Structural relations of harmonic sums and Mellin transforms up to weight $w = 5$

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**Abstract**

We derive the structural relations between the Mellin transforms of weighted Nielsen integrals emerging in the calculation of massless or massive single-scale quantities in QED and QCD, such as anomalous dimensions and Wilson coefficients, and other hard scattering cross sections depending on a single scale. The set of all multiple harmonic sums up to weight five cover the sums needed in the calculation of the 3-loop anomalous dimensions. The relations extend the set resulting from the quasi-shuffle product between harmonic sums studied earlier. Unlike the shuffle relations, they depend on the value of the quantities considered. Up to weight $w = 5$, 242 nested harmonic sums contribute. In the present physical applications it is sufficient to consider the subset of harmonic sums not containing an index $i = -1$, which consists out of 69 sums. The algebraic relations reduce this set to 30 sums. Due to the structural relations a final reduction of the number of harmonic sums to 15 basic functions is obtained. These functions can be represented in terms of factorial series, supplemented by harmonic sums which are algebraically reducible. Complete analytic representations are given for these 15 meromorphic functions in the complex plane deriving their asymptotic- and recursion relations. A general outline is presented on the way nested harmonic sums and multiple zeta values emerge in higher order calculations of zero- and single scale quantities.

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1. Introduction

Finite harmonic sums [1–3] and associated to them, by a Mellin transform, Nielsen-type integrals [4], emerge in perturbative calculations of massless and massive single scale problems in Quantum Field-Theory. The Wilson coefficients and anomalous dimensions in deeply inelastic scattering to three loops [5], the massive quark Wilson coefficients in the limit $Q^2 \gg m^2$ [6,7], as well as the Wilson coefficients for the Drell–Yan process, hadronic Higgs production in the heavy mass limit, the time-like coefficient functions for parton fragmentation into hadrons, cf. [8], the soft- and virtual corrections to Bhabha scattering [9], and various processes more belong to this class. At 2-loop order the respective expressions in terms of harmonic sums were given in [10] using the algebraic and structural relations between these quantities of weight $w \leq 4$. Due to the complexity of higher order calculations the knowledge of as many as possible relations between the finite harmonic sums is of importance to simplify the calculations and to obtain compact analytic results. It turns out that, up to isomorphisms, the basic functions, which express the physical quantities mentioned above, are always the same and form a basis of an algebra, over which the observables can be expressed. These basic functions therefore form central objects in the description of a wide range of physical quantities.

To derive the basic functions we first consider the multiple finite harmonic sums $S_{a_1,...,a_n}(N)$. They provide a unique language to express single scale quantities, which emerge in field theoretic calculations. They are defined by

$$ S_{a_1,...,a_n}(N) = \sum_{k_1=1}^{N} \cdots \sum_{k_n=1}^{N} \frac{\text{sign}(a_1)^{k_1}}{k_1^{a_1}} \cdots \frac{\text{sign}(a_n)^{k_n}}{k_n^{a_n}}. \quad (1.1) $$

Here, $a_k$ are positive or negative integers and $N$ is a positive even or odd number. One calls $n$ the depth and $\sum_{k=1}^{n} |a_k|$ the weight of a harmonic sum. Harmonic sums are associated to Mellin transforms of real functions $f(x)$

$$ S_{a_1,...,a_n}(N) = \int_0^1 dx x^N f_{a_1,...,a_n}(x) = M[f_{a_1,...,a_n}(x)](N). \quad (1.2) $$

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Here $\mathcal{M}$ denotes the Mellin transform. The functions $f_{a_1,\ldots,a_w}(x)$ are usually linear combinations of harmonic polylogarithms $H_{b_1,\ldots,b_l}(x)$ [11–13], weighted by the factor $1/(1 \pm x)$. $f(x)$ may be distribution-valued [14]. One example for this class is

$$\int_0^1 dx x^N f_{a_1,\ldots,a_w}(x) = \int_0^1 dx (x^N - 1) f_{a_1,\ldots,a_w}(x).$$

(1.3)

The number of harmonic sums grows exponentially with the weight $w$ and amounts to $3^{w-1}$ for all sums of weight $w' \leq w$. The finite harmonic sums are not independent objects but obey relations. In view of their rapidly growing number for higher weight it is worthwhile to reveal all their relations to express all harmonic sums in terms of a small set of basic elements only. In a foregoing paper [15] we investigated the shuffle relations [16] between general finite alternating or non-alternating harmonic sums. There all shuffle relations for harmonic sums up to depth and weight $w = 6$ were derived in general form and the counting relations for the number of basis elements spanning the algebra of harmonic sums after the shuffle relations are used have been given. For a certain class of indices $\{a_1,\ldots,a_w\}$, where $n_{|j| = 1,\ldots,a_w}$ elements are equal and $n = \sum_{j=1}^N n_j$, the total number of harmonic sums is

$$n(n_1,\ldots,n_q) = \frac{n!}{n_1! \cdots n_q!}.$$  

(1.4)

The shuffle relations allow to express these sums in terms of

$$l_q(n_1,\ldots,n_q) = \frac{1}{n} \sum_{d|n_q} \mu(d) \left(\frac{d}{n_q}\right)! \left(\frac{n_q}{n}\right)! \cdots \left(\frac{n_q}{n_q}\right)!.$$  

(1.5)

basis elements and polynomials out of objects of lower weight. Here Eq. (1.5) is the 2nd Witt formula, cf. [17], and $\mu(k)$ denotes the Möbius function [18]. $l_q$ also counts the number of Lyndon words [19] associated to $\{a_1,\ldots,a_q\}$, since all harmonic sums belonging to this index set are freely generated by the Lyndon words as a consequence of Radford's theorem [20].

In the limit $N \to \infty$ harmonic sums turn into multiple zeta values (MZVs) [21]. Since multiple zeta values obey many more relations, e.g. [22,23], than the shuffle relations the question arises which other relations may hold for multiple harmonic sums. A series of relations emerges due to the integral representations of the harmonic sums which were derived in Ref. [2]. Furthermore, some sums have a completely symmetric index set and do therefore decompose into polynomials of single harmonic sums. This also implies relations between the Mellin transforms of certain Nielsen-type integrals weighted with the denominators 1/(1 ± x).

In the present paper we will not limit the consideration to harmonic sums with $N \in \mathbb{N}$ but will allow for $N \in \mathbb{C}$ and derive the complex analysis for these quantities. Along with this, new relations between these objects will emerge. In this generalized case we consider rational fractions of $N$, $N/q$, and allow to differentiate for the index $N$, which both yield new relations. The harmonic sums turn out to be meromorphic functions. They can be represented through factorial series [27,28] up to polynomials of $S_1(N)$ and harmonic sums of lower degree. The analytic continuation of $S_1(N)$ is given by Euler's di-gamma function $\psi(z)$.

The weight $w = 1$ harmonic sums $S_{1,\pm}(N)$ may all be traced back to the $\psi$-function for $N \in \mathbb{C}$. At the beginning of the 20th century Nielsen [27] studied the respective functions belonging to the class of weight $w = 2$, from which the corresponding analytic continuations can be derived. Due to the fact, that harmonic sums, with the exception of factors of $S_1(N)$, can be represented as factorial series, allows to derive their analytic continuations. The recursion relations for $(N + 1) \to N$, $N \in \mathbb{C}$, and the asymptotic representation for $|N| \to \infty$ are obtained in analytic form. The singularities are poles located at the non-positive integers. Due to the presence of factors $S_1(N)$ in some cases the respective sums behave $\sim \ln^k(N)$ as $|N| \to \infty$. Since we derive the analytic continuations in analytic form, also all derivatives are easily determined. In the definition of the basic functions we chose representations in the past, in which the functions to be Mellin-transformed may possess a branch point at $x = 1$. To express the Mellin transforms $\mathcal{M}[f(x)](N)$ in terms of factorial series it is required that the functions $f(x)$ are analytic at $x = 1$, which can be obtained using well-known mirror relations for the corresponding Nielsen integrals or harmonic polylogarithms transforming $x \leftrightarrow (1 - x)$.

The paper is organized as follows. In Section 2 a brief general outline is presented on the way finite nested harmonic sums emerge in higher order calculations for single scale processes. Some basic definitions are given in Section 3. Classes of harmonic sums are discussed in Section 4. In Sections 5–9 we consider the Mellin transforms being associated to the sums of weight $w = 1$ to $w = 5$ in detail and derive the structural relations for the harmonic sums. Here we will first refer to the set of Mellin transforms chosen formerly [2,15,30]. The basis found in this way will be reordered by a linear transformation into another one which is consistent with the representation in terms of factorial series. Section 10 contains the conclusions. The algebraic relations to weight $w = 5$ used are given in Appendix A. Appendix B contains the relations necessary to express the basic functions in the complex plane. Some useful integrals which emerge in this context are given in Appendix C.

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1 Various mathematical terms used in the following were defined in Ref. [15] to which we refer readers from the physics community who are not yet used to this terminology.

2 If $a_1 = 1$, the corresponding multiple sums diverge for $N \to \infty$ but can be considered symbolically. Actually they are expressible in terms of a polynomial of the (divergent) harmonic sums $\sigma_i = \sum_{k=1}^{\infty}(1/k)$ and the finite basis elements of multiple zeta values, see [3,15,24].

3 The relations between the alternating MZVs to weight $w = 12$ and non-alternating MZVs to weight $w = 24$ based on the shuffle-, stuffle-, and new relations have been determined in [24] recently. Generalizations of finite harmonic sums and harmonic polylogarithms have been given for other applications, cf. [25] and [26].

4 Precise analytic continuations of the basic functions [22,29] based on semi-numerical representations were given in [30,31]. Here we made use of the MINIMAX method [32,33]. This method has also been applied to derive the analytic continuation for the heavy flavor Wilson coefficients up to 2-loop order [34]. For another proposal for the analytic continuation of harmonic sums to $N \in \mathbb{R}$, for which some simple examples were presented, cf. [35]. For other effective parameterizations see [36].

5 The structural relations of $w = 6$ are presented in Ref. [37].
2. The emergence of harmonic sums

In the following we give a brief outline on the way finite nested harmonic sums emerge in higher order calculations for single scale processes. These processes contain a scale, such as a momentum fraction $z$, which relates a parton momentum $p = z P$ collinearly to the hadron momentum $P$ in the massless limit, $0 \leq z \leq 1$. Examples for this case are space- and time-like splitting and coefficient functions, cf. [5,8]. The representation also appears to massive calculations in the limit $Q^2/m^2 \gg 1$, cf. e.g. [6,7]. Likewise this variable may be viewed as the ratio of two Lorentz-invariants $z = t/s$, as the case for the soft and virtual corrections to Bhabha-scattering [9], or the initial state radiation to $e^+ e^-$ annihilation [38], where the respective ratio is $z = s'/s$ with $s'$ the cms energy of the virtual gauge boson exchanged. In the latter two processes the electrons are massive but are dealt with in the limit $s/m^2 \gg 1$. $s$, $s'$ and $t$ are Mandelstam-variables, i.e. Lorentz-products of linear combinations of 4-momenta. The factions $z$ do always obey $0 \leq z \leq 1$.

There are two principle approaches, which can be followed in these calculations. Either one uses the light-cone expansion [39] for space-like and the cut-vertex method [40] in the time-like case or one follows a partonic description in the massless case, resp. the case extended over the $\sigma$ Lorentz-products of linear combinations of 4-momenta. The factions moments, cf. [41], depending on the physical process. In the partonic approach one may form these moments accordingly, transforming immediately. Here, furthermore, the corresponding current crossing relations have to be observed, which single out even or odd integer as the ratio of two Lorentz-invariants

Mellin transforms of the new polylogarithms, which one may call e radiation to performed and lead to a further factor of the kind

We refer to this method, since it uniquely allows to create the structures emerging. All the Feynman-parameter integrals can now be performed and lead to a further factor of the kind

$\Gamma(a_1 N + b_1 (\sigma_a) + \bar{\Gamma} \varepsilon) \ldots \Gamma(a_k N + b_k (\sigma_a) + \bar{\Gamma} \varepsilon) \bigg|_{\sigma_a \ldots \varepsilon}$

leaving the non-trivial Feynman parameter integrals. In carrying out theses integrals scalar and tensor integrals have to be performed.

The Feynman parameter integrals contain the Mellin variable in the numerator only. The denominator is given by the Kirchhoff-polynomial of the respective graph consisting out of $k$ monomials raised to a real non-integer power. A possible next step consists in expressing the Feynman-parameter integrals in terms of Mellin–Barnes integrals [43] for each of these monomials,

\[
\frac{1}{(A + B)^\gamma} = \frac{1}{2\pi i} \int_{y-i\infty}^{y+i\infty} \frac{\Gamma(-\sigma) \Gamma(q + \sigma)}{\Gamma(q)} d\sigma B^{-q-\sigma} A^\sigma. \tag{2.4}
\]

The use of Mellin–Barnes integrals usually leads to rather large set of sums if compared to the sums needed to express the physics results. We refer to this method, since it uniquely allows to create the structures emerging. All the Feynman-parameter integrals can now be performed and lead to a further factor of the kind

\[
\frac{\Gamma(c_1 N + d_1 (\sigma_a) + q_1 \varepsilon) \ldots \Gamma(c_l N + d_l (\sigma_a) + q_l \varepsilon)}{\Gamma(c_1 N + d_1 (\sigma_a) + q_1 \varepsilon) \ldots \Gamma(c_l N + d_l (\sigma_a) + q_l \varepsilon)} \bigg|_{\sigma_a \ldots \varepsilon}.
\]
Now the $k$ Mellin–Barnes integrals have to be performed. This can be done applying the residue theorem, after the according contours have to be properly fixed. In this way one obtains $k$ or more infinite sums over the above rational function of $I'$-functions, with according replacement of the sum-index in place of the variables $a_k $.

For these multiple sum expressions one may seek representations which are generalized hypergeometric series [7,44] and generalizations thereof. Going to ever higher orders not all of these functions may be known by now but have to be introduced newly. They are naturally generated by the above integrals.

At this stage one may wish to expand in $\varepsilon$. If quantities without infrared singularities are considered, the maximal negative power in $\varepsilon$ is given by the loop-order of the diagram. Infrared singularities may enhance this order. The expansion has to be carried out up to the respective order required in the calculation. As only $I'$-functions are expanded, which partly contain $a_k k_i $ with $a_i, k_i \in \mathbb{N}$, single harmonic sums of the type $S_2(a_k k_i )$ emerge in products. The various infinite sums with index $k_i $ nest these products, which finally leads to nested harmonic sums and multiple $\zeta$-values or their respective generalizations in higher orders, as described above. The according sums can be uniquely found investigating the corresponding recurrences in $N$ over $\Pi \Sigma$-fields, as possible with the code Sigma [46].

The harmonic sums, which occur in the calculations of single scale quantities up to a given weight can be represented over a basis of functions, which is independent of the respective quantity being considered. In the following we identify these basis elements up to weight $w = 5$.

### 3. Basic definitions

We will consider one-parameter real-valued functions $x \in \lbrack 0, 1 \rbrack $. Partly this set will be extended to special distributions $f(x) \in D'([0, 1])$ occurring in field theoretic calculations. Their Mellin transform is defined by Eq. (1.2), where $N$ is a positive, suitably large integer. According to the emergence of the respective Mellin transform in quantum field theoretic calculations, such as the local light cone expansion [39], $N $ is either an even or odd integer. Factors of $(-1)^N $, which emerge in the following, have therefore a definite meaning and are either equal to $+1$ or $-1$. Both branches may be continued analytically in $N$ from $\mathbb{N}$ to $\mathbb{C}$ according to Carlson’s theorem [47]. The distributions $f(x)$ considered in the following are differentiable functions in the class $C^\infty([0, 1])$ or $\delta$-distributions $\delta^{(k)}(1-x), k \geq 0$ in $D'([0, 1])$ [14]. Furthermore, we consider functions with a $+\langle\rangle$-prescription,

$$
\frac{1}{0} \int dx x^N f(x) = \frac{1}{0} \int dx (x^N - 1) f(x),
$$

with $f \in C^\infty([0, 1])$. The Mellin transform of the latter functions are harmonic sums in case the functions $f(x)$ are harmonic polylogarithms [12] weighted by a factor $1/(1 \pm x)$, which we will consider throughout the present paper. The Mellin transform of the $\delta^{(k)}(1-x)$-distributions yield

$$
\frac{1}{0} \int dx x^N \delta^{(k)}(1-x) = (-1)^k \prod_{l=0}^{k} (N-l).
$$

In all cases below which are not of the form $f(x) = \ln^n(x) \tilde{f}(x)$, or a linear combination of these terms, the function can be expanded into a Taylor series for $x \in [0, 1]$.

$$
f(x) = \sum_{k=0}^{\infty} a_k x^k, \quad a_k = \frac{f^{(k)}(0)}{k!}, \quad \forall a_k \in \mathbb{R}.
$$

The Mellin transform of $f(x)$ is

$$
\frac{1}{0} \int dx x^N f(x) = \sum_{k=0}^{\infty} \frac{a_k}{N + 1 + k}.
$$

All the above Mellin transforms are meromorphic functions in $N$. For the case $f(x) = \ln^n(x) \tilde{f}(x)$

$$
\frac{1}{0} \int dx x^N \ln^n(x) \tilde{f}(x) = \frac{n!}{N^n} \frac{1}{0} \int dx x^N \tilde{f}(x)
$$

holds accordingly.

The class of functions $\tilde{f}(x)$ is formed out of polynomials of harmonic polylogarithms [12]. For physical applications in the massless case it will turn out that all contributing harmonic sums up to weight $w = 5$ can be represented by polynomials out of Mellin transforms of the type

$$
M \left[ \frac{\tilde{f}(x)}{x-1} \right]_+ (N), \quad \text{or} \quad M \left[ \frac{\tilde{f}(x)}{x+1} \right] (N).
$$

---

7 First non-harmonic sums were found in individual diagrams in [45]. They canceled, however, in the final result in the $\overline{\text{MS}}$-scheme within each color factor.
where \( f(x) \) is a polynomial of Nielsen integrals. In the analytic continuation one may consider Mellin transforms at rational arguments, like \( N/2 \) and study the mapping

\[
M\left[ \frac{\hat{f}(x^2)}{1-x^2} \right](N) \rightarrow M\left[ \frac{\hat{f}(x)}{1-x} \right]\left( \frac{N-1}{2} \right),
\]

for \( \hat{f}(1) = 0 \). The factor decomposition of the denominators yields

\[
\frac{1}{1-x^2} = \frac{1}{\Phi_1(x)\Phi_2(x)} = \frac{1}{2} \left[ \frac{1}{1+x} + \frac{1}{1-x} \right],
\]

where \( \Phi_{1,2}(x) \) denote the first two cyclotomic polynomials \([48,8]\). The representation of a harmonic polylogarithm \( f(x^2) \) in terms of other harmonic polylogarithms \( f(x) \) may be worked out for non-negative indices, \([12]\). We will give the explicit relation for the case of the Nielsen integrals \( S_n(x) \) \([4]\)

\[
S_{n,p}(x) = \frac{(-1)^{n+p-1}}{(n-1)! p!} \int_0^1 \frac{dz}{z} \ln^{n-1}(z) \ln^p(1-xz).
\]

The following relation holds

\[
S_{n,p}(x^2) = 2^n \frac{(-1)^{n+p-1}}{(n-1)! p!} \sum_{l=0}^{p} \binom{p}{l} \frac{1}{p!} \int_0^x \frac{dz}{z} \ln^{n-l-1}(z) \ln^p(1-z) \ln^l(1+z).
\]

For \( n = 1 \) one obtains

\[
\frac{1}{2} S_{1,p}(x^2) = S_{1,p}(x) + S_{1,p}(-x) + \frac{(-1)^p}{p!} \sum_{l=1}^{p-1} \binom{p}{l} \frac{1}{p!} \int_0^x \frac{dz}{z} \ln^{n-l-1}(1-zx) \ln^l(1+zx).
\]

Even in this simple case for Nielsen integrals, which are not classical polylogarithms, the mapping of the argument \( x \rightarrow x^2 \) does not give a closed relation in the same class of functions anymore. However, relations of this type may be used to express certain Mellin transforms, cf. \([2]\), for examples up to \( w = 4 \).

4. Classes of harmonic sums

The number of all possible alternating and non-alternating harmonic sums of weight \( w \), \( N(w) \), is

\[
N(w) = 2 \cdot 3^{w-1}.
\]

The number of basic sums in the case of all permutations can be calculated using the 1st Witt formula \([17]\) for an alphabet of length \( l = 3 \) for \( w > 1 \), \([15]\).

\[
N_{\text{basic}}(1) = 2,
\]

\[
N_{\text{basic}}(w) = \frac{1}{w} \sum_{d|w} \mu\left( \frac{w}{d} \right) 3^d, \quad w \geq 2.
\]

The alternating and non-alternating harmonic sums \([2,3]\) are generated by Mellin transforms of nested integrals based on the three \( w = 1 \) functions

\[
\frac{1}{1+x}, \quad \frac{1}{x}, \quad \frac{1}{1-x}.
\]

Therefore, the alphabet out of which the index of the respective harmonic sums is formed as a word is of length \( l = 3 \). The harmonic sums form a subset w.r.t. all possible index-sets over the alphabet \( \{-1, 0, 1\} \), since the letter 0 cannot appear first. The counting relation is given by Eq. (4.1).

Investigating the structure of the single-scale quantities in QCD and QED, cf. \([6,7,10,29,31,50]\) to 2- and 3-loop order in more detail, it turns out that harmonic sums with index \( i = -1 \) do not contribute. One finds that the number of all harmonic sums of weight \( w \), which do not contain any index \( i = -1 \), is obtained by expanding the following generating function \([51]\)

\[
\frac{1-x}{1-2x-x^2} = \sum_{w=0}^{\infty} N_{-(-1)}(w)x^w,
\]

with

\[
N_{-(-1)}(w) = \frac{1}{2} \left[ (1-\sqrt{2})^w + (1+\sqrt{2})^w \right] = \sum_{k=0}^{\lfloor w/2 \rfloor} \binom{w}{2k} 2^{w}.
\]

\---

*8 In massive calculations higher cyclotomic polynomials may occur as well. Examples are the fractional values of the \( \beta \)-function \((5.8)\), as \( \beta((x+1)/2) = 2M[1/(1+z^2)](x), \beta((x+1)/3) = \beta(x+1) - M((z-2)/(z^2-z+1))(x) \) for the 4th and 6th cyclotomic polynomial, cf. \([27]\). See also \([49]\).*
5. Sums of weight one

This relation modifies in case of \( \gamma \) by \( \gamma = \psi(N + 1) - \gamma_E \).

Table 1
Number of harmonic sums, number of sums, which do not contain the index \([-1]\), number of sums with positive indices and the respective numbers of basic sums by which all sums can be expressed using the algebraic relations (a-basic sums) [15] in dependence of their weight.

<table>
<thead>
<tr>
<th>Weight</th>
<th>Sums</th>
<th>a-basic sums</th>
<th>Sums ([-1])</th>
<th>a-basic sums</th>
<th>Sums (i &gt; 0)</th>
<th>a-basic sums</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
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<td>3</td>
<td>2</td>
<td>2</td>
<td>1</td>
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<td>7</td>
<td>4</td>
<td>4</td>
<td>2</td>
</tr>
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<td>17</td>
<td>8</td>
<td>8</td>
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<td>312</td>
<td>239</td>
<td>68</td>
<td>64</td>
<td>18</td>
</tr>
<tr>
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<td>810</td>
<td>577</td>
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<td>30</td>
</tr>
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<td>2184</td>
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<td>56</td>
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<td>5880</td>
<td>3363</td>
<td>664</td>
<td>512</td>
<td>99</td>
</tr>
</tbody>
</table>

\( N_{[-1]}(w) \) obeys the recursion relation

\[
N_{[-1]}(w) = 2 \cdot N_{[-1]}(w - 1) + N_{[-1]}(w - 2)
\]

with the starting values \( N_{[-1]}(1) = 1 \), \( N_{[-1]}(2) = 3 \). Another interesting subclass of the harmonic sums is that of the non-alternating harmonic sums. These sums are formed over an alphabet of length \( l = 2 \). Similarly to (4.2) one obtains

\[
N_{l > 0}(w) = 2^{w - 1}, \quad N_{l > 0}^{\text{basic}}(1) = 1,
\]

\[
N_{l > 0}^{\text{basic}}(w) = \frac{1}{w} \sum_{d|w} \mu \left( \frac{w}{d} \right) 2^d, \quad w \geq 2.
\]

In Table 1 the number of sums is given in dependence of the weight \( w \). Here the number of a-basic sums is the number of sums obtained using the algebraic relations [15] \(^9\). As shown in Table 1 the number of a-basic sums for all harmonic sums, \( N_{\text{basic}}(w) \), is larger or equal then the number of a harmonic sum, which do not contain \([-1]\) as an index. The corresponding number of basic sums is given by:

\[
N_{[-1]}^{\text{basic}}(w) = \frac{2}{w} \sum_{d|w} \mu \left( \frac{w}{d} \right) N_{[-1]}^{\text{basic}}(d).
\]

Values of \( N_{[-1]}^{\text{basic}}(w) \) are partly connected to the number of a non-rooted tree studied in [52] for \( w = 2 \ldots 7 \), but obey a different counting rule otherwise.

We mention that relation (4.2) applies also to other objects, as the harmonic polylogarithms, where the respective numbers up to \( w = 8 \) were determined empirically in [12]. Here we may apply it even for \( w = 1 \), unlike the case for harmonic sums.

5. Sums of weight one

The harmonic sums of weight \( w = 1 \) are generated by the Mellin transform of the first two cyclotomic polynomials \([48]^{10}\) (after regularization of the integral)

\[
\frac{1}{1 - x} \quad \text{and} \quad \frac{1}{1 + x}
\]

by

\[
M \left[ \frac{1}{1 - x} \right](N) = -S_1(N) = -\psi(N + 1) - \gamma_E, \quad (5.2)
\]

\[
M \left[ \frac{1}{1 + x} \right](N) = (-1)^N [S_{-1}(N) + \ln(2)] = \beta(N + 1). \quad (5.3)
\]

Here \( \gamma_E \) denotes the Euler–Mascheroni constant. The representation of the integral in Eq. (5.2) in terms of the \( \psi \)-function was first given by Legendre [53]. The Mellin transform for an integrable function \( x^a f(x) \) obeys the identity

\[
M[ f(x^a) ](N) = \frac{1}{a} M[ f(x) ] \left( \frac{N + 1 - a}{a} \right), \quad a \in \mathbb{R}, \quad a > 0. \quad (5.4)
\]

This relation modifies in case of \( f(x) \) being a \( + \)-distribution. For \( a = 2 \) one obtains

\(^9\) Later on we will derive a basis representation for the harmonic sums including the structural relations. Since in this representation we make a special choice, we list the corresponding algebraic relations w.r.t. to this basis for the dependent sums in Appendix A.

\(^{10}\) These polynomials are the real-valued factors of \( x^N - 1 \) with \( N \geq 1, N \in \mathbb{N} \).
\[
\frac{1}{1-x^2} = \frac{1}{2} \left[ \frac{1}{1-x} + \frac{1}{1+x} \right].
\]  
(5.5)

\[
M \left( \left( \frac{1}{1-x} \right)_+ \right)^{N-1/2} = M \left( \left( \frac{1}{1-x} \right)_+ \right) (N) + M \left( \frac{1}{1+x} \right) (N) + \ln(2).
\]  
(5.6)

The latter relation can even be analytically continued in closed form since, see [2],
\[
-\psi \left( \frac{N}{2} \right) - \gamma_E = -\psi(N) - \gamma_E + \beta(N) + \ln(2),
\]  
(5.7)

with
\[
\beta(N) = \frac{1}{2} \left[ \psi \left( \frac{N+1}{2} \right) - \psi \left( \frac{N}{2} \right) \right].
\]  
(5.8)

cf. [27,54]. The duplication relation for the \( \psi \)-function yields
\[
\psi(N) = \frac{1}{2} \left[ \psi \left( \frac{N}{2} \right) + \psi \left( \frac{N+1}{2} \right) \right] + \ln(2).
\]  
(5.9)

Here fractional arguments in the \( \psi \)-function emerge quite naturally. For \( k > 1 \) the harmonic sums \( S_{-k}(N) \) and \( S_k(N) \) obey, respectively:
\[
S_{-k}(N) = \frac{(-1)^{k-1}}{(k-1)!} (-1)^N \beta^{(k-1)}(N+1) - \left[ 1 - \frac{1}{2^{k-1}} \zeta(k) \right],
\]  
(5.10)
\[
S_k(N) = \frac{(-1)^{k-1}}{(k-1)!} \psi^{(k-1)}(N+1) + \zeta(k),
\]  
(5.11)

with \( \zeta \) the Riemann \( \zeta \)-function. All these sums are expressed by the \( \psi \)-function and its derivatives. We therefore conclude that due to the above rational-argument and differential relations there is only one basic single harmonic sum, \( S_1(N) \).

One may wonder whether differentiation relations can also be of importance for multiple zeta values. This is indeed the case [55]. The multiple zeta values can be generalized to multiple Hurwitz zeta values [56] defined by
\[
\zeta^{a,d}_{c} = \sum_{k_1=1}^{\infty} \frac{(\text{sign}(c))^{k_1}}{(a + k_1)c} \zeta^{H,a}_{d}(k_1),
\]  
(5.12)

iteratively with
\[
\zeta^{H,a}_{d}(k_1) = \sum_{k_2=1}^{k_1} \frac{(\text{sign}(d_{1}))^{k_2}}{(a + k_2)d_{1}} \zeta^{H,a}_{d_{2}...d_{m}}(k_2).
\]  
(5.13)

Here \( a \in \mathbb{C} \) so that the above sums are defined. One may differentiate for \( a \) and perform then the limit \( a \to 0 \). Multiple Hurwitz zeta values obey stuffle relations, using the diction of Ref. [23]. Furthermore, one may form shuffle, duplication and more general algebraic relations among them, similar to the case studied for the multiple zeta values in Ref. [24]. Differentiating these relations builds classes of these relations which may be somewhat easier obtained as working out the relations directly for the multiple zeta values. It is not excluded that at very high weights even more relations between multiple zeta values can be found than obtained in [24], although for lower weights, i.e. \( w \leq 12 \) this is not expected.

The differential quotient of a harmonic sum is always of the form
\[
\frac{d}{dN} S_{\varphi}^{a}(N) = S_{\varphi}^{a}(N) - \zeta_{\varphi}, \quad \lim_{N \to \infty} S_{\varphi}^{a}(N) = \zeta_{\varphi}.
\]  
(5.14)

This is due to the fact that (5.14) can be represented by a Mellin transform which contains \( x^N \) as a factor of the integrand being continuous in \( x \in [0,1] \). The Mellin transform vanishes for \( N \to \infty \).

As an example we consider single harmonic sums. Differentiation yields
\[
\frac{d}{dN} S_k(N) = -k \left[ S_{k+1}(N) - \zeta(k+1) \right],
\]  
(5.15)
\[
\frac{d}{dN} \left[ (-1)^N S_k(N) \right] = -(-1)^N k \left[ S_{-(k+1)}(N) + \left( 1 - \frac{1}{2^{k-1}} \right) \zeta(k+1) \right].
\]  
(5.16)

Differentiating the Hurwitz zeta value \( \zeta^{a}(k_1) \) and taking the limit \( a \to 0 \) yields
\[
\lim_{a \to 0} \frac{d}{da} \zeta^{a} = -c \zeta_{+(c+1)}, \quad c > 0,
\]  
(5.17)
\[
\lim_{a \to 0} \frac{d}{da} \zeta^{a} = c \zeta_{-(c-1)}, \quad c < 0.
\]  
(5.18)
6. Sums of weight two

Among the six harmonic sums four decompose into polynomials of single sums, which may be expressed through the \( \psi^{(k)}(z) \) functions as shown in the previous section. Two sums, \( S_{-1,1}(N) \) and \( S_{1,-1}(N) \) remain. Due to the simplest shuffle relation by Euler [57]

\[
S_{a,b}(N) + S_{b,a}(N) = S_a(N)S_b(N) + S_{a \oplus b}(N)
\]

(6.1)

with

\[
a \wedge b := \text{sign}(a) \text{ sign}(b) \left| a \right| + \left| b \right|
\]

(6.2)

these sums are connected, which implies the following relation for the Mellin transforms

\[
\mathcal{M}\left[ \frac{\ln(1-x)}{1-x} \right](N) = -\mathcal{M}\left[ \frac{\ln(1+x)}{1+x} \right](N) + (-1)^{N+1}\left[ S_1(N)S_{-1}(N) + S_{-2}(N) \right.
\]

\[
\left. + \left[ S_1(N) - S_{-1}(N) \right]\ln(2) - \ln^2(2) + \frac{1}{2}\zeta_2 \right].
\]

(6.3)

cf. [2]. Similar to (5.5) one may decompose

\[
\frac{\ln(1-x^2)}{1-x^2} = 2 \left\{ \frac{\ln(1-x)}{1-x} + \frac{\ln(1-x)}{1+x} + \frac{\ln(1+x)}{1-x} + \frac{\ln(1+x)}{1+x} \right\},
\]

(6.4)

which yields

\[
\mathcal{M}\left[ \left( \frac{\ln(1-x)}{1-x} \right)_+ \right](N) = \mathcal{M}\left[ \left( \frac{\ln(1-x)}{1-x} \right)_+ \right](N) + \mathcal{M}\left[ \frac{\ln(1-x)}{1+x} \right](N)
\]

\[
+ \mathcal{M}\left[ \frac{\ln(1+x)}{1+x} \right](N) + \mathcal{M}\left[ \frac{\ln(1+x)}{1-x} \right](N) - \frac{1}{2}\zeta_2 + \ln^2(2).
\]

(6.5)

Since the l.h.s. of (6.5) and the first and fourth term in the r.h.s. are polynomials of single sums, the remainder two terms are related. However, (6.4) does not yield a new relation. Therefore

\[
F_1(N) := \mathcal{M}\left[ \frac{\ln(1+x)}{1+x} \right](N)
\]

(6.6)

is the first non-trivial Mellin transform beyond the single harmonic sum \( S_1(N) \). Although \( F_1(N) \) expresses a harmonic sum containing \(-1\) as index, which belongs to a class being absent in the final results in physics applications, it may be of use to derive compact expressions in other cases later.

As a historic remark, we mention that Nielsen [27] considered these functions as well using the notation \( \xi(N), \eta(N), \xi_1(N) \) and \( \xi_2(N) \),

\[
\xi(N) = \mathcal{M}\left[ \frac{\ln(1-x)}{x-1} \right](N-1) = \frac{1}{2}\left[ \psi'(N) - \xi_2 - (\psi(N) + \gamma_E)^2 \right] = -S_{1,1}(N-1),
\]

(6.7)

\[
\eta(N) = \mathcal{M}\left[ \frac{\ln(1+x) - \ln(2)}{x-1} \right](N-1),
\]

(6.8)

\[
\xi_1(N) = \mathcal{M}\left[ \frac{\ln(1+x)}{x+1} \right](N-1),
\]

(6.9)

\[
-\xi_2(N) = \mathcal{M}\left[ \frac{\ln(1-x)}{x+1} \right](N-1).
\]

(6.10)

They obey the relations

\[
\left[ \psi(z) + \gamma_E \right]\left[ \psi(1-z) + \gamma_E \right] = 2\xi_2 - \xi(z) - \xi(1-z),
\]

(6.11)

\[
\beta(z)\left[ \psi(1-z) + \gamma_E \right] = -\beta(1-z)\ln(2) - \xi_1(z) - \xi_2(1-z),
\]

(6.12)

\[
\beta(z)\left[ \psi(z) + \gamma_E \right] = \beta'(z) + \beta(z)\ln(2) + \frac{1}{2}\psi\left( \frac{z}{2} \right) - \frac{1}{2}\psi\left( \frac{z+1}{2} \right),
\]

(6.13)

\[
\beta(z) + \beta(1-z) = \frac{\pi}{\sin(\pi z)},
\]

(6.14)

\[
\beta(z)\beta(1-z) = \eta(z) + \eta(1-z),
\]

(6.15)

\[
\beta^2(z) = \psi'(z) - 2\eta(z),
\]

(6.16)

for \( z \in ]0,1[ \). Most of them were given in Ref. [27]. They result from algebraic relations between harmonic sums and corresponding integral representations. Let us illustrate this for (6.12). One may represent

\[
\beta(N+1)\left[ \psi(N+1) + \gamma_E \right] = (-1)^NS_1(N)\left[ S_{-1}(N) + \ln(2) \right].
\]

(6.17)
cf. [2]. Using Euler’s relation (6.1) one obtains
\[
\beta(N + 1)[\psi(N + 1) + \gamma_E] = (-1)^N[S_{1,-1}(N) + S_{-1,1}(N) - S_{-2}(N) + \ln(2)S_1(N)],
\]
(6.18)
which can be expressed referring to the functions \( \beta(N), \beta'(N), \xi_1(N) \) and \( \xi_2(N) \). Relation (6.13) is a consequence of the properties of the logarithm.11

7. Sums of weight three

There are eighteen harmonic sums of weight \( w = 3 \) [2]. Twelve of these sums are related to the remaining six harmonic sums by shuffle relations [15]. The latter are represented by the Mellin transforms
\[
M \left[ \frac{\ln^2(1+x)}{1-x} \right]_+(N), \quad M \left[ \frac{\ln^2(1+x)}{1+x} \right]_+(N),
\]
\[
M \left[ \frac{\text{Li}_2(-x)}{1-x} \right]_+(N), \quad M \left[ \frac{\text{Li}_2(x)}{1-x} \right]_+(N),
\]
\[
M \left[ \frac{\text{Li}_2(-x)}{1+x} \right]_+(N), \quad M \left[ \frac{\text{Li}_2(x)}{1+x} \right]_+(N).
\]
(7.1)
The first two functions in (7.1) correspond to the harmonic sums of the type \( S_{-1,1,-1}(N) \) and \( S_{1,1,-1}(N) \), which are not connected algebraically. Using the general relation
\[
M[\ln^{(n)} f(x)](N) = \frac{d^n}{dn^N} M[f(x)](N),
\]
(7.2)
the Mellin transform \( M[\ln(x)\ln(1+x)/(1+x)](N) \) can be calculated from \( F_1(N) \). We exploit Euler’s relation for the sums \( S_{1,-2}(N) \) and \( S_{-2,1}(N) \), [2], to express \( M[\text{Li}_2(-x)/(1+x)](N) \) in terms of \( M[\text{Li}_2(x)/(1+x)](N) \),
\[
M \left[ \frac{\text{Li}_2(-x)}{1+x} \right]_+(N) = (-1)^{N+1} \left\{ \ln(2) [S_2(N) - S_{-2}(N)] + \frac{1}{2} \text{Li}_2 S_{-1}(N) + \frac{3}{4} \zeta_3 \right. \\
+ S_{-1}(N) S_2(N) + S_{-3}(N) \left. \right\} + M \left[ \frac{\text{Li}_2(x) + \ln(x)\ln(1-x)}{1+x} \right]_+(N).
\]
(7.3)
Furthermore, the identity
\[
\frac{1}{2^{n-2}} \frac{\text{Li}_n(x^2)}{1-x^2} = \frac{\text{Li}_n(x)}{1-x} + \frac{\text{Li}_n(x)}{1+x} + \frac{\text{Li}_n(-x)}{1-x} + \frac{\text{Li}_n(-x)}{1+x}
\]
holds and one obtains
\[
M \left[ \frac{\text{Li}_2(-x)}{x-1} \right]_+(N) = \frac{1}{2} M \left[ \frac{\text{Li}_2(x)}{x-1} \right]_+(N) - \frac{1}{2} M \left[ \frac{\text{Li}_2(x)}{x+1} \right]_+(N) - \frac{3}{8} \zeta_3 + \frac{1}{2} \text{Li}_2 \ln(2).
\]
(7.5)
Eq. (7.5) can be used to express
\[
M[\{(\text{Li}_2(-x)/(1-x))_+\}](N)
\]
in terms of the remaining Mellin transforms.

Four basic functions emerge at weight \( w = 3 \)
\[
F_2(N) := M \left[ \frac{\ln^2(1+x) - \ln^2(2)}{1-x} \right]_+(N),
\]
(7.6)
\[
F_3(N) := M \left[ \frac{\ln^2(1+x)}{1+x} \right]_+(N),
\]
(7.7)
\[
F_4(N) := M \left[ \frac{\text{Li}_2(x)}{x-1} \right]_+(N),
\]
(7.8)
\[
F_5(N) := M \left[ \frac{\text{Li}_2(x)}{x+1} \right]_+(N).
\]
(7.9)
Here we have chosen a form for \( F_2(N) \) which yields a particular simple asymptotic representation as \( N \in \mathbb{C}, |N| \to \infty \). The basic sums at weight \( w = 3 \) which do not contain the index \( \{-1\} \) are thus given by
\[
S_{-2,1}(N) = (-1)^{N+1} F_4(N) + \zeta_2 S_{-1}(N) - \frac{5}{8} \zeta_3 + \zeta_2 \ln(2),
\]
(7.10)
\[
S_{2,1}(N) = F_4(N) + \zeta_2 S_{1}(N).
\]
(7.11)
11 We correct misprints in Ref. [27], §75, third equation. The minus sign in front of \( \beta'(x) \) has to be removed. The equation below Eq. (8) has to be replaced by (6.12).
8. Sums of weight four

Out of the 54 harmonic sums which emerge at weight \( w = 4 \), 38 harmonic sums can be expressed by 16 sums through shuffle relations [15]. The latter sums are related to one Mellin transform for each index set \((-1, 1, 1), (1, -1, 1), (1, 1, -1), (1, -1, -1), (1, 1, 1), (1, 1, 1), (3, 1), (3, -1), (3, 1), (1, -1, 2), (1, 1, -2), (1, 1, 2)\) and to two Mellin transforms for the sets \((-1, 1, 2)\) and \((-1, -1, 2)\). Various of these harmonic sums contain an index \((-1)\). Since sums of this type do not occur in the known physics applications we will discuss sums without this index only from here on. After the algebraic relations are exploited, the seven sums with index sets \((2, 1, 1), (-2, 1, 1), (3, 1), (-3, 1), (-2, 2), (4), \) and \((-2, 4)\) remain at this weight.

Unlike the case for weight \( w = 2 \), the harmonic sums with symmetric index pattern at weight \( w = 4 \), \( S_{-2,-2}(N) \) and \( S_{2,2}(N) \) relate two of the above Mellin transforms. They have the representation, [2],

\[
S_{-2,-2}(N) = \mathcal{M}\left[ \frac{\text{Li}_2(x) - 2\text{Li}_3(x)}{x-1} \right](N) + \frac{\zeta_2}{2} [S_2(N) - S_{-2}(N)] - \frac{3}{2} \zeta_3 S_1(N) \quad (8.1)
\]

\[
S_{2,2}(N) = \mathcal{M}\left[ \frac{\text{Li}_2(x) - 2\text{Li}_3(x)}{x-1} \right](N) + 2\zeta_3 S_1(N)
= \frac{1}{2} \left\{ \left[ \psi'(N + 1) + (-1)^N \frac{1}{2} \zeta_2 \right]^2 - \frac{1}{6} \psi^{(3)}(N + 1) + \frac{2}{5} \zeta_2^2 \right\}.
\quad (8.2)
\]

Since the Mellin transform of the distribution \([\text{Li}_3(-x)/(x-1)]_+\), \((7.5)\), depends on \( F_{1,2,4}(N) \) and \( \mathcal{M}[\text{Li}_2(x)/(x-1)]_+ \) is a basic function their derivative w.r.t. \( N \) is known and the Mellin transforms of \([\text{Li}_3(-x)/(x-1)]_+\) and \([\text{Li}_3(x)/(x-1)]_+\) can be expressed by \((8.1), (8.2)\).

One may use the relation

\[
S_{3,-1}(N) + S_{-1,3}(N) = S_{-1}(N) S_3(N) + S_{-4}(N)
\quad (8.3)
\]

to express \( \mathcal{M}[\text{Li}_3(-x)/(1 + x)]_+(N) \)

\[
\mathcal{M}\left[ \text{Li}_3(-x) \right]_+(1 + x) \quad (N) = -\mathcal{M}\left[ \text{Li}_3(x) \right]_+(1 + x) \quad (N) + \mathcal{M}\left[ \text{Li}_2(x) + \text{Li}_3(x) \right](N)
+ (-1)^N \frac{3}{5} \zeta_2^2 - \frac{5}{2} \zeta_3 \ln 2 + S_{-1}(N) S_3(N) + S_{-4}(N)
\]

\[
- \ln(2) [S_{-3}(N) - S_3(N)] + \frac{1}{2} \zeta_2 S_{-2}(N) - \frac{7}{4} \zeta_3 S_1(N)
\]

\[
- (S_{-1}(N) + \ln(2)) \zeta_3.
\quad (8.4)
\]

Furthermore, the relation

\[
\frac{1}{4} \mathcal{M}\left[ \text{Li}_3(x) \right]_+(1 - x)^+ \left( \frac{N}{2} \right) = \mathcal{M}\left[ \text{Li}_3(x) \right]_+(1 - x)^+ \quad (N) + \mathcal{M}\left[ \text{Li}_3(x) \right]_+(1 + x)^+ \quad (N)
+ \mathcal{M}\left[ \text{Li}_3(-x) \right]_+(1 + x)^+ \quad (N) + \mathcal{M}\left[ \text{Li}_3(-x) \right]_+(1 - x)^+ \quad (N)
\]

\[
+ \frac{29}{40} \zeta_2^2 - 2 \zeta_4 \left( \frac{1}{2} \right) = \frac{3}{2} \zeta_3 \ln 2 + \frac{1}{2} \zeta_3 \ln^2 2 - \frac{1}{12} \ln^4 2
\quad (8.5)
\]

holds. However, similar to \((6.5)\), it does not lead to a further reduction since \( \mathcal{M}[\text{Li}_3(-x)/(1 + x)]_+(N) \) and \( \mathcal{M}[\text{Li}_3(x)/(1 + x)]_+(N) \) enter in the same way as in \((8.4)\).

Square argument relations may be considered for more general Nielsen integrals as well. For \( S_{1,2}(x)/(1 - x) \) one obtains the relation

\[
\frac{1}{2} \mathcal{M}\left[ S_{1,2}(x) \right]_+(1 - x)^+ \left( \frac{N}{2} - 1 \right) = \mathcal{M}\left[ S_{1,2}(x) \right]_+(1 - x)^+ \quad (N)
+ \mathcal{M}\left[ S_{1,2}(x) \right]_+(1 + x)^+ \quad (N)
+ \mathcal{M}\left[ S_{1,2}(-x) \right]_+(1 + x)^+ \quad (N)
+ \mathcal{M}\left[ S_{1,2}(-x) \right]_+(1 - x)^+ \quad (N)

+ \int_0^1 dx \frac{S_{1,2}(x^2)}{1 + x}.
\quad (8.6)
\]

which refers to the functions \( S_{1,2}(\pm x)/(1 \pm x) \) and \( I_1(x)/(1 \pm x) \). \( I_1(x) \) is given by, cf. [30],

\[
I_1(x) = \frac{1}{2} S_{1,2}(x^2) - S_{1,2}(x) - S_{1,2}(-x).
\quad (8.7)
\]
The function \( I_1(x)/(1 - x) \) does not occur up to \( w = 6 \) for single scale quantities. Therefore, we do not consider square argument relations beyond those for \( \text{Li}_k(x) \) in the following.

At weight \( w = 4 \) the following basic functions contribute:

\[
\begin{align*}
F_{6a}(N) := & M \left[ \frac{\text{Li}_3(x)}{1 - x} \right]_+(N), \\
F_{6b}(N) := & M \left[ \frac{\text{Li}_3(x)}{1 + x} \right]_+(N), \\
F_7(N) := & M \left[ \frac{S_{1,2}(x)}{x - 1} \right]_+(N), \\
F_8(N) := & M \left[ \frac{S_{1,2}(x)}{1 + x} \right]_+(N).
\end{align*}
\]

The number of basic Mellin transform occurring in physical processes turns out to be even smaller. In the case of the one-loop anomalous dimensions and the Wilson coefficients in first order in the coupling constant, at most single harmonic sums contribute. In the case of the two-loop anomalous dimensions \( F_2(N) \) emerges as the first non-trivial function, cf. [1]. The case of the 2-loop coefficient functions has been analyzed systematically in Ref. [10] for all Wilson coefficients in polarized and unpolarized deeply inelastic scattering, the polarized and unpolarized Drell–Yan process and the fragmentation functions, as well as the coefficient functions for hadronic Higgs- and pseudoscalar Higgs-production. In particular Mellin transforms being associated to harmonic sums with an index set formed of chains of the elements \(-1\) and \(+1\) do not contribute at this level. This does not exclude that functions of this type do not emerge in higher orders.

9. Sums of weight five

We will consider the sums of different depth separately and assume that the algebraic relations have been exploited already.

9.1. Twofold sums

The following sums contribute: \( S_{4,4,1}(N), S_{4,3,4,2}(N) \). We obtain the representations

\[
\begin{align*}
S_{4,4,1}(N) & = -M \left( \frac{\text{Li}_4(x)}{x - 1} \right)_+(N) + S_1(N) \zeta_4 - S_2(N) \zeta_3 + S_3(N) \zeta_2, \\
S_{4,3,4,2}(N) & = (-1)^{N+1} M \left( \frac{\text{Li}_4(x)}{x + 1} \right)_+(N) + S_{-1}(N) \zeta_4 - S_{-2}(N) \zeta_3 + S_{-3}(N) \zeta_2 + \frac{3}{4} \zeta_3 \zeta_4 - \frac{59}{32} \zeta_5. \\
S_{2,3,4}(N) & = M \left( \frac{\ln(x)[S_{1,2}(1 - x) - \zeta_3] + 3[S_{1,3}(1 - x) - (\zeta_3)]}{x - 1} \right)_+(N) + 3 \zeta_4 S_1(N), \\
S_{2,2,3}(N) & = (-1)^N M \left( \frac{\ln(x)[S_{1,2}(1 - x) - \zeta_3] + 3[S_{1,3}(1 - x) - (\zeta_3)]}{1 + x} \right)_+(N) \\
& + 3 \zeta_4 S_{-1}(N) + \frac{21}{32} \zeta_5 + 3 \zeta_4 \ln(2) - \frac{3}{4} \zeta_2 \zeta_3, \\
S_{2,1,3}(N) & = (-1)^{N+1} M \left( \frac{1}{1 + x} \left[ \frac{1}{2} \ln^2(x) \text{Li}_2(-x) - 2 \ln(x) \text{Li}_3(-x) + 3 \text{Li}_4(-x) \right] \right)_+(N) \\
& + \frac{3}{4} \zeta_3 [S_{-2}(N) - S_{2}(N)] - \frac{21}{8} \zeta_4 S_{-1}(N) - \frac{41}{32} \zeta_5 - \frac{21}{8} \zeta_4 \ln(2) + \zeta_2 \zeta_3, \\
S_{1,2,3}(N) & = -M \left( \frac{1}{x - 1} \left[ \frac{1}{2} \ln^2(x) \text{Li}_2(-x) - 2 \ln(x) \text{Li}_3(-x) + 3 \text{Li}_4(-x) \right] \right)_+(N) \\
& + \frac{3}{4} \zeta_3 [S_{2}(N) - S_{-2}(N)] - \frac{21}{8} \zeta_4 S_1(N).
\end{align*}
\]

In the above integrands we use the relations

\[
\begin{align*}
S_{1,2}(1 - x) & = - \text{Li}_3(x) + \ln(x) \text{Li}_2(x) + \frac{1}{2} \ln(1 - x) \ln^2(x) + \zeta_2, \\
S_{1,3}(1 - x) & = - \text{Li}_4(x) + \ln(x) \text{Li}_3(x) - \frac{1}{2} \ln^2(x) \text{Li}_2(x) - \frac{1}{6} \ln^3(x) \ln(1 - x) + \zeta_4,
\end{align*}
\]

which reduce the representation. Since all Mellin transforms

\[
\frac{\text{Li}_k(\pm x)}{\pm 1}, \quad k \leq 3,
\]

are known, the only new ones are those of the functions

\[
\frac{\text{Li}_4(\pm x)}{\pm 1}
\]
and the other terms follow by differentiation. Due to

\[
S_{1,-4}(N) = (-1)^N M \left[ \frac{\text{Li}_4(-x) - \ln(x) \text{Li}_3(-x) + \ln^2(x) \text{Li}_2(-x)/2 + \ln^3(x) \ln(1+x)/6}{x+1} \right](N)
\]

+ \frac{7}{8} \zeta_4 \left[ S_{-1}(N) - S_1(N) \right] - \frac{1}{2} \zeta_2 \zeta_3 + \frac{7}{8} \zeta_4 \ln(2) + \frac{29}{32} \zeta_5.
\]

(9.11)

\[
S_{1,4}(N) = -M \left[ \frac{S_{1,3}(1-x)}{x-1} \right] + \frac{2}{5} \zeta_2^2 S_1(N) + \zeta + 2 \zeta_3 - 2 \zeta_5.
\]

(9.12)

Eqs. (9.2), (9.11) allow to express

\[
M \left[ \frac{\text{Li}_4(-x)}{1+x} \right](N),
\]

(9.13)

but (9.12) does not lead to a new relation.

In some of the harmonic sums Mellin transforms of the functions

\[
\text{Li}_k(-x)
\]

(9.14)

emerge. For odd values of \(k = 2l + 1\) the harmonic sums \(S_{1,-(k-1)}(N), S_{-(k-1),1}(N)\) and \(S_{-l-1}(N)\) allow to substitute the Mellin transforms of these functions in terms of Mellin transforms of basic functions and derivatives thereof. For even values of \(k\) this argument applies to \(M[\text{Li}_k(-x)/(1+x)](N)\) but not to \(M[\text{Li}_k(-x)/(1+x)](N)\). In the latter case one may use relation (7.4). Since in massless quantum field-theoretic calculations both denominators occur, one may use this decomposition based on the first two cyclotomic polynomials, cf. [48], and the decomposition relation for \(\text{Li}_k(x^2)\). The corresponding Mellin transforms also require half-integer arguments. The relation

\[
\frac{1}{2^{k-1}} M \left[ \frac{(\text{Li}_k(x^2))}{x^2-1} \right] \left[ \frac{N-1}{2} \right] = M \left[ \frac{(\text{Li}_k(x))}{x-1} \right] \left[ \frac{N-1}{2} \right] + M \left[ \frac{(\text{Li}_k(x))}{x+1} \right] \left[ \frac{N-1}{2} \right] + M \left[ \frac{(\text{Li}_k(-x))}{x-1} \right] \left[ \frac{N}{2} \right] - M \left[ \frac{(\text{Li}_k(-x))}{x+1} \right] \left[ \frac{N}{2} \right] - \int_0^1 dx \frac{\text{Li}_k(x^2)}{1+x}
\]

(9.15)

determines \(M[\text{Li}_k(-x)/(1+x)](N)\). For \(k = 4\) the last integral in (9.15) is given by

\[
\int_0^1 dx \frac{\text{Li}_4(x^2)}{1+x} = \frac{2}{5} \ln(2) \zeta_2^2 + 3 \zeta_2 \zeta_3 - \frac{25}{4} \zeta_5
\]

(9.16)

and one obtains

\[
M \left[ \frac{\text{Li}_4(-x)}{x+1} \right](N) = -\frac{1}{8} M \left[ \frac{(\text{Li}_4(x))}{x-1} \right] \left[ \frac{N-1}{2} \right] + M \left[ \frac{(\text{Li}_4(x))}{x+1} \right] \left[ \frac{N-1}{2} \right] + M \left[ \frac{(\text{Li}_4(-x))}{x-1} \right] \left[ \frac{N}{2} \right] - M \left[ \frac{(\text{Li}_4(-x))}{x+1} \right] \left[ \frac{N}{2} \right] - \frac{1}{20} \zeta_2^2 \ln(2) - \frac{3}{8} \zeta_2 \zeta_3 + \frac{25}{32} \zeta_5.
\]

(9.17)

The new functions are:

\[
F_9(N) = M \left[ \frac{(\text{Li}_4(x))}{x-1} \right](N),
\]

(9.18)

\[
F_{10}(N) = M \left[ \frac{\text{Li}_4(x)}{1+x} \right](N).
\]

(9.19)

9.2. Threefold sums

At this depth the sums \(S_{\pm 3,1,1}(N), S_{2,2,1}(N), S_{-2,2,1}(N), S_{-2,2,1}(N)\) and \(S_{2,2,1}(N)\) contribute. One derives the following representations.

\[
S_{3,1,1}(N) = M \left[ \frac{S_{2,2,1}(x)}{x-1} \right] \left[ \frac{N}{2} \right] + \zeta_3 S_2(N) - \frac{\zeta_4}{4} S_1(N),
\]

(9.20)

\[
S_{-3,1,1}(N) = (-1)^N M \left[ \frac{S_{2,2,1}(x)}{1+x} \right] \left[ \frac{N}{2} \right] + \zeta_3 S_2(-N) - \frac{\zeta_4}{4} S_{-1}(N) + \frac{7}{8} \zeta_3 \zeta_2 - \frac{1}{4} \zeta_2 \ln(2) - \frac{7}{8} \zeta_3 \ln^2(2) + \frac{1}{3} \zeta_2 \ln^3(2)
\]

+ \frac{15}{32} \zeta_5 - 2 \ln(2) \text{Li}_4(\frac{1}{2}) - 2 \text{Li}_5(\frac{1}{2}) - \frac{1}{15} \ln^5(2).
\]

(9.21)
S_{2,1,1} = -M\left(\frac{2S_{2,1}(x)}{x-1}\right)_+ (N) + \zeta_2 S_{2,1}(N) - \frac{3}{10} \zeta_2^2 S_1(N).

(9.22)

S_{-2,1,2} = M\left(\frac{\ln(x)S_{1,2}(-x) - Li_2^2(-x)/2}{x-1}\right)_+ (N)
- \frac{1}{2} \zeta_2\left[S_{-2,1}(N) - S_{-2,1}(-N)\right] \left[\frac{1}{8} \zeta_3 - \frac{1}{2} \ln(2) \zeta_2\right]\left[S_{-2}(N) - S_{2}(N)\right]
+ \frac{1}{8} \zeta_2^2 S_1(N).

(9.23)

S_{-2,2,1} = (-1)^{N+1} M\left[\frac{2S_{2,1}(x) - Li_2^2(x)/2}{1+x}\right] (N) + \zeta_2 S_{-2,1}(N) - \frac{3}{10} \zeta_2^2 S_{-1}(N)
+ 4 \ln(x)\left(\frac{1}{2}\right) + 4 \ln(x)\left(\frac{1}{2}\right) \ln(2) - \frac{89}{64} \zeta_3 - \frac{9}{8} \zeta_2 \zeta_3 + \frac{2}{15} \ln^5(2) - \frac{2}{3} \zeta_2 \ln^3(2)
+ \frac{7}{4} \zeta_3 \ln^2(2) - \frac{3}{16} \zeta_2^2 \ln(2).

(9.24)

S_{2,1,2} = (-1)^N M\left[\frac{\ln(x)S_{1,2}(-x) - Li_2^2(-x)/2}{1+x}\right] (N)
- \frac{1}{2} \zeta_2\left[S_{2,1}(N) - S_{-2,1}(N)\right] \left[\frac{1}{8} \zeta_3 - \frac{1}{2} \ln(2) \zeta_2\right]\left[S_{2}(N) - S_{-2}(N)\right]
+ \frac{1}{8} \zeta_2^2 S_{-1}(N) - \frac{177}{64} \zeta_3 + \frac{11}{8} \zeta_2 \zeta_3 + \frac{1}{8} \zeta_2^2 \ln(2).

(9.25)

Here also the sums $S_{2,2,1}(N)$ emerge, which is a consequence of the representation chosen. The associated Mellin transforms are accounted for, however, by the $w = 3$ basic functions, cf. [2]. In the threefold sums the basic functions

$F_{11}(N) = M\left(\frac{S_{2,1}(x)}{x-1}\right)_+ (N),

(9.26)

F_{12}(N) = M\left[\frac{S_{2,1}(x)}{1+x}\right] (N),

(9.27)

F_{13}(N) = M\left[\frac{Li_2^2(x)}{x-1}\right] (N),

(9.28)

F_{14}(N) = M\left[\frac{Li_2^2(x)}{1+x}\right] (N),

(9.29)

F_{15}(N) = M\left[\frac{ln(x)S_{1,2}(-x) - Li_2^2(-x)/2 + \zeta_2^2/8}{x-1}\right] (N),

(9.30)

F_{16}(N) = M\left[\frac{ln(x)S_{1,2}(-x) - Li_2^2(-x)/2}{1+x}\right] (N),

(9.31)

emerge.

9.3. Fourfold sums

Here the two sums $S_{2,2,1,1,1}(N)$ contribute. They obey the representation

$S_{2,2,1,1,1} = -M\left[\frac{S_{1,1,1}(x)}{x-1}\right]_+ (N) + \zeta_4 S_1(N),

(9.32)

S_{-2,2,1,1,1} = (-1)^{N+1} M\left[\frac{S_{1,1,1}(x)}{1+x}\right] (N) + \zeta_4 S_{-1}(N) + \zeta_4 \ln(2) - \frac{7}{16} \zeta_2 \zeta_3 - \frac{1}{6} \zeta_2 \ln^3(2)
+ \frac{7}{16} \zeta_3 \ln^2(2) - \frac{27}{32} \zeta_3 + \ln(2) \ln(2) \frac{1}{2} + \frac{1}{30} \ln^5(2) + \ln(2) \ln(2) \frac{1}{2}.

(9.33)

The final basic functions contributing up to weight $w = 5$ are thus

$F_{17}(N) = M\left[\frac{S_{1,1,1}(x)}{x-1}\right]_+ (N),

(9.34)

F_{18}(N) = M\left[\frac{S_{1,1,1}(x)}{1+x}\right] (N).

(9.35)
Let us summarize the basic functions, which contribute up to the level of the 3-loop anomalous dimensions, which are \( w = 5 \) quantities. They are given by

\[
\begin{align*}
\text{w = 1:} & \quad 1/(x - 1), \\
\text{w = 2:} & \quad \ln(1 + x)/(x + 1), \\
\text{w = 3:} & \quad \text{Li}_2(x)/(x \pm 1), \\
\text{w = 4:} & \quad \text{Li}_3(x)/(x + 1), \quad S_{1,2}(x)/(x \pm 1), \\
\text{w = 5:} & \quad \text{Li}_4(x)/(x \pm 1), \quad S_{1,3}(x)/(x + 1), \quad S_{2,2}(x)/(x \pm 1), \\
& \quad \text{Li}_2^5(x)/(x + 1), \quad \left[ \ln(x)S_{1,2}(-x) - \text{Li}_2^2(-x)/2 \right]/(x \pm 1).
\end{align*}
\]

The five-fold sum \( S_{1,1,1,1,1}(N) \) decomposes algebraically into a polynomial out of single sums, [2]. The representation of the regularized Mellin transforms of the basic functions for complex argument is given in Appendix B.

10. Conclusions

We investigated the relations between harmonic sums, which are related to their functional value. They extend the set of algebraic relations being implied by their quasi-shuffle property related to the index pattern. In quantum field theoretic calculations of massless single scale quantities up to 3-loop order and for massive quantities to 2-loop order only harmonic sums with indices \( i \neq -1 \) occur. We derived the structural relations for this sub-algebra up to weight \( w = 5 \). These are fractional argument-, integration-by-parts- and differentiation relations. The set of 69 harmonic sums is reduced to 30 sums by the algebraic relations. The structural relations imply a further reduction to 15 basic harmonic sums. In physical applications these sums have to be known for complex arguments. We showed that these functions can be analytically continued to meromorphic functions with poles at the non-positive integers referring to their representation in terms of Mellin-integrals. The basic sums obey recurrence relations for complex arguments given by corresponding harmonic sums of lower weight. Separating divergent contributions for \( |N| \to \infty, \propto S^k_1(N), k \geq 0, k \in \mathbb{N} \), algebraically, the asymptotic representation of the harmonic sums was derived in analytic form. The recursion relations and asymptotic representations allow to calculate the basic functions for complex arguments analytically. In the physical applications to \( w = 5, 15 \) basic functions contribute, as the example of the 3-loop anomalous dimensions shows. This set is extended to 37 functions at \( w = 6 \) in case of the 3-loop Wilson coefficients, cf. [37]. Here, 20 functions emerge for \( w = 6 \) and two \( w = 5 \) functions \( M(\text{Li}_2(x)/(x - 1)) \) and \( M(S_{1,3}(x)/(x - 1)) \) do also occur. They do not contribute to the 3-loop anomalous dimensions. We included their representation in the present paper. The investigation of a large number of massless and massive 2-loop problems showed that the basic functions are universal up to isomorphies. This is expected also for the 3-loop case.

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Appendix A. Algebraic relations

In this appendix we list the algebraic relations w.r.t. the basis derived in the present paper. As the two-fold sums obey the simple relation \( (6.1) \) we list the sums of higher depth only. In the following we give the explicit representation of the harmonic sums without an index \([-1]\), which contribute in physical single-scale processes up to \( w = 5 \). The single sums are given in (5.10), (5.11). In the following we drop the common argument \( N \).

Weight 2 sums:

\[
S_{1,1} = \frac{1}{2} \left[ S_1^2 + S_2 \right].
\]  

Weight 3 sums:

\[
S_{1,1,1} = \frac{1}{6} S_1^3 + \frac{1}{2} S_1 S_2 + \frac{1}{3} S_3.
\]  

Weight 4 sums:

\[
\begin{align*}
S_{1,-2,1} &= -2S_{-2,1,1} + S_1 S_{-2,1} + S_{-3,1} + S_{-2,2}, \\
S_{1,1,-2} &= -S_{-2,1,1} - S_1 S_{-2,1} - S_{-3,1} - S_{-2,2} + S_1 S_{-3} + S_{-4} + \frac{1}{2} S_{-2} \left[ S_1^2 + S_2 \right], \\
S_{1,2,1} &= -2S_{2,1,1} + S_1 S_{2,1} + S_1 S_{1,1} + S_{2,2}, \\
S_{1,1,2} &= S_{2,1,1} - S_1 S_{2,1} - S_{3,1} - S_{2,2} + S_3 S_1 + S_4 + \frac{1}{2} S_2 \left[ S_1^2 + S_2 \right], \\
S_{1,1,1,1} &= \frac{1}{4} S_4 + \frac{1}{8} S_2^2 + \frac{1}{3} S_1 S_3 + \frac{1}{4} S_1^2 S_2 + \frac{1}{24} S_1^4.
\end{align*}
\]
Weight 5 sums:

\[
S_{1,-3,1} = -2S_{-3,1,1} + S_{1}S_{-3,1} + S_{-4,1} + S_{-3,2},
\]

\[
S_{1,1,-3} = S_{-3,1,1} - S_{1}S_{-3,1} - S_{-4,1} - S_{-3,2} + S_{1}S_{-4} + S_{-5} + \frac{1}{2}S_{-3}[S_{1}^{2} + S_{2}],
\]

\[
S_{1,3,1} = -2S_{3,1,1} + S_{1}S_{3,1} + S_{4,1} + S_{3,2},
\]

\[
S_{1,1,3} = S_{3,1,1} - S_{1}S_{3,1} - S_{4,1} - S_{3,2} + S_{1}S_{4} + S_{5} + \frac{1}{2}S_{3}[S_{1}^{2} + S_{2}],
\]

\[
S_{-2,-2,1} = \frac{1}{2}[-S_{-2,1,-2} + S_{-2}S_{-2,1} + S_{4,1} + S_{-2,3}],
\]

\[
S_{1,-2,-2} = \frac{1}{2}[-S_{1,-2,-2} + S_{-2}S_{1,-2} + S_{-3,-2} + S_{1,4}],
\]

\[
S_{2,-2,1} = -S_{2,1,-2} - S_{-2,2,1} + S_{3,-2} - S_{1,-4} - S_{-2}S_{1,2} + S_{1}S_{2,-2} + S_{2,-3} + S_{1}S_{-2,2} + S_{-2,3},
\]

\[
S_{-2,1,2} = S_{2}S_{-2,1} + S_{-4,1} + S_{2,1,-2} - S_{3,-2} + S_{1,-4} + S_{-2}S_{1,2} - S_{1}S_{2,-2} - S_{2,-3} - S_{1}S_{-2,2},
\]

\[
S_{1,-2,2} = -S_{2}S_{-2,1} - S_{-4,1} - S_{2,1,-2} - S_{-2,2,1} + S_{3,-2} - S_{1,-4} - S_{-2}S_{1,2} + S_{1}S_{2,-2} + S_{2,-3} + S_{3,-2},
\]

\[
S_{1,2,-2} = -S_{2}S_{1,2} + S_{1,-4} - S_{1}S_{-2,2} - S_{-2,3} + S_{-2,2,1},
\]

\[
S_{2,1,2} = -2S_{2,2,1} + S_{2}S_{2,1} + S_{4,1} + S_{2,3},
\]

\[
S_{1,2,2} = S_{2,2,1} + \frac{1}{2}[S_{2}S_{1,2} + S_{3,2} + S_{1,4} - S_{2}S_{2,1} - S_{4,1} - S_{2,3}],
\]

\[
S_{1,1,-2,1} = -3S_{-2,1,1,1} + S_{1}S_{-2,1,1} + S_{-3,1,1} + S_{-2,2,1} + S_{-2,1,2},
\]

\[
S_{1,1,-2,1} = 3S_{2,-1,1,1} - S_{1}S_{-2,1,1} - S_{-3,1,1} - S_{-2,2,1} - S_{-2,1,2}
\]

\[
\frac{1}{2}[S_{1}S_{-2,1} + S_{2,-2,1} + S_{1,-3,1} + S_{1,-2,2}],
\]

\[
S_{1,1,1,-2} = -S_{2,-1,1,1} + \frac{1}{3}S_{1}S_{1,1,-2} + S_{-2,1,1} - \frac{1}{2}S_{1,-2,1},
\]

\[
\frac{1}{3}(S_{2,1,-2} + S_{1,2,-2} + S_{1,1,-3} + S_{-3,1,1} + S_{-2,2,1} + S_{-2,1,2})
\]

\[
- \frac{1}{6}(S_{2,2,-1} + S_{1,-3,1} + S_{1,-2,2}).
\]

\[
S_{1,2,1,1} = -3S_{2,1,1,1} + S_{1}S_{2,1,1} + S_{3,1,1} + S_{2,2,1} + S_{2,1,2},
\]

\[
S_{1,1,2,1} = 3S_{2,1,1,1} + S_{1}\left[\frac{1}{2}S_{1,2,-1} - S_{2,1,1}\right] + \frac{1}{2}[S_{1,3,1,1} + S_{2,2,1} - S_{2,2,1}] + S_{1,1,-1} - S_{2,1,2},
\]

\[
S_{1,1,1,2} = -S_{2,1,1,1} + S_{1}\left[2S_{1,2,1} + S_{1,2,2} + S_{1,1,3} - \frac{1}{2}S_{1,3,1} + S_{3,1,1}\right]
\]

\[
- \frac{1}{3}\left[2S_{2,1,2} + \frac{1}{2}S_{2,2,1} + \frac{1}{2}S_{2,2,1} + S_{1,1,3} - \frac{1}{2}S_{1,3,1} + S_{3,1,1}\right].
\]

\[
S_{1,1,1,1,1}(N) = \frac{1}{120}S_{1}^{5} + \frac{1}{12}S_{2}^{3} + \frac{1}{6}S_{3}^{2} + \frac{1}{4}S_{4}S_{1} + \frac{1}{2}S_{1}^{2}S_{2} + \frac{1}{6}S_{2}S_{3} + \frac{1}{5}S_{5}.
\]

Some of the sums of lower complexity can be further expressed using algebraic relations.

**Appendix B. The basic functions for complex arguments**

To derive the analytic representation of the Mellin transforms of the basic functions we first express them in terms of factorial series and a rest part which can be decomposed algebraically.\(^{12}\) We show that both parts are meromorphic functions with poles at the nonpositive integers. They obey recursion relations in which functions of the same class but lower complexity occur. Finally we derive the associated asymptotic representations in analytic form. To make use of this formalism the basic functions have to be mapped. The corresponding functions lay in the same equivalence class. First we remind some properties of factorial series. Then we define the functions associated to the basic Mellin transforms and derive their recursion relations and asymptotic representations.

\(^{12}\) In [58] asymptotic relations for non-alternating harmonic sums to low orders in \(1/N^A\) were derived. Our algorithm given below is free of these restrictions. The main ideas were presented in January 2004 [59], see also [29].
B.1. Asymptotic representations of factorial series

The Mellin transforms
\[ \Omega(z) = \int_0^1 dt \varphi(t)t^{z-1} \]  
(B.1)

with \( \varphi(t) \) one of the above basic functions, suitably transformed, is an integral representation of a factorial series \( \Omega(z) \) [27,28] in the complex plane \( z \in \mathbb{C} \). The basic functions are mapped such that \( \varphi(t) \) can be expanded into a Taylor series around \( t = 1 \),
\[ \varphi(1-t) = \sum_{k=0}^{\infty} a_k t^k. \]  
(B.2)

As will be shown below, the remainder terms can be expressed in terms of known harmonic sums of lower complexity. For \( \Re(z) > 0 \), \( \Omega(z) \) is given by the factorial series
\[ \Omega(z) = \sum_{k=0}^{\infty} \frac{a_{k+1}}{z(z+1)\ldots(z+k)}. \]  
(B.3)

\( \Omega(z) \) has poles at the non-positive integers and one may continue \( \Omega(z) \) analytically to values of \( z \in \mathbb{C} \) as a meromorphic function. Let us now derive the asymptotic representation
\[ \Omega(z) \sim \sum_{k=1}^{\infty} \frac{a_k}{z^k}. \]  
(B.4)

As shown in [27] the coefficients \( a_k \) are obtained by
\[ a_1 = a_1, \]
\[ a_k = \sum_{l=0}^{k-2} (-1)^l c^l_{k-1} a_{k-l}. \]  
(B.5)

where \( c^l_k \) are the Stirling numbers of 2nd kind,
\[ c^l_k = \frac{1}{(k-1)!} \sum_{n=0}^{k-2} (-1)^n \binom{k-1}{n} (k-n-1)^{k+l-1}, \]  
(B.6)
\[ c^0_k = 1, \]
\[ c^1_k = c^1_{k+1} - kc^0_{k+1}. \]  
(B.7)

Not for all harmonic sums the asymptotic representation can be found in the way outlined above using the associated Mellin transform [2,15]. In the case of \( S_1(N) \) the function \( \psi(N+1) \) contains a logarithmic contribution
\[ \psi(1+z) = -\gamma_E + \sum_{k=1}^{\infty} \frac{z}{k(k+z)} \ln(z) + \frac{1}{2z} - \sum_{k=1}^{\infty} \frac{B_{2k}}{2kz^{2k}}. \]  
(B.9)

Here \( B_k \) denote the Bernoulli numbers, which can be obtained from the generating function [60]
\[ \frac{x}{\exp(x)-1} = \sum_{k=0}^{\infty} \frac{B_k x^k}{k!}. \]  
(B.10)

Also \( \psi(z) \) and its derivatives are meromorphic functions with poles at the non-positive integers. One may show that nested harmonic sums with an index pattern
\[ [1, 1, \ldots, 1, a, \ldots], \quad |a| > 1 \]  
(B.11)
contain a term \( \propto S^t_1(N) \) as \( |N| \to \infty \), where \( k \) is the number of 1’s left to \( a \). These terms can always be separated algebraically and result in a growth \( \propto \ln^k(z) \) similar to the behavior in (B.9). After this separation was performed the remainder terms can be expressed by factorial series.

The function \( \nu(z) \) is associated to \( \psi(z) \) by
\[ \nu(z) = \ln(z) - \psi(z) \]  
(B.12)
and removes the logarithm in (B.9). It obeys the following factorial series [27]
\[ \nu(z) = \sum_{s=0}^{\infty} \frac{s! \psi(s+1)}{z(z+1)\ldots(z+s)}, \]  
(B.13)
where \( \psi_n(x) \) denotes the Stirling polynomial which obeys the recursion
\[
(x + 2)\psi_n(x + 1) = (x - n)\psi_n(x) + (x + 1)\psi_{n-1}(x),
\]
with the initial values
\[
\psi_0(x) = \frac{1}{2}, \quad \psi_1(x) = \frac{1}{4\pi}(3x + 2).
\]
The function \( \beta(N) \) associated to the harmonic sum \( S_{-1}(N - 1) \) is represented by the factorial series
\[
\beta(z) = \sum_{k=0}^{\infty} \frac{k!}{z(z+1) \ldots (z+k)} \cdot \frac{1}{2^{k+1}} = \sum_{k=0}^{\infty} \frac{(-1)^k}{z+k}.
\]

To derive asymptotic representations for the basic function \( F_i(z)|_{i=1..18} \) some of the functions have to be mapped into a form, which is regular at \( z = 1 \), which is indicated by a hat below. We consider the following Mellin transforms:

\[
F_1(z) = \mathcal{M} \left[ \frac{\ln(1+x)}{1+x} \right] (z),
\]
\[
F_2(z) = \mathcal{M} \left[ \frac{\ln^2(1+x) - \ln^2(2)}{1-x} \right] (z),
\]
\[
F_3(z) = \mathcal{M} \left[ \frac{\ln^2(1+x)}{1+x} \right] (z),
\]
\[
\hat{F}_4(z) = \mathcal{M} \left[ \frac{\Li_2(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_5(z) = \mathcal{M} \left[ \frac{\Li_2(1-x)}{1+x} \right] (z),
\]
\[
\hat{F}_{60}(z) = \mathcal{M} \left[ \frac{S_{1,2}(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_{60}(z) = \mathcal{M} \left[ \frac{S_{1,2}(1-x)}{1+x} \right] (z),
\]
\[
\hat{F}_7(z) = \mathcal{M} \left[ \frac{\Li_3(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_8(z) = \mathcal{M} \left[ \frac{\Li_3(1-x)}{1+x} \right] (z),
\]
\[
\hat{F}_9(z) = \mathcal{M} \left[ \frac{S_{1,3}(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_{10}(z) = \mathcal{M} \left[ \frac{S_{1,3}(1-x)}{1+x} \right] (z),
\]
\[
\hat{F}_{11}(z) = \mathcal{M} \left[ \frac{S_{2,2}(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_{12}(z) = \mathcal{M} \left[ \frac{S_{2,2}(1-x)}{1+x} \right] (z),
\]
\[
\hat{F}_{13}(z) = \mathcal{M} \left[ \frac{\Li_2^2(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_{14}(z) = \mathcal{M} \left[ \frac{\Li_2^2(1-x)}{1+x} \right] (z),
\]
\[
F_{15}(z) = \mathcal{M} \left[ \frac{\ln(x)S_{1,2}(-x) - \Li_2^2(-x)/2 + \zeta_2^2/8}{1-x} \right] (z),
\]
\[
F_{16}(z) = \mathcal{M} \left[ \frac{\ln(x)S_{1,2}(-x) - \Li_2^2(-x)/2}{1+x} \right] (z),
\]
\[
\hat{F}_{17}(z) = \mathcal{M} \left[ \frac{\Li_4(1-x)}{1-x} \right] (z),
\]
\[
\hat{F}_{18}(z) = \mathcal{M} \left[ \frac{\Li_4(1-x)}{1+x} \right] (z).
\]
B.2. Representation of the basic functions

The numerator functions are related to the original basic functions, cf. [61], by

\[ \text{Li}_2(x) = -\text{Li}_2(1-x) - \ln(x) \ln(1-x) + \zeta_2, \quad (B.36) \]

\[ \text{Li}_3(x) = -S_{1,2}(1-x) - \ln(x) \text{Li}_2(1-x) - \frac{1}{2} \ln^2(x) \ln(1-x) + \frac{1}{2} \ln^2(x) \ln(x) + \zeta_3, \quad (B.37) \]

\[ S_{1,2}(x) = -\text{Li}_4(1-x) + \ln(1-x) \text{Li}_2(1-x) + \frac{1}{2} \ln^2(1-x) \ln(x) + \zeta_3, \quad (B.38) \]

\[ \text{Li}_4(x) = S_{1,3}(1-x) - \ln(x) S_{1,2}(1-x) - \frac{1}{2} \ln^2(x) \text{Li}_2(1-x) \]

\[-\frac{1}{6} \ln^3(x) \ln(1-x) + \frac{1}{2} \ln^2(x) \zeta_2 + \ln(x) \zeta_3 + \zeta_4. \quad (B.39) \]

\[ S_{1,3}(x) = -\text{Li}_4(1-x) + \ln(1-x) \text{Li}_3(1-x) - \frac{1}{2} \ln^2(1-x) \text{Li}_2(1-x) \]

\[-\frac{1}{6} \ln^3(x) \ln(x) + \zeta_4. \quad (B.40) \]

\[ \text{Li}_5^2(x) = \text{Li}_2^2(1-x) + 2 \text{Li}_2(1-x) \ln(1-x) \ln(x) - 2 \text{Li}_2(1-x) \zeta_2 \]

\[+ \ln^2(1-x) \ln^2(x) - 2 \ln(1-x) \ln(x) \zeta_2 + \zeta_2^2. \quad (B.41) \]

\[ S_{2,2}(x) = -S_{2,2}(1-x) + \ln(1-x) S_{1,2}(1-x) + \frac{\zeta_4}{4} \]

\[-\left[ \text{Li}_5(1-x) - \ln(1-x) \text{Li}_2(1-x) - \zeta_3 \right] \ln(x) + \frac{1}{4} \ln^2(1-x) \ln^2(x). \quad (B.42) \]

In the above we arranged the representations such, that the remainder Mellin transforms can be obtained either by algebraic relations or differentiation of Mellin transforms being derived above or are known otherwise, cf. [2,31,62]. We remind the following relations:

\[ M[\ln(1-x) \text{Li}_2(1-x)](N) = \frac{2}{N+1} \left[ S_1(N+1)S_2(N+1) + S_3(N+1) - \zeta_2 S_1(N+1) - \frac{1}{2} S_{2,1}(N+1) \right]. \quad (B.43) \]

\[ M[\ln^2(1-x) \text{Li}_2(1-x)](N) = -\frac{1}{N+1} \left[ 6S_{1,1,2}(N+1) + 4S_{1,2,1}(N+1) + 2S_{2,1,1}(N) \right] \]

\[-6\zeta_2 S_{1,1}(N+1) - 2\zeta_3 S_1(N+1) \right]. \quad (B.44) \]

\[ M[\ln(1-x) \text{Li}_3(1-x)](N) = -\frac{1}{N+1} \left[ 3S_{1,1,2}(N+1) + S_{1,2,1}(N+1) \right] \]

\[-\frac{3}{2} \zeta_2 \left( S_1^2(N+1) + S_2(N+1) \right) + \zeta_3 S_1(N+1) \right]. \quad (B.45) \]

\[ M[\ln(1-x) S_{1,2}(1-x)](N) = \frac{1}{N+1} \left[ 2S_{1,3}(N+1) + S_{3,1}(N+1) + S_{2,2}(N+1) \right] \]

\[-\zeta_2 S_2(N+1) - 2\zeta_3 S_1(N+1) \right]. \quad (B.46) \]

By summation one obtains from (B.43)-(B.46)
\[(-1)^N M \left[ \frac{\ln(1-x) \text{Li}_2(1-x)}{x+1} \right] \] \( = 2S_{-1,1,2}(N) + S_{-1,2,1}(N) - 2\zeta_2 S_{-1,1}(N) \]
\[ - \frac{7}{8} \zeta_2^2 + \frac{1}{8} \ln^4(2) + 3 \text{Li}_4 \left( \frac{1}{2} \right) + \frac{3}{4} \ln^2(2). \] (B.51)

\[(-1)^N M \left[ \frac{\ln^2(1-x) \text{Li}_2(1-x)}{x+1} \right] \] \( = -6S_{-1,1,2}(N) - 4S_{-1,1,2,1}(N) - 2S_{-1,2,1,1}(N) \]
\[ + 6\zeta_2 S_{-1,1,1}(N) + 2\zeta_3 S_{-1,1}(N) \]
\[ - \frac{21}{4} \zeta_2 \zeta_3 - \frac{1}{2} \zeta_2^2 \ln^3(2) + \frac{57}{20} \zeta_3^2 \ln(2) - \frac{1}{10} \ln^5(2) \]
\[ - \frac{29}{32} \zeta_5 + 12 \text{Li}_5 \left( \frac{1}{2} \right). \] (B.52)

\[(-1)^N M \left[ \frac{\ln(1-x) \text{Li}_3(1-x)}{x+1} \right] \] \( = -3S_{-1,1,1,2}(N) - S_{-1,1,2,1}(N) + 3\zeta_2 S_{-1,1,1,1}(N) \]
\[ - \zeta_3 S_{-1,1,1}(N) + \frac{35}{16} \zeta_2 \zeta_3 + \frac{5}{12} \zeta_2 \ln^3(2) \]
\[ - \frac{53}{40} \zeta_2^2 \ln(2) + \frac{7}{16} \zeta_3 \ln^2(2) - \frac{29}{64} \zeta_5 + \frac{1}{30} \ln^5(2) - 4 \text{Li}_5 \left( \frac{1}{2} \right). \] (B.53)

\[(-1)^N M \left[ \frac{\ln(1-x)S_{1,2}(1-x)}{x+1} \right] \] \( = 2S_{-1,1,3}(N) + S_{-1,3,1}(N) + S_{-1,2,2}(N) - \zeta_2 S_{-1,2}(N) - 2\zeta_3 S_{-1,1}(N) \]
\[ - \frac{15}{8} \zeta_2 \zeta_3 + \frac{1}{6} \zeta_2 \ln^3(2) - \frac{11}{46} \zeta_3^2 \ln(2) + \frac{7}{8} \zeta_3 \ln^2(2) \]
\[ + \frac{159}{64} \zeta_5 - \frac{1}{60} \ln^5(2) + 2 \text{Li}_5 \left( \frac{1}{2} \right). \] (B.54)

The above expressions depend on harmonic sums, for which we derive the following relations. They are used to derive the asymptotic representations only.

\[ S_{-1,1,1}(N) = S_{1,1,-1}(N) + \frac{1}{2} \left[ S_1(N) S_{-1,1}(N) + S_{-1,2,1}(N) + S_{-1,1,2}(N) \right] \]
\[ - S_1(N) S_{-1,1}(N) - S_{-2,1}(N) - S_{-1,2}(N) \] \( \right]. \) (B.55)

\[ S_{1,1,1}(N) = (-1)^N \frac{1}{2} \tilde{F}_3(N) + \ln(2) \left[ S_{1,1,1}(N) - S_{-1,1}(N) \right] + \frac{1}{2} \ln^2(2) \left[ S_1(N) - S_{-1}(N) \right] - \frac{1}{6} \ln^3(2). \] (B.56)

\[ S_{1,1,2}(N) = -\tilde{F}_7(N) + \zeta_2 S_{1,1}(N) - \zeta_3 S_1(N) + \frac{2}{5} \zeta_2^2. \] (B.57)

\[ S_{-1,1,2}(N) = (-1)^N \tilde{F}_8(N) + \zeta_2 S_{-1,1}(N) - \zeta_3 S_{-1}(N) - \text{Li}_4 \left( \frac{1}{2} \right) + \frac{9}{20} \zeta_2^2 - \frac{7}{8} \zeta_3 \ln(2) \]
\[ - \frac{1}{2} \zeta_2 \ln^2(2) - \frac{1}{24} \ln^4(2). \] (B.58)

\[ S_{1,2,-1}(N) = (-1)^N M \left[ 2S_{1,2}(x) + \ln(1+x) \text{Li}_2(-x) \right] \frac{1}{1+x} \]
\[ - \frac{1}{2} \zeta_2 S_{1,-1}(N) + \left[ \frac{1}{4} \zeta_3 - \frac{1}{2} \zeta_2 \ln(2) \right] \left[ S_1(N) - S_{-1}(N) \right] + \frac{6}{5} \zeta_2^2 - 3 \text{Li}_4 \left( \frac{1}{2} \right) \]
\[ - \frac{23}{8} \zeta_3 \ln(2) + \zeta_2 \ln^2(2) - \frac{1}{8} \ln^4(2). \] (B.59)

\[ S_{1,1,3}(N) = -\tilde{F}_{12}(N) + \zeta_3 S_{1,1}(N) - \frac{\zeta_2^2}{10} S_1(N) + 2\zeta_5 - \zeta_2 \zeta_3. \] (B.60)

\[ S_{1,2,2}(N) = -\frac{1}{2} \tilde{F}_{13}(N) - 2S_{1,3,3}(N) + \zeta_2 S_{1,2}(N) + 2\zeta_3 S_{1,1}(N) - \frac{\zeta_2^2}{2} S_1(N) + \zeta_2 \zeta_3 - \frac{3}{2} \zeta_5. \] (B.61)

\[ S_{-1,1,3}(N) = (-1)^N \tilde{F}_{12}(N) + \zeta_3 S_{-1,1}(N) - \frac{\zeta_2^2}{10} S_{-1}(N) + 2 \left[ \text{Li}_5 \left( \frac{1}{2} \right) + \text{Li}_4 \left( \frac{1}{2} \right) \ln(2) \right] \]
\[ + \frac{1}{15} \ln^5(2) - \frac{1}{3} \zeta_2 \ln^3(2) + \frac{3}{8} \zeta_2^2 \ln(2) + \frac{1}{16} \zeta_2 \zeta_3 - \frac{151}{64} \zeta_5. \] (B.62)

\[ S_{-1,3,1}(N) = S_{1,3,-1}(N) + S_1(N) S_{-1,3}(N) + S_{-1,4}(N) - S_{-1}(N) S_{1,3}(N) - S_{1,-4}(N). \] (B.63)
The above relations require the function

\[ M \left[ \frac{\ln^3(1-x)}{1+x} \right] (N), \] (B.69)

which is related to \( M[\ln^3(1+x)/(1+x)](N) \) by

\[ S_{-1,1,1,1}(N) = (-1)^{N+1} \frac{1}{6} M \left[ \frac{\ln^3(1-x)}{1+x} \right] (N) - \text{Li}_4\left(\frac{1}{2}\right), \] (B.70)

\[ S_{1,1,1,-1}(N) = (-1)^{N+1} \frac{1}{6} M \left[ \frac{\ln^3(1+x)}{1+x} \right] (N) + \text{Li}_4\left(\frac{1}{2}\right), \] (B.71)

\[ S_{-1,1,1,1}(N) = -S_{1,1,1,-1}(N) + S_1(N) \frac{1}{3} \left[ S_{-1,1,1}(N) + S_{1,1,-1}(N) - \frac{1}{2} S_{1,-1,1}(N) \right] \]

\[ - \frac{1}{6} \left[ S_{2,-1,1}(N) + S_{1,-2,1}(N) + S_{1,-1,2}(N) \right] + \frac{1}{3} \left[ S_{-1,2,1}(N) + S_{-2,1,1}(N) \right. \]

\[ + S_{-1,2,1}(N) + S_{1,1,-2}(N) + S_{2,1,-1}(N) + S_{1,2,-1}(N). \] (B.72)

The sums associated to the index sets \( [1,1,-1] \) and \( [1,2,-1] \) are represented by \( F_2(N) \), resp. \( S_{1,2,-1}(N) \) and \( S_{-1,1,2}(N) \), using the algebraic relations [15]. We use the subsidiary functions

\[ H_1(N) = M \left[ \frac{2\text{Li}_2(-x)}{1+x} + \ln(1+x) \right] (N), \] (B.73)

\[ H_2(N) = M \left[ \frac{\ln(1+x) \text{Li}_3(-x) + \text{Li}_2^2(-x)}{1+x} \right] (N), \] (B.74)

\[ H_3(N) = M \left[ \frac{\ln^3(1+x)}{1+x} \right] (N). \] (B.75)
to obtain the asymptotic representations, cf. Section B.4. The other sums are two-fold and their explicit representations were given in [2] and in the previous sections.

Changing the arguments from $z$ to $1 - z$ in the numerator functions leads to relations like

\[
M \left[ \frac{\text{Li}_2(z) - \zeta_2}{z + 1} \right] (N) = -M \left[ \frac{\text{Li}_2(1 - z)}{z + 1} \right] (N) - \frac{d}{dN} M \left[ \ln(1 - z) \right] (N), \tag{B.76}
\]

\[
M \left[ \frac{\text{Li}_3(z) - \zeta_3}{z + 1} \right] (N) = -M \left[ \frac{\text{Li}_3(1 - z)}{z + 1} \right] (N) - \frac{d}{dN} M \left[ \frac{\text{Li}_2(1 - z) + \zeta_2}{z + 1} \right] (N) - d^2 \frac{1}{dN^2} \frac{M}{2} \left[ \ln(1 - z) \right] (N), \tag{B.77}
\]

\[
M \left[ \frac{S_{1,2}(z) - \zeta_3}{z + 1} \right] (N) = -M \left[ \frac{\text{Li}_3(1 - z)}{z + 1} \right] (N) + M \left[ \ln(1 - x) \text{Li}_2(1 - z) \right] (N) + \frac{d}{dN} M \left[ \ln^2(1 - z) \right] (N), \tag{B.78}
\]

\[
M \left[ \frac{\text{Li}_4(z) - \zeta_4}{z + 1} \right] (N) = -M \left[ \frac{S_{1,3}(1 - z)}{z + 1} \right] (N) - \frac{d}{dN} M \left[ S_{1,2}(1 - z) - \zeta_3 \right] (N) - d^2 \frac{1}{dN^2} \frac{M}{2} \left[ \ln(1 - z) \right] (N), \tag{B.79}
\]

\[
M \left[ \frac{S_{1,3}(z) - \zeta_4}{z + 1} \right] (N) = -M \left[ \frac{\text{Li}_4(1 - z)}{z + 1} \right] (N) - \frac{1}{6} M \left[ \ln^3(1 - z) \right] (N) + M \left[ \ln(1 - z) \text{Li}_2(1 - z) \right] (N) - \frac{d}{dN} M \left[ \ln^2(1 - z) \text{Li}_2(1 - z) \right] (N), \tag{B.80}
\]

\[
M \left[ \frac{\text{Li}_2^2(z) - \zeta_2^2}{z + 1} \right] (N) = M \left[ \frac{\text{Li}_2(1 - z)}{z + 1} \right] (N) - 2\zeta_2 M \left[ \frac{\text{Li}_2(1 - z)}{z + 1} \right] (N) - 2\zeta_2 \frac{d}{dN} M \left[ \ln(1 - z) \right] (N) + 2 \frac{d}{dN} M \left[ \ln(1 - z) \text{Li}_2(1 - z) \right] (N), \tag{B.81}
\]

which are used to express the asymptotic representations, Section B.4.

B.3. Recursion relations

The following recursion relations hold for the basic functions:

\[
\psi(z) = \psi(z) + \frac{1}{z}, \tag{B.82}
\]

\[
\psi^{(n)}(z) = \psi^{(n)}(z) + (-1)^n \frac{n!}{2^{n+1}}, \tag{B.83}
\]

\[
\beta(z) = -\beta(z) + \frac{1}{z}, \tag{B.84}
\]

\[
\beta^{(n)}(z) = -\beta^{(n)}(z) + (-1)^n \frac{n!}{2^{n+1}}, \tag{B.85}
\]

\[
F_1(z) = -F_1(z - 1) + \frac{1}{z} \left[ \ln(2) - \beta(z + 1) \right], \tag{B.86}
\]

\[
F_2(z) = F_2(z - 1) + \frac{2}{z} F_1(z), \tag{B.87}
\]

\[
F_3(z) = -F_3(z - 1) + \frac{1}{z} \left[ \ln^2(2) - 2F_1(z + 1) \right]. \tag{B.88}
\]
\[ F_4(z) = F_4(z - 1) - \frac{1}{z} \left[ \zeta_2 - \frac{S_1(z)}{z} \right], \quad (B.89) \]

\[ F_5(z) = -F_5(z - 1) - \frac{1}{z} \left[ \zeta_2 - \frac{S_1(z)}{z} \right], \quad (B.90) \]

\[ F_{6a}(z) = F_{6a}(z - 1) - \frac{\zeta_3}{z} + \frac{1}{z^2} \left[ \zeta_2 - \frac{S_1(z)}{z} \right], \quad (B.91) \]

\[ F_{6b}(z) = -F_{6b}(z - 1) + \frac{\zeta_3}{z} + \frac{1}{z^2} \left[ \zeta_2 - \frac{S_1(z)}{z} \right], \quad (B.92) \]

\[ F_7(z) = F_7(z - 1) + \frac{\zeta_3}{z} - \frac{1}{2z^2} \left[ 2S_1(z) + S_2(z) \right], \quad (B.93) \]

\[ F_8(z) = -F_8(z - 1) - \frac{\zeta_3}{z} + \frac{1}{2z^2} \left[ 2S_1(z) + S_2(z) \right], \quad (B.94) \]

\[ F_9(z) = F_9(z - 1) + \frac{\zeta_4}{z} - \frac{\zeta_3}{z^2} + \frac{\zeta_2}{z^3} - \frac{1}{z^4} S_1(z), \quad (B.95) \]

\[ F_{10}(z) = -F_{10}(z - 1) - \frac{\zeta_4}{z} + \frac{\zeta_3}{z^2} - \frac{\zeta_2}{z^3} + \frac{1}{z^4} S_1(z), \quad (B.96) \]

\[ F_{11}(z) = F_{11}(z - 1) + \frac{\zeta_4}{4z} - \frac{\zeta_3}{z^2} + \frac{1}{2z^3} \left[ 2S_1(z) + S_2(z) \right], \quad (B.97) \]

\[ F_{12}(z) = -F_{12}(z - 1) + \frac{\zeta_4}{4z} - \frac{\zeta_3}{z^2} + \frac{1}{2z^3} \left[ 2S_1(z) + S_2(z) \right], \quad (B.98) \]

\[ F_{13}(z) = F_{13}(z - 1) + \frac{\zeta_2^2}{z} - \frac{4\zeta_3}{z^2} - \frac{2\zeta_2}{z^3} + \frac{2S_1(z)}{z^2} - \frac{2zS_1(z)}{z^2} + \frac{2zS_1(z)}{z^2} \left[ 2S_1(z) + S_2(z) \right], \quad (B.99) \]

\[ F_{14}(z) = -F_{14}(z - 1) + \frac{\zeta_2^2}{z} - \frac{4\zeta_3}{z^2} + \frac{2\zeta_2}{z^3} + \frac{2zS_1(z)}{z^2} - \frac{2zS_1(z)}{z^2} \left[ 2S_1(z) + S_2(z) \right], \quad (B.100) \]

\[ F_{15}(z) = F_{15}(z - 1) - R_1(z), \quad (B.101) \]

\[ F_{16}(z) = -F_{16}(z - 1) + R_1(z), \quad (B.102) \]

\[ F_{17}(z) = F_{17}(z - 1) + \frac{\zeta_4}{z} - \frac{1}{6z^2} \left[ 3S_1(z) + 3S_1(z)S_2(z) + 2S_3(z) \right], \quad (B.103) \]

\[ F_{18}(z) = -F_{18}(z - 1) + \frac{\zeta_4}{6z^2} \left[ 3S_1(z) + 3S_1(z)S_2(z) + 2S_3(z) \right], \quad (B.104) \]

with

\[ R_1(z) = M \left[ \ln(z)S_{1,2}(-x) - \frac{1}{2} \ln^2(-x) + \frac{\zeta_2^2}{8} \right](z), \quad (B.105) \]

\[ M[\ln^2(-x)](z) = -\frac{\zeta_2^2}{4(z+1)} - \frac{\ln^2(z)}{(z+1)^3} + \frac{4}{(z+1)^3} F_1(z+1) \]

\[ - \frac{2}{(z+1)^2} \left[ \ln(x)S_{1,2}(-x) - \frac{\zeta_3}{8(z+1)^2} + \frac{1}{2(z+1)^3} \right] F_1(z+1) \]

\[ - \frac{1}{2(z+1)} \frac{\partial}{\partial z} \left[ \ln^2(z) - \frac{2}{z+1} F_1(z+1) \right]. \quad (B.106) \]

\[ M[\ln^2(z)](z) = -\frac{\zeta_3}{8(z+1)^2} + \frac{1}{2(z+1)^3} - \frac{1}{(z+1)^3} F_1(z+1) \]

\[ - \frac{1}{2(z+1)} \frac{\partial}{\partial z} \left[ \ln^2(z) - \frac{2}{z+1} F_1(z+1) \right]. \quad (B.107) \]

cf. (7.3).

The recursion relations can be obtained from the integral-representations of the Mellin transforms. Any point in the analytic region of the basic functions is connected by the recursions which have to be applied until the asymptotic region \(|z| \gtrsim z_{\text{asympt}}\) with \(z_{\text{asympt}} \approx 15 \ldots 20\) is reached.

### B.4. Asymptotic representations

The asymptotic representations of functions contributing to the single harmonic sums and the basic functions \(F_t(z)\) and \(F_t(z)\) are given in the following. We maintain contributions up to \(O(1/z^{19})\), to reach double precision accuracy in a fully analytic representation. Higher order terms can calculated if needed in more special numerical applications.

\[ \psi(z) \sim \ln(z) - \frac{1}{2z} - \sum_{k=1}^{\infty} \frac{B_{2k}}{2kz^{2k}}. \quad (B.108) \]
\[ \psi^{(n)}(z) \sim (-1)^{n-1} \left[ \frac{(n-1)!}{z^{n+1}} + \sum_{k=1}^{\infty} \frac{n!}{2^{2k+n+1}} T_{k} (2k+n-1)! \frac{B_{2k}}{2^{2k}(2k+1)!} \right]. \]  

\[ \psi(z) \sim \ln(z) - \frac{1}{2z^2} - \frac{1}{12z^4} + \frac{1}{240z^6} - \frac{1}{132z^{10}} + \frac{691}{12z^{14}} + O\left( \frac{1}{z^{18}} \right). \]  

\[ \psi'(z) \sim 1 + \frac{1}{12z^2} + \frac{1}{8z^4} + \frac{1}{6z^6} + \frac{1}{2z^{10}} - \frac{1}{6z^{12}} + \frac{5}{6z^{14}} + \frac{691}{6z^{18}} + 2730z^{13} + O\left( \frac{1}{z^{17}} \right). \]  

\[ \psi''(z) \sim \frac{1}{z^2} - \frac{1}{12z^4} - \frac{1}{6z^6} - \frac{1}{2z^{10}} - \frac{3}{10z^{12}} + \frac{5}{6z^{14}} + \frac{691}{210z^{14}} - \frac{35}{2z^{16}} + O\left( \frac{1}{z^{20}} \right). \]  

\[ \psi'''(z) \sim \frac{2}{z^3} + \frac{3}{2z^5} + \frac{3}{2z^7} + \frac{3}{2z^9} - \frac{21}{10z^{11}} + \frac{10}{15z^{13}} + \frac{280}{15z^{15}} + O\left( \frac{1}{z^{19}} \right). \]  

\[ \psi^{(4)}(z) \sim -\frac{6}{z^4} - \frac{12}{z^6} - \frac{12}{z^8} - \frac{33}{12z^{10}} + \frac{130}{2z^{12}} + \frac{691}{16z^{14}} - 4760z^{18} + 85680z^{22} + 82476z^{26} + O\left( \frac{1}{z^{30}} \right). \]  

\[ \beta(z) \sim \frac{1}{2z} + \sum_{k=1}^{\infty} \frac{(-1)^{k-1} T_{k}}{(2z)^{2k}}. \]  

\[ \beta^{(n)}(z) \sim (-1)^{n} \left[ \frac{n!}{2^{2n+1}} + \sum_{k=1}^{\infty} \frac{(-1)^{k-1} T_{k}}{(2n)z^{2k+n+1}} (2k+n-1)! \right]. \]  

\[ \beta(z) \sim \frac{1}{2z} + \frac{1}{4z^2} + \frac{1}{8z^3} - \frac{17}{16z^4} + \frac{31}{4z^6} - \frac{691}{8z^{10}} + \frac{5461}{4z^{12}} + \frac{929569}{32z^{16}} + \frac{3202291}{4z^{18}} + 221930581z^{20} + O\left( \frac{1}{z^{24}} \right). \]  

\[ \beta'(z) \sim \frac{1}{2z} - \frac{1}{4z^2} + \frac{1}{2z^3} + \frac{1}{4z^4} - \frac{17}{16z^5} + \frac{155}{2z^7} + \frac{2073}{2z^9} - \frac{38227}{2z^{11}} + \frac{929569}{2z^{13}} + \frac{28820619}{2z^{15}} + \frac{1109652905}{2z^{17}} + O\left( \frac{1}{z^{19}} \right). \]  

\[ \beta''(z) \sim \frac{1}{2z^2} + \frac{3}{2z^4} - \frac{5}{2z^6} - \frac{21}{2z^8} + \frac{153}{2z^{10}} + \frac{1705}{2z^{12}} + 26949z^{14} + \frac{573405}{2z^{16}} + \frac{15802673}{2z^{18}} + \frac{547591761}{2z^{20}} + O\left( \frac{1}{z^{22}} \right). \]  

\[ \beta'''(z) \sim -\frac{3}{z^3} + \frac{6}{z^4} - \frac{15}{z^5} - \frac{84}{z^6} + \frac{207}{z^7} - \frac{10230}{z^8} - \frac{188643}{z^9} - 4587240z^{10} + \frac{142224057}{z^{12}} + \frac{5475917610}{z^{14}} + O\left( \frac{1}{z^{16}} \right). \]  

\[ \beta^{(4)}(z) \sim \frac{12}{z^4} + \frac{30}{z^6} - \frac{105}{z^8} - \frac{756}{z^{10}} + \frac{8415}{z^{12}} + \frac{132990}{z^{14}} + \frac{2829645}{z^{16}} + \frac{77983080}{z^{18}} + \frac{2702257083}{z^{20}} + O\left( \frac{1}{z^{22}} \right). \]  

\[ \beta^{(5)}(z) \sim -\frac{60}{z^5} + \frac{180}{z^7} - \frac{840}{z^9} + \frac{7560}{z^{11}} - \frac{100980}{z^{13}} - \frac{1861860}{z^{15}} + \frac{45274320}{z^{17}} + \frac{1403695440}{z^{19}} + \frac{54045141660}{z^{21}} + O\left( \frac{1}{z^{23}} \right). \]
$F_1(z - 1) = \mathcal{M} \left[ \frac{\ln(1 + x)}{1 + x} \right] (z - 1)$

\[
\approx \frac{1}{2} \left[ \frac{1}{z} - \frac{1}{z^2} \right] + \frac{1}{4} \left[ \frac{1}{z^2} - \frac{1}{z^4} \right] + \frac{1}{8} \left[ \frac{1}{z^4} - \frac{1}{z^6} \right] + \frac{1}{16} \left[ \frac{1}{z^6} - \frac{1}{z^8} \right] + \cdots 
\]

\[
\approx \frac{1}{2} \ln(2) 
\]

$F_2(z - 1) = \mathcal{M} \left[ \frac{\ln^2(1 + x) - \ln^2(2z)}{1 - x} \right] (z - 1)$

\[
\approx \frac{1}{2} \left[ \frac{1}{z} - \frac{1}{z^2} \right] + \frac{1}{4} \left[ \frac{1}{z^2} - \frac{1}{z^4} \right] + \frac{1}{8} \left[ \frac{1}{z^4} - \frac{1}{z^6} \right] + \cdots 
\]

\[
\approx \frac{1}{2} \ln^2(2) 
\]

$F_3(z - 1) = \mathcal{M} \left[ \frac{\ln^2(1 + x)}{1 + x} \right] (z - 1)$

\[
\approx \frac{1}{2} \left[ \frac{1}{z} - \frac{1}{z^2} \right] + \frac{1}{4} \left[ \frac{1}{z^2} - \frac{1}{z^4} \right] + \frac{1}{8} \left[ \frac{1}{z^4} - \frac{1}{z^6} \right] + \cdots 
\]

\[
\approx \frac{1}{2} \ln^2(2) 
\]

$\hat{F}_4(z - 1) = \mathcal{M} \left[ \frac{\text{L}_2(1 - x)}{1 - x} \right] (z - 1)$

\[
\approx \frac{1}{2} \left[ \frac{1}{z} - \frac{1}{z^2} \right] + \frac{1}{4} \left[ \frac{1}{z^2} - \frac{1}{z^4} \right] + \frac{1}{8} \left[ \frac{1}{z^4} - \frac{1}{z^6} \right] + \cdots 
\]

\[
\approx \frac{1}{2} \ln^2(2) 
\]

$\hat{F}_5(z - 1) = \mathcal{M} \left[ \frac{\text{L}_2(1 - x)}{1 + x} \right] (z - 1)$

\[
\approx \frac{1}{2} \left[ \frac{1}{z} - \frac{1}{z^2} \right] + \frac{1}{4} \left[ \frac{1}{z^2} - \frac{1}{z^4} \right] + \frac{1}{8} \left[ \frac{1}{z^4} - \frac{1}{z^6} \right] + \cdots 
\]

\[
\approx \frac{1}{2} \ln^2(2) 
\]
\[ \hat{F}_{6a}(z-1) = M \left[ \frac{S_1 z (1-x)}{1-x} \right] (z-1) \]
\[ \approx \frac{1}{4 z^2} + \frac{8}{z^2} - \frac{3}{z^2} - \frac{5}{z^2} + \frac{29}{z^2} + \frac{133}{z^2} + \frac{133}{z^2} - \frac{163}{z^2} + \frac{163}{z^2} + \frac{251}{z^2} \]
\[ = \frac{3058125}{8 z^2} - \frac{590412261}{120 z^{18}} + \frac{1422236953}{120 z^{18}} + O \left( \frac{1}{z^{20}} \right). \]
\[
\hat{F}_{11}(z - 1) = M \left[ \frac{S_{2,2}(1 - x)}{1 - x} \right] (z - 1)
\]

\[
\hat{F}_{12}(z - 1) = M \left[ \frac{S_{2,2}(1 - x)}{1 + x} \right] (z - 1)
\]

\[
\hat{F}_{13}(z - 1) = M \left[ \frac{\ln(x)S_{1,2}(-x) - \ln(x)S_{1,2}(-x)/2 + \zeta_2^2/8}{1 - x} \right] (z - 1)
\]
\[
\hat{F}_{16}(z-1) = M \left[ \frac{\text{Li}_4(1-x) - \text{Li}_4(-x)}{1+x} \right](z-1)
\]

\[
\hat{F}_{17}(z-1) = M \left[ \frac{\text{Li}_4(1-x)}{1-x} \right](z-1)
\]

\[
\hat{F}_{18}(z-1) = M \left[ \frac{\text{Li}_4(1-x)}{1+x} \right](z-1)
\]
The asymptotic representations of the subsidiary functions $H, H(z)$ are given by:

$$H_1(z) = M \left[ 251_1(-x) + \ln(1 + x) \right] \left( x - O \left( \frac{1}{z^{20}} \right) \right). \quad (B.142)$$

$$H_2(z) = M \left[ \frac{1 + x}{\ln(1 + x)} \right] \left( x - O \left( \frac{1}{z^{20}} \right) \right). \quad (B.143)$$
They are related to the Bernoulli numbers by

\[
H_0 = \int_0^1 \int_0^1 \exp(x+y) \, dx \, dy
\]

where the tangent numbers or Euler zigzag numbers, \([27,60]\), with the generating function

\[
x = \sum_{k=0}^{\infty} \frac{T_k}{k!} x^k = \frac{2}{\tan(x/2)}
\]

are given by

\[
T_k = \frac{2}{\pi} \int_0^{\pi/2} \sin^{2k-1}(x) \, dx
\]

In the above \(T_k\) denotes the tangent numbers or Euler zigzag numbers, \([27,60]\), with the generating function

\[
\frac{\exp(x) - \exp(-x)}{\exp(x) + \exp(-x)} = \sum_{k=1}^{\infty} \frac{(-1)^{k-1}}{(2k-1)!} T_k x^{2k-1}.
\]

They are related to the Bernoulli numbers by

\[
T_k = \frac{2^{2k}(2^{2k}-1)}{2k} (-1)^{k-1} B_{2k}.
\]

### Appendix C. Some integrals of \(w = 5\)

In this appendix a series of integrals used in the present calculation is presented. Other integrals of this type were given in \([63]\).

\[
\int_0^1 \frac{\text{Li}_4(z)}{1+z} \, dz = \ln(2) \zeta_4 + \frac{3}{4} \zeta_2 \zeta_3 - \frac{59}{32} \zeta_5.
\]

\[
\int_0^1 \frac{\text{Li}_4(x^2)}{1+x} \, dx = \frac{2}{5} \zeta_2^2 \ln(2) + 3 \zeta_2 \zeta_3 - \frac{25}{4} \zeta_5.
\]
\[ \int_0^1 dz \frac{S_{1.2}(z)}{1 + z} = \ln(2) \zeta_4 - \frac{7}{16} \zeta_2 \zeta_3 - \frac{1}{6} \zeta_2 \ln^3(2) + \frac{7}{16} \zeta_3 \ln^2(2) - \frac{27}{32} \zeta_5 + \ln(2) \text{Li}_4 \left( \frac{1}{2} \right) + \frac{1}{30} \ln^5(2) + \text{Li}_5 \left( \frac{1}{2} \right). \] (C.3)

\[ \int_0^1 dz \frac{S_{2.2}(z)}{1 + z} = \frac{1}{4} \zeta_4 \ln(2) - \frac{7}{8} \zeta_2 \zeta_3 - \frac{1}{3} \zeta_2 \ln^3(2) + \frac{7}{8} \zeta_3 \ln^2(2) - \frac{15}{32} \zeta_5 + 2 \left[ \ln(2) \text{Li}_4 \left( \frac{1}{2} \right) + \text{Li}_5 \left( \frac{1}{2} \right) \right] + \frac{1}{15} \ln^5(2), \] (C.4)

\[ \int_0^1 dz \frac{S_{2.2}(-z)}{1 + z} = -2 \text{Li}_5 \left( \frac{1}{2} \right) + \frac{125}{64} \zeta_5 - \frac{3}{4} \zeta_2 \ln(2) + \frac{7}{8} \zeta_1 \ln^2(2) - \frac{1}{6} \zeta_2 \ln^3(2) + \frac{1}{60} \ln^5(2). \] (C.5)

\[ \int_0^1 dz \frac{\text{Li}_2^2(z)}{1 + z} = \ln(2) \zeta_2^2 - \frac{5}{4} \zeta_2 \zeta_3 + \frac{29}{32} \zeta_5. \] (C.6)

\[ \int_0^1 dz \frac{\text{Li}_2^2(-z)}{1 + z} = \frac{1}{4} \zeta_2^2 \ln(2) + \frac{7}{2} \zeta_1 \ln^2(2) - \frac{4}{3} \zeta_2 \ln^3(2) - \frac{1}{4} \zeta_2 \zeta_3 - \frac{125}{16} \zeta_5 + \frac{4}{15} \ln^5(2) + 8 \left[ \text{Li}_4 \left( \frac{1}{2} \right) \ln(2) + \text{Li}_5 \left( \frac{1}{2} \right) \right]. \] (C.7)

\[ \int_0^1 dx \frac{\ln(x) \text{Li}_3(x)}{1 + x} = \frac{21}{8} \zeta_2 \zeta_3 - \frac{83}{16} \zeta_5. \] (C.8)

\[ \int_0^1 dx \frac{\ln^3(x) \ln(1 - x)}{1 + x} = -\frac{9}{2} \zeta_2 \left[ \zeta_3 + \zeta_2 \ln(2) \right] + \frac{273}{16} \zeta_5. \] (C.9)

\[ \int_0^1 dx \frac{\ln(x) \text{Li}_3(-x)}{1 + x} = \frac{51}{32} \zeta_5 - \frac{3}{4} \zeta_2 \zeta_3. \] (C.10)

\[ \int_0^1 dx \frac{\text{Li}_3(-x) \ln(1 + x)}{1 + x} = \frac{1}{16} \zeta_2 \zeta_3 + \frac{3}{4} \zeta_2 \ln^2(2) - \frac{5}{4} \zeta_1 \ln^2(2) + \frac{125}{64} \zeta_5 - \frac{1}{15} \ln^5(2) - 2 \left[ \text{Li}_4 \left( \frac{1}{2} \right) \ln(2) + \text{Li}_5 \left( \frac{1}{2} \right) \right]. \] (C.11)

\[ \int_0^1 dx \frac{\text{Li}_2(-x) \ln^2(1 + x)}{x} = \frac{7}{4} \zeta_3 \ln^2(2) - \frac{1}{8} \zeta_2 \zeta_3 - \frac{2}{3} \zeta_2 \ln^3(2) - \frac{125}{32} \zeta_5 + 4 \left[ \ln(2) \text{Li}_4 \left( \frac{1}{2} \right) + \text{Li}_5 \left( \frac{1}{2} \right) \right] + \frac{2}{15} \ln^5(2). \] (C.12)

\[ \int_0^1 dx \frac{\text{Li}_2(-x) \ln^2(1 - x)}{x} = -\frac{7}{4} \zeta_3 \ln^2(2) + \frac{3}{4} \zeta_2 \zeta_3 + \frac{2}{3} \zeta_2 \ln^3(2) + \frac{15}{16} \zeta_5 - 4 \left[ \ln(2) \text{Li}_4 \left( \frac{1}{2} \right) + \text{Li}_5 \left( \frac{1}{2} \right) \right] - \frac{2}{15} \ln^5(2). \] (C.13)

\[ \int_0^1 dx \frac{\ln(x) \delta_{1,2}(x)}{1 + x} = \frac{41}{32} \zeta_5 - \frac{11}{16} \zeta_2 \zeta_3. \] (C.14)

\[ \int_0^1 dx \frac{\ln(x) \ln(1 + x) \ln^2(1 - x)}{x} = -\frac{7}{2} \zeta(5) - \frac{3}{8} \zeta(2) \zeta(3) + 4 \left[ \text{Li}_3 \left( \frac{1}{2} \right) + 4 \text{Li}_4 \left( \frac{1}{2} \right) \ln(2) \right] + \frac{7}{4} \zeta_3 \ln(2) - \frac{2}{3} \zeta_2 \ln^3(2) + \frac{2}{15} \ln^5(2). \] (C.15)
\[
\begin{align*}
\int_0^1 \frac{dx}{x} \ln(x)(1-x) \ln^2(1+x) &= -\frac{25}{16} \zeta_5 + \frac{7}{8} \zeta_2, \\
\int_0^1 \frac{dx I_2(x^2)}{1+x} &= -\frac{3}{4} \zeta_3 + \zeta_2 \ln(2), \\
\int_0^1 \frac{dx I_1(x)}{1+x} &= -\frac{5}{8} \zeta_2 \ln(2) + \frac{3}{20} \zeta_2^2, \\
\int_0^1 \frac{dx S_1, z(x^2)}{1+x} &= -\frac{9}{2} \zeta_2 \ln(2) - \frac{37}{20} \zeta_2^2 + 4 \ln \left(\frac{1}{2}\right) - \zeta_2 \ln^2(2) + \frac{1}{6} \ln^4(2).
\end{align*}
\]