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Structural Relations between Nested Harmonic Sums *

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We describe the structural relations between nested harmonic sums emerging in the description of physical single scale quantities up to the 3–loop level in renormalizable gauge field theories. These are weight w=6 harmonic sums. We identify universal basic functions which allow to describe a large class of physical quantities and derive their complex analysis. For the 3–loop QCD Wilson coefficients 35 basic functions are required, whereas a subset of 15 describes the 3–loop anomalous dimensions.

1. Introduction

Scattering cross sections in renormalizable Quantum Field Theories which depend on a single kinematic or mass scale obey a particularly simple form if dealt with in Mellin space. Contrary to the case in momentum-fraction space, where the variable $z = p/P$ is referred to, or a representation depending on $z = s/t$, with s and t Mandelstam variables, the results are expressed in terms of nested harmonic sums with an outer summation index N [1]. In this way a unique language is available in which the integrals emerging in higher order calculations can be expressed. Although it is not expected that even in this case the representation will be sufficient, cf. [2], it holds for all 3-loop calculations having been performed so far [3]. Furthermore, this representation holds independent of the processes considered.

The nested harmonic sums are recursively defined by

$$S_{b,\vec{a}}(N) = \sum_{k=1}^{N} \frac{\text{sign}(b)^k}{k^{|b|}} S_{\vec{a}}(k) \ , \qquad (1)$$

where $\vec{a} = (a_1, ..., a_l)$ and $b, a_i \ \in \ \mathbb{Z}\backslash\{0\}$. The weight w and depth d of a harmonic sum $S_{\vec{a}}(N)$ are given by $\mathsf{w} = \sum_{k=1}^{l} |a_k|$ and $\mathsf{d} = l$. At each weight w there are $2 \cdot 3^{\mathsf{w}-1}$ harmonic sums. In the limit $N \rightarrow \infty$ the nested harmonic sums turn into multiple zeta values $\zeta_{\vec{a}}$, [4]. As well known, there is a large number of algebraic relations between the multiple zeta values due to the shuffle- and stuffle relations, cf. [5]. The nested harmonic sums form a quasi–shuffle algebra, [6], with the shuffle product $\sqcup\!\sqcup$, which maps two index sets in all possible orders preserving the order of the original sets. The algebraic relations of the harmonic sums are well known, [7], and are related to the shuffle product and the structure of the index sets. The number of the respective basis elements are counted by the Lyndon words or due to the Witt relations [8]. Let us consider the harmonic sums up to weight w=6. The reduction obtained cumulatively by the algebraic relations $\#_r$ compared to the original number $\#_c$ is

w	1	2	3	4	5	6
$\#_c$	2	8	26	80	242	728
$\#_r$	2	5	13	31	79	195

In the physical applications we observe [2, 9, 10] that one may find representations in which the index $\{-1\}$ never appears in a nested harmonic sum. The number of harmonic sums of this type $N_{\neg\{-1\}}(w)$ and the corresponding number of basis elements $N^{\text{basis}}_{\neg\{-1\}}(w)$ are given by

$$N_{\neg\{-1\}}(w) = \frac{1}{2}\left[\left(1-\sqrt{2}\right)^w + \left(1+\sqrt{2}\right)^w\right]$$
$$N^{\text{basis}}_{\neg\{-1\}}(w) = \frac{2}{w}\sum_{d|w}\mu\left(\frac{w}{d}\right)N_{\neg\{-1\}}(d) \ , \qquad (2)$$

with $\mu(d)$ the Möbius function. This leads to the following reduction

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w	1	2	3	4	5	6
$\#_c$	1	4	11	28	69	168
$\#_r$	1	3	7	14	30	60

Note that already the numbers at input are lower than the numbers after the algebraic reduction in the former case.

All further relations between the nested harmonic sums are called structural relations. They result from the mathematical structure of these objects beyond that given by their indices.

2. Structural Relations

In the physical application nested harmonic sums emerge as a consequence of the light-cone expansion [11] and related techniques, observing the crossing relations for the respective processes, cf. e.g. [12]. The physical quantities are thus defined at either even or odd integers N. To use these expressions in experimental data analyzes it is, however, necessary to map these representations back to momentum-fraction space. This requires an analytic continuation of the nested harmonic sums from the even, resp. odd, values of N to $N \in \mathbb{C}$. Eventually one has to derive the complex analysis for the nested harmonic sums. In passing, N takes values $N \in \mathbb{Q}$ and $N \in \mathbb{R}$, which leads to new relations, as we will outline below. From a practical point of view, the most complicated part consists in deriving the corresponding representations for $N \in \mathbb{C}$ for a large number of harmonic sums. Whenever possible, we will seek equivalence classes for these sums, the elements of which can be easily accessed applying some operator, which can be straightforwardly realized even in the final numerical precision representations.

Harmonic sums can be represented in terms of Mellin integrals, cf. [1],

$$S_{\vec{a}}(N) = \mathrm{M}[f_{\vec{a}}(x)](N) = \int_0^1 dx \frac{\hat{f}_{\vec{a}'}(x)}{1 \pm x}|_{\mathrm{reg}} x^{N-1} \ .$$

The first structural relation one obtains at w=1 by decomposing

$$\frac{1}{1-x^2} = \frac{1}{2}\left[\frac{1}{1-x} + \frac{1}{1+x}\right] \qquad (3)$$

which yields

$$\begin{aligned} -\psi\left(\frac{N}{2}\right) &= -\psi(N) + \beta(N) + \ln(2) \\ \beta(N) &= \frac{1}{2}\left[\psi\left(\frac{N+1}{2}\right) - \psi\left(\frac{N}{2}\right)\right] \end{aligned} \qquad (4)$$

Since $S_{-1}(N) = (-1)^N \beta(N+1) - \ln(2), S_1(N) = \psi(N+1) + \gamma_E$, the sum $S_{-1}(N)$ is not algebraically independent of $S_1(N)$ for $N \in \mathbb{Q}$. At higher weights (3) can be generalized using

$$\ln(1-x^2) = \ln(1-x) + \ln(1+x) \qquad (5)$$

$$\frac{1}{2^{k-2}}\mathrm{Li}_k(x^2) = \mathrm{Li}_k(x) + \mathrm{Li}_k(-x) \qquad (6)$$

as numerator function.

Considering $N \in \mathbb{R}$ one may define the differentiation of harmonic sums via

$$\frac{d}{dN} S_{\vec{a}}(N) = \mathrm{M}[\ln(x) f_{\vec{a}}(x)](N) \ . \qquad (7)$$

In this way we obtain

$$S_2(N) = -\frac{d}{dN} S_1(N) + \zeta_2 \ . \qquad (8)$$

In general one observes that the set of harmonic sums, extended by the multiple zeta values, is closed under differentiation. In particular one may form equivalence classes through differentiation and consider the harmonic sum with the lowest weight of this class as its representative. A consequence of these two relations is, that all single harmonic sums may be traced back to $S_1(N)$. The complex analysis of the whole class derives from that of $S_1(N)$.

A third class of structural relations emerges through the respective iterated integral representation [13], combined with algebraic relations. At w=2 one obtains

$$\begin{aligned} \mathrm{M}\left[\frac{\ln(1-x)}{1+x}\right](N) &= -\mathrm{M}\left[\frac{\ln(1+x)}{1+x}\right](N) \\ &- [\psi(N) + \gamma_E + \ln(2)]\beta(N) + \beta'(N) \end{aligned} \qquad (9)$$

In this way we identify the first basic function

$$F_1(x) = \frac{\ln(1+x)}{1+x} \ , \qquad (10)$$

which is related to the harmonic sum $S_{-1,1}(N)$. Although in physics problems the index $\{-1\}$ is not emerging, $F_1(x)$ is still useful to express a series of harmonic sums. All w=2 harmonic sums reduce algebraically or are related to $F_1(x)$ and single harmonic sums.

At w=3 we apply (6) for the first time. Together with a relation similar to (9) all sums which do not contain $\{-1\}$ as index reduce to the Mellin transforms of

$$F_{2,3}(x) = \frac{\mathrm{Li}_2(x)}{1 \pm x} \ . \qquad (11)$$

Let us now study the double sums in general. Using the above relations one may show that Nielsen integrals [14] are sufficient to express all double sums in terms of Mellin transformations of the functions

$$\hat{F}_{k,\pm}(x) = \frac{\mathrm{Li}_k(x)}{1 \pm x} \ . \qquad (12)$$

For even weight w there is an Euler relation and only $\mathrm{Li}_k(x)/(1+x)$ contributes. Let us illustrate this for $S_{2,3}(N)$. One derives

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

where the functions $S_{1,k}(1-x)$ are polynomials of $\ln(x), \ln(1-x)$ and $\mathrm{Li}_k(x)$. Therefore $S_{2,3}(N)$ is related to $S_{4,1}(N)$ up to derivatives of known harmonic sums of lower weight.

In the following we only have to consider sums with depth $\mathsf{d} \geq 3$. We derive all one-dimensional integral representations for the harmonic sums up to w=6 which do not contain an index $\{-1\}$ and use the above relations. We obtain the following set of basic functions, [2, 15].

$$\begin{aligned}
\mathsf{w}=1:&\quad 1/(x-1)_+\\
\mathsf{w}=2:&\quad \ln(1+x)/(x+1)\\
\mathsf{w}=3:&\quad \mathrm{Li}_2(x)/(x\pm1)\\
\mathsf{w}=4:&\quad \mathrm{Li}_3(x)/(x+1),\\
&\quad S_{1,2}(x)/(x\pm1)\\
\mathsf{w}=5:&\quad \mathrm{Li}_4(x)/(x\pm1),\\
&\quad S_{1,3}(x)/(x\pm1)\\
&\quad S_{2,2}(x)/(x\pm1),\\
&\quad \mathrm{Li}_2^2(x)/(x\pm1)\\
&\quad [\ln(x)S_{1,2}(-x) - \mathrm{Li}_2^2(-x)/2]/(x\pm1)\\
\mathsf{w}=6:&\quad \mathrm{Li}_5(x)/(x+1),\\
&\quad S_{1,4}(x)/(x\pm1)\\
&\quad S_{2,3}(x)/(x\pm1),\\
&\quad S_{3,2}(x)/(x\pm1)\\
&\quad \mathrm{Li}_2(x)\mathrm{Li}_3(x)/(x\pm1)\\
&\quad S_{1,2}(x)\mathrm{Li}_2(x)/(x\pm1)\\
&\quad A_1(x)/(x+1)\\
&\quad A_2(x)/(x\pm1)\\
&\quad A_3(x)/(x+1)\\
&\quad H_{0,-1,0,1,1}(x)/(x-1)\\
&\quad [A_1(-x)+N_\alpha(x)]/(x+1)\ ,
\end{aligned} \qquad (13)$$

where

$$\begin{aligned}
A_1(x) &= \int_0^x \frac{dy}{y}\mathrm{Li}_2^2(y)\\
A_2(x) &= \int_0^x \frac{dy}{y}\ln(1-y)S_{1,2}(y)\\
A_3(x) &= \int_0^x \frac{dy}{y}[\mathrm{Li}_4(y) - \zeta_4]\ ,
\end{aligned} \qquad (14)$$

and $N_\alpha(x)|_{\alpha=1...3}$ are polynomials of Nielsen integrals. Up to w=5 the numerator functions are Nielsen integrals, while at w=6 some of the numerator functions are general harmonic polylogarithms over the alphabet $\{0, 1, -1\}$ [16] in the representation we derived. Yet it may still be, that an equivalent representation can be found over a two-letter alphabet, which will be investigated further. [2]

The Mellin transforms of the basic functions in (13) span the space of the harmonic sums which occur in higher order calculations for single scale quantities in Quantum Chromodynamics. Examples are the anomalous dimensions and Wilson coefficients in deeply-inelastic scattering up to 3-loops [3, 18]. With rising order in the coupling constant α_s the number of contributing basic functions is given by

$O(\alpha_s)$	Wilson coeff./anom. dim.	#	1
$O(\alpha_s^2)$	anomalous dimensions	#	2

[2]Structures of this type have been found at least in case of the multiple zeta values recently [17].

$$
\begin{array}{llll}
O(\alpha_s^2) & \text{Wilson coefficients} & \# & \leq 5 \\
O(\alpha_s^3) & \text{anomalous dimensions} & \# & 15 \\
O(\alpha_s^3) & \text{Wilson coefficients} & \# & 35
\end{array}
\qquad (15)
$$

We represented a wide class of massless and massive 2-loop quantities in terms of harmonic sums, among them the unpolarized and polarized Drell-Yan cross section and the hard scattering cross sections for hadronic Higgs-boson and pseudoscalar-boson production in the heavy top quark limit [19], the unpolarized and polarized time-like anomalous dimensions and Wilson coefficients [20], the polarized anomalous dimensions and Wilson coefficients [21], the heavy flavor deep-inelastic Wilson coefficients in the limit $Q^2 \gg m^2$ [22], including the $O(\varepsilon)$ terms, as well as the virtual- and soft corrections to Bhabha scattering [10]. All these quantities fall into the third class above and are represented by the respective basic functions and simple polynomial factors in the Mellin variable. The same structure is obtained for other similar processes more.

3. Complex Analysis

Finally we have to derive the analytic continuation of the nested harmonic sums $N \in \mathbb{N} \to N \in \mathbb{C}$. In the past precise numerical representations were derived in [23]. [3] Here the integrand is dealt with using the `MINIMAX`-method [25], which leads to an adaptive representation in the complex plane in terms of a rational function. We seek, however, for a rigorous representation.

It is well-known [26] that Mellin transforms of the type

$$
\begin{aligned}
\Omega(z) &= \int_0^1 dt\; t^{z-1}\; \varphi(t); \\
\varphi(1-t) &= \sum_{k=0}^{\infty} a_k t^k \;,
\end{aligned}
\qquad (16)
$$

are factorial series,

$$
\Omega(z) = \sum_{k=0}^{\infty} \frac{a_{k+1} k!}{z(z+1)\dots(z+k)} \;. \qquad (17)
$$

[3] This is also possible in the case of the heavy quark Wilson coefficients, including power corrections, cf. [24].

$\varphi(t)$ has to be analytic at $t = 1$. $\Omega(z)$ is a meromorphic function for $z \in \mathbb{C}$, with poles at the non-positive integers. It obeys a recursion for $z \to z+1$ and has an analytic asymptotic representation. The choice of the basic functions in (13) is not immediately suited in all cases, as some of the functions possess branch points at $t = 1$. However, one may map this behaviour using relations for the basic functions, as for the change of the argument $t \to (1-t)$. Let us consider the example

$$
F_3(N) = \mathrm{M}[\mathrm{Li}_2(x)/(1+x)](N) \;. \qquad (18)
$$

The recursion relation is given by

$$
\begin{aligned}
F_3(z+1) &= -F_3(z) \\
&\quad + \frac{1}{z}\left[\zeta_2 - \frac{\psi(z+1)+\gamma_E}{z}\right] \;.
\end{aligned}
\qquad (19)
$$

We map

$$
\mathrm{Li}_2(z) \to -\mathrm{Li}_2(1-z) - \ln(z)\ln(1-z) + \zeta_2 \;, \qquad (20)
$$

and derive the asymptotic representation for

$$
\begin{aligned}
\mathrm{M}\left[\frac{\mathrm{Li}_2(1-z)}{1+z}\right](N) &\sim \frac{1}{2N^2} + \frac{1}{4N^3} - \frac{7}{24}\frac{1}{N^4} \\
&\quad - \frac{1}{3}\frac{1}{N^5} + \frac{73}{120}\frac{1}{N^6} \dots
\end{aligned}
\qquad (21)
$$

We still need to consider $\mathrm{M}[\ln(z)\ln(1-z)/(1+z)](N)$, which is a derivative of the function $F_1(N)$ and a few simpler terms. Representations like this can be obtained for all the basic functions. In this way analytic expressions for the Mellin transforms, resp. nested harmonic sums, which are needed up to the level w=6, are obtained. The above relations can be tuned to any numerical accuracy by analytic means.

4. Conclusions

In perturbative higher order calculations in renormalizable Quantum Field Theories nested harmonic sums form an appropriate way of representation for single-scale quantities, at least up to 3–loop orders. The number of multiple nested harmonic sums grows exponentially with the weight

w. The harmonic sums obey algebraic and structural relations, which reduce the number of objects to a small set of basic functions. The quantities are meromorphic functions in $\mathbb{C}$ with poles at the non-positive integers, obey recursion relations and possess an analytic asymptotic representation. Due to this these functions are known in analytic form. The basic functions emerge as unique quantities in a large variety of higher order calculations and hint to a rather simple mathematical structure behind Feynman diagrams. The simple pattern, known in case of zero-scale quantities, where only a few basis elements span the space of all multiple zeta values, is rediscovered for the next more complicated class of processes and found to be of quite similar structure. It is an observation that harmonic sums with an index $\{-1\}$ can be avoided in the physical quantities, for yet unknown reason. Due to this the complexity of 728 objects at w=6, anticipated originally, reduces to 168. The latter ones can now be represented by 35 basic functions, which is an essential compactification.

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