with iterated integrals leading to harmonic polylogarithms. Corresponding terms occur in massive higher order calculations. The Mellin transform associates the nested sums and the iterated integrals. Both classes form quasi-shuffle resp. shuffle algebras and obey structural resp. argument-induced relations. Similar relations hold for the different sets of special numbers. One expects an even richer structure in case of multi-leg integrals at higher loop orders, a territory which is widely unexplored still. In this way Feynman diagrams generate a still growing number of new classes of mathematical structures. Knowing their relations greatly helps to simplify the theoretical calculations and also allows for better numerical representations.

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