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November 2023

RISC Report Series No. 23-12

ISSN: 2791-4267 (online)

Available at `https://doi.org/10.35011/risc.23-12`

JOHANNES KEPLER UNIVERSITY LINZ
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4040 Linz, Austria
www.jku.at
DVR 0093696

DO–TH 23/12
DESY 23–142
CERN-TH-2023-164
ZU-TH 60/23

arXiv:2311.00644 [hep-ph]
October 2023
RISC Report series 23–12
MSUHEP-23-025

The first–order factorizable contributions to the three–loop massive operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$

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Abstract

The unpolarized and polarized massive operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$ contain first–order factorizable and non–first–order factorizable contributions in the determining difference or differential equations of their master integrals. We compute their first–order factorizable contributions in the single heavy mass case for all contributing Feynman diagrams. Moreover, we present the complete color–ζ factors for the cases in which also non–first–order factorizable contributions emerge in the master integrals, but cancel in the final result as found by using the method of arbitrary high Mellin moments. Individual contributions depend also on generalized harmonic sums and on nested finite binomial and inverse binomial sums in Mellin N–space, and correspondingly, on Kummer–Poincaré and square–root valued alphabets in Bjorken–x space. We present a complete discussion of the possibilities of solving the present problem in N–space analytically and we also discuss the limitations in the present case to analytically continue the given N–space expressions to $N \in \mathbb{C}$ by strict methods. The representation through generating functions allows a well synchronized representation of the first–order factorizable results over a 17–letter alphabet. We finally obtain representations in terms of iterated integrals over the corresponding alphabet in x–space, also containing up to weight $\mathsf{w} = 5$ special constants, which can be rationalized to Kummer–Poincaré iterated integrals at special arguments. The analytic x–space representation requires separate analyses for the intervals $x \in [0, 1/4], [1/4, 1/2], [1/2, 1]$ and $x > 1$. We also derive the small and large x limits of the first–order factorizable contributions. Furthermore, we perform comparisons to a number of known Mellin moments, calculated by a different method for the corresponding subset of Feynman diagrams, and an independent high–precision numerical solution of the problems.

1 Introduction

Precision data on deep–inelastic scattering structure functions allow precision measurements of the strong coupling constant $a_s(Q^2) = \alpha_s(Q^2)/(4\pi)$ [1–4], the extraction of the parton distribution functions (PDFs), cf. e.g. [5, 6], and the measurement of the charm quark mass m_c [7]. To suppress higher twist effects [8–10] one chooses $Q^2 \gtrsim 25\text{GeV}^2$, which is also the asymptotic region for the charm contribution to the structure function $F_2(x, Q^2)$ [11]. Besides the detailed knowledge of the evolution of the PDFs in Quantum Chromodynamics (QCD) [12–34] one needs the massless [14, 32] and massive Wilson coefficients in the single–mass [17–19, 35–39] and two–mass cases [40–44] to three–loop order for neutral current interactions.

While many of the contributing massive operator matrix elements (OMEs) have been calculated both in the unpolarized and polarized case [15–19, 29, 31, 32, 35–45], the constant part to the unrenormalized OMEs $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, denoted by $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$, are still missing. All logarithmic contributions are known, however, [35, 37]. Furthermore, the massive OMEs provide the transition matrix elements in the variable–flavor number scheme in the single–mass [46] and the two–mass case [40]. The transitions of heavy flavors becoming light to two–loop order were studied in Refs. [47, 48], also including two–mass effects.

The OMEs can be expressed in terms of a basis of Feynman integrals called master integrals. These master integrals fulfill systems of first–order differential equations. Equivalently, one can uncouple these to scalar linear higher–order differential operators. One important question, for example to classify which function spaces occur in the solutions, is whether the differential operators can be factorized into first–order factors. In the following we call those parts of the final result which are determined by master integrals that fulfill first–order factorizable differential equations *first–order factorizable contributions* and the remaining part *non–first–order factorizable contributions*.

In this paper we present all first–order factorizable contributions (also called d'Alembertian solutions) for the Feynman diagrams contributing to $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$. We compute the polarized OMEs in the Larin scheme [49].[1] The results for the complete OMEs in Mellin N–space can also be subdivided according to color factors and ζ values, which are multiplied by functions that evaluate to rational numbers for fixed values of N. These rational numbers fulfill recurrence relations that can be determined by using the method of arbitrarily high Mellin moments [51]. In this way, we find solutions to complete color–ζ factors, even in some cases where non–first–order factorizable master integrals emerge, since their contributions cancel in the final result. Out of 25 color–ζ values, 10 remain to be computed and we will deal with their first–order factorizable terms here for all contributing diagrams. The remaining terms, containing also non–first–order factorizable contributions, are the subject of a forthcoming paper [52], since the algorithms to compute them are rather different from the ones of the present paper.

Furthermore, we also present the solutions in Mellin N–space we have obtained for the complete project. In a series of color–ζ terms with non–first–order factorizable contributions we computed closed form difference equations at very high degree and order. These define recurrent functions which may be used for shift relations of the analytic continuations from $N \in \mathbb{N}$ to $N \in \mathbb{C}$ within the analyticity region of the problems. Moreover, one may calculate the asymptotic solutions of difference equations of this kind and of individual building blocks also in the first–order factorizable case, such as generalized harmonic sums [53] and nested finite binomial sums [54]. These serve as numeric initial conditions for the shift relations in $N \in \mathbb{C}$.

[1] To describe the scale dependence of the polarized structure function $g_1(x, Q^2)$, the Wilson coefficients have to be computed in the same scheme [32] and one needs to refer to parton distributions in this scheme, the evolution of which is ruled by the anomalous dimensions in the Larin scheme [20, 31]. For the non–singlet case see Ref. [50].

The asymptotic expansions for harmonic sums [55,56] were derived in Refs. [57,58]. Besides the results in the first–order factorizable case, we will also present details of the technologies used in the present calculation.

The paper is organized as follows. In Section 2 we present the basic computation steps to obtain the results in Mellin N–space. A subset of Feynman diagrams turns out to be given in terms of master integrals which are first–order factorizable and therefore lead to product–sum representations using the algorithms of Refs. [59–72] implemented in the package `Sigma` [73,74]. As we mentioned above, it is also possible to compute a series of complete color–ζ values, even though their master integrals may contain non–first–order factorizable contributions, as long as these contributions cancel in the determining recurrence, which then turns out to be first–order factorizable. In Section 3 we present these contributions to $a_{Qg}^{(3)}(N)$ and $\Delta a_{Qg}^{(3)}(N)$, except for irreducible diagrams resulting in purely rational and ζ_3 terms. The structure of the first–order factorizable contributions to Feynman diagrams contributing to the purely rational and ζ_3 terms in N–space is discussed in Section 4. Here we also consider the principal structure of high moments to all contributions. In Section 5 we compute the t–space representation of the first–order factorizable contributions of the OMEs from the associated set of differential equations to the required depth in the dimensional parameter $\varepsilon = D - 4$. Here $t \in \mathbb{R}$ denotes a resummation variable, cf. Eq. (2.1). From this representation we perform the analytic continuation to x–space. The final expressions are given by G–functions, see Eq. (2.3), over root–valued alphabets and corresponding G–constants at special values $x = x_0$. The contributing G–functions of x over the root–valued alphabet can be rationalized and mapped to Kummer–Poincaré iterated integrals [75–81], at the expense of a root–valued main argument. We expand the G–functions of x into series around $x = 0, 1/2$ and 1 and give precise numerical representations for the G–functions at special values of x_0. The letters of the latter quantities can be rationalized.[2] In Section 6 we perform the expansions around $x = 0$ and $x = 1$ for the first–order factorizable terms to determine their contributions to the most singular terms of $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$. This requires the calculation of a series of G–functions, Eq. (2.3), with root valued letters at $x = 1$. We also investigate color rescaling relations. In Section 7 we present numerical results, and Section 8 contains the conclusions. In the Appendices A–D we summarize a series of technical aspects, such as the asymptotic expansions of contributing generalized harmonic sums, of characteristic aspects of nested (inverse) binomial sums and their asymptotic expansion, the calculation of special G–constants, and the analytic continuation to N–space.

2 The main steps of the calculation

The Feynman diagrams of the OMEs $(\Delta)A_{Qg}^{(3)}$ are generated by `QGRAF` [82] using the Feynman rules of Refs. [83,84]. The Lorentz- and Dirac algebra has been performed with `Form` [85,86], the color algebra by using `color` [87], and the integration by parts reduction [88–93] by using the package `Reduze 2` [94,95]. The diagrams have been calculated in Mellin N–space using different techniques which are described in Refs. [96, 97] for the first–order–factorizable contributions. These included summation technologies based on difference ring theory [59–72], encoded in the package `Sigma` [73, 74], the solution of differential equations [98, 99] and using `SolveDE` of the package `HarmonicSums` [53–57, 100–112] as well as the differential equation solver for first–order factorizable systems of Ref. [99]. Differential equations are decoupled using the package `OreSys` [113–115]. Finally, we applied also the multiple Almkvist–Zeilberger algorithm [116, 117] as implemented in the package `MultiIntegrate` [118]. We thus obtain first a representation in

[2] We will also say that the corresponding G–functions are rationalized.

N–space for all first–order factorizable contributions.

One may even envisage the complete solution of the problem in N–space. Here the first step is to obtain closed form difference equations for all color–ζ values by using the method of arbitrary high Mellin moments [51] and guessing algorithms [119,120] implemented in `Sage` [121,122]. For the color factors $C_{F,A}^2 T_F$ and $C_F C_A T_F$ this task is very demanding in terms of computer time and requires an amount of moments far beyond 15000, which is the level currently obtained for other color factors in the unpolarized case. In the polarized case we computed 11000 moments. At present it is only possible to solve those color–ζ contributions which are related to first–order factorizable difference equations. Solving them leads to nested product–sum representations. Even though individual Feynman diagrams may contain master integrals that fulfill non–first–order factorizable differential equations, in some cases it is still possible to solve the corresponding color–ζ contribution if the non–first–order factorizable terms cancel in the sum over all Feynman diagrams.

Because of the fact that we cannot easily solve some of the large difference equations, which will also apply to the yet missing ones, we have chosen a different strategy in the cases of non–first–order factorizable difference equations by referring to x–space directly. The N–space expressions are first resummed into the t–space representations [123, 124] by

$$F(t) = \sum_{N=1}^{\infty} t^N F(N), \text{ with } t \in \mathbb{R}. \tag{2.1}$$

Likewise, we can do this also for the master integrals directly and express the first–order factorizable master integrals as functions of t. This covers 1009 of the total 1233 Feynman diagrams which contain only first–order factorizable master integrals. We obtain the corresponding x–space representation $\tilde{F}(x)$ from $F(t)$ using the method described in Ref. [125] by computing the discontinuity of $F(1/x)$,

$$\tilde{F}(x) = -\frac{1}{2\pi i} \mathrm{Disc}_x F\left(\frac{1}{x}\right). \tag{2.2}$$

This leads to G–functions, which are defined by

$$G(\{f_1(\tau), \vec{f}(\tau)\}, x) = \int_0^x dy f_1(y) G(\{\vec{f}(\tau)\}, y). \tag{2.3}$$

Here the letters f_i belong to an associated alphabet $\mathfrak{A}$ of length m,

$$\mathfrak{A} = \{f_i(x)\}|_{i=1}^{m}. \tag{2.4}$$

In general some of the letters are given by higher transcendental functions. Both the G–functions in t–and x–space have to have representations as Riemann integrals individually, which requires to remove singularities if they are present in some letters. In the course of the calculation different constants will emerge as G–functions, (2.3), evaluated at a series of special values of $x \in [0, 1]$. All G–functions of x and the constants shall be further reduced algebraically at the end of the calculation and, if possible, simplified to known special functions, using algorithms of the package `HarmonicSums`. As it turns out later, it will also be useful to apply the t–space representation to the nested binomial sum contributions.

The results in N– and in x–space are related by a Mellin transform [126–130]

$$\mathbf{M}[f(x)](N) = \int_0^1 dx x^{N-1} f(x). \tag{2.5}$$

In the following we will present the results in Mellin N–space. The unrenormalized OME $\hat{\hat{A}}_{Qg}$ has the following structure [84] both in the unpolarized and polarized cases[3]

$$\hat{\hat{A}}_{Qg}\left(\frac{\hat{m}^2}{\mu^2}, \hat{a}_s, \varepsilon, N\right) = \sum_{l=1}^{\infty} \hat{a}_s^l \hat{\hat{A}}_{Qg}^{(l)}\left(\frac{\hat{m}^2}{\mu^2}, \varepsilon, N\right), \tag{2.6}$$

$$\hat{\hat{A}}_{Qg}^{(1)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2}\left[\frac{\hat{\gamma}_{qg}^{(0)}}{\varepsilon} + a_{qg,Q}^{(1)} + \varepsilon\overline{a}_{qg,Q}^{(1)} + \varepsilon^2\overline{\overline{a}}_{qg,Q}^{(1)}\right] + O(\varepsilon^3), \tag{2.7}$$

$$\hat{\hat{A}}_{Qg}^{(2)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon}\left[\frac{1}{\varepsilon^2}c_{Qg,(2)}^{(-2)} + \frac{1}{\varepsilon}c_{Qg,(2)}^{(-1)} + c_{Qg,(2)}^{(0)} + \varepsilon c_{Qg,(2)}^{(1)}\right] + O(\varepsilon^2), \tag{2.8}$$

$$\hat{\hat{A}}_{Qg}^{(3)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2}\left[\frac{1}{\varepsilon^3}c_{Qg,(3)}^{(-3)} + \frac{1}{\varepsilon^2}c_{Qg,(3)}^{(-2)} + \frac{1}{\varepsilon}c_{Qg,(3)}^{(-1)} + a_{Qg}^{(3)}\right] + O(\varepsilon)\ , \tag{2.9}$$

with $\hat{m}$ the unrenormalized mass, $\hat{a}_s = \hat{g}_s^2/(16\pi^2)$ the unrenormalized strong coupling constant and μ the renormalization and factorization scale. The renormalization of the OMEs proceeds in four steps, cf. [84]: the renormalization of the heavy quark mass, of the strong coupling [131–147], of the local composite operators, and the subtraction of the collinear singularities due to massless sub–graphs [84].

3 First-order factorizable recurrences for complete color-ζ contributions

In the following we will consider the constant parts of the unrenormalized unpolarized and polarized OMEs, $a_{Qg}^{(3)}(N)$ and $\Delta a_{Qg}^{(3)}(N)$. The additional contributions resulting from lower–order terms due to renormalization were given in Refs. [36, 37].

The calculation of 2000 Mellin moments has been sufficient to determine all color–ζ contributions to $a_{Qg}^{(3)}(N)$ and $\Delta a_{Qg}^{(3)}(N)$ obeying first–order–factorizable recurrences by using the methods of Refs. [51, 119, 120] for generating the recurrences and the methods of Refs. [59–72] for computing the closed form solutions. These are all contributions $\propto N_F$, with N_F the number of massless flavors,[4] and all other terms except the purely rational ones and those $\propto \zeta_3$ of $O(T_F)$ and $O(T_F^2)$ of the irreducible Feynman diagrams, which contain ${}_2F_1$ terms [125, 148] in x–space. This implies that their recurrences are not first–order factorizable. Here we include also the reducible contributions[5], which leads to a part of the rational and ζ_3 terms. In the unpolarized case also the Feynman diagrams with external Faddeev–Popov ghosts [149] contribute to the first–order factorizable terms. The yet missing part concerns only irreducible Feynman diagrams.

For the color-ζ structures which can be obtained fully in closed form, we obtain

$$a_{Qg}^{(3)} = \frac{1}{2}[1+(-1)^N] \times\Biggl\{C_F\Biggl\{C_A T_F\Biggl[\frac{8S_1^2\zeta_2 P_{13}}{3(N-1)N^2(1+N)^2(2+N)^2} - \frac{288\zeta_2^2 P_{14}}{5(N-1)N^2(1+N)^2(2+N)^2}$$

[3]In the polarized case the symbol Δ is put in front of the respective coefficient. Structurally the relations are the same as those of (2.7–2.9).

[4]A direct computation of the N_F terms in the unpolarized case using summation methods has been performed before in [15].

[5]These are self–energy insertions on external lines of the Feynman diagrams.

$$+\frac{\zeta_2 P_{25}}{18(N-1)N^3(1+N)^3(2+N)^3}-\frac{4S_1\zeta_2 P_{29}}{9(N-1)N^3(1+N)^3(2+N)^3}$$

$$+\mathsf{B}_4\Biggl[\frac{32P_{14}}{(N-1)N^2(1+N)^2(2+N)^2}+32p_{qg}^{(0)}S_1\Biggr]+p_{qg}^{(0)}\Biggl[-\frac{12S_2\zeta_2 P_1}{(N-1)N(1+N)(2+N)}$$

$$+\Biggl[-\frac{8\bigl(1+3N+3N^2\bigr)\zeta_2}{N(1+N)}+16S_1\zeta_2\Biggr]S_{-2}+\bigl(32S_1^3-8S_3-8S_{-3}+16S_{-2,1}\bigr)\zeta_2$$

$$-\frac{288}{5}S_1\zeta_2^2\Biggr]\Biggr]+T_F^2\Biggl[\frac{2\zeta_2 P_{34}}{9(N-1)N^4(1+N)^4(2+N)^3}+N_F\Biggl[-\frac{32S_1^2P_7}{81N^2(1+N)^2(2+N)}$$

$$-\frac{16S_3P_{24}}{81(N-1)N^3(1+N)^3(2+N)^2}+\frac{2(N-2)\zeta_2 P_{30}}{9(N-1)N^4(1+N)^4(2+N)^3}$$

$$+\frac{8S_2P_{33}}{27(N-1)N^4(1+N)^4(2+N)^3}+\frac{P_{37}}{243(N-1)N^6(1+N)^6(2+N)^5}$$

$$+p_{qg}^{(0)}\Biggl[-\frac{56\zeta_3 P_{15}}{9(N-1)N^2(1+N)^2(2+N)}+\Biggl[-\frac{256}{27}S_3-\frac{128}{3}S_{2,1}+\frac{224\zeta_3}{9}\Biggr]S_1+\Biggl[-\frac{64}{9}S_2$$

$$-\frac{16\zeta_2}{3}\Biggr]S_1^2-\frac{32}{27}S_1^4-\frac{128}{9}S_2^2+\frac{256}{9}S_4-\frac{128}{3}S_{3,1}+\frac{256}{3}S_{2,1,1}\Biggr]$$

$$+\Biggl[-\frac{16P_{12}}{243N^2(1+N)^3(2+N)}+\frac{32\bigl(24+83N+49N^2+10N^3\bigr)S_2}{27N^2(1+N)(2+N)}$$

$$+\frac{16\bigl(12+28N+11N^2+5N^3\bigr)\zeta_2}{9N^2(1+N)(2+N)}\Biggr]S_1+\frac{32\bigl(24+83N+49N^2+10N^3\bigr)S_1^3}{81N^2(1+N)(2+N)}$$

$$-\frac{128\bigl(-2-3N+N^2\bigr)S_{2,1}}{3N^2(1+N)(2+N)}\Biggr]+\frac{80\bigl(6+11N+4N^2+N^3\bigr)S_1\zeta_2}{9N^2(1+N)(2+N)}+p_{qg}^{(0)}\Biggl[-\frac{40}{3}S_1^2\zeta_2$$

$$+8S_2\zeta_2\Biggr]\Biggr]\Biggr\}+C_A^2T_F\Biggl\{\frac{144(N-2)(3+N)\zeta_2^2P_2}{5(N-1)N^2(1+N)^2(2+N)^2}$$

$$-\frac{4S_1^2\zeta_2 P_{18}}{3(N-1)N^2(1+N)^2(2+N)^2}+\frac{4S_1\zeta_2 P_{31}}{9(N-1)^2N^3(1+N)^3(2+N)^3}$$

$$+\frac{2\zeta_2 P_{35}}{9(N-1)^2N^4(1+N)^4(2+N)^4}+\mathsf{B}_4\Biggl[-\frac{4P_{17}}{(N-1)N^2(1+N)^2(2+N)^2}-16p_{qg}^{(0)}S_1\Biggr]$$

$$+p_{qg}^{(0)}\Biggl[-\frac{4S_2\zeta_2 P_8}{3(N-1)N(1+N)(2+N)}+\Biggl[-32S_2\zeta_2+\frac{288\zeta_2^2}{5}\Biggr]S_1$$

$$+\Biggl[-\frac{8\zeta_2 P_9}{3(N-1)N(1+N)(2+N)}-48S_1\zeta_2\Biggr]S_{-2}+\bigl(-16S_1^3-8S_3-8S_{-3}$$

$$+16S_{-2,1}\bigr)\zeta_2\Biggr]\Biggr\}+C_AT_F^2\Biggl[-\frac{4\zeta_2 P_{28}}{9(N-1)N^3(1+N)^3(2+N)^3}$$

$$+N_F\Biggl[-\frac{64S_{2,1}P_4}{27N(1+N)^2(2+N)^2}-\frac{160S_{-3}P_5}{27N(1+N)^2(2+N)^2}-\frac{16S_1^3P_{10}}{81N(1+N)^2(2+N)^2}$$

$$
\begin{aligned}
&+\frac{64 S_{-2,1} P_{16}}{9(N-1)N^2(1+N)^2(2+N)^2}+\frac{8 S_1^2 P_{20}}{81 N(1+N)^3(2+N)^3}\\
&-\frac{32 S_3 P_{22}}{81(N-1)N^2(1+N)^2(2+N)^2}+\frac{8 S_2 P_{26}}{81(N-1)N^3(1+N)^3(2+N)^3}\\
&-\frac{4\zeta_2 P_{27}}{9(N-1)N^3(1+N)^3(2+N)^3}-\frac{8 P_{36}}{243(N-1)N^5(1+N)^5(2+N)^5}\\
&+p_{qg}^{(0)}\Biggl[\Biggl[\Biggl[\frac{1888}{27}S_3+\frac{224}{9}S_{2,1}-64 S_{-2,1}-\frac{224}{9}\zeta_3\Biggr]S_1+\frac{160}{3}S_{-3}S_1+\Biggl[\frac{176}{9}S_2+\frac{16\zeta_2}{3}\Biggr]S_1^2\\
&+\frac{32}{27}S_1^4+\frac{80}{9}S_2^2+\frac{640}{9}S_4+\Biggl[-\frac{64(-1+2N)S_1}{(N-1)N}+32 S_1^2+\frac{160}{3}S_2+\frac{32}{3}\zeta_2\Biggr]S_{-2}\\
&+\frac{352}{9}S_{-4}-\frac{32}{9}S_{3,1}+\frac{64(-1+2N)S_{-2,1}}{(N-1)N}-\frac{128}{3}S_{-2,2}-\frac{160}{3}S_{-3,1}-\frac{416}{9}S_{2,1,1}\\
&+64 S_{-2,1,1}+\frac{16}{3}S_2\zeta_2+\frac{448\bigl(1+N+N^2\bigr)\zeta_3}{9(N-1)N(1+N)(2+N)}\Biggr]+\Biggl[-\frac{16\zeta_2 P_6}{9N(1+N)^2(2+N)^2}\\
&-\frac{16 S_2 P_{11}}{27N(1+N)^2(2+N)^2}+\frac{16 P_{32}}{243(N-1)N^2(1+N)^4(2+N)^4}\Biggr]S_1\\
&+\Biggl[-\frac{64 S_1(N) P_{16}}{9(N-1)N^2(1+N)^2(2+N)^2}+\frac{32 P_{21}}{81N(1+N)^3(2+N)^3}\Biggr]S_{-2}\Biggr]\\
&+p_{qg}^{(0)}\Biggl[\frac{40}{3}S_1^2\zeta_2+\frac{40}{3}S_2\zeta_2+\frac{80}{3}S_{-2}\zeta_2\Biggr]+\frac{160\bigl(4-N+N^2+4N^3+N^4\bigr)S_1\zeta_2}{9N(1+N)^2(2+N)^2}\Biggr]\\
&+C_F^2 T_F\Biggl[-\frac{16\mathsf{B}_4(N-1)\bigl(-2+3N+3N^2\bigr)}{N^2(1+N)^2}+\frac{4 S_1^2\zeta_2 P_3}{N^2(1+N)^2(2+N)}\\
&+\frac{8 S_1\zeta_2 P_{19}}{N^3(1+N)^3(2+N)}+\frac{\zeta_2 P_{23}}{2N^4(1+N)^4(2+N)}+p_{qg}^{(0)}\Biggl[\Biggl[-\frac{16\zeta_2}{N(1+N)}+32 S_1\zeta_2\Biggr]S_{-2}\\
&-16 S_1^3\zeta_2-\frac{8\bigl(2+3N+3N^2\bigr)S_2\zeta_2}{N(1+N)}+(32 S_1 S_2+16 S_3+16 S_{-3}-32 S_{-2,1})\zeta_2\Biggr]\\
&+\frac{144(N-1)\bigl(-2+3N+3N^2\bigr)\zeta_2^2}{5N^2(1+N)^2}\Biggr]-\frac{64}{9}p_{qg}^{(0)}T_F^3\zeta_3\Biggr\}+O(\mathrm{rat})+O(\zeta_3),
\end{aligned}
\tag{3.1}
$$

with the polynomials P_i

$$P_1 = N^4+2N^3-3N^2-4N-4, \tag{3.2}$$
$$P_2 = 3N^4+6N^3+7N^2+4N+4, \tag{3.3}$$
$$P_3 = 3N^4+14N^3+43N^2+48N+20, \tag{3.4}$$
$$P_4 = 5N^4+11N^3+50N^2+85N+20, \tag{3.5}$$
$$P_5 = 5N^4+14N^3+53N^2+82N+20, \tag{3.6}$$
$$P_6 = 5N^4+20N^3+59N^2+76N+20, \tag{3.7}$$
$$P_7 = 10N^4+185N^3+789N^2+521N+141, \tag{3.8}$$
$$P_8 = 11N^4+22N^3-59N^2-70N-48, \tag{3.9}$$
$$P_9 = 11N^4+22N^3-47N^2-58N-36, \tag{3.10}$$

$$
\begin{aligned}
P_{10} &= 20N^4+107N^3+344N^2+439N+134, && (3.11)\\
P_{11} &= 40N^4+151N^3+544N^2+779N+214, && (3.12)\\
P_{12} &= 230N^5-924N^4-5165N^3-7454N^2-10217N-2670, && (3.13)\\
P_{13} &= N^6-9N^5-120N^4-137N^3+29N^2+56N+36, && (3.14)\\
P_{14} &= 3N^6+9N^5-5N^4-25N^3-14N^2-16, && (3.15)\\
P_{15} &= 3N^6+9N^5-N^4-17N^3-38N^2-28N-24, && (3.16)\\
P_{16} &= 5N^6-9N^5-24N^4-61N^3-143N^2-20N+36, && (3.17)\\
P_{17} &= 9N^6+27N^5-15N^4-75N^3-62N^2-20N-56, && (3.18)\\
P_{18} &= 11N^6+33N^5-87N^4-85N^3+4N^2-116N-48, && (3.19)\\
P_{19} &= 13N^6+36N^5+39N^4+8N^3-21N^2-29N-10, && (3.20)\\
P_{20} &= 22N^6+271N^5+2355N^4+6430N^3+6816N^2+3172N+1256, && (3.21)\\
P_{21} &= 47N^6+278N^5+1257N^4+2552N^3+1794N^2+284N+448, && (3.22)\\
P_{22} &= 65N^6+429N^5+1155N^4+725N^3+370N^2+496N+648, && (3.23)\\
P_{23} &= -153N^8-612N^7-1196N^6-1374N^5-947N^4-222N^3+176N^2+184N\\
&\quad +48, && (3.24)\\
P_{24} &= 29N^8-976N^7-2382N^6+1736N^5+9129N^4+7472N^3+6832N^2+5376N\\
&\quad +3888, && (3.25)\\
P_{25} &= -261N^9-1566N^8+2506N^7+27752N^6+65115N^5+88078N^4+76456N^3\\
&\quad +46032N^2+17200N+3552, && (3.26)\\
P_{26} &= 4N^9-117N^8+806N^7+6901N^6+15770N^5+7720N^4-6644N^3-3128N^2\\
&\quad -4032N-1728, && (3.27)\\
P_{27} &= 15N^9+90N^8+146N^7-32N^6-501N^5-610N^4-244N^3-48N^2\\
&\quad +224N+96, && (3.28)\\
P_{28} &= 69N^9+414N^8+1148N^7+2134N^6+3171N^5+5180N^4+6500N^3+5352N^2\\
&\quad +3008N+672, && (3.29)\\
P_{29} &= 337N^9+2088N^8+4868N^7+5338N^6+1523N^5-3602N^4-5768N^3-3392N^2\\
&\quad +48N+288, && (3.30)\\
P_{30} &= 45N^{10}+405N^9+1606N^8+3842N^7+6717N^6+9325N^5+10888N^4+9804N^3\\
&\quad +6232N^2+3264N+864, && (3.31)\\
P_{31} &= 103N^{10}+515N^9+1124N^8+1298N^7-809N^6-601N^5+3078N^4+2820N^3\\
&\quad +680N^2-2160N-864, && (3.32)\\
P_{32} &= 491N^{10}+5292N^9+23603N^8+61598N^7+87216N^6+29418N^5-73982N^4\\
&\quad -73764N^3-11408N^2-2672N+864, && (3.33)\\
P_{33} &= 57N^{11}+547N^{10}+1416N^9-398N^8-6819N^7-13965N^6-19422N^5\\
&\quad -31384N^4-39024N^3-27808N^2-16992N-5184, && (3.34)\\
P_{34} &= 333N^{11}+2331N^{10}+6142N^9+6930N^8+617N^7-6377N^6-4900N^5\\
&\quad +4444N^4+11680N^3+8944N^2+4992N+1728, && (3.35)\\
P_{35} &= 69N^{13}+552N^{12}+1190N^{11}-997N^{10}-8937N^9-17658N^8-16952N^7\\
&\quad -19177N^6-36634N^5-54000N^4-57200N^3-39184N^2-17184N-3456, && (3.36)\\
P_{36} &= 3597N^{15}+44514N^{14}+237011N^{13}+692290N^{12}+1139033N^{11}+849246N^{10}
\end{aligned}
$$

$$
\begin{aligned}
& -377441N^9-1484940N^8-1459136N^7-806374N^6-465872N^5-281016N^4 \\
& -22912N^3+33504N^2+18432N+3456, \qquad (3.37)\\
P_{37} \; = \; & 15777N^{17}+186525N^{16}+879391N^{15}+1874085N^{14}+575913N^{13}-5568833N^{12} \\
& -10465411N^{11}-2970289N^{10}+11884298N^9+12640320N^8-10343664N^7 \\
& -40750480N^6-55711424N^5-53947712N^4-42534912N^3-23256576N^2 \\
& -7865856N-1244160 \qquad (3.38)
\end{aligned}
$$

and

$$
p_{qg}^{(0)}=\frac{N^2+N+2}{N(N+1)(N+2)}. \qquad (3.39)
$$

The above expressions can all be represented in terms of nested harmonic sums [55, 56]

$$
S_{b,\vec{a}}(N)=\sum_{k=1}^{N}\frac{(\mathrm{sign}(b))^k}{k^{|b|}}S_{\vec{a}}(k), \quad S_{\emptyset}=1, \quad b,a_i\in\mathbb{Z}\backslash\{0\}, \qquad (3.40)
$$

for which we use the shorthand notation $S_{\vec{a}}(N)\equiv S_{\vec{a}}$. The constant B_4 is given by

$$
\mathsf{B}_4 \;=\; -4\zeta_2\ln^2(2)+\frac{2}{3}\ln^4(2)-\frac{13}{2}\zeta_4+16\mathrm{Li}_4\left(\frac{1}{2}\right), \qquad (3.41)
$$

and

$$
\mathrm{Li}_n(x)=\sum_{k=1}^{\infty}\frac{x^k}{k^n}, \quad |x|\le 1. \qquad (3.42)
$$

The constants $\zeta_n,\;\; n\ge 2$, denote the Riemann ζ [126,150] function evaluated at integer argument n,

$$
\zeta_n=\sum_{k=1}^{\infty}\frac{1}{k^n}. \qquad (3.43)
$$

The $SU(N_c)$ color factors are given by $C_A=N_c, C_F=(N_c^2-1)/(2N_c), T_F=1/2$, with $N_c=3$ for QCD.

The contribution to the constant part[6] $\Delta a_{Qg}^{(3)}(N)$ of the polarized three–loop OME $\Delta A_{Qg}^{(3)}$ in the Larin scheme is given by

$$
\begin{aligned}
\Delta a_{Qg}^{(3)} = & \frac{1}{2}[1-(-1)^N]\Biggl\{C_F\Biggl[T_F^2\Biggl[N_F\Biggl[\frac{8S_2Q_{18}}{27N^4(1+N)^4(2+N)}-\frac{16S_3Q_{12}}{81N^3(1+N)^3(2+N)} \\
& +\frac{Q_{20}}{243N^6(1+N)^6(2+N)}+\Biggl(\frac{32\bigl(10N^3+49N^2+19N-24\bigr)S_2}{27N^2(1+N)(2+N)}-\frac{16Q_5}{243N^2(1+N)^2(2+N)} \\
& -\frac{256}{27}\Delta p_{qg}^{(0)}S_3-\frac{128}{3}\Delta p_{qg}^{(0)}S_{2,1}\Biggr)S_1-\Biggl(\frac{32\bigl(651+442N+175N^2+10N^3\bigr)}{81N^2(1+N)(2+N)}+\frac{64}{9}\Delta p_{qg}^{(0)}S_2\Biggr)S_1^2 \\
& +\frac{32\bigl(-24+19N+49N^2+10N^3\bigr)S_1^3}{81N^2(1+N)(2+N)}+\Delta p_{qg}^{(0)}\Biggl(-\frac{32}{27}S_1^4-\frac{128}{9}S_2^2-\frac{128}{3}S_{3,1}+\frac{256}{3}S_{2,1,1}
\end{aligned}
$$

[6] Here the same conditions as for Eq. (3.1) apply.

$$
+\frac{256}{9}S_4\Bigg) - \frac{128 S_{2,1}}{3N^2} + \Delta p_{qg}^{(0)}\Bigg(\frac{2Q_{13}}{9N^3(1+N)^3} + \frac{16(6+5N)S_1}{9N} - \frac{16}{3}S_1^2\Bigg)\zeta_2
$$

$$
+\Delta p_{qg}^{(0)}\Bigg(-\frac{56Q_1}{9N^2(1+N)^2} + \frac{224 S_1}{9}\Bigg)\zeta_3\Bigg] + \Delta p_{qg}^{(0)}\Bigg(\frac{2Q_{15}}{9N^3(1+N)^3} + \frac{80(3+N)S_1}{9N}
$$

$$
-\frac{40}{3}S_1^2 + 8S_2\Bigg)\zeta_2\Bigg] + C_A T_F\Bigg[\mathsf{B}_4\Delta p_{qg}^{(0)}\Bigg(\frac{32\big(-5+3N+3N^2\big)}{N(1+N)} + 32S_1\Bigg) + \Bigg(-\frac{4S_1 Q_9}{9N^3(1+N)^3}
$$

$$
+\frac{Q_{16}}{18N^4(1+N)^4} + \frac{8\big(27-40N-12N^2+N^3\big)S_1^2}{3N^2(1+N)^2} + 32\Delta p_{qg}^{(0)}S_1^3 - 12\Delta p_{qg}^{(0)^2}(2+N)S_2
$$

$$
-8\Delta p_{qg}^{(0)}S_3 + \Delta p_{qg}^{(0)}\Bigg(-\frac{8\big(1+3N+3N^2\big)}{N(1+N)} + 16S_1\Bigg)S_{-2} - 8\Delta p_{qg}^{(0)}S_{-3} + 16\Delta p_{qg}^{(0)}S_{-2,1}\Bigg)\zeta_2
$$

$$
+\Bigg(-\frac{288\Delta p_{qg}^{(0)}\big(-5+3N+3N^2\big)}{5N(1+N)} - \frac{288}{5}\Delta p_{qg}^{(0)}S_1\Bigg)\zeta_2^2\Bigg]\Bigg]
$$

$$
+C_A T_F^2\Bigg[N_F\Bigg[-\frac{32S_3Q_4}{81N^2(1+N)^2(2+N)} + \frac{8S_2Q_{11}}{81N^3(1+N)^3(2+N)} - \frac{8Q_{19}}{243N^5(1+N)^5(2+N)}
$$

$$
+\Bigg(\frac{16Q_{10}}{243N(1+N)^4(2+N)} - \frac{16\big(139+38N+71N^2+40N^3\big)S_2}{27N(1+N)^2(2+N)} + \frac{1888}{27}\Delta p_{qg}^{(0)}S_3
$$

$$
+\frac{224}{9}\Delta p_{qg}^{(0)}S_{2,1} - 64\Delta p_{qg}^{(0)}S_{-2,1}\Bigg)S_1 + \Bigg(\frac{8Q_3}{81N(1+N)^3(2+N)} + \frac{176}{9}\Delta p_{qg}^{(0)}S_2\Bigg)S_1^2
$$

$$
-\frac{16\big(83+82N+67N^2+20N^3\big)S_1^3}{81N(1+N)^2(2+N)} + \Delta p_{qg}^{(0)}\Bigg(\frac{32}{27}S_1^4 + \frac{80}{9}S_2^2 + \frac{640}{9}S_4\Bigg) + \Bigg(32\Delta p_{qg}^{(0)}S_1^2
$$

$$
+\frac{160}{3}\Delta p_{qg}^{(0)}S_2 + \frac{32\big(-296+49N-40N^2+47N^3\big)}{81N(1+N)^3} - \frac{64\big(7-6N+5N^2\big)S_1}{9N(1+N)^2}\Bigg)S_{-2}
$$

$$
+\Bigg(-\frac{160\big(7-6N+5N^2\big)}{27N(1+N)^2} + \frac{160}{3}\Delta p_{qg}^{(0)}S_1\Bigg)S_{-3} + \frac{352}{9}\Delta p_{qg}^{(0)}S_{-4} - \frac{64\big(7-9N+5N^2\big)S_{2,1}}{27N(1+N)^2}
$$

$$
-\frac{32}{9}\Delta p_{qg}^{(0)}S_{3,1} + \frac{64\big(7-6N+5N^2\big)S_{-2,1}}{9N(1+N)^2} + \Delta p_{qg}^{(0)}\Bigg(-\frac{128}{3}S_{-2,2} - \frac{160}{3}S_{-3,1} - \frac{416}{9}S_{2,1,1}
$$

$$
+64S_{-2,1,1}\Bigg) + \Bigg(-\frac{4Q_6}{9N^3(1+N)^3} - \frac{16\big(7+5N^2\big)S_1}{9N(1+N)^2} + \Delta p_{qg}^{(0)}\big(\frac{16}{3}S_1^2 + \frac{16}{3}S_2 + \frac{32}{3}S_{-2}\big)\Bigg)\zeta_2
$$

$$
+\Delta p_{qg}^{(0)}\Bigg(\frac{448}{9N(1+N)} - \frac{224S_1}{9}\Bigg)\zeta_3\Bigg] + \Bigg(-\frac{4Q_7}{9N^3(1+N)^3} + \frac{160(-2+N)(2+N)S_1}{9N(1+N)^2}
$$

$$
+\Delta p_{qg}^{(0)}\Bigg(\frac{40}{3}S_1^2 + \frac{40}{3}S_2 + \frac{80}{3}S_{-2}\Bigg)\Bigg)\zeta_2\Bigg] + C_F^2 T_F\Bigg[-\frac{16\mathsf{B}_4\Delta p_{qg}^{(0)}\big(-2+3N+3N^2\big)}{N(1+N)}
$$

$$
+\Delta p_{qg}^{(0)}\Bigg(-\frac{Q_{14}}{2N^3(1+N)^3} + \Bigg(\frac{8Q_2}{N^2(1+N)^2} + 32S_2\Bigg)S_1 + \frac{4(2+N)(5+3N)S_1^2}{N(1+N)} - 16S_1^3
$$

$$
-\frac{8\big(2+3N+3N^2\big)S_2}{N(1+N)}+16S_3+\left(\left(-\frac{16}{N(1+N)}+32S_1\right)S_{-2}+16S_{-3}-32S_{-2,1}\right)\zeta_2
$$
$$
+\frac{144\Delta p_{qg}^{(0)}\big(-2+3N+3N^2\big)}{5N(1+N)}\zeta_2^2\Bigg]+C_A^2T_F\Bigg[\mathsf{B}_4\left(-36\Delta p_{qg}^{(0)^2}(2+N)-16\Delta p_{qg}^{(0)}S_1\right)
$$
$$
+\left(\frac{2Q_{17}}{9N^4(1+N)^4}+\left(\frac{4Q_8}{9N^3(1+N)^3}-32\Delta p_{qg}^{(0)}S_2\right)S_1-\frac{4\big(24-83N+11N^3\big)S_1^2}{3N^2(1+N)^2}\right.
$$
$$
-16\Delta p_{qg}^{(0)}S_1^3-\frac{4\Delta p_{qg}^{(0)}\big(-48+11N+11N^2\big)S_2}{3N(1+N)}-8\Delta p_{qg}^{(0)}S_3-8\Delta p_{qg}^{(0)}S_{-3}
$$
$$
+\left(\left(-\frac{8\Delta p_{qg}^{(0)}\big(-36+11N+11N^2\big)}{3N(1+N)}-48\Delta p_{qg}^{(0)}S_1\right)S_{-2}+16\Delta p_{qg}^{(0)}S_{-2,1}\right)\zeta_2
$$
$$
+\Delta p_{qg}^{(0)}\left(\frac{144\big(-8+3N+3N^2\big)}{5N(1+N)}+\frac{288}{5}S_1\right)\zeta_2^2\Bigg]-\frac{64}{9}\Delta p_{qg}^{(0)}T_F^3\zeta_3\Bigg\}+O(\mathrm{rat})+O(\zeta_3), \qquad (3.44)
$$

with the polynimials

$$
\begin{aligned}
Q_1 &= 3N^4+6N^3-N^2-4N+12, && (3.45)\\
Q_2 &= 13N^4+23N^3+4N^2-14N-5, && (3.46)\\
Q_3 &= 22N^4+183N^3+1027N^2+2022N+580, && (3.47)\\
Q_4 &= 65N^4+364N^3+883N^2+614N-648, && (3.48)\\
Q_5 &= 230N^4-1154N^3-2405N^2-709N-66, && (3.49)\\
Q_6 &= 15N^5+15N^4-103N^3+33N^2-20N-36, && (3.50)\\
Q_7 &= 69N^5+69N^4-55N^3+51N^2-338N-36, && (3.51)\\
Q_8 &= 103N^5+103N^4-79N^3+317N^2-612N-144, && (3.52)\\
Q_9 &= 337N^5+403N^4-541N^3-583N^2-300N+108, && (3.53)\\
Q_{10} &= 491N^5+2837N^4+6440N^3+10244N^2+10934N+1328, && (3.54)\\
Q_{11} &= 4N^6-201N^5-143N^4+246N^3-1328N^2+1368N+1296, && (3.55)\\
Q_{12} &= 29N^6-1005N^5-3859N^4-5139N^3-4486N^2-2172N+1944, && (3.56)\\
Q_{13} &= 45N^6+135N^5+211N^4+101N^3-68N^2+384N+216, && (3.57)\\
Q_{14} &= 153N^6+459N^5+527N^4+217N^3-4N^2-48N+8, && (3.58)\\
Q_{15} &= 333N^6+999N^5+805N^4-7N^3-14N^2-300N-216, && (3.59)\\
Q_{16} &= -261N^7-522N^6+3712N^5+5362N^4-5623N^3-7144N^2-276N\\
&\quad +144, && (3.60)\\
Q_{17} &= 69N^7+138N^6-667N^5-541N^4+952N^3-1277N^2+990N+432, && (3.61)\\
Q_{18} &= 57N^8+376N^7+1488N^6+1958N^5-461N^4-510N^3+1676N^2-1656N\\
&\quad -1296, && (3.62)\\
Q_{19} &= 3597N^{10}+19335N^9+36218N^8+27506N^7-1294N^6-13534N^5\\
&\quad +12977N^4-7N^3-4122N^2-8388N-3240, && (3.63)\\
Q_{20} &= 15777N^{12}+76086N^{11}+111457N^{10}-96922N^9-540757N^8-841318N^7\\
&\quad -810709N^6-26710N^5+826216N^4+92256N^3-345888N^2-289440N\\
&\quad -77760 && (3.64)
\end{aligned}
$$

and

$$\Delta p_{qg}^{(0)} = \frac{N-1}{N(N+1)}. \tag{3.65}$$

The first moment of $\Delta a_{Qg}^{(3)}$ vanishes for the computed color–ζ contributions, as it does at first [151] and second order [48, 152]. At first order, this is even true for general values of m^2/Q^2, cf. [48, 152].[7] The available parts of $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$ are expressed in terms of the following set of 14 harmonic sums

$$\left\{S_{-4}, S_{-3}, S_{-2}, S_1, S_2, S_3, S_4, S_{-3,1}, S_{-2,1}, S_{-2,2}, S_{2,1}, S_{3,1}, S_{-2,1,1}, S_{2,1,1}\right\}. \tag{3.66}$$

Correspondingly, the following set of 21 harmonic polylogarithms [101] spans the expressions in x–space

$$\begin{aligned}&\left\{\mathrm{H}_{-1}, \mathrm{H}_0, \mathrm{H}_1, \mathrm{H}_{0,-1}, \mathrm{H}_{0,1}, \mathrm{H}_{0,-1,-1}, \mathrm{H}_{0,-1,1}, \mathrm{H}_{0,0,-1}, \mathrm{H}_{0,0,1}, \mathrm{H}_{0,1,-1}, \mathrm{H}_{0,1,1}, \mathrm{H}_{0,-1,-1,-1}, \mathrm{H}_{0,-1,0,1},\right.\\ &\left.\mathrm{H}_{0,0,-1,-1}, \mathrm{H}_{0,0,-1,1}, \mathrm{H}_{0,0,0,-1}, \mathrm{H}_{0,0,0,1}, \mathrm{H}_{0,0,1,-1}, \mathrm{H}_{0,0,1,1}, \mathrm{H}_{0,1,1,1}, \mathrm{H}_{0,0,0,0,1}\right\},\end{aligned} \tag{3.67}$$

after algebraic reduction [102]. The harmonic polylogarithms are defined by

$$\mathrm{H}_{b,\vec{a}}(x) = \int_0^x dy f_b(y) \mathrm{H}_{\vec{a}}(y), \quad f_b(y) \in \left\{\frac{1}{y}, \frac{1}{1-y}, \frac{1}{1+y}\right\}. \tag{3.68}$$

The corresponding expressions in N– and x–space are given in ancillary files in computer readable form.

4 The N-space structure of the remaining diagrams

In the following we summarize the results we have obtained in Mellin N–space, both for the cases of first–order factorizable and non–first–order factorizable recurrences. One possible strategy to follow is to obtain closed form recursion relations for all color–ζ contributions and to perform an analytic continuation to $N \in \mathbb{C}$. One has to derive the asymptotic expansion of these recurrences and use their shift properties

$$N+1 \rightarrow N \tag{4.1}$$

to reach any point in the analyticity region for $N \in \mathbb{C}$. It finally turns out that it is very time–consuming to obtain the recurrences for the purely rational terms of $O(T_F)$, while those of $O(T_F\zeta_3)$ still can be obtained on the basis of up to 15000 Mellin moments, see Table 3 below. In the polarized case a maximal number of 11000 Mellin moments has been computed.

Analyzing the sequences of Mellin moments for the purely rational terms of the color factors $T_F C_F^2$, $T_F C_A^2$, $T_F C_F C_A$, $T_F^2 C_F$ and $T_F^2 C_A$ one observes that these contributions to $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$

[7] For other OMEs and Wilson coefficients, as e.g. in the polarized non–singlet case, the first moment (corresponding to the polarized Bjorken sum rule) is not vanishing [153, 154] and also obtains power corrections of $O((m^2/Q^2)^k)$ [155].

c_i	200	1000	2000
$C_F T_F^2$	$-5.89 \cdot 10^{-5}$	$-2.14 \cdot 10^{-43}$	$-1.65 \cdot 10^{-93}$
$C_A T_F^2$	$-1.38 \cdot 10^{-6}$	$-8.12 \cdot 10^{-45}$	$-6.89 \cdot 10^{-95}$
$C_F^2 T_F$	$1.96 \cdot 10^{-58}$	$9.83 \cdot 10^{-299}$	$1.41 \cdot 10^{-599}$
$C_F C_A T_F$	$9.84 \cdot 10^{-59}$	$4.29 \cdot 10^{-299}$	$5.93 \cdot 10^{-600}$
$C_A^2 T_F$	$2.91 \cdot 10^{-58}$	$1.16 \cdot 10^{-298}$	$1.59 \cdot 10^{-599}$
Δc_i	200	1000	2000
$C_F T_F^2$	$-5.53 \cdot 10^{-5}$	$-2.82 \cdot 10^{-43}$	$-3.68 \cdot 10^{-93}$
$C_A T_F^2$	$-1.06 \cdot 10^{-6}$	$-4.48 \cdot 10^{-43}$	$-5.57 \cdot 10^{-93}$
$C_F^2 T_F$	$-1.52 \cdot 10^{-57}$	$-3.51 \cdot 10^{-297}$	$9.90 \cdot 10^{-598}$
$C_F C_A T_F$	$-8.21 \cdot 10^{-57}$	$-1.68 \cdot 10^{-296}$	$-1.19 \cdot 10^{-597}$
$C_A^2 T_F$	$2.71 \cdot 10^{-58}$	$2.61 \cdot 10^{-294}$	$1.14 \cdot 10^{-597}$

Table 1: Relative approximation of the ratio of color factors, cf. Eq. (4.2), as a function of $N = 200, 1000, 2000$ for $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$. The corresponding coefficients are c_i and Δc_i.

N	$a_{Qg}^{(3),\mathrm{sol,irr}}$	N	$\Delta a_{Qg}^{(3),\mathrm{sol,irr}}$
2	–201.6595414		
4	–1525.640364	3	–847.6187716
6	–1715.840721	5	–1460.511965
10	–1741.066914	9	–1687.025772
100	–966.5291789	99	–969.8344024
200	–737.1136471	199	–738.5607476
1000	–358.5858699	999	–358.7549068
2000	–254.2324483	1999	–254.2957895
5000	–156.9872766	4999	–157.0039294

Table 2: Values of some moments of the irreducible contributions of the first–order factorizable diagrams $(\Delta)a_{Qg}^{(3)}(N)$ in QCD for $N_F = 0$.

individually diverge strongly for large values of N. The coefficients of the same color factors with an additional factor of ζ_3 show the same behavior. The sum over the purely rational terms and the ζ_3 terms for each color factor separately, however, tends to zero, i.e.

$$\lim_{N\to\infty} \frac{r[c_i](N)}{r[c_i\zeta_3](N)} + \zeta_3 = 0. \tag{4.2}$$

Here $r[c_i]$ denotes the corresponding rational pre–factor of the color factors, which we illustrate in Table 1. Therefore, the respective recurrences are not independent. On the other hand, they cannot be easily joined in an exact manner, but only approximately by rationalizing ζ_3 with a high number of digits in the numerator and denominator. One therefore would have to deal with diverging asymptotic representations, which have to be handled analytically.

In N–space individual terms rise with factors 2^N or 4^N and it is hard to see how these contributions cancel analytically. We therefore list a series of moments for the sum of the first–order factorizable diagrams to the irreducible contribution to $(\Delta)a_{Qg}^{(3)}(N)$ in the unpolarized and polarized cases, setting the known N_F–terms to zero and the color factors to those of QCD in Table 2. They are first rising and then slowly falling towards $N\to\infty$, which suggests that intermediate contributions rising $\propto 2^N$ or larger do finally cancel in the set of the first–order factorizable terms. Similar to what has been observed in Ref. [38] for $A_{gg}^{(3)}$, even the values of the irreducible contributions of the first–order factorizable diagrams in the unpolarized and polarized cases approach each other for large values of N. As will be shown in Section 6, both $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$ tend to zero as $N\to\infty$ for the first–order–factorizable contributions. In x–space the most singular contributions are $\propto \ln^k(1-x),\quad k>0, k\in\mathbb{N}$. Because the Qg–channel is off–diagonal, no $\delta(1-x)$ and $\left[\ln^k(1-x)/(1-x)\right]_+$–distributions, with $k\geq 0$, will be present in x–space.

Unpolarized	Color/ζ	Moments	Order	Degree	First order factors	Size of rec. [Mbyte]
	$C_FT_F^2$	3150	27	654	15	11.75
	$C_AT_F^2$	9858	46	1407	30	105.08
	$C_FT_F^2\zeta_3$	1092	15	238	7	0.89
	$C_AT_F^2\zeta_3$	2156	24	447	14	5.52
	$C_F^2T_F\zeta_3$	9858	58	2024		304.79
	$C_FC_AT_F\zeta_3$	12826	65	2602		563.50
	$C_A^2T_F\zeta_3$	14036	68	2848		709.63
Polarized						
	$C_FT_F^2$	1395	18	279	9	1.69
	$C_FT_F^2\zeta_3$	480	10	104	4	0.15
	$C_AT_F^2\zeta_3$	1702	21	352	11	3.46
	$C_F^2T_F\zeta_3$	8787	55	1803		233.36
	$C_FC_AT_F\zeta_3$	10340	60	2146		363.35

Table 3: Characteristics of non–first–order factorizable recurrences in the unpolarized and polarized cases, by the required number of moments, their order and degree, their first–order factors, and their size.

A further problem is given by the fact that the asymptotic representation is not easily obtainable to a sufficient number of terms for non-first-order factorizable recurrences if the recurrences are very large. On the other hand, in the first–order factorizable cases, analytic techniques are available to compute the asymptotic representations as will be outlined in Appendices A and B. While for non–first–order factorizable recurrences their first–order factors can all be split off, the respective factors of higher than first–order cannot be algorithmically determined yet. Therefore one is left with some recurrences of a larger order, the final solution of which is not given by product–sum representations, but by higher transcendental functions to be determined.[8] In Table 3 we summarize the characteristics of the cases of non–first–order factorizable recurrences we have computed.

To illustrate the complexity of the problem, the largest rational number in the input for the determination of the recurrences has a size of 31k digits in the numerator and of 26.6k in the denominator. The largest recursion obtained has a size of ~ 0.7 GB.

The first–order factors are split off by using algorithms of `Sigma` [73, 74] leaving a non–first–order factorizable remainder. For very large recurrences this process can take several months of computation time, and we did not perform this computation in these cases, since a very large remainder recurrence is obtained for which the analytic solution cannot be given at present.

One may consider asymptotic solutions of the non–first–order factorizable difference equations following Refs. [157–160]. For the color factors $C_F T_F^2 \zeta_3$ related to the smallest corresponding recurrences we calculated the fundamental system of order $\mathsf{o} = 15$ and $\mathsf{o} = 10$ in the unpolarized and polarized case, respectively. These systems are computed by the `HarmonicSums` command `REAsymptotics[rec,f[n],7]`,[9] where `f[n]` is the function obeying the homogeneous recurrence `rec` and 7 is the desired expansion depth. The systems of the asymptotic solutions are given by

$$\left\{ T_k^{C_F T_F^2 \zeta_3} \Big|_{k=1}^{15} \right\} =$$

$$\Bigg\{ \left[\frac{1}{N^4} + \frac{174}{197N^5} - \frac{115915}{197N^6} - \frac{10928670}{197N^7} \right] \left(-\frac{9}{8} \right)^N, \frac{(-1)^N}{N},$$

$$\left[-\frac{158191326}{19272263N^5} + \frac{3264014438}{57816789N^6} - \frac{449608338428}{1561053303N^7} + \frac{1}{N^2} \right] (-1)^N,$$

$$\left[\frac{1}{N^3} - \frac{321703313}{19272263N^5} + \frac{7167720182}{57816789N^6} - \frac{1124854321331}{1561053303N^7} \right] (-1)^N,$$

$$\left[\frac{1}{N^4} - \frac{156571794}{19272263N^5} + \frac{2861638081}{57816789N^6} - \frac{431900140522}{1561053303N^7} \right] (-1)^N,$$

$$\Bigg[-\frac{3486911695}{77089052N^5} + \frac{3980355789289}{6938014680N^6} - \frac{859592977355719}{187326396360N^7}$$

$$+ \left(\frac{1}{N^2} - \frac{3}{N^3} + \frac{7}{N^4} - \frac{15}{N^5} + \frac{31}{N^6} - \frac{63}{N^7} \right) \ln(N) \Bigg] (-1)^N,$$

$$\Bigg[-\frac{1}{10} + \frac{1260823915355237}{1046073508500N^6} - \frac{244509992621968565 71}{296561839659750N^7} + \Bigg(\frac{1}{N} - \frac{370565089177}{34869116950N^2}$$

[8] There exist only very few studies for solutions of this kind, cf. [156].

[9] Commands described here and in the following refer to the package `HarmonicSums`, unless denoted otherwise.

$$
\begin{aligned}
&+\frac{1286040852281}{34869116950N^3}-\frac{7299389618221}{52303675425N^4}+\frac{1795444741338}{3486911695N^5}-\frac{124663841290259}{69738233900N^6}\\
&+\frac{412778573182657}{69738233900N^7}\Bigg)\ln(N)+\left(\frac{1}{N^2}-\frac{3}{N^3}+\frac{7}{N^4}-\frac{15}{N^5}+\frac{31}{N^6}-\frac{63}{N^7}\right)\ln^2(N)\Bigg](-1)^N,\\
&\left[\frac{1}{N^3}+\frac{162553}{18054N^4}+\frac{388414}{9027N^5}+\frac{29532113}{162486N^6}+\frac{571451720}{731187N^7}\right]\left(-\frac{1}{8}\right)^N,\\
&\left[\frac{1}{N^3}+\frac{191225}{26118N^4}+\frac{147338}{4353N^5}+\frac{31187665}{235062N^6}+\frac{591255400}{1057779N^7}\right]\left(\frac{1}{8}\right)^N,\\
&\frac{1}{N}+\frac{10178885}{237654N^4}-\frac{42829585}{118827N^5}+\frac{1605361621}{712962N^6}-\frac{122618276090}{9624987N^7},\\
&\frac{1}{N^2}+\frac{46443703}{475308N^4}-\frac{197209085}{237654N^5}+\frac{7403011091}{1425924N^6}-\frac{282535272647}{9624987N^7},\\
&\frac{1}{N^3}+\frac{2528753}{158436N^4}-\frac{11998345}{79218N^5}+\frac{460898245}{475308N^6}-\frac{17701180264}{3208329N^7},\\
&\frac{76310107}{633744N^4}-\frac{845948561}{792180N^5}+\frac{66371498737}{9506160N^6}-\frac{36692791628777}{898332120N^7}\\
&+\left(\frac{1}{N}-\frac{1}{N^2}+\frac{3}{N^3}-\frac{7}{N^4}+\frac{15}{N^5}-\frac{31}{N^6}+\frac{63}{N^7}\right)\ln(N),\\
&-\frac{1}{10}-\frac{551687998205741}{824149155600N^5}+\frac{7787774926751531}{824149155600N^6}-\frac{1181014629051224017}{77882095204200N^7}\\
&+\Bigg(\frac{2317251527}{3433954815N}-\frac{19487025602}{3433954815N^2}+\frac{29435287829}{2289303210N^3}-\frac{546390092023}{6867909630N^4}\\
&+\frac{1751952232097}{4578606420N^5}-\frac{20751649513859}{13735819260N^6}+\frac{514700153390909}{96150734820N^7}\Bigg)\ln(N)+\Bigg(\frac{1}{N}-\frac{1}{N^2}\\
&-\frac{7}{N^4}+\frac{15}{N^5}+\frac{3}{N^3}-\frac{31}{N^6}+\frac{63}{N^7}\Bigg)\ln^2(N),\\
&\left[\frac{1}{N^4}+\frac{11886}{325N^5}+\frac{111473}{65N^6}+\frac{27764898}{325N^7}\right]\left(\frac{9}{8}\right)^N\Bigg\}+O\left(\left(\frac{9}{8}\right)^N\frac{1}{N^8}\right),
\end{aligned}
\tag{4.3}
$$

$$
\begin{aligned}
&\left\{\Delta T_k^{C_F T_F^2\zeta_3}\Big|_{k=1}^{10}\right\}=\\
&\quad\Bigg\{\left(-\frac{9}{8}\right)^N\left[\frac{1}{N^4}+\frac{183}{4N^5}+\frac{2123}{2N^6}+\frac{369303}{4N^7}\right],\\
&\quad\left[\frac{1}{N}-\frac{6167375}{2538N^4}+\frac{251053021}{2538N^5}-\frac{6845892761}{2538N^6}+\frac{269421699821}{4374N^7}\right](-1)^N,\\
&\quad\left[\frac{1}{N^2}-\frac{1377791}{2538N^4}+\frac{49777453}{2538N^5}-\frac{1270724105}{2538N^6}+\frac{47946548525}{4374N^7}\right](-1)^N,\\
&\quad\left[\frac{1}{N^3}-\frac{205031}{5076N^4}+\frac{5548237}{5076N^5}-\frac{125746313}{5076N^6}+\frac{4443239285}{8748N^7}\right](-1)^N,
\end{aligned}
$$

$$
\Bigg[\frac{44549521}{60912N^4}-\frac{9803624797}{304560N^5}+\frac{281386223183}{304560N^6}-\frac{80403763171913}{3674160N^7}
+\left(\frac{1}{N}-\frac{14}{N^2}+\frac{194}{N^3}-\frac{2666}{N^4}+\frac{36386}{N^5}-\frac{493754}{N^6}+\frac{6667634}{N^7}\right)\ln(N)\Bigg](-1)^N,
$$

$$
\Bigg[\frac{176076128920087}{32075655120N^5}-\frac{2170077025499773}{8018913780N^6}+\frac{1538555009752949330 63}{18186896453040N^7}
$$

$$
+\Bigg(-\frac{96551923}{44549521N}+\frac{2198167821}{44549521N^2}-\frac{205984981993}{267297126N^3}+\frac{1479535025071}{133648563N^4}
-\frac{409866696159859}{2672971260N^5}+\frac{926453767962681}{445495210N^6}-\frac{390121843311426469}{14033099115N^7}\Bigg)\ln(N)
$$

$$
+\left(\frac{1}{N}-\frac{14}{N^2}+\frac{194}{N^3}-\frac{2666}{N^4}+\frac{36386}{N^5}-\frac{493754}{N^6}+\frac{6667634}{N^7}\right)\ln^2(N)\Bigg](-1)^N,
$$

$$
\left[\frac{263556904}{8019N^7}-\frac{5053141}{891N^6}+\frac{47194}{99N^5}-\frac{2765}{99N^4}+\frac{1}{N^3}\right]\left(-\frac{1}{8}\right)^N,
$$

$$
\left[-\frac{299001079}{729N^7}+\frac{1211485}{81N^6}-\frac{2521}{9N^5}-\frac{97}{9N^4}+\frac{1}{N^3}\right]\left(\frac{1}{8}\right)^N,
$$

$$
\frac{1}{N}-\frac{403557}{1346N^3}+\frac{1066131187}{109026N^4}-\frac{25497634607}{109026N^5}+\frac{1600616428213}{327078N^6}
-\frac{838217215706339}{8831106N^7},
$$

$$
\frac{1}{N^2}-\frac{664689}{18844N^3}+\frac{1356819775}{1526364N^4}-\frac{29465309123}{1526364N^5}+\frac{1762154712985}{4579092N^6}
-\frac{897121773060599}{123635484N^7}\Bigg\}+O\left(\left(\frac{9}{8}\right)^N\frac{1}{N^8}\right). \tag{4.4}
$$

More efforts are needed to compute the respective systems for the larger recurrences. In a final numerical step one has to combine these solutions. This combination is not unique, as the result is necessarily approximate. Details on this will be given in a later publication. Here the problem is also that a series of particular solutions strongly diverges as $N \rightarrow \infty$. These contributions cancel against contributions in other color–ζ factors as outlined above.

Let us now turn back to the first–order factorizable contributions and consider the Feynman diagrams which are solely determined by these. Still one may use the techniques available for first–order factorizable problems for individual Feynman diagrams contributing to the sets of color–ζ factors not yet being covered by the results in Section 3. The final strategy is then to transform these results to x–space where also the non–first–order factorizable contributions will be solved, cf. [52]. Working on a diagram–by–diagram basis we have obtained the N–space solutions for the first–order factorizable cases, which we will discuss now.

The results are given in terms of generalized harmonic sums [53, 161, 162], cyclotomic sums [100], and finite (inverse) binomial sums [54] in form of polynomials over $\mathbb{Q}(N)$ in Mellin N–space, beyond the harmonic sums. The cyclotomic sums can be shown to be reducible to harmonic sums in all contributing Feynman diagrams. The generalized harmonic sums are defined by

$$S_{b,\vec{a}}(\{c,\vec{d}\},N) = \sum_{k=1}^{N} \frac{c^k}{k^b} S_{\vec{a}}(\{\vec{d}\},k), \quad b, a_i \in \mathbb{N}\backslash\{0\}, \quad c, d_i \in \mathbb{Z}\backslash\{0\}. \tag{4.5}$$

All these quantities obey first–order shift relations in a hierarchy of terms, such as

$$S_{b,\vec{a}}(\{c,\vec{d}\},N+1) - S_{b,\vec{a}}(\{c,\vec{d}\},N) = \frac{c^N}{N^b} S_{\vec{a}}(\{\vec{d}\},N) \tag{4.6}$$

for the harmonic and generalized harmonic sums and synonymous relations for nested (inverse) binomial sums. Their recurrences are of the type

$$\mathsf{BS}_1(N) = \sum_{k=1}^{N} f(k), \tag{4.7}$$

$$\mathsf{BS}_2(N) = \sum_{k=1}^{N} g(k) \mathsf{BS}_3(k), \tag{4.8}$$

and one obtains

$$\mathsf{BS}_1(N) - \mathsf{BS}_1(N-1) = f(N), \tag{4.9}$$

$$\mathsf{BS}_2(N) - \mathsf{BS}_2(N-1) = g(N) \mathsf{BS}_3(N). \tag{4.10}$$

Using Eqs. (4.6, 4.9, 4.10) the respective outermost sum is removed. What remains is to provide these sums in the asymptotic region $N \in \mathbb{C}, \quad |N| \to \infty$.

The following sums contribute to the first–order factorizable contributions. In the linear representation these are 72 harmonic sums up to weight $\mathsf{w} = 5$, while the following 33 harmonic sums remain after algebraic reduction [102],

$$\Big\{ S_{-1}, S_1, S_{-2}, S_2, S_{-3}, S_3, S_{-4}, S_4, S_{-5}, S_5, S_{-2,-1}, S_{-2,1}, S_{2,-1}, S_{2,1}, S_{-2,2}, S_{-2,-3}, S_{-2,3}, S_{2,-3},$$
$$S_{2,3}, S_{-3,1}, S_{3,1}, S_{-4,1}, S_{4,1}, S_{2,1,1}, S_{-2,1,-2}, S_{-2,1,1}, S_{-2,2,1}, S_{2,1,-2}, S_{2,2,1}, S_{-3,1,1}, S_{3,1,1}, S_{-2,1,1,1},$$
$$S_{2,1,1,1} \Big\}. \tag{4.11}$$

Their asymptotic representations have been given in Ref. [57].

Furthermore, the following 45 generalized harmonic sums

$$\Big\{ S_1(\{-2\}), S_1\left(\left\{\frac{1}{2}\right\}\right), S_1(\{2\}), S_2(\{-2\}), S_2\left(\left\{\frac{1}{2}\right\}\right), S_3(\{2\}), S_4(\{2\}), S_{1,1}\left(\left\{\frac{1}{2}, 2\right\}\right),$$
$$S_{1,1}\left(\left\{1, \frac{1}{2}\right\}\right), S_{1,1}\left(\{1, 2\}\right), S_{1,2}\left(\left\{\frac{1}{2}, -1\right\}\right), S_{1,2}\left(\left\{\frac{1}{2}, 1\right\}\right), S_{1,2}(\{2, 1\}), S_{1,3}\left(\left\{\frac{1}{2}, 2\right\}\right),$$
$$S_{1,3}(\{2, 1\}), S_{1,4}\left(\left\{\frac{1}{2}, 2\right\}\right), S_{2,1}(\{2, 1\}), S_{2,3}\left(\left\{\frac{1}{2}, 2\right\}\right), S_{1,1,1}\left(\left\{\frac{1}{2}, 1, 1\right\}\right), S_{1,1,1}(\{2, 1, 1\}),$$
$$S_{1,1,2}\left(\left\{-2, \frac{1}{2}, -1\right\}\right), S_{1,1,2}\left(\left\{-2, \frac{1}{2}, 1\right\}\right), S_{1,1,2}\left(\left\{\frac{1}{2}, 2, 1\right\}\right), S_{1,1,2}\left(\left\{2, \frac{1}{2}, -1\right\}\right),$$

$$S_{1,1,2}\left(\left\{2,\frac{1}{2},1\right\}\right), S_{1,1,3}\left(\left\{\frac{1}{2},2,1\right\}\right), S_{1,1,3}\left(\left\{1,\frac{1}{2},2\right\}\right), S_{1,2,1}\left(\left\{\frac{1}{2},2,1\right\}\right),$$
$$S_{2,1,1}(\{2,1,1\}), S_{2,1,2}\left(\left\{-2,\frac{1}{2},-1\right\}\right), S_{2,1,2}\left(\left\{-2,\frac{1}{2},1\right\}\right), S_{2,1,2}\left(\left\{\frac{1}{2},2,1\right\}\right),$$
$$S_{2,2,1}\left(\left\{\frac{1}{2},2,1\right\}\right), S_{1,1,1,1}\left(\left\{\frac{1}{2},2,1,1\right\}\right), S_{1,1,1,1}\left(\left\{2,\frac{1}{2},1,1\right\}\right), S_{1,1,1,1}(\{2,1,1,1\}),$$
$$S_{1,1,1,2}\left(\left\{1,\frac{1}{2},2,1\right\}\right), S_{1,1,1,2}\left(\left\{1,2,\frac{1}{2},-1\right\}\right), S_{1,1,1,2}\left(\left\{1,2,\frac{1}{2},1\right\}\right),$$
$$S_{1,1,2,1}\left(\left\{1,\frac{1}{2},2,1\right\}\right), S_{1,2,1,1}\left(\left\{\frac{1}{2},2,1,1\right\}\right), S_{2,1,1,1}\left(\left\{\frac{1}{2},2,1,1\right\}\right),$$
$$S_{1,1,1,1,1}\left(\left\{\frac{1}{2},2,1,1,1\right\}\right), S_{1,1,1,1,1}\left(\left\{1,\frac{1}{2},2,1,1\right\}\right), S_{1,1,1,1,1}\left(\left\{1,2,\frac{1}{2},1,1\right\}\right)\Bigg\} \quad (4.12)$$

contribute.

The asymptotic expansion of these sums can be performed by using the `HarmonicSums` commands `SExpansion` and `BSExpansion`, respectively. In course of this the following additional 17 sums emerge, which have to be dealt with in the same way

$$\Bigg\{S_2(\{2\}), S_{1,1}(\{2,1\}), S_{1,1,3}\left(\left\{\frac{1}{2},1,2\right\}\right), S_{1,2,2}\left(\left\{\frac{1}{2},2,1\right\}\right), S_{1,3,1}\left(\left\{\frac{1}{2},2,1\right\}\right),$$
$$S_{1,1,1,2}\left(\left\{\frac{1}{2},2,1,1\right\}\right), S_{1,1,1,2}\left(\left\{2,1,1,\frac{1}{2}\right\}\right), S_{1,1,2,1}\left(\left\{\frac{1}{2},2,1,1\right\}\right),$$
$$S_{1,1,1,1,1}\left(\left\{\frac{1}{2},1,2,1,1\right\}\right), S_{2,2}(\{2,1\}), S_{1,3}(\{1,2\}), S_{1,1,2}(\{1,2,1\}), S_{1,1,1,1}(\{2,1,1,1\}),$$
$$S_{2,1}(\{2,1\}), S_{1,1,1,2}\left(\left\{1,\frac{1}{2},2,1\right\}\right), S_{1,1,1,2}\left(\left\{\frac{1}{2},1,2,1\right\}\right), S_{1,1,1,2}\left(\left\{1,\frac{1}{2},2,1\right\}\right)\Bigg\}. \quad (4.13)$$

In some cases a certain generalized harmonic sum has to be re–shuffled before by using `SRemoveLeadingIndex`, `SRemoveTrailingIndex`, or by using more general shuffling relations. The set of constants, which are multiple zeta values in the case of harmonic sums [112], is now extended to those of generalized harmonic sums at infinity with the additional numerator weights

$$\left\{-\frac{1}{2},-2,\frac{1}{2},2\right\}. \quad (4.14)$$

One may map these constants to G–functions at argument $x = 1$ or the associated generalized harmonic polylogarithmic constants [53]. Here one applies first the command `GLRemovePole[fct,a]` with $a \in [0,1]$ the pole positions, to obtain the Cauchy principal value of the respective integrals. Examples for constants even reducing to multiple zeta values [112] are

$$\mathrm{H}_{0,0,0,1/2}(1) = -\mathrm{Li}_4\left(\frac{1}{2}\right) - \frac{1}{24}\ln^4(2) + \ln^2(2)\zeta_2 + \frac{4}{5}\zeta_2^2, \quad (4.15)$$
$$\mathrm{H}_{1/2,0,1,1,1}(1) = \mathrm{Li}_5\left(\frac{1}{2}\right) - \frac{1}{120}\ln^5(2) + \frac{1}{3}\ln^3(2)\zeta_2 + \frac{4}{5}\ln(2)\zeta_2^2 + \frac{21}{16}\zeta_2\zeta_3 - \frac{155}{32}\zeta_5. \quad (4.16)$$

The generalized harmonic polylogarithms are defined by

$$\mathrm{H}_{a,\vec{b}}(x) = \int_0^x dy f_a(y)\mathrm{H}_{\vec{b}}(y), \quad \text{with} \quad f_a(y) = \frac{1}{y-a}. \tag{4.17}$$

One example of an asymptotic expansion of a contributing generalized harmonic sum occurring in the calculation of $a_{Qg}^{(3)}$ is given by

$$\begin{aligned}
T_1 &= -\frac{32C_A T_F(C_A-2C_F)(N-4)}{N(1+N)(2+N)} S_{2,1,1,1}\left(\left\{\frac{1}{2},2,1,1\right\},N\right) \\
&= C_A T_F(C_A-2C_F)\Biggl\{\mathrm{Li}_5\left(\frac{1}{2}\right)\left[\frac{64}{N^2}-\frac{448}{N^3}+\frac{1216}{N^4}-\frac{2752}{N^5}+\frac{5824}{N^6}-\frac{11968}{N^7}\right] \\
&\quad +\frac{8}{N^4}-\frac{1832}{27N^5}+\frac{6632}{27N^6}-\frac{2135236}{3375N^7}+\ln^5(2)\biggl[-\frac{8}{15N^2}+\frac{56}{15N^3}-\frac{152}{15N^4}+\frac{344}{15N^5} \\
&\quad -\frac{728}{15N^6}+\frac{1496}{15N^7}\biggr]+\ln^3(2)\left[\frac{88}{3N^2}-\frac{616}{3N^3}+\frac{1672}{3N^4}-\frac{3784}{3N^5}+\frac{8008}{3N^6}-\frac{16456}{3N^7}\right]\zeta_2 \\
&\quad +\left[\frac{16}{N^4}-\frac{352}{3N^5}+\frac{1072}{3N^6}-\frac{12832}{15N^7}+\left[-\frac{14}{N^2}+\frac{98}{N^3}-\frac{266}{N^4}+\frac{602}{N^5}-\frac{1274}{N^6}+\frac{2618}{N^7}\right]\zeta_3\right]\zeta_2 \\
&\quad +\ln(2)\left[\frac{196}{5N^2}-\frac{1372}{5N^3}+\frac{3724}{5N^4}-\frac{8428}{5N^5}+\frac{17836}{5N^6}-\frac{36652}{5N^7}\right]\zeta_2^2+\ln^2(2)\biggl[-\frac{14}{N^2}+\frac{98}{N^3} \\
&\quad -\frac{266}{N^4}+\frac{602}{N^5}-\frac{1274}{N^6}+\frac{2618}{N^7}\biggr]\zeta_3+\biggl[-\frac{279}{2N^2}+\frac{1953}{2N^3}-\frac{5301}{2N^4}+\frac{11997}{2N^5}-\frac{25389}{2N^6} \\
&\quad +\frac{52173}{2N^7}\biggr]\zeta_5+\left[\frac{16}{N^4}-\frac{1040}{9N^5}+\frac{2648}{9N^6}-\frac{142112}{225N^7}\right]L+\biggl[\frac{16}{N^4}-\frac{352}{3N^5}+\frac{1072}{3N^6} \\
&\quad -\frac{12832}{15N^7}\biggr]L^2\Biggr\}+O\left(\frac{1}{N^8}\right).
\end{aligned} \tag{4.18}$$

with

$$L = \ln(N) + \gamma_E, \tag{4.19}$$

and γ_E the Euler–Mascheroni constant. The asymptotic expansions of the contributing generalized harmonic sums are discussed in Appendix A and are given in an ancillary file in computer–readable form. Here also generalized harmonic polylogarithms beyond multiple zeta values contribute.

Now we turn to the remaining sums, which are nested binomial or inverse binomial sums. We derive linear representations and eliminate algebraic relations between the binomial sums. Moreover, they are reduced to a standard form removing summation index shifts. By these operations also sums of lower kind are generated. The following 58 sums contribute

$$\Biggl\{\sum_{\tau_1=1}^N \frac{(\tau_1!)^2}{(2\tau_1)!}, \sum_{\tau_1=1}^N \frac{(2\tau_1)!}{(\tau_1!)^2}, \sum_{\tau_1=1}^N \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)!}{(\tau_2!)^2}}{(2\tau_1)!}, \sum_{\tau_1=1}^N \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2}(2\tau_2)!}{(\tau_2!)^2\tau_2^3}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3}}{(\tau_2!)^2 \tau_2^2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)!}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)!}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3}}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3}}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{\sum_{\tau_4=1}^{\tau_3} \frac{1}{\tau_4}}{\tau_3}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-2)^{\tau_2} (2\tau_2)! \tau_2^2}{(\tau_2!)^2}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! \tau_2^2}{(\tau_2!)^2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! \left(\sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3^2}\right) \tau_2^2}{(\tau_2!)^2}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! S_{-2}(\tau_3) \tau_2^2}{(\tau_2!)^2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-2)^{\tau_2} (2\tau_2)! \left(\sum_{\tau_3=1}^{\tau_2} \frac{2^{-\tau_3} S_2(\tau_3)}{\tau_3}\right) \tau_2^2}{(\tau_2!)^2}}{(2\tau_1)!},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-2)^{\tau_2} (2\tau_2)! \left(\sum_{\tau_3=1}^{\tau_2} \frac{2^{-\tau_3} \sum_{\tau_4=1}^{\tau_3} \frac{(-1)^{\tau_4}}{\tau_4^2}}{\tau_3}\right) \tau_2^2}{(\tau_2!)^2}}{(2\tau_1)!}, \sum_{\tau_1=1}^{N} \frac{(-1)^{\tau_1} (2\tau_1)!}{(\tau_1!)^2 \tau_1^4}, \sum_{\tau_1=1}^{N} \frac{(-1)^{\tau_1} (2\tau_1)!}{(\tau_1!)^2 \tau_1^3},$$

$$\sum_{\tau_1=1}^{N} \frac{(2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{1}{\tau_2}}{(\tau_1!)^2 \tau_1^3}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2}{(2\tau_1)! \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)!}{(\tau_2!)^2}}{(2\tau_1)! \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)!}{(\tau_2!)^2 \tau_2^3}}{(2\tau_1)! \tau_1^2},$$

$$\sum_{\tau_1=1}^{N} \frac{(2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2}}{\tau_2^2}}{(\tau_1!)^2 \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(-1)^{\tau_1} (2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2}}{\tau_2^2}}{(\tau_1!)^2 \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3}}{(\tau_2!)^2 \tau_2^2}}{(2\tau_1)! \tau_1^2},$$

$$\sum_{\tau_1=1}^{N} \frac{(2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{1}{\tau_2}}{(\tau_1!)^2 \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)!}{(\tau_2!)^2 \tau_2}}{(2\tau_1)! \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)!}{(\tau_2!)^2 \tau_2}}{(2\tau_1)! \tau_1^2},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)! \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)! \tau_1^2},$$

$$\sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3}}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)! \tau_1^2}, \sum_{\tau_1=1}^{N} \frac{(\tau_1!)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2} (2\tau_2)! \sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3}}{\tau_3^2}}{(\tau_2!)^2 \tau_2}}{(2\tau_1)! \tau_1^2},$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{\big(2\tau_2\big)!\sum_{\tau_3=1}^{\tau_2}\frac{\sum_{\tau_4=1}^{\tau_3}\frac{1}{\tau_4}}{\tau_3}}{\big(\tau_2!\big)^2\tau_2}}{\big(2\tau_1\big)!\tau_1^2},\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{(-2)^{\tau_2}\big(2\tau_2\big)!\tau_2^2}{\big(\tau_2!\big)^2}}{\big(2\tau_1\big)!\tau_1^2},
$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}\big(2\tau_2\big)!\tau_2^2}{\big(\tau_2!\big)^2}}{\big(2\tau_1\big)!\tau_1^2},\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}\big(2\tau_2\big)!S_2(\tau_2)\tau_2^2}{\big(\tau_2!\big)^2}}{\big(2\tau_1\big)!\tau_1^2},
$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}\big(2\tau_2\big)!S_{-2}(\tau_2)\tau_2^2}{\big(\tau_2!\big)^2}}{\big(2\tau_1\big)!\tau_1^2},\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{(-2)^{\tau_2}\big(2\tau_2\big)!\Big(\sum_{\tau_3=1}^{\tau_2}\frac{2^{-\tau_3}\sum_{\tau_4=1}^{\tau_3}\frac{1}{\tau_4^2}}{\tau_3}\Big)\tau_2^2}{\big(\tau_2!\big)^2}}{\big(2\tau_1\big)!\tau_1^2},
$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(\tau_1!\big)^2\sum_{\tau_2=1}^{\tau_1}\frac{(-2)^{\tau_2}\big(2\tau_2\big)!\Big(\sum_{\tau_3=1}^{\tau_2}\frac{2^{-\tau_3}\sum_{\tau_4=1}^{\tau_3}\frac{(-1)^{\tau_4}}{\tau_4^2}}{\tau_3}\Big)\tau_2^2}{\big(\tau_2!\big)^2}}{\big(2\tau_1\big)!\tau_1^2},\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{(-1)^{\tau_1}\big(2\tau_1\big)!}{\big(\tau_1!\big)^2\tau_1},
$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{1}{\tau_2^3}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}}{\tau_2^3}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{1}{\tau_2^2}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{(-1)^{\tau_1}\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{1}{\tau_2^2}}{\big(\tau_1!\big)^2\tau_1},
$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}}{\tau_2^2}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{(-1)^{\tau_1}\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}}{\tau_2^2}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3}}{\tau_2^2}}{\big(\tau_1!\big)^2\tau_1},
$$

$$
\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{\sum_{\tau_3=1}^{\tau_2}\frac{(-1)^{\tau_3}}{\tau_3^2}}{\tau_2}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{\big(2\tau_1\big)!\sum_{\tau_2=1}^{\tau_1}\frac{\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3}}{\tau_2}}{\big(\tau_1!\big)^2\tau_1},\sum_{\tau_1=1}^{N}\frac{(-2)^{\tau_1}\big(2\tau_1\big)!\tau_1^2}{\big(\tau_1!\big)^2},
$$

$$
\sum_{\tau_1=1}^{N}\frac{(-1)^{\tau_1}\big(2\tau_1\big)!\tau_1^2}{\big(\tau_1!\big)^2},\sum_{\tau_1=1}^{N}\frac{(-1)^{\tau_1}\big(2\tau_1\big)!\Big(\sum_{\tau_2=1}^{\tau_1}\frac{1}{\tau_2^2}\Big)\tau_1^2}{\big(\tau_1!\big)^2},\sum_{\tau_1=1}^{N}\frac{(-1)^{\tau_1}\big(2\tau_1\big)!\Big(\sum_{\tau_2=1}^{\tau_1}\frac{(-1)^{\tau_2}}{\tau_2^2}\Big)\tau_1^2}{\big(\tau_1!\big)^2},
$$

$$
\sum_{\tau_1=1}^{N}\frac{(-2)^{\tau_1}\big(2\tau_1\big)!\Big(\sum_{\tau_2=1}^{\tau_1}\frac{2^{-\tau_2}\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3^2}}{\tau_2}\Big)\tau_1^2}{\big(\tau_1!\big)^2},\sum_{\tau_1=1}^{N}\frac{(-2)^{\tau_1}\big(2\tau_1\big)!\Big(\sum_{\tau_2=1}^{\tau_1}\frac{2^{-\tau_2}\sum_{\tau_3=1}^{\tau_2}\frac{(-1)^{\tau_3}}{\tau_3^2}}{\tau_2}\Big)\tau_1^2}{\big(\tau_1!\big)^2}\Bigg\}. \tag{4.20}
$$

The nested binomial sums do not obviously have such a systematic representation like the case for harmonic, generalized harmonic and cyclotomic sums. This is implied by the different building blocks entering the different summands, which are central binomials in the numerators and denominators, lower sums of different kind, rational expressions and powers of $m^k, m \in \mathbb{N}, k \in \mathbb{Z}$. Yet one may find a basis set by summation technologies of `Sigma` [73, 74] using the underlying difference ring theory [69,70] and additional term synchronization with algorithms in `HarmonicSums`.

A more synchronized picture emerges in t–space, as is outlined in Section 5. The corresponding generating functions will then have a representation in terms of letters smoothing out the more involved structures in the sum representations.

One may compute the asymptotic expansion of most of these binomial sums using the command `BSExpansion`, which relies on the inverse Mellin transform of the respective binomial sum. This may not be easily derived because regularizations beyond the one given by the +-operation are necessary. In these cases one needs to reformulate the corresponding expressions by individual partial integrations first. By considering the Mellin inversion for the nested binomial sums only, one needs to account for Mellin convolutions with the corresponding pre–factors, cf. [54]. In Appendix B we will list a series of expansions of nested binomial sums in the asymptotic region. More expansions are given in an ancillary file.

Finally, we are going to use a different strategy to deal with the nested binomial sum contributions to the unpolarized and polarized amplitudes in Section 5. In the end our goal is to obtain first the x–space representation for all first–order factorizable contributions.[10] At the end of the calculation analytic structures are obtained in x–space which can be finally Mellin–transformed and allow for representations in Mellin N–space evolution programs [163], see Appendix D.

5 From t-space to x-space

To obtain an even more uniform approach to the present problem, in particular for the nested binomial sum contributions, we went back to the amplitude representation in t–space, the resummation of the N–space representation into a generating function, cf. Eq. (2.1), in the unpolarized and polarized case. We solved the first–order factorizable contributions in terms of G–functions in the region around $t = 0$. The t–representation in the unpolarized case is even in t and in the polarized case odd in t, [164, 165]. I.e. it is sufficient to consider one of the regions

$$(-\infty, 0] \qquad \text{or} \qquad [0, \infty). \tag{5.1}$$

The following alphabet of 17 letters spans the contributing master integrals to the required order in the dimensional parameter ε in the basis originally obtained by the integration–by–parts reduction [94, 95]

$$\begin{aligned} \mathfrak{A} \;=\; & \Biggl\{\frac{1}{t}, \frac{1}{1-t}, \frac{1}{1+t}, \frac{1}{2-t}, \frac{1}{2+t}, \frac{1}{4-t}, \frac{1}{4+t}, \frac{1}{1-2t}, \frac{1}{1+2t}, \sqrt{t(4-t)}, \sqrt{t(4+t)}, \\ & \frac{\sqrt{t(4-t)}}{1-t}, \frac{\sqrt{t(4+t)}}{1+t}, \frac{\sqrt{t(4-t)}}{1+t}, \frac{\sqrt{t(4+t)}}{1-t}, \frac{\sqrt{t(4-t)}}{1+2t}, \frac{\sqrt{t(4+t)}}{1-2t}\Biggr\}. \end{aligned} \tag{5.2}$$

The alphabet exhibits the symmetry

$$t \leftrightarrow -t, \tag{5.3}$$

which is essential for the occurrence of either only even or only odd moments. With the exception of $1/t$, there are therefore only eight essential letters. The t–space representation is still very close to the N–space representation, since the latter is obtained by performing a formal Taylor expansion of the former one. In this way now also the finite nested (inverse) binomial sums received a more systematic representation. As can be seen in the alphabet $\mathfrak{A}$, Eq. (5.2), there are letters for harmonic polylogarithms, Kummer–Poincaré integrals and root–valued letters, as well as products of those with the former ones. Furthermore, the corresponding G–functions in t contain respective combinations of subsets of all these letters.

We will consider the region $t \in [0, \infty)$, containing the following (pseudo)thresholds

$$t_0 \in \left\{\frac{1}{2}, 1, 2, 4\right\}. \tag{5.4}$$

[10] Let us note that also in the two–mass case the unpolarized and polarized pure singlet OMEs could not be computed in terms of first–order factorizable structures in N–space, but it has been possible in x–space, cf. Refs. [41, 43].

The differential equations have to be solved in the regions $t \in [0, 1/2], [1/2, 1], [1, 2], [2, 4]$, and $[4, \infty)$, corresponding in x to the potential ranges for $x \in [2, \infty), [1, 2], [1/2, 1], [1/4, 1/2], [0, 1/4]$. Finally, it will turn out that $x \in [0, 1]$, because the amplitude will exhibit an imaginary part after the transformation

$$t \to \frac{1}{x} \tag{5.5}$$

in the physical region only.

We begin by solving the amplitude in the region $t \in [0, 1/2]$. Here 10, 20, 44, and up to 1046 G–functions contribute for the terms $O(1/\varepsilon^k), \quad k = -3, ..., 0$, referring to the G–basis representation after algebraic reduction. On the other hand, there are only 730 contributing G–functions at $O(\varepsilon^0)$ in the original unpolarized and polarized amplitudes, where products of iterated integrals are expanded into their linear representations. This is typical for large alphabets, cf. also Ref. [124]. Therefore we did not perform the algebraic reduction in the present case.

The formal Taylor series expansion in t reproduces the moments computed by `MATAD` [84,166] for $N = 2, 4, 6, 8, 10$ in the unpolarized case and for $N = 3, 5, 7, 9$ in the polarized case.[11] The solution in terms of G–functions shows that after the transformation (5.5) the amplitude both in the unpolarized and the polarized case has no imaginary parts and, furthermore, no singularity at $t = 1/2$. The solution of the differential equations in the present case and for the subsequent regions are obtained as follows. As we have the solutions in terms of G–functions, we can establish a hirachical system of coupled differential equations by differentiating with respect to t. To base the iterated integrals at a new point t_0, we can now transform the system to a new variable $t' = t_0 + t$ and integrate the differential equation again. The boundary values at the point $t' = 0$ can be obtained by evaluating the previous representation at $t = t_0$. If the leftmost letter is singular at $t = t_0$ we can shuffle this letter to the right and obtain logarithmic singularities at $t = t_0$ which have to match the ones generated by the expansion around $t' = 0$ of the new representation. The hierarchical structure of the system allows to proceed from iterated integrals of weight 1 up to the ones with weight 6. One then inserts the G–functions into the amplitudes and checks whether an imaginary part remains. For t = 1/2 this is not the case and the real part turns out to be non–singular. This implies that there are no contributions to the amplitude for $x > 1$.

In the next step we use the representation at $t = 1/2$ and solve the corresponding differential equations in the region $t \in [1/2, 1]$ repeating the above steps, with initial values at $t = 1/2$ and correspondingly for the thresholds $t = 1, 2, 4$. One may test the result in x–space by computing Mellin moments and by comparing with the results above by `MATAD`.

The analytic continuation at $t = 2$ and at $t = 4$ does not generate additional imaginary parts, which we established by flagging the respective imaginary parts occurring at each new threshold for individual integrals and found that these contributions vanish in the amplitudes. This requires the precise calculation of the contributing constants. The analytic proof of the vanishing of the combination of the G–functions with different main arguments would be much more difficult. This means that the result in x–space is continuous in $x \in (0, 1]$.

The results in x–space are given by G–functions over the 14 letter alphabet $\mathfrak{A}_x$,

$$\begin{aligned} \mathfrak{A}_x \quad = \quad & \Biggl\{ \frac{1}{x}, \frac{1}{1-x}, \frac{1}{1+x}, \frac{1}{1-2x}, \frac{1}{2+x}, \frac{1}{2-x}, \frac{\sqrt{1-4x}}{x}, \frac{\sqrt{1-4x}}{1-x}, \frac{\sqrt{1-4x}}{1+x}, \frac{\sqrt{1-4x}}{2+x}, \\ & \frac{\sqrt{1+4x}}{x}, \frac{\sqrt{1+4x}}{1-x} \frac{\sqrt{1+4x}}{1+x}, \frac{\sqrt{1+4x}}{2-x} \Biggr\}. \end{aligned} \tag{5.6}$$

[11] We did not compute the moment for $N = 1$.

For the G–functions at argument x we perform algebraic reductions. This reduces 386 original G–functions in the unpolarized case to 322, and 360 G–functions in the polarized case to 315. The number of letters of the contributing G–constants is larger than the one in $\mathfrak{A}_x$. There are 697 constants in the unpolarized case and 659 in the polarized case given by root–valued G–functions at main argument $x = 1/4, 1/2, 3/4$ and 1. The algebraic reduction to a basis would enlarge the number of contributing constants.

Since in all cases only one type of square–root factor appears in the letters, the letters for all contributing G–functions can be rationalized. In a series of cases one has to remove poles in the integration domain at $x = 1/2$. The letter $1/(1-2x)$ emerges for `GL[{...},1/2]` only, i.e. at the integration boundary, which can be removed by `GLRemovePole`.[12]

In the unpolarized case, 155 G–constants at $x = 1/4$ emerge, 161 at $x = 1/2$, 112 at $x = 3/4$ and 269 at $x = 1$, while in the polarized case 155 G–constants at $x = 1/4$, 127 at $x = 1/2$, 112 at $x = 3/4$ and 265 at $x = 1$ contribute. The constants with main argument $x = 1/2$ are all generalized harmonic polylogarithms. These constants reduce to

$$\Biggl\{\ln(2)\zeta_2, \zeta_3, \mathrm{Li}_4\left(\frac{1}{2}\right), \zeta_5, \mathrm{Li}_5\left(\frac{1}{2}\right), \mathrm{H}_{0,0,-2,1}(1), \mathrm{H}_{0,0,1,-2}(1), \mathrm{H}_{0,1,0,-2}(1), \mathrm{H}_{0,3,1,-1}(1),$$
$$\mathrm{H}_{3,0,1,-1}(1), \mathrm{H}_{3,1,0,-1}(1), \mathrm{H}_{0,1,0,0,-2}(1), \mathrm{H}_{3,1,-1,0,-1}(1), \mathrm{H}_{3,1,-1,0,1}(1), \mathrm{H}_{3,1,1,0,-1}(1)\Biggr\}. \quad (5.7)$$

For the generalized harmonic polylogarithms which do not reduce to multiple zeta values or logarithms and polylogarithms of different argument, we present numerical values in an ancillary file.

For the G–constants of main argument $x = 1/4, 3/4$ one has first to rescale the letters such that the main argument is $x = 1$. An example is

$$T_2 = \mathrm{G}\left[\left\{\frac{1}{1-\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{1-\tau}\right\}, \frac{1}{4}\right] = \mathrm{G}\left[\left\{\frac{1}{4-\tau}, \frac{\sqrt{1-\tau}}{\tau}, \frac{\sqrt{1-\tau}}{4-\tau}\right\}, 1\right]. \quad (5.8)$$

Then the command `SpecialGLToH` rationalizes the G-function. Furthermore, denominators containing quadratic forms need to be decomposed by the command `LToGL[GLToL[GL[{....},c]]` which yields a proper input form for a numerical precision calculation. One obtains

$$\begin{aligned}
T_2 = {} & 6 + \sqrt{3}i \\
& \times \Biggl[\mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}\right\}, 1\right]\Biggl[-4 - \mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}, \frac{1}{-1+\tau}\right\}, 1\right] + \mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}, \frac{1}{1+\tau}\right\}, 1\right] \\
& + \mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}, \frac{1}{-1+\tau}\right\}, 1\right] - \mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}, \frac{1}{1+\tau}\right\}, 1\right]\Biggr] + \sqrt{3}i\mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}\right\}, 1\right]\Biggl[4 \\
& - \mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}, \frac{1}{-1+\tau}\right\}, 1\right] + \mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}, \frac{1}{1+\tau}\right\}, 1\right] + \mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}, \frac{1}{-1+\tau}\right\}, 1\right] \\
& - \mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}, \frac{1}{1+\tau}\right\}, 1\right]\Biggr] + 2i\sqrt{3}\Biggl\{\mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}, \frac{1}{-i\sqrt{3}+\tau}, \frac{1}{-1+\tau}\right\}, 1\right] \\
& - \mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}, \frac{1}{-i\sqrt{3}+\tau}, \frac{1}{1+\tau}\right\}, 1\right] - \mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}, \frac{1}{i\sqrt{3}+\tau}, \frac{1}{-1+\tau}\right\}, 1\right]
\end{aligned}$$

[12]Here `GL[...]` denotes the respective G–function in the notation of `HarmonicSums`.

$$+\mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau},\frac{1}{i\sqrt{3}+\tau},\frac{1}{1+\tau}\right\},1\right]\Bigg\}+\left(-8+4\ln(2)+12\mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}\right\},1\right]\right)$$
$$\times\mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau}\right\},1\right]+4(-2+\ln(2))\mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau}\right\},1\right]-4\mathrm{G}\left[\left\{\frac{1}{-i\sqrt{3}+\tau},\frac{1}{1+\tau}\right\},1\right]$$
$$-4\mathrm{G}\left[\left\{\frac{1}{i\sqrt{3}+\tau},\frac{1}{1+\tau}\right\},1\right], \tag{5.9}$$

with

$$\mathrm{G}\left[\left\{\frac{1}{\pm i\sqrt{3}+\tau}\right\},1\right]=\ln(2)-\frac{1}{2}\ln(3)\mp\frac{i}{6}\pi. \tag{5.10}$$

In this example no poles in $x \in [0,1]$ are present. The G–constants are given in terms of Kummer–Poincaré integrals. Their amount is more than an order of magnitude larger than the number of original constants. Kummer–Poincaré integrals can be evaluated by using methods of `Pari GP` [167] or by [168], using the method of Hölder convolution from Ref. [161].

Finally, we performed formal Taylor series expansions of the results in x around $x = 0, 1/2$ and 1 with 100 terms. The number of G–constants which emerge in the expansions around $x = 0$ and are not multiple zeta values [112] is 604, corresponding to 12719 terms after rationalization and decomposition into Kummer–Poincaré integrals. For $x = 1/2$, 502 constants contribute, and for $x = 1$ the number of constants is 213, see Appendix C. The set of the necessary constants in the polarized case are a subset of those in the unpolarized case. The representations of the expansions are given by

$$\mathbb{F}_0(x) = \sum_{k=-1}^{100}\sum_{l=0}^{5} a_{k,l}^{(0)} \ln^l(x) x^k, \tag{5.11}$$
$$\mathbb{F}_{1/2}(x) = \sum_{k=0}^{100} a_k^{(1/2)} \left(x-\frac{1}{2}\right)^k, \tag{5.12}$$
$$\mathbb{F}_1(x) = \sum_{k=0}^{100}\sum_{l=0}^{5} a_{k,l}^{(1)} \ln^l(1-x)(1-x)^k. \tag{5.13}$$

These representations can be matched at $x = 2/10$ and $x = 7/10$ and one may compute a series of lower Mellin moments numerically at high precision, and also compare with the direct numerical solution, see also Refs. [169–171]. The representations (5.11–5.13) can also be Mellin transformed to construct a N–space representation for $N \in \mathbb{C}$, see Appendix D. The method of iterated integrals in G–space shows the cancellation of diverging terms in the large N limit as $a^N, a > 1$. The largest number of constants contributes for the representation around $x = 0$, and those for the expansion around $x = 1$ are, apart from very few new constants, a subset of those around $x = 0$. The contributing constants are the same in the unpolarized and polarized cases.

6 The small and large x expansions

We can now perform the expansion of the results for the already solved parts of $a_{Qg}^{(3)}$ and $\Delta a_{Qg}^{(3)}$ and for the first–order factorizable contributions both for $x \to 0$ and $x \to 1$. The final result is not obtained directly, but will require a series of technical steps to be carried out because of the emergence of quite a series of Kummer–Poincaré integrals at special numbers, cf. Appendix C. In the polarized case, even terms that cannot contribute seem to be present. It will, however, turn out that the corresponding coefficients in front of the respective structures will arrange to zero, requiring to solve three–fold iterated integrals with letters in root–valued alphabets.

In the small x limit there is a prediction in the unpolarized case from Ref. [172], given by

$$a_{Qg}^{(3),x\to 0}(x) = \frac{64}{243} C_A^2 T_F \left[1312 + 135\zeta_2 - 189\zeta_3\right] \frac{\ln(x)}{x}. \tag{6.1}$$

This expression rescales with C_F/C_A in the pure singlet case, first calculated in Ref. [19]. The contribution $\propto \zeta_2$ has been computed in Eq. (3.1) and agrees with the corresponding term in Eq. (6.1).

In the polarized case the leading singularity is located at $N = 0$ and does not derive from the same dynamics as in the unpolarized case. Instead, one uses so–called infrared evolution equations or similar techniques [173, 174] in the massless case.[13] Whether in this case also color rescaling works is not clear a priori. From Eq. (3.44) we obtain the small x contribution

$$\frac{4}{3} C_F T_F^2 N_F \ln^5(x). \tag{6.2}$$

This term cannot be color rescaled by C_F/C_A to the pure singlet contribution, cf. Ref. [39], which after color rescaling would yield

$$\Delta a_{Qg}^{(3),x\to 0,\text{resc.}}(x) = \frac{2}{15} C_A T_F \left[8C_A + 9C_F\right] \ln^5(x). \tag{6.3}$$

but no term $\propto N_F$. This situation is similar to the case of $\Delta a_{qq,Q}^{(3)}$ and $\Delta a_{qq,Q}^{\text{PS},(3)}$, cf. [37], where the leading singularity at small x of $\Delta a_{qq,Q}^{\text{PS},(3)}$ is $\propto \ln^4(x)$, while one obtains $\Delta a_{qq,Q}^{(3)} \propto (8/3) C_F T_F^2 N_F \ln^5(x)$, due to which there is no color rescaling in this case either. The corresponding color factors in Eq. (6.3) can still receive contributions from the non–first–order factorizable contributions.

In deriving the small x limit of the irreducible contributions to the first order factorizable terms in the polarized case, also potential contributions of $O(\ln(x)/x)$ and $O(1/x)$ emerge. Their pre–factor has to be proven to vanish, which requires the calculation of special constants over root–valued alphabets. This is shown in Appendix C. While the vanishing of the coefficient in front of the $O(\ln(x)/x)$ term can be shown analytically, we decided to show the cancellation of the pre–factor of the $O(1/x)$ term numerically to a precision of ~ 1000 digits, which is equivalent to methods used in 'experimental mathematics', cf. e.g. [175]. There are terms $\propto \ln^5(x)$ in the irreducible first–order factorizing terms to color factors which also contribute to the non–first–order factorizing contributions. Since it has been known for longer that it is very difficult to determine the small x behavior of a single scale quantity from a limited set of moments, we will not intend this here, but solely rely on the analytic calculation in x–space for all contributions.

In the large x limit the first–order factorizable contributions of the irreducible diagrams have the structure indicated in Eq. (5.13).

In Mellin space the most singular term behaves like

$$\propto \frac{S_1^5(N)}{N} \tag{6.4}$$

[13] The corresponding massive calculation has not been performed.

and all other terms also vanish as $N \to \infty$. The corresponding decrease with N proceeds only slowly as is illustrated in Table 4. One obtains

$$a_{Qg}^{(3),x\to 1}(x) = \frac{8}{3}(C_A - C_F)^2 \ln^5(1-x) + O(\ln^4(1-x)) \quad (6.5)$$

and

$$\Delta a_{Qg}^{(3),x\to 1}(x) = a_{Qg}^{(3),x\to 1}(x) \quad (6.6)$$

in the leading order. This equality holds numerically for $x \gtrsim 0.95$ at the level of up to 2.5 %.

Both the above large and small x limits correspond to the first–order factorizable terms only and will receive additions from the diagrams which also receive contributions due to non–first–order factorizable master integrals in part, being dealt with in a forthcoming paper [52].

N	$S_1^5(N)/N$
10^1	21.556
10^2	37.561
10^3	23.502
10^4	8.982
10^5	2.583
10^6	0.618
10^7	0.130

Table 4: Numerical illustration of the decrease of the most singular part of the first–order factorizable contributions in the large x limit.

7 Numerical Results

In the following we illustrate numerically the analytic results obtained for the contributing irreducible Feynman diagrams which are first–order–factorizable. In Figures 1 and 2 the sum of these contributions to $a_{Qg}^{(3)}(x)$ are illustrated in the whole x region and in the region of larger values of x setting $N_F = 3$. Here we use the expansions around $x = 0, 1/2$ and 1, which are matched in their respective overlap regions. In Figures 3 and 4 we show the corresponding results for the contributions to $\Delta a_{Qg}^{(3)}(x)$. These partial results of the analytic calculation are shown as quantitative illustrations, but they cannot be used for phenomenological analyses yet.

Let us define

$$(\Delta)r(N) = \frac{\mathbf{M}[(\Delta)a_{Qg}^{(3)}(x)](N)}{(\Delta)\mathrm{MOM}(N)} - 1, \quad (7.1)$$

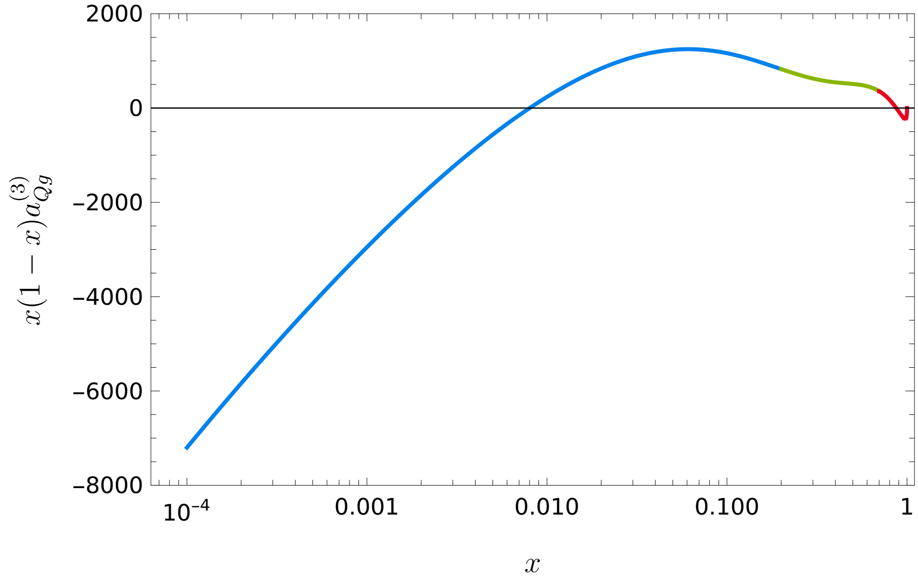

Figure 1: The contributions due to the first–order factorizable Feynman diagrams to $a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$. Full line (blue): expansion around $x = 0$; full line (green): expansion around $x = 1/2$; full line (red): expansion around $x = 1$.

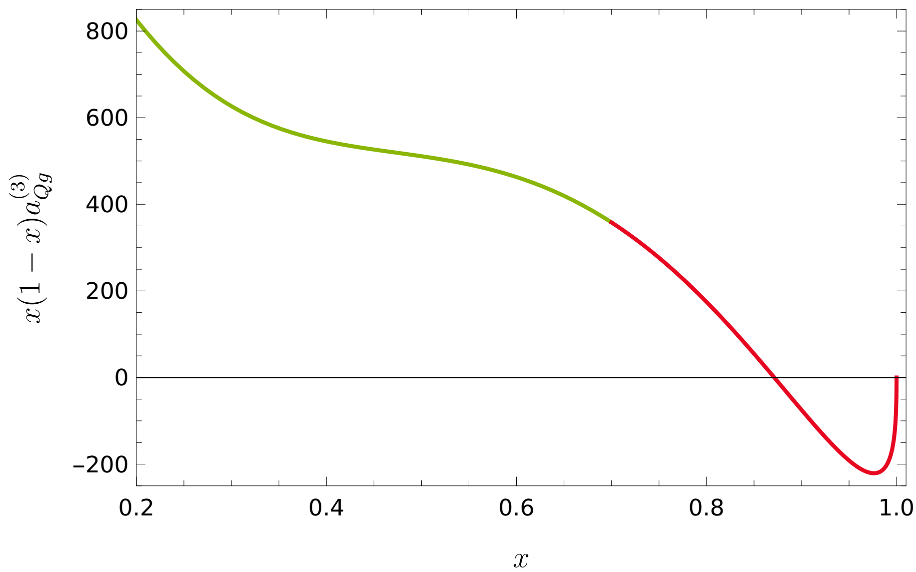

Figure 2: The contributions due to the first–order factorizable Feynman diagrams to $a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$ for larger values of x. Full line (green): expansion around $x = 1/2$; full line (red): expansion around $x = 1$.

with MOM denoting the moments calculated analytically in Mellin space. We have compared the moments based on the analytic results with the sum of the Mellin moments of the first–order–factorizable irreducible Feynman diagrams for $N = 2, \ldots, 20$ in the unpolarized case obtaining

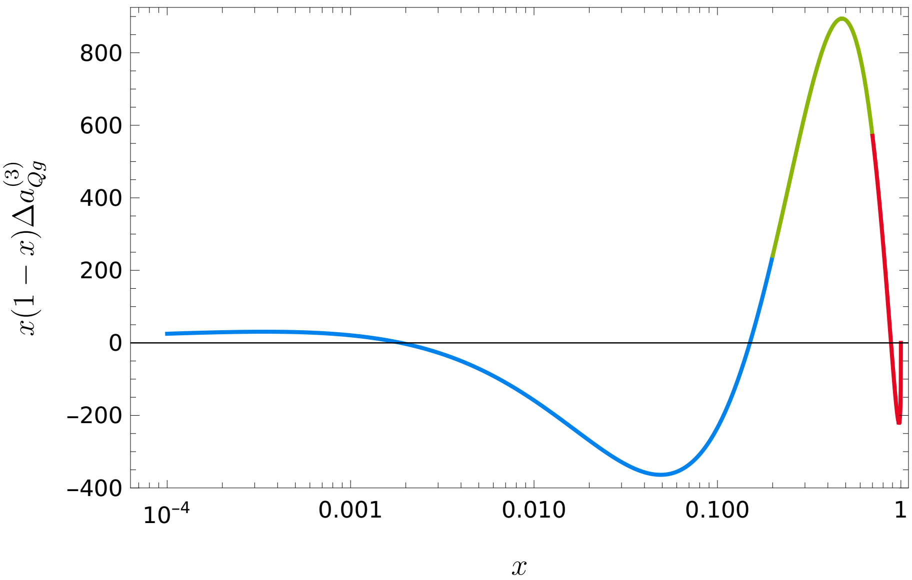

Figure 3: The contributions due to the first–order factorizable Feynman diagrams to $\Delta a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$. Full line (blue): expansion around $x = 0$; full line (green): expansion around $x = 1/2$; full line (red): expansion around $x = 1$.

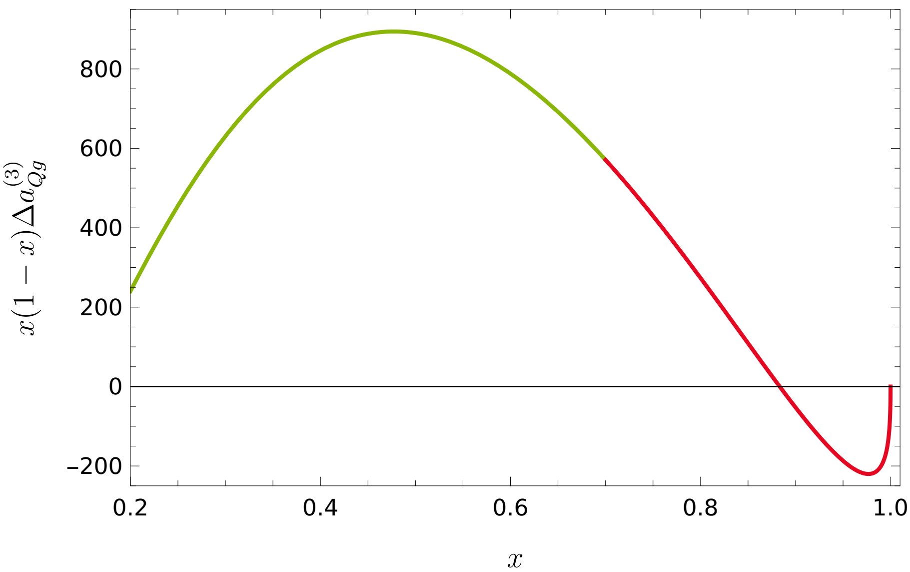

Figure 4: The contributions due to the first–order factorizable Feynman diagrams to $\Delta a_{Qg}^{(3)}(x)$ as a function of x rescaled by the factor $x(1-x)$ for larger values of x. Full line (green): expansion around $x = 1/2$; full line (red): expansion around $x = 1$.

$$
\begin{aligned}
r(N) \;=\; & \{-1.74353 \cdot 10^{-8}, 4.73887 \cdot 10^{-10}, -2.03360 \cdot 10^{-12}, -1.05471 \cdot 10^{-14}, \\
& -5.99520 \cdot 10^{-15}, -6.88338 \cdot 10^{-15}, -6.77236 \cdot 10^{-15}, -6.77236 \cdot 10^{-15}, \\
& -7.21645 \cdot 10^{-15}, -7.43849 \cdot 10^{-15}\}. \qquad (7.2)
\end{aligned}
$$

Similarly, in the polarized case we obtain for $N = 3, \dots, 21$

$$\begin{aligned}\Delta r(N) &= \{-5.44219 \cdot 10^{-9}, -2.52013 \cdot 10^{-11}, -1.39555 \cdot 10^{-13}, -6.99441 \cdot 10^{-15}, \\ &\quad -6.10623 \cdot 10^{-15}, -6.66134 \cdot 10^{-15}, -6.55032 \cdot 10^{-15}, -7.32747 \cdot 10^{-15}, \\ &\quad -7.43849 \cdot 10^{-15}, -7.32747 \cdot 10^{-15}\}. \end{aligned} \tag{7.3}$$

We have also solved the system of first order differential equations by calculating symbolic series expansions around different values of t and numerically matching these at points where two neighboring expansions converge, choosing $t = 0, 1/7, 1/4, 3/4, 4/3, 2, 4$ and ∞ More details regarding this method can be found in Refs. [170, 171]. For the solution of large linear systems of equations, which we encounter here, we make use of finite field techniques implemented in `FireFly` [176, 177]. A comparison to the analytic solution has been performed at the points

$$x \in \{10^{-4}, 10^{-3}, 10^{-2}, 2 \cdot 10^{-2}, 7 \cdot 10^{-2}, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 0.95, 0.99\} \tag{7.4}$$

for the quantity

$$(\Delta) r_{\text{num./an}} = \frac{(\Delta) a_{Qg}^{(3),\text{irr. numeric}}}{(\Delta) a_{Qg}^{(3),\text{irr. analytic}}} - 1. \tag{7.5}$$

One obtains

$$\begin{aligned} r_{\text{num./an}} &= \{7.75 \cdot 10^{-16}, 1.86 \cdot 10^{-15}, \; 1.96 \cdot 10^{-14}, 4.27 \cdot 10^{-15}, 2.57 \cdot 10^{-15}, \; 7.01 \cdot 10^{-15}, \\ &\quad 5.49 \cdot 10^{-10}, 8.08 \cdot 10^{-18}, 8.92 \cdot 10^{-18}, 1.04 \cdot 10^{-17}, 1.29 \cdot 10^{-17}, 2.39 \cdot 10^{-19}, \\ &\quad 3.85 \cdot 10^{-19}, 2.46 \cdot 10^{-19}, 1.39 \cdot 10^{-19}, 6.61 \cdot 10^{-20}\} \end{aligned} \tag{7.6}$$

and

$$\begin{aligned} \Delta r_{\text{num./an}} &= \{1.35 \cdot 10^{-15}, 9.32 \cdot 10^{-15}, 4.34 \cdot 10^{-15}, 3.63 \cdot 10^{-15}, 1.45 \cdot 10^{-14}, 4.03 \cdot 10^{-14}, \\ &\quad 9.13 \cdot 10^{-10}, 5.22 \cdot 10^{-18}, 5.42 \cdot 10^{-18}, 6.22 \cdot 10^{-18}, 7.62 \cdot 10^{-20}, 9.15 \cdot 10^{-19}, \\ &\quad 1.78 \cdot 10^{-19}, 3.86 \cdot 10^{-19}, 1.51 \cdot 10^{-19}, 6.80 \cdot 10^{-20}\}. \end{aligned} \tag{7.7}$$

Both the above numerical checks confirm our analytic results.

8 Conclusions

The massive OMEs $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$ receive contributions from non–first–order and first–order factorizable terms. In the present paper we have calculated the latter contributions. In Mellin N–space these are given by harmonic sums, generalized harmonic sums and nested (inverse) binomial sums. The Mellin inversion to x–space, in particular for the terms containing binomial contributions, is most efficiently done by using the t–space representation. This requires to study the five different regions $t \in (0, 1/2], [1/2, 1], [1, 2], [2, 4]$ and $t \in [4, \infty)$. In transforming to x–space, only at $x = 1$ an imaginary part is implied, which is not changed at the pseudo–thresholds $x = 1/4, 1/2$ and the amplitudes vanish for $x > 1$. This implies continuity of the amplitudes in $x \in (0, 1]$. The result in x–space, either obtained by direct Mellin inversion or by the t–space method, are given by G–functions over a 14 letter alphabet and a large set of G–constants at special numbers in the main argument. The integral representations of these constants can all be rationalized and cast into Kummer–Poincaré type Riemann–integrals of complex–valued letters after regularization, if needed. These constants are calculated to 100 digits numerically. The amplitudes are finally expanded into logarithmic–modulated Taylor series up to 100 terms around $x = 0, x = 1/2$ and $x = 1$.

We also discussed a series of results for the representations in Mellin N–space, including non–first–order factorizable contributions. We determined all recurrences which required 15000 moments in the unpolarized case and 11000 moments in the polarized case, not covering a smaller number of recurrences requiring an even larger number of moments, such as the purely rational color–ζ terms $\propto T_F$. This allowed us to compute all non–purely rational terms and non ζ_3 terms, despite the fact that the contributing diagrams partly contain non–first–order factorizable contributions. The latter canceled in the sum when using the method of arbitrary high moments and one obtains nested sum–product representations. For the purely rational terms and their associated terms $\propto \zeta_3$ we have observed that the corresponding recurrences are highly divergent in the limit $N \to \infty$, while the sum of these contributions vanishes in this limit. The rational terms generate a factor of ζ_3 dynamically for $N \to \infty$. One may calculate the fundamental systems of the asymptotic representations of the non–first–order factorizable recurrences, although this requires quite some effort for large recurrences. Furthermore, a series of representations in N–space diverge $\propto a^N, \quad a = 2, 4$. These divergences have to be arranged to cancel analytically.

We have also calculated the leading small and large x contributions from the first–order factorizable terms to the singularities of $O(\ln(x)/x)$ in the unpolarized and of $O(\ln^5(x))$ in the polarized case, as well as of $O(\ln^5(1-x))$ for $x \to 1$. In the unpolarized case our results agree with those for the ζ_2 term given in the literature. In the polarized case we obtained the leading small x contribution $\propto N_F$. This term cannot be obtained by color rescaling from the pure singlet term.

The master integrals computed for the present part of the project form analytic base case integrals of the second part of the calculation of $(\Delta)a_{Qg}^{(3)}$, in which the non–first–order factorizable contributions are computed. The corresponding ${}_2F_1$ solutions have already been calculated in Ref. [125] to $O(\varepsilon^0)$. Ancillary files to this paper contain larger formulae and a series of technical results.

A The asymptotic expansions of the contributing generalized harmonic sums

In the following we list a series of examples of different depth of the asymptotic expansions of the generalized harmonic sums which contribute to the present calculations. We present the terms up to $O(1/N^{10})$. The complete set of expressions is given in an ancillary file. The asymptotic representations are required in N–space programs, cf. [163]. Some of the contributions are suppressed by a factor of 2^{-N} and a series of terms diverges like $\propto 2^N$. The latter behavior cancels in the amplitude, including contributions from the terms containing finite binomial sums. The derivation of theses asymptotic expansions is not straightforward even using the package `HarmonicSums`. In a series of cases the use of shuffle relations is required before these expansions are performed. This is one reason to present the corresponding expressions in explicit form. For $|N| = 50$ the relative accuracy of the representations amounts to values between $2.48 \cdot 10^{-26}$ and $0.95 \cdot 10^{-6}$.

Examples for asymptotic expansions are given by

$$S_1(\{-2\}, N) \approx$$

$$
-\ln(3)+(-2)^N\left[\frac{2}{3N}-\frac{2}{9N^2}-\frac{2}{27N^3}+\frac{2}{27N^4}+\frac{10}{81N^5}\right.
$$
$$
\left.-\frac{14}{243N^6}-\frac{98}{243N^7}-\frac{106}{729N^8}+\frac{4430}{2187N^9}+\frac{2518}{729N^{10}}-\frac{28402}{2187N^{11}}\right], \tag{A.1}
$$
$$
S_{1,2}\left(\left\{\frac{1}{2},-1\right\},N\right)\approx
$$
$$
2^{-N}\left[(-1)^N\left[\frac{1}{6N^3}-\frac{1}{2N^4}+\frac{2}{3N^5}+\frac{1}{6N^6}-\frac{7}{3N^7}+\frac{11}{6N^8}+\frac{12}{N^9}\right.\right.
$$
$$
\left.-\frac{57}{2N^{10}}-\frac{229}{3N^{11}}\right]+\left[\frac{1}{2N}-\frac{1}{N^2}+\frac{3}{N^3}-\frac{13}{N^4}+\frac{75}{N^5}-\frac{541}{N^6}\right.
$$
$$
\left.\left.+\frac{4683}{N^7}-\frac{47293}{N^8}+\frac{545835}{N^9}-\frac{7087261}{N^{10}}+\frac{102247563}{N^{11}}\right]\zeta_2\right]
$$
$$
+\mathrm{H}_{0,-2,-1}(1)+\mathrm{H}_{-2,0,-1}(1)-\frac{1}{2}\zeta_2\ln(3), \tag{A.2}
$$
$$
S_{1,1,2}\left(\left\{-2,\frac{1}{2},-1\right\},N\right)\approx
$$
$$
-\frac{1}{18N^3}+\frac{5}{24N^4}-\frac{79}{180N^5}+\frac{37}{72N^6}+\frac{1}{9N^7}-\frac{59}{36N^8}
$$
$$
+\frac{763}{540N^9}+\frac{941}{120N^{10}}+L\left[-\mathrm{H}_{0,-2,-1}(1)-\mathrm{H}_{-2,0,-1}(1)\right.
$$
$$
\left.-\mathrm{H}_{-2,-1,0}(1)\right]+\left[\left[\frac{2}{3N}-\frac{2}{9N^2}-\frac{2}{27N^3}+\frac{2}{27N^4}+\frac{10}{81N^5}\right.\right.
$$
$$
\left.-\frac{14}{243N^6}-\frac{98}{243N^7}-\frac{106}{729N^8}+\frac{4430}{2187N^9}+\frac{2518}{729N^{10}}\right][\mathrm{H}_{0,-2,-1}(1)
$$
$$
\left.+\mathrm{H}_{-2,0,-1}(1)]\right](-2)^N+\left[-\frac{1}{2N}+\frac{1}{12N^2}-\frac{1}{120N^4}-\frac{1}{240N^8}\right.
$$
$$
\left.+\frac{1}{252N^6}+\frac{1}{132N^{10}}\right][\mathrm{H}_{0,-2,-1}(1)+\mathrm{H}_{-2,0,-1}(1)+\mathrm{H}_{-2,-1,0}(1)]
$$
$$
-\frac{1}{2}\ln^2(2)\zeta_2+\frac{1}{2}\left[\mathrm{H}_{-1,2}(1)+\mathrm{H}_{-2,1}(1)\right]\zeta_2+\ln(3)\left[-\frac{1}{3N}+\frac{1}{9N^2}\right.
$$
$$
+\frac{1}{27N^3}-\frac{1}{27N^4}-\frac{5}{81N^5}+\frac{7}{243N^6}+\frac{49}{243N^7}+\frac{53}{729N^8}
$$
$$
\left.-\frac{2215}{2187N^9}-\frac{1259}{729N^{10}}\right](-2)^N\zeta_2+\left[\frac{1}{4N^2}-\frac{3}{4N^3}+\frac{9}{4N^4}-\frac{37}{4N^5}\right.
$$
$$
\left.+\frac{105}{2N^6}-\frac{1505}{4N^7}+\frac{25893}{8N^8}-\frac{130101}{4N^9}+\frac{748035}{2N^{10}}\right](-1)^N\zeta_2
$$
$$
+\mathrm{H}_{-2,1,-1,0}(1)+\mathrm{H}_{-2,-1,0,1}(1)+\mathrm{H}_{-2,-1,1,0}(1)-\left[\mathrm{H}_{0,-2,-1}(1)\right.
$$

$$+\mathrm{H}_{-2,0,-1}(1)\Bigg]\ln(3)+\frac{1}{2}\zeta_2\ln^2(3), \tag{A.3}$$

$$S_{1,1,1,2}\left(\left\{1,2,\frac{1}{2},-1\right\}\right)(N)\approx$$

$$\ln(2)\Bigg[\Bigg[\frac{1}{2N}-\frac{1}{12N^2}+\frac{1}{120N^4}-\frac{1}{252N^6}+\frac{1}{240N^8}-\frac{1}{132N^{10}}\Bigg]$$
$$\times\mathrm{H}_{0,-2,-1}(1)+\Bigg[\frac{1}{2N}-\frac{1}{12N^2}+\frac{1}{120N^4}-\frac{1}{252N^6}+\frac{1}{240N^8}$$
$$-\frac{1}{132N^{10}}\Bigg]\mathrm{H}_{-2,0,-1}(1)-\mathrm{H}_{0,-1,-2,-1}(1)-\mathrm{H}_{-1,0,-2,-1}(1)$$
$$-\mathrm{H}_{-1,-2,0,-1}(1)+\ln(3)\Bigg[-\frac{1}{4N}+\frac{1}{24N^2}-\frac{1}{240N^4}+\frac{1}{504N^6}$$
$$-\frac{1}{480N^8}+\frac{1}{264N^{10}}\Bigg]\zeta_2+\frac{1}{2}\mathrm{H}_{-1,-2}(1)\zeta_2\Bigg]+L\Bigg[\ln(2)$$
$$\times\Bigg[\mathrm{H}_{0,-2,-1}(1)+\mathrm{H}_{-2,0,-1}(1)-\frac{1}{2}\ln(3)\zeta_2\Bigg]-\mathrm{H}_{0,-1,-2,-1}(1)$$
$$-\mathrm{H}_{-1,0,-2,-1}(1)-\mathrm{H}_{-1,-2,0,-1}(1)+\frac{1}{2}\ln^2(2)\zeta_2+\frac{1}{2}\mathrm{H}_{-1,-2}(1)$$
$$\times\zeta_2+\frac{1}{4}\zeta_2^2\Bigg]+\ln^2(2)\Bigg[\frac{1}{2}\mathrm{H}_{0,-2,-1}(1)+\frac{1}{2}\mathrm{H}_{-2,0,-1}(1)+\Bigg[\frac{1}{4N}$$
$$-\frac{1}{24N^2}+\frac{1}{240N^4}-\frac{1}{504N^6}+\frac{1}{480N^8}-\frac{1}{264N^{10}}\Bigg]\zeta_2$$
$$-\frac{1}{4}\zeta_2\ln(3)\Bigg]+\Bigg[\frac{1}{24N^5}-\frac{5}{16N^6}+\frac{53}{48N^7}-\frac{25}{16N^8}-\frac{359}{96N^9}$$
$$+\frac{3763}{192N^{10}}\Bigg](-1)^N+\Bigg[\Bigg[\Bigg[\frac{4}{N^2}+\frac{12}{N^3}+\frac{60}{N^4}+\frac{380}{N^5}+\frac{2940}{N^6}$$
$$+\frac{26908}{N^7}+\frac{284508}{N^8}+\frac{3413628}{N^9}+\frac{45832380}{N^{10}}\Bigg]$$
$$\times\mathrm{H}_{0,-2,-1}(1)+\Bigg[\frac{4}{N^2}+\frac{12}{N^3}+\frac{60}{N^4}+\frac{380}{N^5}+\frac{2940}{N^6}+\frac{26908}{N^7}$$
$$+\frac{284508}{N^8}+\frac{3413628}{N^9}+\frac{45832380}{N^{10}}\Bigg]\mathrm{H}_{-2,0,-1}(1)+\ln(3)$$
$$\times\Bigg[-\frac{2}{N^2}-\frac{6}{N^3}-\frac{30}{N^4}-\frac{190}{N^5}-\frac{1470}{N^6}-\frac{13454}{N^7}-\frac{142254}{N^8}$$
$$-\frac{1706814}{N^9}-\frac{22916190}{N^{10}}\Bigg]\zeta_2\Bigg]2^N+\Bigg[-\frac{1}{2N}+\frac{1}{12N^2}-\frac{1}{120N^4}$$

$$
\begin{aligned}
&+\frac{1}{252N^6}-\frac{1}{240N^8}+\frac{1}{132N^{10}}\Bigg][\mathrm{H}_{0,-1,-2,-1}(1)+\mathrm{H}_{-1,0,-2,-1}(1)\\
&+\mathrm{H}_{-1,-2,0,-1}(1)]+\frac{1}{4}\ln^3(2)\zeta_2+\Bigg[\frac{1}{2N}-\frac{5}{8N^2}+\frac{71}{72N^3}\\
&-\frac{107}{48N^4}+\frac{6757}{900N^5}-\frac{8503}{240N^6}+\frac{478466}{2205N^7}-\frac{549383}{336N^8}\\
&+\frac{10242761}{700N^9}-\frac{36407611}{240N^{10}}+\Bigg[\frac{1}{4N}-\frac{1}{24N^2}+\frac{1}{240N^4}\\
&-\frac{1}{504N^6}+\frac{1}{480N^8}-\frac{1}{264N^{10}}\Bigg]\mathrm{H}_{-1,-2}(1)-\frac{1}{2}\mathrm{H}_{-1,-1,-2}(1)\\
&-\frac{3}{8}\zeta_3\Bigg]\zeta_2+\Bigg[\frac{1}{8N}-\frac{1}{48N^2}+\frac{1}{480N^4}-\frac{1}{1008N^6}+\frac{1}{960N^8}\\
&-\frac{1}{528N^{10}}\Bigg]\zeta_2^2+\mathrm{H}_{0,-1,-1,-2,-1}(1)+\mathrm{H}_{-1,0,-1,-2,-1}(1)\\
&+\mathrm{H}_{-1,-1,0,-2,-1}(1)+\mathrm{H}_{-1,-1,-2,0,-1}(1),
\end{aligned}
\tag{A.4}
$$

$$
\begin{aligned}
&S_{1,1,1,2}\left(\left\{1,2,\frac{1}{2},1\right\}\right)(N)\approx\\
&\quad\frac{67}{16}\zeta_5+\frac{1}{4N^2}-\frac{11}{12N^3}+\frac{295}{96N^4}-\frac{953}{80N^5}+\frac{250711}{4320N^6}\\
&\quad-\frac{359743}{1008N^7}+\frac{162670639}{60480N^8}-\frac{36393227}{1512N^9}+\frac{15720627001}{63000N^{10}}\\
&\quad+\Bigg[-\frac{9}{16}\zeta_3-\frac{1}{N}+\frac{5}{4N^2}-\frac{71}{36N^3}+\frac{107}{24N^4}-\frac{6757}{450N^5}\\
&\quad+\frac{8503}{120N^6}-\frac{956932}{2205N^7}+\frac{549383}{168N^8}-\frac{10242761}{350N^9}+\frac{36407611}{120N^{10}}\Bigg]\zeta_2\\
&\quad+\Bigg[-\frac{17}{40}L-\frac{17}{80N}+\frac{17}{480N^2}-\frac{17}{4800N^4}+\frac{17}{10080N^6}\\
&\quad-\frac{17}{9600N^8}+\frac{17}{5280N^{10}}\Bigg]\zeta_2^2+\Bigg[\frac{5}{2N^2}+\frac{15}{2N^3}+\frac{75}{2N^4}\\
&\quad+\frac{475}{2N^5}+\frac{3675}{2N^6}+\frac{33635}{2N^7}+\frac{355635}{2N^8}+\frac{4267035}{2N^9}\\
&\quad+\frac{57290475}{2N^{10}}\Bigg]2^N\zeta_3,
\end{aligned}
\tag{A.5}
$$

$$
\begin{aligned}
&S_{1,1,1,1,1}\left(\left\{\frac{1}{2},2,1,1,1\right\}\right)(N)\approx\\
&\quad 4\mathrm{Li}_5\left(\frac{1}{2}\right)+\frac{1}{120}\ln^5(2)-\frac{2}{N}+\frac{1}{4N^2}+\frac{17}{324N^3}-\frac{3}{4N^4}\\
&\quad-\frac{29171}{45000N^5}+\frac{17837}{2160N^6}+\frac{13192844957}{62233920N^7}+\frac{3835123}{1120N^8}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{858280391021}{16329600N^9}+\frac{940261784593}{1134000N^{10}}+L^2\Bigg[-\frac{1}{N}+\frac{25}{36N^3}+\frac{5}{2N^4}\\
&+\frac{2993}{200N^5}+\frac{314}{3N^6}+\frac{3823133}{4410N^7}+\frac{500479}{60N^8}+\frac{1385608621}{15120N^9}\\
&+\frac{1428138841}{1260N^{10}}\Bigg]+L^3\Bigg[-\frac{1}{3N}-\frac{2}{9N^3}-\frac{2}{3N^4}-\frac{142}{45N^5}-\frac{58}{3N^6}\\
&-\frac{9146}{63N^7}-\frac{1294}{N^8}-\frac{601342}{45N^9}-\frac{470906}{3N^{10}}\Bigg]+L\Bigg[-\frac{2}{N}+\frac{1}{2N^2}\\
&-\frac{19}{108N^3}-\frac{1}{3N^4}-\frac{190517}{18000N^5}-\frac{18941}{180N^6}-\frac{5946741}{5488N^7}\\
&-\frac{3813722}{315N^8}-\frac{134889193063}{907200N^9}-\frac{25291803223}{12600N^{10}}+\Bigg[-\frac{1}{N}-\frac{2}{3N^3}\\
&-\frac{2}{N^4}-\frac{58}{N^6}-\frac{9146}{21N^7}-\frac{142}{15N^5}-\frac{3882}{N^8}-\frac{601342}{15N^9}-\frac{470906}{N^{10}}\Bigg]\\
&\times\zeta_2\Bigg]+\ln(2)\Bigg[\mathrm{Li}_4\left(\frac{1}{2}\right)+\frac{12}{5}\zeta_2^2\Bigg]+\Bigg[\mathrm{Li}_4\left(\frac{1}{2}\right)\Bigg[-\frac{1}{N}+\frac{2}{N^2}\\
&-\frac{6}{N^3}+\frac{26}{N^4}-\frac{150}{N^5}+\frac{1082}{N^6}-\frac{9366}{N^7}+\frac{94586}{N^8}-\frac{1091670}{N^9}\\
&+\frac{14174522}{N^{10}}\Bigg]+\ln^4(2)\Bigg[-\frac{1}{24N}+\frac{1}{12N^2}-\frac{1}{4N^3}+\frac{13}{12N^4}\\
&-\frac{25}{4N^5}+\frac{541}{12N^6}-\frac{1561}{4N^7}+\frac{47293}{12N^8}-\frac{181945}{4N^9}+\frac{7087261}{12N^{10}}\Bigg]\\
&+\ln^2(2)\Bigg[\frac{1}{N}-\frac{2}{N^2}+\frac{6}{N^3}-\frac{26}{N^4}+\frac{150}{N^5}-\frac{1082}{N^6}+\frac{9366}{N^7}\\
&-\frac{94586}{N^8}+\frac{1091670}{N^9}-\frac{14174522}{N^{10}}\Bigg]\zeta_2+\Bigg[\frac{4}{5N}-\frac{8}{5N^2}+\frac{24}{5N^3}\\
&-\frac{104}{5N^4}+\frac{120}{N^5}-\frac{4328}{5N^6}+\frac{37464}{5N^7}-\frac{378344}{5N^8}+\frac{873336}{N^9}\\
&-\frac{56698088}{5N^{10}}\Bigg]\zeta_2^2\Bigg]2^{-N}+\frac{1}{3}\ln^3(2)\zeta_2+\Bigg[-\frac{1}{N}+\frac{25}{36N^3}+\frac{5}{2N^4}\\
&+\frac{2993}{200N^5}+\frac{314}{3N^6}+\frac{3823133}{4410N^7}+\frac{500479}{60N^8}+\frac{1385608621}{15120N^9}\\
&+\frac{1428138841}{1260N^{10}}\Bigg]\zeta_2+\Bigg[-\frac{2}{3N}-\frac{4}{9N^3}-\frac{4}{3N^4}-\frac{284}{45N^5}-\frac{116}{3N^6}\\
&-\frac{18292}{63N^7}-\frac{2588}{N^8}-\frac{1202684}{45N^9}-\frac{941812}{3N^{10}}\Bigg]\zeta_3, \qquad \text{(A.6)}
\end{aligned}
$$

Some of the above constants can be expressed in terms of polylogarithms. We present the relations up to depth three, since from depth 4 classical polylogarithms do not usually provide a good basis. One obtains

$$\mathrm{H}_{-1,-2}(1) = \frac{1}{2}\zeta_2 - \ln^2(2) + \ln(2)\ln(3) - \frac{1}{2}\ln^2(3) - \mathrm{Li}_2\left[\frac{1}{3}\right], \tag{A.7}$$

$$\mathrm{H}_{-1,2}(1) = \ln^2(2) - \ln^2(3) - 2\mathrm{Li}_2\left[\frac{1}{3}\right] + \zeta_2, \tag{A.8}$$

$$\mathrm{H}_{-2,1}(1) = \mathrm{Li}_2\left[\frac{1}{3}\right], \tag{A.9}$$

$$\mathrm{H}_{0,4}(1) = -2\ln^2(2) + 2\ln(2)\ln(3) - \ln^2(3) + \zeta_2 - 2\mathrm{Li}_2\left[\frac{1}{3}\right], \tag{A.10}$$

$$\begin{aligned}\mathrm{H}_{0,4,2}(1) = & -\frac{3}{2}\zeta_2\ln(2) - \frac{5}{6}\ln^3(2) + 2\ln^2(2)\ln(3) - \ln(2)\ln^2(3) + \frac{7}{2}\zeta_3 \\ & -2\ln(2)\mathrm{Li}_2\left[\frac{1}{3}\right] + 4\mathrm{Li}_3\left[-\frac{1}{2}\right],\end{aligned} \tag{A.11}$$

$$\mathrm{H}_{0,0,-2}(1) = -\mathrm{Li}_3\left[-\frac{1}{2}\right], \tag{A.12}$$

$$\mathrm{H}_{0,0,4}(1) = -2\zeta_2\ln(2) + \frac{2}{3}\ln^3(2) + \frac{7}{2}\zeta_3 + 4\mathrm{Li}_3\left[-\frac{1}{2}\right], \tag{A.13}$$

$$\begin{aligned}\mathrm{H}_{0,1,-2}(1) = & -2\zeta_2(\ln(2) - \ln(3)) - \frac{1}{2}\ln^2(2)\ln(3) + \ln(2)\ln^2(3) - \frac{1}{2}\ln^3(3) \\ & +(\ln(2) - \ln(3))\mathrm{Li}_2\left[\frac{1}{3}\right] - \mathrm{Li}_3\left[\frac{1}{3}\right] + \mathrm{Li}_3\left[\frac{2}{3}\right] - \zeta_3,\end{aligned} \tag{A.14}$$

$$\mathrm{H}_{0,-2,1}(1) = -\zeta_2\ln\left(\frac{3}{2}\right) - \frac{1}{6}\ln^3\left(\frac{3}{2}\right) - \mathrm{Li}_3\left[-\frac{1}{2}\right] + \mathrm{Li}_3\left[\frac{1}{3}\right], \tag{A.15}$$

$$\begin{aligned}\mathrm{H}_{0,-2,-1}(1) = & -\frac{4}{3}\ln^3(2) + 3\zeta_2(\ln(2) - \ln(3)) + \ln^2(2)\ln(3) - \frac{1}{2}\ln(2)\ln^2(3) + \frac{1}{2}\ln^3(3) \\ & + \ln(2)\mathrm{Li}_2\left[\frac{1}{3}\right] + \mathrm{Li}_3\left[-\frac{1}{3}\right] - 2\mathrm{Li}_3\left[\frac{1}{3}\right] - 2\mathrm{Li}_3\left[\frac{2}{3}\right] + \mathrm{Li}_3\left[\frac{3}{4}\right] \\ & + \frac{21}{8}\zeta_3,\end{aligned} \tag{A.16}$$

$$\mathrm{H}_{-1,2,-1}(1) = \zeta_2\ln(2) + \ln^2(2)\ln(3) - \ln(2)\ln^2(3) + 2\mathrm{Li}_3\left[\frac{1}{3}\right] - 2\mathrm{Li}_3\left[\frac{2}{3}\right], \tag{A.17}$$

$$\begin{aligned}\mathrm{H}_{-1,0,2}(1) = & \frac{5}{6}\ln^3(2) - \ln(2)\ln^2(3) + \frac{1}{6}\ln^3(3) + \frac{1}{2}\zeta_2\Big[-\ln(2) + 2\ln(3)\Big] \\ & -2\ln(2)\mathrm{Li}_2\left[\frac{1}{3}\right] - \mathrm{Li}_3\left[-\frac{1}{3}\right] - \mathrm{Li}_3\left[\frac{3}{4}\right] + \frac{1}{4}\zeta_3,\end{aligned} \tag{A.18}$$

$$\begin{aligned}\mathrm{H}_{-2,0,-1}(1) = & \frac{4}{3}\ln^3(2) - \ln^2(2)\ln(3) + \frac{1}{2}\ln(2)\ln^2(3) - \frac{1}{3}\ln^3(3) + \frac{1}{2}\zeta_2\Big[-6\ln(2) \\ & +5\ln(3)\Big] - \ln(2)\mathrm{Li}_2\left[\frac{1}{3}\right] + 2\mathrm{Li}_3\left[\frac{2}{3}\right] - \mathrm{Li}_3\left[\frac{3}{4}\right] - \zeta_3.\end{aligned} \tag{A.19}$$

Here we used the relation

$$\mathrm{Li}_2\left[\frac{1}{3}\right] = -\frac{1}{2}\ln^2\left(\frac{2}{3}\right) - \mathrm{Li}_2\left[-\frac{1}{2}\right] \tag{A.20}$$

and other ones for $\mathrm{Li}_2(x)$, cf. [178–180]. The remaining generalized polylogarithms at argument $x = 1$ can be calculated numerically, e.g. with the program of Ref. [168], and we have listed their numerical values in ancillary files at an accuracy of 100 digits for completeness.

B The asymptotic expansions of nested binomial sums

We will give only some examples for the asymptotic expansion of nested binomial sums in the following.[14] Also here aspects summarized in Ref. [57] play a central role, see also [181]. In N–space one first splits off lower–order factors and expands them individually asymptotically. Then one considers the t–representations and splits off potential distribution–valued contributions, cf. [125]. The asymptotic expansion of these contributions is known [56]. After this the respective quantities $F(N)$ are viewed as Mellin transforms of functions $f(x)$, which are either analytic in the vicinity of $x = 1$, or have to be first rewritten to obey this condition, [57]. These Mellin transforms can then be expanded into asymptotic series, because they have representations in terms of factorial series [182–184],

$$\Omega(N) = \sum_{k=0}^{\infty} a_{k+1} \frac{k!}{N(N+1)\dots(N+k)}. \tag{B.1}$$

Terms $\propto S_1^k(N), k \geq 1, k \in \mathbb{N}$, are no factorial series, but their asymptotic series are known. Contributing Γ–functions of non–integer arguments may imply other powers of N, as e.g. factors of $\sqrt{N}$ and also factors a^N with $a \in \mathbb{Z}\backslash\{0\}$. A comprehensive treatment of these contributions is better given by the t–space representation, being more systematic. The examples for asymptotic representations given in the following were obtained by using the command `BSExpansion`. Usually the resulting expressions have an involved form. One obtains the following asymptotic expansions up to $O(1/N^{10})$

$$\begin{aligned}
\tilde{F}_1(N) = \sum_{\tau_1=1}^{N} \frac{\left(\tau_1!\right)^2}{\left(2\tau_1\right)!} \approx& \\
& \frac{1}{3} + \frac{2\pi}{9\sqrt{3}} + \Biggl[-\frac{1}{3} - \frac{19}{72N} + \frac{407}{3456N^2} - \frac{3587}{27648N^3} + \frac{612727}{2654208N^4} \\
& -\frac{36974287}{63700992N^5} + \frac{640361849}{339738624N^6} - \frac{60994830787}{8153726976N^7} + \frac{54910715707991}{1565515579392N^8} \\
& -\frac{2376532755785617}{12524124635136N^9} + \frac{699435110164273561}{601157982486528N^{10}} - \frac{115034280046636642783}{14427791579676672N^{11}}\Biggr] \\
& \times 2^{-2N}\sqrt{N}\sqrt{\pi},
\end{aligned} \tag{B.2}$$

$$\begin{aligned}
\tilde{F}_2(N) = \sum_{\tau_1=1}^{N} \frac{\left(2\tau_1\right)!}{\left(\tau_1!\right)^2} \approx& \\
& \Biggl[\frac{4}{3} + \frac{1}{18N} + \frac{59}{288N^2} + \frac{2425}{6912N^3} + \frac{576793}{663552N^4} + \frac{5000317}{1769472N^5} + \frac{953111599}{84934656N^6} \\
& +\frac{107249721865}{2038431744N^7} + \frac{37133194953283}{130459631616N^8} + \frac{5464331904405803}{3131031158784N^9}
\end{aligned}$$

[14] A series of representations has been given in Refs. [38, 54].

$$
+\frac{1797410945424609151}{150289495621632 N^{10}}\Bigg]\frac{4^N}{\sqrt{N}\sqrt{\pi}}, \tag{B.3}
$$

$$
\tilde{F}_3(N) = \sum_{\tau_1=1}^{N} \frac{\left(\tau_1!\right)^2 \sum_{\tau_2=1}^{\tau_1} \frac{(-1)^{\tau_2}\left(2\tau_2\right)!}{\left(\tau_2!\right)^2 \tau_2^3}}{\left(2\tau_1\right)!} \approx
$$

$$
\begin{aligned}
&-\frac{16}{9} - \left[\frac{4}{9}\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}\right\}, 1\right] + \frac{2}{9}\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}, \frac{1}{\tau}\right\}, 1\right]\right]\mathrm{G}\left[\left\{\frac{\sqrt{1-\tau}}{4-\tau}\right\}, 1\right] \\
&-\left[\frac{4}{9}\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}\right\}, 1\right] + \frac{2}{9}\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}, \frac{1}{\tau}\right\}, 1\right]\right]\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{1+\tau}\right\}, 1\right] \\
&+\frac{4}{9}\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{1+\tau}, \frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}\right\}, 1\right] + \frac{2}{9}\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{1+\tau}, \frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}, \frac{1}{\tau}\right\}, 1\right] \\
&+\Bigg[\frac{2}{5N^3} - \frac{22}{25N^4} + \frac{24}{125N^5} + \frac{1188}{625N^6} - \frac{947}{3125N^7} - \frac{57253}{6250N^8} - \frac{28938}{15625N^9} \\
&+\frac{5225906}{78125N^{10}}\Bigg](-1)^N + \Bigg\{\Bigg[-\frac{2}{3}\sqrt{N} - \frac{19}{36}\frac{1}{\sqrt{N}} + \frac{407}{1728}\frac{1}{N^{3/2}} - \frac{3587}{13824}\frac{1}{N^{5/2}} \\
&+\frac{612727}{1327104}\frac{1}{N^{7/2}} - \frac{36974287}{31850496}\frac{1}{N^{9/2}} + \frac{640361849}{169869312}\frac{1}{N^{11/2}} - \frac{60994830787}{4076863488}\frac{1}{N^{13/2}} \\
&+\frac{54910715707991}{782757789696}\frac{1}{N^{15/2}} - \frac{2376532755785617}{6262062317568}\frac{1}{N^{17/2}} \\
&+\frac{699435110164273561}{300578991243264}\frac{1}{N^{19/2}} - \frac{11503428004663664 2783}{7213895789838336}\frac{1}{N^{21/2}}\Bigg] \\
&\times\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}\right\}, 1\right]\sqrt{\pi} + \Bigg[-\frac{1}{3}\sqrt{N} - \frac{19}{72}\frac{1}{\sqrt{N}} + \frac{407}{3456}\frac{1}{N^{3/2}} - \frac{3587}{27648}\frac{1}{N^{5/2}} \\
&+\frac{612727}{2654208}\frac{1}{N^{7/2}} - \frac{36974287}{63700992}\frac{1}{N^{9/2}} + \frac{640361849}{339738624}\frac{1}{N^{11/2}} - \frac{60994830787}{8153726976}\frac{1}{N^{13/2}} \\
&+\frac{54910715707991}{1565515579392}\frac{1}{N^{15/2}} - \frac{2376532755785617}{12524124635136}\frac{1}{N^{17/2}} \\
&+\frac{699435110164273561}{601157982486528}\frac{1}{N^{19/2}} - \frac{115034280046636642783}{14427791579676672}\frac{1}{N^{21/2}}\Bigg] \\
&\times\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau}, \frac{1}{\tau}, \frac{1}{\tau}\right\}, 1\right]\sqrt{\pi}\Bigg\}2^{-2N}.
\end{aligned} \tag{B.4}
$$

The different G–constants at $x = 1$ have to be regulated in general and should be rationalized, whenever possible. Then their letters should be partial fractioned, prior to calculating them numerically.

To perform the inverse Mellin transform, one can compute first the t–representation by using the command `ComputeGeneratingFunction`

$$
F_1(t) = t\left\{-\frac{1}{2(t-1)} - \frac{1}{(4-t)^{3/2}\sqrt{t}(t-1)}\mathrm{G}\left[\left\{\sqrt{4-\tau}\sqrt{\tau}\right\}, t\right]\right\}, \tag{B.5}
$$

$$
\begin{aligned}
F_2(t) &= \frac{1}{t-1}\left[1-\frac{1}{\sqrt{1-4t}}\right], && \text{(B.6)}\\
F_3(t) &= t\Biggl\{-\frac{5}{2(t-1)}+\frac{\mathrm{H}_{-1}(t)}{t-1}-\frac{\mathrm{H}_{0,-1}(t)}{2(t-1)}+\frac{(2+t)\mathrm{H}_{0,0,-1}(t)}{2(t-1)t}+\frac{1}{(4-t)^{3/2}(t-1)\sqrt{t}}\\
&\times\Biggl[-4\mathrm{G}\left[\left\{\sqrt{(4-\tau)\tau}\right\},t\right]+5\mathrm{G}\left[\left\{\frac{\sqrt{4-\tau}}{\sqrt{\tau(1+\tau)}}\right\},t\right]+\frac{3}{2}\mathrm{G}\left[\left\{\sqrt{(4-\tau)\tau},\frac{1}{1+\tau}\right\},t\right]\\
&-\frac{1}{2}\mathrm{G}\left[\left\{\sqrt{(4-\tau)\tau},\frac{1}{\tau},\frac{1}{1+\tau}\right\},t\right]+\mathrm{G}\left[\left\{\sqrt{(4-\tau)\tau},\frac{1}{\tau},\frac{1}{\tau},\frac{1}{1+\tau}\right\},t\right]\Biggr]\Biggr\}. && \text{(B.7)}
\end{aligned}
$$

The binomial sums above can be represented by regularized Mellin transforms over an extended support

$$
\begin{aligned}
\tilde{F}_1(N) &= \left[\frac{1}{3}+\frac{2\pi}{9\sqrt{3}}\right]\left(1-\frac{1}{4^N}\right)+\frac{1}{2\cdot 4^N}\int_0^1 dy\frac{y^N-1}{(1-y)^{3/2}}\frac{y}{4-y}, && \text{(B.8)}\\
\tilde{F}_2(N) &= \frac{1}{\pi}\int_0^4 dy\frac{y^N-1}{y-1}\frac{\sqrt{y}}{\sqrt{4-y}}, && \text{(B.9)}\\
\tilde{F}_3(N) &= -\frac{16}{9}+\left(\frac{7}{9}2^{1-2N}+\frac{1}{9}(4^N-1)4^{1-N}\mathrm{G}\left[\left\{\frac{\sqrt{1-\tau}}{4-\tau}\right\},1\right]\right)\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right]\\
&+\frac{4}{9}\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau},\frac{\sqrt{1+4\tau}}{1+\tau}\right\},1\right]-\frac{2}{9}\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau},\frac{\sqrt{1+4\tau}}{1+\tau}\right\},1\right]\\
&-\frac{1}{9}(4^N-1)\mathrm{G}\left[\left\{\frac{\sqrt{1-\tau}}{4-\tau}\right\},1\right]\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right]2^{1-2N}\\
&-\frac{7}{9}4^{-N}\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right]+f_{a3}2^{-1-2N}\int_0^1 dx\frac{x(x^N-1)}{(1-x)^{3/2}(4-x)}\\
&+\int_0^1 dx\frac{x^{N+1}f_{b3}(x)2(-1)^N}{(1+x)(1+4x)^{3/2}}, && \text{(B.10)}
\end{aligned}
$$

with

$$
\begin{aligned}
f_{a3} &= 2\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right]-\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right], && \text{(B.11)}\\
f_{b3}(x) &= 2\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right]+2\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau},\frac{1}{\tau}\right\},x\right]\\
&-\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right]+\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau},\frac{1}{\tau},\frac{1}{\tau}\right\},x\right]. && \text{(B.12)}
\end{aligned}
$$

While these functions of N evaluate to rational numbers for $N\in\mathbb{N}$, the N dependence cannot be simply factored out as in the usual Mellin transforms.

The above constants have the following representation,

$$
\mathrm{G}\left[\left\{\frac{\sqrt{1-\tau}}{4-\tau},\right\},1\right] = 2-\frac{\pi}{\sqrt{3}}, \qquad \text{(B.13)}
$$

$$\mathrm{G}\left[\left\{\frac{\sqrt{1+4\tau}}{\tau},\frac{1}{\tau}\right\},1\right] = -\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right], \tag{B.14}$$

$$\begin{aligned}\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right] &= -4-4\ln(2)-\ln^2(2)+4\sqrt{5}+4\ln\left(\sqrt{5}-1\right)\\ &\quad +2\ln(2)\ln\left(\sqrt{5}-1\right)-\ln^2\left(\sqrt{5}-1\right)+2\mathrm{Li}_2\left[\frac{1}{2}-\frac{\sqrt{5}}{2}\right],\end{aligned} \tag{B.15}$$

$$\begin{aligned}\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right] &= -8+\frac{2\ln^3(2)}{3}-i\ln^2(2)(-2i+\pi)+\ln(2)\big(-8+2\zeta_2\big)\\ &\quad +8\sqrt{5}+2\zeta_3+\big(8-2\ln^2(2)+2\ln(2)(2+i\pi)-2\zeta_2\big)\\ &\quad \times\ln\left(\sqrt{5}-1\right)+(-2+2\ln(2)-i\pi)\ln^2\left(\sqrt{5}-1\right)\\ &\quad -\frac{2}{3}\ln^3\left(\sqrt{5}-1\right)+4\mathrm{Li}_2\left[\frac{1}{2}\big(1-\sqrt{5}\big)\right]+2\mathrm{Li}_3\left[\frac{1}{2}\big(1-\sqrt{5}\big)\right]\\ &\quad -2\mathrm{Li}_3\left[\frac{1}{2}\big(1+\sqrt{5}\big)\right]\end{aligned} \tag{B.16}$$

$$\begin{aligned}&\mathrm{G}\left[\left\{\frac{1}{\tau},\frac{1}{\tau},\frac{\sqrt{1+4\tau}}{\tau},\frac{\sqrt{1+4\tau}}{\tau}\right\},1\right] =\\ &\quad 24-8\mathrm{Li}_4\left[\frac{1}{2}\right]-\frac{11}{3}\ln^4(2)-\frac{8}{3}i\ln^3(2)(\pi-2i)+\ln(2)\big(16+8i\pi\\ &\quad -16\sqrt{5}-56\zeta_2-16i\pi\zeta_2-7\zeta_3\big)+\ln^2\left(\sqrt{5}-1\right)\Bigg[4+\ln^2(2)\\ &\quad -8i\pi-6i\ln(2)\pi+11\zeta_2-2\mathrm{Li}_2\left[\frac{1-\sqrt{5}}{2}\right]-2\mathrm{Li}_2\left[\frac{1+\sqrt{5}}{2}\right]\Bigg]\\ &\quad +\ln\left(\sqrt{5}-1\right)\Bigg[-16+\frac{14}{3}\ln^3(2)+8\ln^2(2)(1+i\pi)-8i\pi\\ &\quad +\ln(2)\Big[-8+8i\pi+2\zeta_2\Big]+16\sqrt{5}+48\zeta_2+12i\pi\zeta_2+\frac{7}{2}\zeta_3\\ &\quad +4(2+\ln(2))\mathrm{Li}_2\left[\frac{1-\sqrt{5}}{2}\right]+4\ln(2)\mathrm{Li}_2\left[\frac{1+\sqrt{5}}{2}\right]\\ &\quad +4\mathrm{Li}_3\left[\frac{1-\sqrt{5}}{2}\right]-4\mathrm{Li}_3\left[\frac{1+\sqrt{5}}{2}\right]\Bigg]+\ln^2(2)\big(4-14\zeta_2\big)\\ &\quad -16\sqrt{5}-4\mathrm{H}_{-1,-1,-1,1}\big(\sqrt{5}\big)-8\zeta_2-8i\pi\zeta_2+\frac{68}{5}\zeta_2^2\\ &\quad -\frac{2}{3}(4+5\ln(2)-i\pi)\ln^3\left(\sqrt{5}-1\right)+\ln^4\left(\sqrt{5}-1\right)+\big(8i\pi\\ &\quad +4i\ln(2)\pi-12\zeta_2\big)\mathrm{Li}_2\left[\frac{1-\sqrt{5}}{2}\right]+\big(8+4\ln(2)(2+i\pi)\\ &\quad +8i\pi-12\zeta_2\big)\mathrm{Li}_2\left[\frac{1+\sqrt{5}}{2}\right]-4(2+\ln(2))\mathrm{Li}_3\left[\frac{1-\sqrt{5}}{2}\right]\end{aligned}$$

$$+4\ln(2)\mathrm{Li}_3\left[\frac{1+\sqrt{5}}{2}\right]+4\mathrm{Li}_4\left[\frac{1}{2}\right]-4\mathrm{Li}_4\left[\frac{1-\sqrt{5}}{2}\right], \tag{B.17}$$

and

$$\begin{aligned}
\mathrm{H}_{-1,-1,-1,1}(\sqrt{5}) \quad = \quad & -\frac{2}{3}\ln^4(2)+\left[\frac{7}{6}\ln^3(2)+\frac{1}{2}\ln(2)\zeta_2+\frac{7}{8}\zeta_3\right]\ln\left(\sqrt{5}-1\right)-\left[\frac{3}{4}\ln^2(2)\right. \\
& \left.+\frac{1}{4}\zeta_2\right]\ln^2\left(\sqrt{5}-1\right)+\frac{1}{6}\ln(2)\ln^3\left(\sqrt{5}-1\right)-\mathrm{Li}_4\left[\frac{1}{2}\right]+\mathrm{Li}_4\left[\frac{1+\sqrt{5}}{2}\right] \\
& -\frac{7}{4}\ln(2)\zeta_3.
\end{aligned} \tag{B.18}$$

The remaining constants are better calculated numerically, since the space of polylogarithms will normally not suffice, but they have a representation in terms of Kummer–Poincaré iterated integrals, see Appendix C. These G–functions at $x=1$ are real and the imaginary contributions cancel those of $\mathrm{Li}_k(y)$ for $y>1$. If more than two different letters occur, the corresponding expressions become much more involved, but can still be rationalized if the root factor is the same. Then also letters containing general quadratic forms in the denominators occur [103], which can be decomposed into (complex) Kummer–Poincaré type letters [75–78] by partial fractioning. This representation can be obtained by applying the command `GLToL` to the G–functions.

We also mention that the command `SExpansion` may be used for a partial asymptotic expansion of binomial sums, mapping to other binomial sums. An example is given by

$$\begin{aligned}
\sum_{\tau_1=1}^{N}\frac{\left(\tau_1!\right)^2\sum_{\tau_2=1}^{\tau_1}\frac{\left(2\tau_2\right)!\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3}}{\left(\tau_2!\right)^2\tau_2^2}}{\left(2\tau_1\right)!\left(1+\tau_1\right)} \quad \approx \quad & \frac{1}{N^2}+\frac{4}{9N^3}-\frac{5}{3N^4}+\frac{23}{15N^5}-\frac{67}{180N^6}-\frac{299}{630N^7} \\
& +\frac{127}{2520N^8}+\frac{859}{1134N^9}+\frac{587}{6300N^{10}}+\left[\frac{2}{N^2}-\frac{8}{3N^3}+\frac{2}{N^4}\right. \\
& \left.-\frac{2}{3N^5}-\frac{1}{3N^6}+\frac{1}{3N^7}+\frac{1}{3N^8}-\frac{4}{9N^9}-\frac{3}{5N^{10}}\right]L \\
& -2\sum_{\tau_1=1}^{N}\frac{\left(\tau_1!\right)^2\sum_{\tau_2=1}^{\tau_1}\frac{\left(2\tau_2\right)!\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3}}{\left(\tau_2!\right)^2\tau_2^2}}{\left(2\tau_1\right)!\tau_1^2}+\left[\frac{1}{\sqrt{N}}-\frac{7}{8}\frac{1}{N^{3/2}}\right. \\
& +\frac{113}{128}\frac{1}{N^{5/2}}-\frac{909}{1024}\frac{1}{N^{7/2}}+\frac{29067}{32768}\frac{1}{N^{9/2}}-\frac{232137}{262144}\frac{1}{N^{11/2}} \\
& +\frac{3715061}{4194304}\frac{1}{N^{13/2}}-\frac{29759813}{33554432}\frac{1}{N^{15/2}}+\frac{1904293555}{2147483648}\frac{1}{N^{17/2}} \\
& \left.-\frac{15205631037}{17179869184}\frac{1}{N^{19/2}}\right]2^{-2N}\sqrt{\pi}\sum_{\tau_1=1}^{N}\frac{\left(2\tau_1\right)!\sum_{\tau_2=1}^{\tau_1}\frac{1}{\tau_2}}{\left(\tau_1!\right)^2\tau_1^2} \\
& +4\sum_{\tau_1=1}^{N}\frac{\left(\tau_1!\right)^2\sum_{\tau_2=1}^{\tau_1}\frac{\left(2\tau_2\right)!\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3}}{\left(\tau_2!\right)^2\tau_2^2}}{\left(2\tau_1\right)!\tau_1}-2\zeta_2^2-2\zeta_2\zeta_3+6\zeta_5\ .
\end{aligned} \tag{B.19}$$

In some cases, the contributing constants are related to solutions of algebraic equations of fourth order.

In the examples given in an ancillary file the representations contained up to four singularities in the region $x \in [0,1]$ which had to be regularized. Furthermore, one has to algebraically reduce the G–functions at $x = 1$ to remove divergences, resulting from the symbol $G[\{1/(1-\tau)\}, 1]$. The contributing 183 (root–valued) G–constants have a linear representation in terms of 7200 divergence free G–constants of the Kummer–Poincaré type. The asymptotic representations of the binomial sums given in an ancillary file to terms of $O(1/N^{10})$ have absolute accuracies between $4.04 \cdot 10^{-7}$ and $2.85 \cdot 10^{-45}$ at $|N| = 50$. The explicit sum representation of the binomial sums can be obtained by using the command `ToHarmonicSumsSum`.

For the individual asymptotic expansions of the binomial sums also G–constants containing two different root–factors contribute. Terms of this kind are absent in the physical amplitudes. These G–constants can also be rationalized as described in [185], see also [186]. We present a series of examples in Appendix C.

C The calculation of special constants

In the following we describe the technical steps in the calculation of a series of G–constants at $x = 1, 1/4$ determined by Kummer–Poincaré and root–valued letters

$$\left\{\frac{1}{2+x}, \frac{1}{1+3x}, \frac{\sqrt{1-4x}}{x}, \frac{\sqrt{1-4x}}{1-x}, \frac{\sqrt{1-4x}}{1+x}, \frac{\sqrt{5-4x}-1}{1-x}, \frac{\sqrt{5-4x}}{1+x}\frac{\sqrt{5-4x}-1}{2-x}, \frac{\sqrt{5-4x}-1}{2+x}\right\}. \tag{C.1}$$

As for the rationalizations to Kummer–Poincaré integrals, one transforms the square–roots

$$\sqrt{a+bx} \to \sqrt{1-x}. \tag{C.2}$$

An example is

$$\begin{aligned}
&\mathrm{G}\left[\left\{\frac{\sqrt{5-4\tau}}{\tau}\right\}, 1\right] \to \\
&\quad \texttt{GLToStandardForm[TransformGL[GL[\{Sqrt[5 - 4VarGL]/(VarGL)\}, 5/(4x)], x]]/.x} \to \texttt{4/5} \\
&= \sqrt{5}\left[\mathrm{G}\left[\left\{\frac{1}{\tau}\right\}, \frac{5}{4}\right] + \mathrm{G}\left[\left\{\frac{\sqrt{1-\tau}}{\tau}\right\}, \frac{4}{5}\right]\right] \qquad \texttt{//SpecialGLToH} \\
&= 2 - 2\sqrt{5} + 2\sqrt{5}\mathrm{G}(\{-1\}, 1) - \left(1+\sqrt{5}\right)\mathrm{G}\left[\{-1\}, \frac{1}{\sqrt{5}}\right] + \mathrm{G}\left[\{0\}, \frac{4}{5}\right] + \sqrt{5}\mathrm{G}\left[\{0\}, \frac{5}{4}\right] \\
&\quad -\left(1-\sqrt{5}\right)\mathrm{G}\left[\{1\}, \frac{1}{\sqrt{5}}\right] \\
&= 2 - 2\sqrt{5} - 2\ln(2)\sqrt{5} + \sqrt{5}\ln(5) + 2\sqrt{5}\ln\left(\sqrt{5}-1\right),
\end{aligned} \tag{C.3}$$

where we used the notation of [168] in the next to last line. Another example is

$$\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{1-\tau}\right\}, \frac{1}{4}\right] \to \mathrm{G}\left[\left\{\frac{\sqrt{1-\tau}}{\tau}, \frac{1}{1-4\tau}\right\}, 1\right]$$

$$
\begin{aligned}
= \quad & -4+2i\sqrt{3}\mathrm{G}\left[\left\{-i\sqrt{3}\right\},1\right]+2\mathrm{G}\left[\{-1\},1\right]\mathrm{G}\left[\left\{-i\sqrt{3}\right\},1\right]-2i\sqrt{3}\mathrm{G}\left[\left\{i\sqrt{3}\right\},1\right] \\
& +2\mathrm{G}\left[\{-1\},1\right]\mathrm{G}\left[\left\{i\sqrt{3}\right\},1\right]-2\mathrm{G}\left[\left\{-1,-i\sqrt{3}\right\},1\right]-2\mathrm{G}\left[\left\{-1,i\sqrt{3}\right\},1\right] \\
& -\mathrm{G}\left[\left\{-i\sqrt{3},-1\right\},1\right]-\mathrm{G}\left[\left\{-i\sqrt{3},1\right\},1\right]-\mathrm{G}\left[\left\{i\sqrt{3},-1\right\},1\right]-\mathrm{G}\left[\left\{i\sqrt{3},1\right\},1\right].
\end{aligned} \tag{C.4}
$$

Some of the emerging Kummer–Poincaré iterated integrals have to be regularized, for example.

$$
\mathrm{G}\left[\{a\},a\right]=-\ln(a)-S_1(\infty), \quad \text{etc.} \tag{C.5}
$$

Furthermore, also expressions like

$$
\mathrm{G}\left[\{1,1\},1\right] = \frac{1}{2}\mathrm{G}^2\left[\{1\},1\right]=\frac{1}{2}S_1^2(\infty), \tag{C.6}
$$

$$
\mathrm{G}\left[\{1,1,1\},1\right] = \frac{1}{6}\mathrm{G}^3\left[\{1\},1\right]=-\frac{1}{6}S_1^3(\infty), \quad \text{etc.} \tag{C.7}
$$

emerge, cf. also [112], where $S_1(\infty)$ drops out in the amplitude.

By using the relations

$$
\mathrm{H}_{-2}(1) = \ln(3)-\ln(2), \tag{C.8}
$$

$$
\mathrm{H}_{0,-2}(1) = -\mathrm{Li}_2\left(-\frac{1}{2}\right), \tag{C.9}
$$

$$
\mathrm{H}_{-1,-3}(1) = \frac{1}{2}\zeta_2+\ln^2(2)-\ln(2)\ln(3)+\mathrm{Li}_2\left(-\frac{1}{2}\right), \tag{C.10}
$$

one shows that the contribution of $O(\ln(x)/x)$ to $\Delta a_{Qg}^{(3)}$ vanishes.

In the $O(1/x)$–term also G–functions at argument $x=1/4,\ 1/2$ and 1 occur. Their combination has to be shown to vanish too. Since these constants are of higher weight than in the case of the $O(\ln(x)/x)$–term, we will rationalize these constants to Kummer–Poincaré iterated integrals as has been outlined above. Of course, one can seek for basis representations of this type of integrals, cf. [53, 103], but in the end also the specific relations of these numbers have to be exploited, since the G–functions will occur at different main argument in any of these representations. The first constants are

$$
\mathrm{G}\left[\left\{\frac{\sqrt{5-4\tau}-1}{1-\tau}\right\},1\right] = -2-2\ln(2)+2\sqrt{5}+2\ln\left(\sqrt{5}-1\right), \tag{C.11}
$$

$$
\mathrm{G}\left[\left\{\frac{\sqrt{5-4\tau}}{1+\tau}\right\},1\right] = 2-2\sqrt{5}+3\ln(2)-6\ln\left(3-\sqrt{5}\right), \tag{C.12}
$$

$$
\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\},\frac{1}{4}\right] = -2, \tag{C.13}
$$

$$
\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{2+\tau}\right\},\frac{1}{4}\right] = -2+3\ln(2), \tag{C.14}
$$

$$
\mathrm{H}_{0,-1,-2}(1) = -\frac{13}{8}\zeta_3-\frac{1}{2}\zeta_2\ln(2)+\zeta_2\ln(3)-\frac{1}{6}\ln^3(3)-\mathrm{Li}_3\left(-\frac{1}{3}\right)
$$

$$+2\mathrm{Li}_3\left(\frac{1}{3}\right), \tag{C.15}$$

$$\mathrm{Li}_2\left(-\frac{1}{3}\right) = -\zeta_2 - \ln^2(2) + 2\ln(2)\ln(3) - \frac{1}{2}\ln^2(3) - 2\mathrm{Li}_2\left(-\frac{1}{2}\right). \tag{C.16}$$

By using the implementation of [168] one shall in general rescale the main argument of the G–functions to $x = 1$ for the numerical calculation. The $O(1/x)$ term contains G–constants with root–valued letters and the above H–constants. It is given by

$$\begin{aligned}
\frac{c_1}{x} = {}& (C_A - 2C_F)^2 T_F \Biggl\{ 48\mathrm{G}\left[\left\{\frac{1}{2-\tau}, \frac{1}{1-\tau}, \frac{-1+\sqrt{5-4\tau}}{1-\tau}\right\}, 1\right] \\
& -32\mathrm{G}\left[\left\{\frac{-1+\sqrt{5-4\tau}}{1-\tau}, \frac{1}{1-\tau}\right\}, 1\right] + 48\mathrm{G}\left[\left\{\frac{1}{2-\tau}, \frac{-1+\sqrt{5-4\tau}}{1-\tau}, \frac{1}{1-\tau}\right\}, 1\right\} \\
& -32\mathrm{G}\left[\left\{\frac{1}{\tau}, \frac{1}{1-\tau}, \frac{-1+\sqrt{5-4\tau}}{1-\tau}\right\}, 1\right] - 32\mathrm{G}\left[\left\{\frac{1}{\tau}, \frac{-1+\sqrt{5-4\tau}}{1-\tau}, \frac{1}{1-\tau}\right\}, 1\right] \\
& +16\mathrm{G}\left[\left\{\frac{-1+\sqrt{5-4\tau}}{1-\tau}, \frac{1}{1-\tau}, \frac{1}{1-\tau}\right\}, 1\right] - 192\ln(2)\left[2 - \frac{\pi}{\sqrt{3}}\right] \\
& -96\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{1-\tau}, \frac{1}{1-\tau}\right\}, \frac{1}{4}\right] + 96\mathrm{G}\left[\left\{\frac{\sqrt{5-4\tau}}{2-\tau}, \frac{1}{1-\tau}\right\}, 1\right] - 96\mathrm{G}\left[\left\{\frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{1-\tau}\right\}, \frac{1}{4}\right] \\
& -64\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{1-\tau}\right\}, \frac{1}{4}\right] - \frac{160}{3}\mathrm{G}\left[\left\{\frac{\sqrt{5-4\tau}}{\tau}, \frac{1}{1-\tau}\right\}, 1\right] \\
& -160\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{1+\tau}, \frac{1}{\tau}\right\}, \frac{1}{4}\right] - 48\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{1-\tau}, \frac{1}{1-\tau}\right\}, \frac{1}{4}\right] \\
& +48\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{1-\tau}, \frac{1}{\tau}\right\}, \frac{1}{4}\right] - 32\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}, \frac{1}{1-\tau}\right\}, \frac{1}{4}\right] \\
& +96\mathrm{G}\left[\left\{\frac{1}{1+\tau}, \frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}\right\}, \frac{1}{4}\right] + 96\mathrm{G}\left[\left\{\frac{1}{1+\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}\right\}, \frac{1}{4}\right] \\
& +\frac{16}{3}\mathrm{G}\left[\left\{\frac{\sqrt{5-4\tau}}{1+\tau}, \frac{1}{\tau}, \frac{1}{1-\tau}\right\}, 1\right] + 16\mathrm{G}\left[\left\{\frac{\sqrt{1-4\tau}}{2+\tau}, \frac{1}{1+\tau}, \frac{1}{\tau}\right\}\frac{1}{4}\right] + \Biggl[-\frac{32}{3} - 16\ln(2) \\
& +16\sqrt{5} + 48\ln(3) - 16\ln\left(3-\sqrt{5}\right) + 48\ln\left(\sqrt{5}-1\right)\Biggr]\zeta_2 - 120\zeta_3 + 384\ln^2(2) - 8\ln^3(3) \\
& -96\ln^2(5) - 192\mathrm{Li}_2\left[\frac{1}{5}\right] - 12\mathrm{Li}_3\left[\frac{1}{9}\right] + 144\mathrm{Li}_3\left[\frac{1}{3}\right]\Biggr\} \stackrel{?}{=} 0.
\end{aligned} \tag{C.17}$$

One may perform the algebraic reduction [102]. After the rationalization there are still quadratic forms in the denominators. The main argument will generally be different from 1. The decomposition into Kummer–Poincaré numbers leads to 197 terms, which are rescaled to main argument $x = 1$. These numbers were calculated to 1000 digits. In this way we showed that the $O(1/x)$ term vanishes at an accuracy of 10^{-998}. This accuracy can be further improved by calculating the G–functions to an even higher precision. We also compared all these constants with the result obtained by using `NumericalValues`, which delivers 6–7 digits only. The numerical values of the constants occurring in (C.17) are given in an ancillary file.

Accordingly, the expansion of the first–order factorizable terms of the amplitude around $x = 0, 1/2$ and 1 to 100 terms lead to a much larger number of G–constants. Their calculation proceeds in the same way.

In the asymptotic expansion of the finite binomial sums also G–functions with two different root–factors out of the set

$$\left\{\sqrt{x(x+1)}, \quad \sqrt{x(1-x)}, \quad \sqrt{1-x^2}\right\} \tag{C.18}$$

emerge. Structures of this kind can be rationalized by the transformation, cf. [185],

$$x = \frac{2y^2}{y^4+1}, \qquad y = \frac{1}{\sqrt{2x}}[\sqrt{1+x} - \sqrt{1-x}]. \tag{C.19}$$

After rationalization, one expects letters of cyclotomy 4, [100], i.e. the emergence of π and the Catalan number C [187], as well as of other cyclotomic constants. For the simplest integrals one obtains

$$\int_0^1 dx \sqrt{x(1+x)} = 4\sqrt{2}\int_0^1 dy \frac{y^2(1+y^2)(1-y^4)}{(1+y^4)^3} = \frac{3}{2\sqrt{2}} - \frac{1}{4}\ln(1+\sqrt{2}) \tag{C.20}$$

$$\int_0^1 dx \sqrt{x(1-x)} = 4\sqrt{2}\int_0^1 dy \frac{y^2(1-y^2)(1-y^4)}{(1+y^4)^3} = \frac{\pi}{8} \tag{C.21}$$

$$\int_0^1 dx \sqrt{1-x^2} = 4\int_0^1 dy \frac{y(1-y^4)^2}{(1+y^4)^3} = \frac{\pi}{4} \tag{C.22}$$

$$\begin{aligned}\int_0^1 dx \sqrt{x(1+x)}\int_0^x dy\sqrt{y(1-y)} &= 32\int_0^1 dx\int_0^x dy \frac{x^2(1-x^2)(1+x^2)^2 y^2(1+y^2)(1-y^2)^2}{\left(1+x^4\right)^3\left(1+y^4\right)^3} \\ &= -\frac{17}{96} + \frac{\mathsf{C}}{16} + \pi\left[\frac{3}{16}\frac{1}{\sqrt{2}} - \frac{1}{32}\ln\left(1+\sqrt{2}\right)\right].\end{aligned} \tag{C.23}$$

$$\begin{aligned}&\int_0^1 dx\sqrt{x(1+x)}\int_0^x dy\sqrt{1-y^2} = \int_0^1 dx \int_0^x dy \frac{16\sqrt{2}x^2(1-x^2)\left(1+x^2\right)^2 y(1-y^4)^2}{\left(1+x^4\right)^3\left(1+y^4\right)^3} \\ &= \pi\left[-\frac{27}{256} + \frac{3}{8}\frac{1}{\sqrt{2}}\right] + \frac{i}{16}\Biggl\{\mathrm{Li}_2\left[1-\sqrt[4]{-1}\right] - \mathrm{Li}_2\left[1+(-1)^{3/4}\right] \\ &+\mathrm{Li}_2\left[\frac{1}{2}\left((1-i)-\sqrt{2}\right)\right] - \mathrm{Li}_2\left[\frac{1}{2}\left((1+i)-\sqrt{2}\right)\right] + \mathrm{Li}_2\left[\frac{1}{2}\left((1+i)-i\sqrt{2}\right)\right] \\ &-\mathrm{Li}_2\left[\frac{1}{2}i\left((-1-i)+\sqrt{2}\right)\right] + \mathrm{Li}_2\left[\frac{2}{(1-i)+\sqrt{2}}\right] - \mathrm{Li}_2\left[\frac{2}{(1+i)+\sqrt{2}}\right] \\ &+2\mathrm{Li}_2\left[\frac{1}{4}(1+i)\left((1-i)+\sqrt{2}\right)\right] - 2i\mathrm{Li}_2\left[\frac{1}{4}(1-i)\left((1+i)+\sqrt{2}\right)\right]\Biggr\}.\end{aligned} \tag{C.24}$$

One may easily write Eq. (C.24) in terms of several generalized hypergeometric functions. However, the representation in terms of polylogarithms and cyclotomic functions is obtained only by rationalizing the integrand.

D Analytic continuation to N-space

One may use the representations of Eq. (5.11–5.13) to perform the analytic continuation to N–space in the analyticity region in $N \in \mathbb{C}$. The following integrals contribute

$$I_1(N,k,l;a) = \int_0^a dx x^{N-1+k} \ln^l(x), \quad k \geq 0, l \leq 5, k, l \in \mathbb{N}, a \in [0,1], \tag{D.1}$$

$$I_2(N,k;b,a) = \int_a^b dx x^{N-1} \left(\frac{1}{2} - x\right)^k, \quad b > \frac{1}{2} > a, a, b \in [0,1], \tag{D.2}$$

$$I_3(N,m;b) = \int_b^1 dx x^{N-1} \ln^m(1-x), \quad m \leq 5, m \in \mathbb{N}, b \in [0,1]. \tag{D.3}$$

These integrals are related to incomplete Beta- and Γ–functions [188]. However, we will use different representations in the following, based on generalized harmonic sums, cf. [53], to allow for simpler representations for $N \in \mathbb{C}$.

One obtains

$$I_1(N,k,l;a) = a^{N+k} \sum_{m=0}^{l} \frac{l!}{(l-m)!} \frac{(-1)^m \ln^{l-m}(a)}{(N+k)^{m+1}} \tag{D.4}$$

and I_1 may be expressed in terms of generalized harmonic sums

$$\frac{a^{N+k}}{(N+k)^\nu} = S_\nu(a)(N+k) - S_\nu(a)(N+k-1), \quad \nu \leq 6, \nu \in \mathbb{N}, a \in [0,1], \tag{D.5}$$

through which its first–order recurrence in N and the asymptotic representations are provided. The function I_2 is written as

$$I_2(N,k;a,b) = \bar{I}_2(N,k;b) - \bar{I}_2(N,k;a); \qquad \bar{I}_2(N,k;a) = I_2(N,k;a,0). \tag{D.6}$$

$\bar{I}_2$ obeys

$$\bar{I}_2(N,k;a) = \frac{a^N}{N}\left(\frac{1}{2} - a\right)^k + \frac{k}{N}\bar{I}_2(N+1,k-1;a), \tag{D.7}$$

$$\bar{I}_2(N,0;a) = \frac{a^N}{N}. \tag{D.8}$$

One may start with the initial condition (D.8) and needs no asymptotic expansion for the representation in $N \in \mathbb{C}$ in this case.

We write I_3 by

$$I_3(N,m;b) = \frac{(-1)^m m!}{N} S_{\underbrace{1,\ldots,1}_{m}} - \bar{I}_3(N,m;b) \tag{D.9}$$

$$\bar{I}_3(N,m;b) = b^N \mathbf{M}[\ln^m(1-xb)](N), \tag{D.10}$$

where

$$\bar{I}_3(N,0;b) = \frac{b^N}{N}, \tag{D.11}$$

$$\bar{I}_3(N,1;b) = -\frac{1}{N}\left[S_1(\{b\}) + \left(1 - b^N\right)\ln(1-b)\right], \tag{D.12}$$

$$
\begin{aligned}
\bar{I}_3(N,2;b) &= \frac{1}{N}\Biggl[2\bigl(S_1 S_1(\{b\}) + S_2(\{b\}) - S_{1,1}(\{b,1\})\bigr) + 2\bigl(S_1 - S_1(\{b\})\bigr)\ln(1-b) \\
&\quad -\bigl(1-b^N\bigr)\ln^2(1-b)\Biggr]. \qquad \text{(D.13)}
\end{aligned}
$$

The higher terms are given in an ancillary file. The recursions for the generalized harmonic sums are given in Eq. (4.6). The asymptotic expansions of the generalized sums for $|N| \rightarrow \infty$ read

$$
\begin{aligned}
S_1(\{b\},N) &= -\ln(1-b) + \Biggl[-\frac{1}{(1-b)N} + \frac{1}{(1-b)^2N^2} - \frac{1+b}{(1-b)^3N^3} + \frac{1+4b+b^2}{(1-b)^4N^4} \\
&\quad -\frac{(1+b)\bigl(1+10b+b^2\bigr)}{(1-b)^5N^5}\Biggr] b^{N+1} + O\left(\frac{1}{N^6}\right), \qquad \text{(D.14)} \\
S_2(\{b\},N) &= \mathrm{Li}_2(b) + \Biggl[-\frac{1}{(1-b)N^2} + \frac{2}{(1-b)^2N^3} - \frac{3(1+b)}{(1-b)^3N^4} + \frac{4\bigl(1+4b+b^2\bigr)}{(1-b)^4N^5}\Biggr] b^{N+1} \\
&\quad +O\left(\frac{1}{N^6}\right), \qquad \text{(D.15)} \\
S_{1,1}(\{b,1\},N) &= \frac{1}{2}\ln^2(1-b) + \mathrm{Li}_2(b) + \Biggl[-\frac{3-b}{2(1-b)^2N^2} + \frac{31+4b+b^2}{12(1-b)^3N^3} - \frac{43+82b+7b^2}{12(1-b)^4N^4} \\
&\quad + -\frac{-549-3414b-1964b^2-74b^3+b^4}{120(1-b)^5N^5} + L\Biggl[-\frac{1}{(1-b)N} + \frac{1}{(1-b)^2N^2} \\
&\quad -\frac{1+b}{(1-b)^3N^3} + \frac{1+4b+b^2}{(1-b)^4N^4} - \frac{(1+b)\bigl(1+10b+b^2\bigr)}{(1-b)^5N^5}\Biggr]\Biggr] b^{N+1} \\
&\quad +O\left(\frac{1}{N^6}\right), \quad \text{etc.} \qquad \text{(D.16)}
\end{aligned}
$$

The representations given in this appendix will also apply to the complete representations for $a_{Qg}^{(3)(N)}$ and $\Delta a_{Qg}^{(3)(N)}$.

Acknowledgments.
We would like to thank S. Klein for calculating a series of Mellin moments in the polarized case [189] by using `MATAD`, which we have used for comparison and thank P. Marquard for discussions. This work was supported by the Austrian Science Fund (FWF) grants P33530 and P34501N.

References

[1] S. Bethke *et al.*, *Workshop on Precision Measurements of α_s*, arXiv:1110.0016 [hep-ph].

[2] S. Moch *et al.*, *High precision fundamental constants at the TeV scale*, arXiv:1405.4781 [hep-ph].

[3] S. Alekhin, J. Blümlein and S.O. Moch, *α_s from global fits of parton distribution functions*, Mod. Phys. Lett. A **31** (2016) no.25, 1630023.

[4] D. d'Enterria et al., *The strong coupling constant: State of the art and the decade ahead*, [arXiv:2203.08271 [hep-ph]].

[5] A. Accardi *et al.*, *A Critical Appraisal and Evaluation of Modern PDFs*, Eur. Phys. J. C **76** (2016) no.8, 471 [arXiv:1603.08906 [hep-ph]].

[6] S. Alekhin, J. Blümlein, S. Moch and R. Placakyte, *Parton distribution functions, α_s, and heavy-quark masses for LHC Run II*, Phys. Rev. D **96** (2017) no.1, 014011 [arXiv:1701.05838 [hep-ph]].

[7] S. Alekhin, J. Blümlein, K. Daum, K. Lipka and S. Moch, *Precise charm-quark mass from deep-inelastic scattering*, Phys. Lett. B **720** (2013) 172–176 [arXiv:1212.2355 [hep-ph]].

[8] J. Blümlein and H. Böttcher, *Higher Twist Contributions to the Structure Functions $F_2^p(x,Q^2)$ and $F_2^d(x,Q^2)$ at Large x and Higher Orders*, Phys. Lett. B **662** (2008) 336–340 [arXiv:0802.0408 [hep-ph]].

[9] J. Blümlein and H. Böttcher, *Higher Twist contributions to the Structure Functions $F_2(x,Q^2)$ and $g_2(x,Q^2)$*, Proc. of DIS 2012, Bonn, 2012, 237–241, DESY-PROC-2012-02, [arXiv:1207.3170 [hep-ph]].

[10] S. Alekhin, J. Blümlein and S. Moch, *Parton Distribution Functions and Benchmark Cross Sections at NNLO*, Phys. Rev. D **86** (2012) 054009 [arXiv: 1202.2281 [hep-ph]].

[11] M. Buza, Y. Matiounine, J. Smith, R. Migneron and W.L. van Neerven, *Heavy quark coefficient functions at asymptotic values $Q^2 \gg m^2$*, Nucl. Phys. B **472** (1996) 611–658 [hep-ph/9601302].

[12] S. Moch, J.A.M. Vermaseren and A. Vogt, *The Three loop splitting functions in QCD: The Nonsinglet case*, Nucl. Phys. B **688** (2004) 101–134 [hep-ph/0403192].

[13] A. Vogt, S. Moch and J.A.M. Vermaseren, *The Three-loop splitting functions in QCD: The Singlet case*, Nucl. Phys. B **691** (2004) 129–181 [hep-ph/0404111].

[14] J.A.M. Vermaseren, A. Vogt and S. Moch, *The Third-order QCD corrections to deep-inelastic scattering by photon exchange*, Nucl. Phys. B **724** (2005) 3–182 [hep-ph/0504242].

[15] J. Ablinger, J. Blümlein, S. Klein, C. Schneider and F. Wißbrock, *The $O(\alpha_s^3)$ Massive Operator Matrix Elements of $O(N_f)$ for the Structure Function $F_2(x,Q^2)$ and Transversity*, Nucl. Phys. B **844** (2011) 26–54 [arXiv:1008.3347 [hep-ph]].

[16] J. Blümlein, A. Hasselhuhn, S. Klein and C. Schneider, *The $O(\alpha_s^3 N_f T_F^2 C_{A,F})$ Contributions to the Gluonic Massive Operator Matrix Elements*, Nucl. Phys. B **866** (2013) 196–211 [arXiv:1205.4184 [hep-ph]].

[17] J. Ablinger, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider and F. Wißbrock, *The Transition Matrix Element $A_{gq}(N)$ of the Variable Flavor Number Scheme at $O(\alpha_s^3)$*, Nucl. Phys. B **882** (2014) 263–288 [arXiv:1402.0359 [hep-ph]].

[18] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider and F. Wißbrock, *The 3-Loop Non-Singlet Heavy Flavor Contributions and Anomalous Dimensions for the Structure Function $F_2(x,Q^2)$ and Transversity*, Nucl. Phys. B **886** (2014) 733–823 [arXiv:1406.4654 [hep-ph]].

[19] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel and C. Schneider, *The 3-loop pure singlet heavy flavor contributions to the structure function $F_2(x,Q^2)$ and the anomalous dimension*, Nucl. Phys. B **890** (2014) 48–151 [arXiv: 1409.1135 [hep-ph]].

[20] S. Moch, J.A.M. Vermaseren and A. Vogt, *The Three-Loop Splitting Functions in QCD: The Helicity-Dependent Case*, Nucl. Phys. B **889** (2014) 351–400 [arXiv: 1409.5131 [hep-ph]].

[21] C. Anastasiou, C. Duhr, F. Dulat, F. Herzog and B. Mistlberger, *Higgs Boson Gluon-Fusion Production in QCD at Three Loops*, Phys. Rev. Lett. **114** (2015) 212001 [arXiv:1503.06056 [hep-ph]].

[22] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel and C. Schneider, *The three-loop splitting functions $P_{qg}^{(2)}$ and $P_{gg}^{(2,N_F)}$*, Nucl. Phys. B **922** (2017) 1–40 [arXiv:1705.01508 [hep-ph]].

[23] B. Mistlberger, *Higgs boson production at hadron colliders at N^3LO in QCD*, JHEP **05** (2018) 028 [arXiv:1802.00833 [hep-ph]].

[24] A. Behring, J. Blümlein, A. De Freitas, A. Goedicke, S. Klein, A. von Manteuffel, C. Schneider and K. Schönwald, *The Polarized Three-Loop Anomalous Dimensions from On-Shell Massive Operator Matrix Elements*, Nucl. Phys. B **948** (2019) 114753 [arXiv:1908.03779 [hep-ph]].

[25] M.X. Luo, T.Z. Yang, H.X. Zhu and Y.J. Zhu, *Quark Transverse Parton Distribution at the Next-to-Next-to-Next-to-Leading Order*, Phys. Rev. Lett. **124** (2020) no.9, 092001 [arXiv:1912.05778 [hep-ph]].

[26] C. Duhr, F. Dulat and B. Mistlberger, *Drell-Yan Cross Section to Third Order in the Strong Coupling Constant*, Phys. Rev. Lett. **125** (2020) no.17 172001 [arXiv: 2001.07717 [hep-ph]].

[27] M.A. Ebert, B. Mistlberger and G. Vita, *Transverse momentum dependent PDFs at N^3LO*, JHEP **09** (2020) 146 [arXiv: 2006.05329 [hep-ph]].

[28] M.A. Ebert, B. Mistlberger and G. Vita, *N-jettiness beam functions at N^3LO*, JHEP **09** (2020) 143 [arXiv:2006.03056 [hep-ph]].

[29] J. Blümlein, P. Marquard, C. Schneider and K. Schönwald, *The three-loop unpolarized and polarized non-singlet anomalous dimensions from off shell operator matrix elements*, Nucl. Phys. B **971** (2021) 115542 [arXiv:2107.06267 [hep-ph]].

[30] M.X. Luo, T.Z. Yang, H.X. Zhu and Y.J. Zhu, *Unpolarized quark and gluon TMD PDFs and FFs at N^3LO*, JHEP **06** (2021) 115 [arXiv:2012.03256 [hep-ph]].

[31] J. Blümlein, P. Marquard, C. Schneider and K. Schönwald, *The three-loop polarized singlet anomalous dimensions from off-shell operator matrix elements*, JHEP **01** (2022) 193 [arXiv: 2111.12401 [hep-ph]].

[32] J. Blümlein, P. Marquard, C. Schneider and K. Schönwald, *The massless three-loop Wilson coefficients for the deep-inelastic structure functions F_2, F_L, xF_3 and g_1*, JHEP **11** (2022) 156 [arXiv:2208.14325 [hep-ph]].

[33] D. Baranowski, A. Behring, K. Melnikov, L. Tancredi and C. Wever, *Beam functions for N-jettiness at N^3LO in perturbative QCD*, JHEP **02** (2023) 073 [arXiv:2211.05722 [hep-ph]].

[34] T. Gehrmann, A. von Manteuffel and T.Z. Yang, *Renormalization of twist-two operators in covariant gauge to three loops in QCD*, JHEP **04** (2023) 041 [arXiv:2302.00022 [hep-ph]].

[35] A. Behring, I. Bierenbaum, J. Blümlein, A. De Freitas, S. Klein and F. Wißbrock, *The logarithmic contributions to the $O(\alpha_s^3)$ asymptotic massive Wilson coefficients and operator matrix elements in deeply inelastic scattering*, Eur. Phys. J. C **74** (2014) no.9, 3033 [arXiv:1403.6356 [hep-ph]].

[36] A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, K. Schönwald and C. Schneider, *The polarized transition matrix element $A_{gq}(N)$ of the variable flavor number scheme at $O(\alpha_s^3)$*, Nucl. Phys. B **964** (2021) 115331 [arXiv:2101.05733 [hep-ph]].

[37] J. Blümlein, A. De Freitas, M. Saragnese, C. Schneider and K. Schönwald, *Logarithmic contributions to the polarized $O(\alpha_s^3)$ asymptotic massive Wilson coefficients and operator matrix elements in deeply inelastic scattering*, Phys. Rev. D **104** (2021) no.3, 034030 [arXiv:2105.09572 [hep-ph]].

[38] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. Goedicke, A. von Manteuffel, C. Schneider and K. Schönwald, *The unpolarized and polarized single-mass three-loop heavy flavor operator matrix elements $A_{gg,Q}$ and $\Delta A_{gg,Q}$*, JHEP **12** (2022) 134 [arXiv:2211.05462 [hep-ph]].

[39] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, C. Schneider and K. Schönwald, *The three-loop single mass polarized pure singlet operator matrix element*, Nucl. Phys. B **953** (2020) 114945 [arXiv:1912.02536 [hep-ph]].

[40] J. Ablinger, J. Blümlein, A. De Freitas, A. Hasselhuhn, C. Schneider and F. Wißbrock, *Three Loop Massive Operator Matrix Elements and Asymptotic Wilson Coefficients with Two Different Masses*, Nucl. Phys. B **921** (2017) 585–688 [arXiv:1705.07030 [hep-ph]].

[41] J. Ablinger, J. Blümlein, A. De Freitas, C. Schneider and K. Schönwald, *The two-mass contribution to the three-loop pure singlet operator matrix element*, Nucl. Phys. B **927** (2018) 339–367 [arXiv:1711.06717 [hep-ph]].

[42] J. Ablinger, J. Blümlein, A. De Freitas, A. Goedicke, C. Schneider and K. Schönwald, *The Two-mass Contribution to the Three-Loop Gluonic Operator Matrix Element* $A_{gg,Q}^{(3)}$, Nucl. Phys. B **932** (2018) 129–240 [arXiv:1804.02226 [hep-ph]].

[43] J. Ablinger, J. Blümlein, A. De Freitas, M. Saragnese, C. Schneider and K. Schönwald, *The three-loop polarized pure singlet operator matrix element with two different masses*, Nucl. Phys. B **952** (2020) 114916 [arXiv:1911.11630 [hep-ph]].

[44] J. Ablinger, J. Blümlein, A. De Freitas, A. Goedicke, M. Saragnese, C. Schneider and K. Schönwald, *The two-mass contribution to the three-loop polarized gluonic operator matrix element* $\Delta A_{gg,Q}^{(3)}$, Nucl. Phys. B **955** (2020) 115059 [arXiv:2004.08916 [hep-ph]].

[45] J. Blümlein, J. Ablinger, A. Behring, A. De Freitas, A. von Manteuffel, and C. Schneider, *Heavy Flavor Wilson Coefficients in Deep-Inelastic Scattering: Recent Results*, PoS (QCDEV2017) 031 [arXiv:1711.07957 [hep-ph]].

[46] M. Buza, Y. Matiounine, J. Smith and W.L. van Neerven, *Charm electroproduction viewed in the variable flavor number scheme versus fixed order perturbation theory*, Eur. Phys. J. C **1** (1998) 301–320 [hep-ph/9612398].

[47] J. Blümlein, A. De Freitas, C. Schneider and K. Schönwald, *The Variable Flavor Number Scheme at Next-to-Leading Order*, Phys. Lett. B **782** (2018) 362–366 [arXiv:1804.03129 [hep-ph]].

[48] I. Bierenbaum, J. Blümlein, A. De Freitas, A. Goedicke, S. Klein and K. Schönwald, $O(\alpha_s^2)$ *polarized heavy flavor corrections to deep-inelastic scattering at* $Q^2 \gg m^2$, Nucl. Phys. B **988** (2023) 116114 [arXiv:2211.15337 [hep-ph]].

[49] S.A. Larin, *The Renormalization of the axial anomaly in dimensional regularization*, Phys. Lett. B **303** (1993) 113–118 [hep-ph/9302240].

[50] J. Blümlein and M. Saragnese, *The* N^3LO *scheme-invariant QCD evolution of the non-singlet structure functions* $F_2^{\rm NS}(x,Q^2)$ *and* $g_1^{\rm NS}(x,Q^2)$, Phys. Lett. B **820** (2021) 136589 [arXiv:2107.01293 [hep-ph]].

[51] J. Blümlein and C. Schneider, *The Method of Arbitrarily Large Moments to Calculate Single Scale Processes in Quantum Field Theory*, Phys. Lett. B **771** (2017) 31–36 [arXiv:1701.04614 [hep-ph]].

[52] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, C. Schneider, and K. Schönwald, *The non–first–order factorizable contributions to the three–loop massive operator matrix elements* $A_{Qg}^{(3)}$ *and* $\Delta A_{Qg}^{(3)}$, DO–TH 23/15.

[53] J. Ablinger, J. Blümlein and C. Schneider, *Analytic and Algorithmic Aspects of Generalized Harmonic Sums and Polylogarithms*, J. Math. Phys. **54** (2013) 082301 [arXiv:1302.0378 [math-ph]].

[54] J. Ablinger, J. Blümlein, C.G. Raab and C. Schneider, *Iterated Binomial Sums and their Associated Iterated Integrals*, J. Math. Phys. **55** (2014) 112301 [arXiv:1407.1822 [hep-th]].

[55] J.A.M. Vermaseren, *Harmonic sums, Mellin transforms and integrals*, Int. J. Mod. Phys. A **14** (1999) 2037–2076 [hep-ph/9806280].

[56] J. Blümlein and S. Kurth, *Harmonic sums and Mellin transforms up to two loop order*, Phys. Rev. D **60** (1999) 014018 [hep-ph/9810241].

[57] J. Blümlein, *Structural Relations of Harmonic Sums and Mellin Transforms up to Weight* $w = 5$, Comput. Phys. Commun. **180** (2009) 2218–2249 [arXiv:0901.3106 [hep-ph]].

[58] J. Blümlein, *Structural Relations of Harmonic Sums and Mellin Transforms at Weight* $w = 6$, Clay Math. Proc. **12** (2010) 167–188 [arXiv:0901.0837 [math-ph]].

[59] M. Karr, *Summation in Finite Terms*, J. ACM **28** (1981) 305–350.

[60] M. Bronstein, *On Solutions of Linear Ordinary Difference Equations in their Coefficient Field*, J. Symbolic Comput. **29** (2000) no. 6 841–877.

[61] C. Schneider, *Symbolic Summation in Difference Fields*, Ph.D. Thesis RISC, Johannes Kepler University, Linz technical report 01–17 (2001).

[62] C. Schneider, *A Collection of Denominator Bounds to Solve Parameterized Linear Difference Equations in* $\Pi\Sigma$*-Extensions*, An. Univ. Timisoara Ser. Mat.-Inform. **42** (2004) 163–179.

[63] C. Schneider, *Solving parameterized linear difference equations in terms of indefinite nested sums and products*, J. Differ. Equations Appl. **11** (2005) 799–821.

[64] C. Schneider, *Degree bounds to find polynomial solutions of parameterized linear difference equations in* $\Pi\Sigma$*–fields*, Appl. Algebra Engrg. Comm. Comput. **16** (1) (2005) 1–32.

[65] C. Schneider, *Simplifying Sums in* $\Pi\Sigma^*$*–Extensions*, J. Algebra Appl. **6** (2007) 415–441.

[66] C. Schneider, *A Symbolic Summation Approach to Find Optimal Nested Sum Representations*, Clay Math. Proc. **12** (2010) 285–308 [arXiv:0904.2323 [cs.SC]].

[67] C. Schneider, *Parameterized Telescoping Proves Algebraic Independence of Sums*, Ann. Comb. **14** (2010) 533–552 [arXiv:0808.2596 [cs.SC]].

[68] C. Schneider, in: *Fast Algorithms for Refined Parameterized Telescoping in Difference Fields*, Computer Algebra and Polynomials, Applications of Algebra and Number Theory, J. Gutierrez, J. Schicho, M. Weimann (ed.), Lecture Notes in Computer Science (LNCS) 8942 (2015) 157–191 [arXiv:1307.7887 [cs.SC]].

[69] C. Schneider, *A Difference Ring Theory for Symbolic Summation*, J. Symb. Comput. **72** (2016) 82–127 [arXiv:1408.2776 [cs.SC]].

[70] C. Schneider, *Summation Theory II: Characterizations of* $R\Pi\Sigma^*$*-extensions and algorithmic aspects*, J. Symb. Comput. **80** (2017) 616–664 [arXiv:1603.04285 [cs.SC]].

[71] S.A. Abramov, M. Bronstein, M. Petkovšek, C. Schneider, *On Rational and Hypergeometric Solutions of Linear Ordinary Difference Equations in* $\Pi\Sigma^*$*–field extensions*, J. Symb. Comput. **107** (2021) 23–66 [arXiv:2005.04944 [cs.SC]].

[72] S.A. Abramov and M. Petkovšek, *D'Alembertian solutions of linear differential and difference equations*, in: Proceedings of ISSAC'94, ed. by J. von zur Gathen (ACM Press, New York, 1994), 169–174.

[73] C. Schneider, *Symbolic Summation Assists Combinatorics*, Sém. Lothar. Combin. **56** (2007) 1–36 article B56b.

[74] C. Schneider, *Simplifying Multiple Sums in Difference Fields*, in: Computer Algebra in Quantum Field Theory: Integration, Summation and Special Functions Texts and Monographs in Symbolic Computation eds. C. Schneider and J. Blümlein (Springer, Wien, 2013) 325–360 [arXiv:1304.4134 [cs.SC]].

[75] E.E. Kummer, J. Reine Angew. Math. (Crelle) *Ueber die Transcendenten, welche aus wiederholten Integrationen rationaler Formeln entstehen*, **21** (1840) 74–90.

[76] E.E. Kummer, J. Reine Angew. Math. (Crelle) *Ueber die Transcendenten, welche aus wiederholten Integrationen rationaler Formeln entstehen (Fortsetzung)*, **21** (1840) 193–225.

[77] E.E. Kummer, J. Reine Angew. Math. (Crelle) *Ueber die Transcendenten, welche aus wiederholten Integrationen rationaler Formeln entstehen (Fortsetzung)*, **21** (1840) 328–371.

[78] H. Poincaré, *Sur les groupes des équations linéaires*, Acta Math. **4** (1884) 201–312.

[79] J.A. Lappo–Danilevsky, Mémoirs sur la Théorie des Systèmes Différentielles Linéaires, (Chelsea Publishing Company, New York, 1953).

[80] K.T. Chen, *Algebras of iterated path integrals and fundamental groups*, Trans. A.M.S. **156** (3) (1971) 359–379.

[81] A.B. Goncharov, *Multiple polylogarithms, cyclotomy and modular complexes*, Math. Res. Lett. **5** (1998) 497–516.

[82] P. Nogueira, *Automatic Feynman graph generation*, J. Comput. Phys. **105** (1993) 279–289.

[83] F. Yndurain, The Theory of Quark and Gluon Interactions, (Springer, Berlin 2006).

[84] I. Bierenbaum, J. Blümlein and S. Klein, *Mellin Moments of the $O(\alpha_s^3)$ Heavy Flavor Contributions to unpolarized Deep-Inelastic Scattering at $Q^2 \gg m^2$ and Anomalous Dimensions*, Nucl. Phys. B **820** (2009) 417–482 [arXiv:0904.3563 [hep-ph]].

[85] J.A.M. Vermaseren, *New features of FORM*, math-ph/0010025.

[86] M. Tentyukov and J.A.M. Vermaseren, *The Multithreaded version of FORM*, Comput. Phys. Commun. **181** (2010) 1419–1427 [hep-ph/0702279].

[87] T. van Ritbergen, A.N. Schellekens and J.A.M. Vermaseren, *Group theory factors for Feynman diagrams*, Int. J. Mod. Phys. A **14** (1999) 41–96 [hep-ph/9802376].

[88] J. Lagrange, Nouvelles recherches sur la nature et la propagation du son, Miscellanea Taurinensis, t. II, 1760-61; Oeuvres t. I, p. 263.

[89] C.F. Gauß, Theoria attractionis corporum sphaeroidicorum ellipticorum homogeneorum methodo novo tractate, Commentationes societas scientiarum Gottingensis recentiores, Vol III, 1813, Werke Bd. **V** pp. 5–7.

[90] G. Green, Essay on the Mathematical Theory of Electricity and Magnetism, Nottingham, 1828 [Green Papers, pp. 1–115].

[91] M. Ostrogradski, *Première note sur la théorie de la chaleur*, Mem. Ac. Sci. St. Peters., **6**, (1831) 129–133.

[92] K.G. Chetyrkin and F.V. Tkachov, *Integration by Parts: The Algorithm to Calculate beta Functions in 4 Loops*, Nucl. Phys. B **192** (1981) 159–204.

[93] S. Laporta, *High precision calculation of multiloop Feynman integrals by difference equations*, Int. J. Mod. Phys. A **15** (2000) 5087–5159 [hep-ph/0102033].

[94] C. Studerus, *Reduze-Feynman Integral Reduction in C++*, Comput. Phys. Commun. **181** (2010) 1293–1300 [arXiv:0912.2546 [physics. comp-ph]].

[95] A. von Manteuffel and C. Studerus, *Reduze 2 - Distributed Feynman Integral Reduction*, arXiv:1201.4330 [hep-ph].

[96] J. Blümlein and C. Schneider, *Analytic computing methods for precision calculations in quantum field theory*, Int. J. Mod. Phys. A **33** (2018) no.17, 1830015 [arXiv:1809.02889 [hep-ph]].

[97] J. Blümlein and C. Schneider, *The SAGEX review on scattering amplitudes Chapter 4: Multi-loop Feynman integrals*, J. Phys. A **55** (2022) no.44, 443005 [arXiv:2203.13015 [hep-th]].

[98] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel and C. Schneider, *Calculating Three Loop Ladder and V-Topologies for Massive Operator Matrix Elements by Computer Algebra*, Comput. Phys. Commun. **202** (2016) 33–112 [arXiv:1509.08324 [hep-ph]].

[99] J. Ablinger, J. Blümlein, P. Marquard, N. Rana and C. Schneider, *Automated Solution of First Order Factorizable Systems of Differential Equations in One Variable*, Nucl. Phys. B **939** (2019) 253–291 [arXiv:1810.12261 [hep-ph]].

[100] J. Ablinger, J. Blümlein and C. Schneider, *Harmonic Sums and Polylogarithms Generated by Cyclotomic Polynomials*, J. Math. Phys. **52** (2011) 102301 [arXiv:1105.6063 [math-ph]].

[101] E. Remiddi and J.A.M. Vermaseren, *Harmonic polylogarithms*, Int. J. Mod. Phys. A **15** (2000) 725–754 [hep-ph/9905237].

[102] J. Blümlein, *Algebraic relations between harmonic sums and associated quantities*, Comput. Phys. Commun. **159** (2004) 19–54 [hep-ph/0311046].

[103] J. Ablinger, J. Blümlein and C. Schneider, *Iterated integrals over letters induced by quadratic forms*, Phys. Rev. D **103** (2021) no.9, 096025 [arXiv:2103.08330 [hep-th]].

[104] J. Ablinger, *A Computer Algebra Toolbox for Harmonic Sums Related to Particle Physics*, Diploma Thesis, JKU Linz, 2009, arXiv:1011.1176[math-ph].

[105] J. Ablinger, *Computer Algebra Algorithms for Special Functions in Particle Physics*, Ph.D. Thesis, Linz U. (2012) arXiv:1305.0687[math-ph].

[106] J. Ablinger, *The package HarmonicSums: Computer Algebra and Analytic aspects of Nested Sums*, PoS (LL2014) 019 [arXiv:1407.6180 [cs.SC]].

[107] J. Ablinger, *Discovering and Proving Infinite Binomial Sums Identities*, Exper. Math. **26** (2016) no.1, 62–71 [arXiv:1507.01703 [math.NT]].

[108] J. Ablinger, *Inverse Mellin Transform of Holonomic Sequences*, PoS (LL2016) 067.

[109] J. Ablinger, *An Improved Method to Compute the Inverse Mellin Transform of Holonomic Sequences*, PoS (LL2018) 063.

[110] J. Ablinger, *Computing the Inverse Mellin Transform of Holonomic Sequences using Kovacic's Algorithm*, PoS (RADCOR2017) 001 [arXiv:1801.01039 [cs.SC]].

[111] J. Ablinger, *Discovering and Proving Infinite Pochhammer Sum Identities*, arXiv:1902.11001 [math.CO].

[112] J. Blümlein, D.J. Broadhurst and J.A.M. Vermaseren, *The Multiple Zeta Value Data Mine*, Comput. Phys. Commun. **181** (2010) 582–625 [arXiv:0907.2557 [math-ph]].

[113] B. Zürcher, *Rationale Normalformen von pseudo-linearen Abbildungen* Ph.D. Thesis Mathematik, ETH Zürich, 1994.

[114] A. Bostan, F. Chyzak and de É. Panafieu, *Complexity estimates for two uncoupling algorithms* Proc. ISSAC'13 (2013), Boston, 85–92, Ed. M. Kauers, [arXiv:1301.5414 [cs.SC]].

[115] S. Gerhold, *Uncoupling Systems of Linear Ore Operator Equations.* Master's thesis, RISC, J. Kepler University, Linz 2002.

[116] G. Almkvist and D. Zeilberger, *The method of differentiating under the integral sign*, J. Symbolic Comput. **10** (1990) 571–591.

[117] M. Apagodu and D. Zeilberger, *Multi-variable Zeilberger and Almkvist-Zeilberger algorithms and the sharpening of Wilf-Zeilberger theory*, Adv. Appl. Math. **37** (2006) 139–152.

[118] J. Ablinger, *Extensions of the AZ-Algorithm and the Package MultiIntegrate*, in: Anti–differentiation and the Calculation of Feynman Amplitudes, J. Blümlein and C. Schneider, Eds., (Springer, Berlin, 2021) [arXiv:2101.11385 [cs.SC]].

[119] M. Kauers, *Guessing Handbook*, JKU Linz, Technical Report RISC 09–07.

[120] J. Blümlein, M. Kauers, S. Klein and C. Schneider, *Determining the closed forms of the $O(a_s^3)$ anomalous dimensions and Wilson coefficients from Mellin moments by means of computer algebra*, Comput. Phys. Commun. **180** (2009) 2143–2165 [arXiv:0902.4091 [hep-ph]].

[121] Sage, `http://www.sagemath.org/`

[122] M. Kauers, M. Jaroschek, and F. Johansson, *Ore polynomials in* Sage, in: Computer Algebra and Polynomials, Editors: J. Gutierrez, J. Schicho, Josef, M. Weimann, Eds.. Lecture Notes in Computer Science **8942** (Springer, Berlin, 2015) 105–125 [arXiv:1306.4263 [cs.SC]].

[123] J. Ablinger, J. Blümlein, A. Hasselhuhn, S. Klein, C. Schneider and F. Wißbrock, *Massive 3-loop Ladder Diagrams for Quarkonic Local Operator Matrix Elements*, Nucl. Phys. B **864** (2012) 52–84 [arXiv:1206.2252 [hep-ph]].

[124] J. Ablinger, J. Blümlein, C. Raab, C. Schneider and F. Wißbrock, *Calculating Massive 3-loop Graphs for Operator Matrix Elements by the Method of Hyperlogarithms*, Nucl. Phys. B **885** (2014) 409–447 [arXiv:1403.1137 [hep-ph]].

[125] A. Behring, J. Blümlein and K. Schönwald, *The inverse Mellin transform via analytic continuation*, JHEP **06** (2023) 062 [arXiv:2303.05943 [hep-ph]].

[126] B. Riemann, *Ueber die Anzahl der Primzahlen unter einer gegebenen Grösse*, in: Berhard Riemann's Gesammelte Mathematische Werke und wissenschaftlicher Nachlass, herausgegeben von Heinrich Weber unter Mitwirkung von Richard Dedekind, (B.G. Teubner, Leipzig, 1876) 136–144, 2nd Edition 1892; (mit den Nachträgen herausgegeben von Max Noether und Wilhelm Wirtinger, Teubner 1902); Reprint Dover 1953.

[127] E. Cahen, *Sur la fonction $\zeta(s)$ de Riemann et sur des fonctions analogues*, Ann. de l'Éc. Norm. (3) **11** (1894) 75–164.

[128] H. Mellin, *Ueber die fundamentale Wichtigkeit des Satzes von Cauchy für die Theorien der Gamma- und der hypergeometrischen Funktionen*, Acta Soc. Fennicae **21** (1896) (1), 1–115.

[129] H. Mellin, *Ueber den Zusammenhang zwischen den linearen Differential- und Differenzengleichungen*, Acta Math. **25** (1902) 139–164.

[130] E.C. Titchmarsh, Introduction to the theory of Fourier integrals, (Oxford, Calendron Press, 1948), 2nd Edition.

[131] O.V. Tarasov, A.A. Vladimirov and A.Y. Zharkov, *The Gell-Mann-Low Function of QCD in the Three Loop Approximation*, Phys. Lett. B **93** (1980) 429–432.

[132] S.A. Larin and J.A.M. Vermaseren, *The Three loop QCD β function and anomalous dimensions*, Phys. Lett. B **303** (1993) 334–336 [hep-ph/9302208].

[133] T. van Ritbergen, J.A.M. Vermaseren and S.A. Larin, *The Four loop β function in quantum chromodynamics* Phys. Lett. B **400** (1997) 379–384 [hep-ph/9701390].

[134] M. Czakon, *The Four-loop QCD β-function and anomalous dimensions*, Nucl. Phys. B **710** (2005) 485–498 [hep-ph/0411261].

[135] K.G. Chetyrkin, *Four-loop renormalization of QCD: Full set of renormalization constants and anomalous dimensions*, Nucl. Phys. B **710** (2005) 499–510 [hep-ph/0405193].

[136] P.A. Baikov, K.G. Chetyrkin and J.H. Kühn, *Five-Loop Running of the QCD coupling constant*, Phys. Rev. Lett. **118** (2017) no.8, 082002 [arXiv:1606.08659 [hep-ph]].

[137] F. Herzog, B. Ruijl, T. Ueda, J.A.M. Vermaseren and A. Vogt, *The five-loop β function of Yang-Mills theory with fermions*, JHEP **02** (2017) 090 [arXiv:1701.01404 [hep-ph]].

[138] T. Luthe, A. Maier, P. Marquard and Y. Schröder, *The five-loop β function for a general gauge group and anomalous dimensions beyond Feynman gauge* JHEP **10** (2017) 166 [arXiv:1709.07718 [hep-ph]].

[139] T. Luthe, A. Maier, P. Marquard and Y. Schröder, *Complete renormalization of QCD at five loops*, JHEP **03** (2017) 020 [arXiv:1701.07068 [hep-ph]].

[140] K.G. Chetyrkin, G. Falcioni, F. Herzog and J.A.M. Vermaseren, *Five-loop renormalisation of QCD in covariant gauges*, JHEP **10** (2017) 179 [arXiv:1709.08541 [hep-ph]].

[141] K.G. Chetyrkin and M. Steinhauser, *Short distance mass of a heavy quark at $O(\alpha_s^3)$*, Phys. Rev. Lett. **83** (1999) 4001–4004 [hep-ph/9907509].

[142] K.G. Chetyrkin and M. Steinhauser, *The Relation between the $\overline{MS}$ and the on-shell quark mass at $O(\alpha_s^3)$*, Nucl. Phys. B **573** (2000) 617–651 [hep-ph/9911434].

[143] K. Melnikov and T. v. Ritbergen, *The Three loop relation between the $\overline{MS}$ and the pole quark masses*, Phys. Lett. B **482** (2000) 99–108 [hep-ph/9912391].

[144] D.J. Broadhurst, N. Gray and K. Schilcher, *Gauge invariant on-shell Z(2) in QED, QCD and the effective field theory of a static quark*, Z. Phys. C **52** (1991) 111–122.

[145] P. Marquard, A.V. Smirnov, V.A. Smirnov and M. Steinhauser, *Four-loop wave function renormalization in QCD and QED*, Phys. Rev. D **97** (2018) no.5, 054032 [arXiv:1801.08292 [hep-ph]].

[146] P. Marquard, A.V. Smirnov, V.A. Smirnov, M. Steinhauser and D. Wellmann, $\overline{\mathrm{MS}}$*-on-shell quark mass relation up to four loops in QCD and a general $SU(N)$ gauge group*, Phys. Rev. D **94** (2016) no.7, 074025 [arXiv:1606.06754 [hep-ph]].

[147] P. Marquard, A.V. Smirnov, V.A. Smirnov and M. Steinhauser, *Quark Mass Relations to Four-Loop Order in Perturbative QCD*, Phys. Rev. Lett. **114** (2015) no.14, 142002 [arXiv:1502.01030 [hep-ph]].

[148] J. Ablinger, J. Blümlein, A. De Freitas, M. van Hoeij, E. Imamoglu, C.G. Raab, C.S. Radu and C. Schneider, *Iterated Elliptic and Hypergeometric Integrals for Feynman Diagrams*, J. Math. Phys. **59** (2018) no.6, 062305 [arXiv:1706.01299 [hep-th]].

[149] L.D. Faddeev and V.N. Popov, *Feynman Diagrams for the Yang-Mills Field*, Phys. Lett. B **25** (1967) 29–30.

[150] E.C. Titchmarsh, The Theory of the Riemann Zeta-Function, (Calendron Press, Oxford, 1986), 2nd Edition, revised by D.R. Heath-Brown.

[151] A.D. Watson, *Spin Spin Asymmetries in Inclusive Muon Proton Charm Production*, Z. Phys. C **12** (1982) 123–125.

[152] M. Buza, Y. Matiounine, J. Smith and W.L. van Neerven, *$O(\alpha_2^2)$ corrections to polarized heavy flavor production at $Q^2 \gg m^2$*, Nucl. Phys. B **485** (1997) 420–456 [hep-ph/9608342].

[153] P.A. Baikov, K.G. Chetyrkin and J.H. Kühn, *Adler Function, Bjorken Sum Rule, and the Crewther Relation to $O(\alpha_s^4)$ in a General Gauge Theory*, Phys. Rev. Lett. **104** (2010) 132004 [arXiv:1001.3606 [hep-ph]].

[154] R.H. Mason and J.A. Gracey, *Kinematic scheme study of the $O(a^4)$ Bjorken sum rule and R ratio*, arXiv:2309.17112 [hep-ph].

[155] J. Blümlein, G. Falcioni and A. De Freitas, *The Complete $O(\alpha_s^2)$ Non-Singlet Heavy Flavor Corrections to the Structure Functions $g_{1,2}^{ep}(x,Q^2)$, $F_{1,2,L}^{ep}(x,Q^2)$, $F_{1,2,3}^{\nu(\bar{\nu})}(x,Q^2)$ and the Associated Sum Rules*, Nucl. Phys. B **910** (2016) 568–617 [arXiv:1605.05541 [hep-ph]].

[156] A. Jiménez-Pastor and M. Petkovsek, *The factorial–basis method for finding definite-sum solutions of linear recurrences with polynomial coefficients*, J. Symb. Comput., **117** (2023) 15–50 [arXiv:2202.05550 [cs.SC]]

[157] G.D. Birkhoff, *Formal theory of irregular difference equations*, Acta Math. **54** (1930) 205–246.

[158] G.D. Birkhoff nd W.J. Trjitzinsky, *Analytic theory of singular difference equations*, Acta Math. **60** (1932) 1–89.

[159] J. Wimp and D. Zeilberger. *Resurrecting the asymptotics of linear recurrences*, J. Math. Anal. Appl., **111** (1985) 162–176.

[160] M. Kauers, *A Mathematica Package for Computing Asymptotic Expansions of Solutions of P-Finite Recurrence Equations*, Technical Report RISC 11-04, JKU Linz.

[161] J.M. Borwein, D.M. Bradley, D.J. Broadhurst and P. Lisonek, *Special values of multiple polylogarithms*, Trans. Am. Math. Soc. **353** (2001) 907–941 [arXiv:math/9910045 [math.CA]].

[162] S. Moch, P. Uwer and S. Weinzierl, *Nested sums, expansion of transcendental functions and multiscale multiloop integrals*, J. Math. Phys. **43** (2002) 3363–3386 [hep-ph/0110083].

[163] J. Blümlein and M. Saragnese, in preparation.

[164] H.D. Politzer, *Asymptotic Freedom: An Approach to Strong Interactions*, Phys. Rept. **14** (1974) 129–180.

[165] J. Blümlein and N. Kochelev, *On the twist -2 and twist - three contributions to the spin dependent electroweak structure functions*, Nucl. Phys. B **498** (1997) 285–309 [hep-ph/9612318].

[166] M. Steinhauser, *MATAD: A Program package for the computation of MAssive TADpoles*, Comput. Phys. Commun. **134** (2001) 335–364 [hep-ph/0009029].

[167] The PARI Group, *PARI/GP version 2.13.4*, 2022, Univ. Bordeaux, F, available from `http://pari.math.u-bordeaux.fr/`.

[168] J. Vollinga and S. Weinzierl, *Numerical evaluation of multiple polylogarithms*, Comput. Phys. Commun. **167** (2005) 177–194 [hep-ph/0410259].

[169] A. Maier and P. Marquard, *Validity of Padé approximations in vacuum polarization at three- and four-loop order*, Phys. Rev. D **97** (2018) no.5, 056016 [arXiv:1710.03724 [hep-ph]].

[170] M. Fael, F. Lange, K. Schönwald and M. Steinhauser, *A semi-analytic method to compute Feynman integrals applied to four-loop corrections to the* $\overline{\rm MS}$*-pole quark mass relation*, JHEP **09** (2021) 152 [arXiv:2106.05296 [hep-ph]].

[171] M. Fael, F. Lange, K. Schönwald and M. Steinhauser, *Singlet and nonsinglet three-loop massive form factors*, Phys. Rev. D **106** (2022) no.3, 034029 [arXiv:2207.00027 [hep-ph]].

[172] S. Catani, M. Ciafaloni and F. Hautmann, *High-energy factorization and small x heavy flavor production*, Nucl. Phys. B **366** (1991) 135–188.

[173] J. Bartels, B.I. Ermolaev and M.G. Ryskin, *Flavor singlet contribution to the structure function* g_1 *at small* x, Z. Phys. C **72** (1996) 627–635 [hep-ph/9603204].

[174] D. Adamiak, Y.V. Kovchegov and Y. Tawabutr, Phys. Rev. D **108** (2023) no.5, 054005 [arXiv:2306.01651 [hep-ph]].

[175] D.H. Bailey, J.M. Borwein, D. Broadhurst and W. Zudilin, *Experimental Mathematics and Mathematical Physics*, Contemp. Math. **517** (2010) 41–58 [arXiv:1005.0414 [math-ph]].

[176] J. Klappert and F. Lange, *Reconstructing rational functions with FireFly*, Comput. Phys. Commun. **247** (2020) 106951 [arXiv:1904.00009 [cs.SC]].

[177] J. Klappert, S.Y. Klein and F. Lange, *Interpolation of dense and sparse rational functions and other improvements in FireFly*, Comput. Phys. Commun. **264** (2021) 107968 [arXiv:2004.01463 [cs.MS]].

[178] L. Lewin, Dilogarithms and associated functions, (Macdonald, London, 1958).

[179] L. Lewin, Polylogarithms and associated functions, (North Holland, New York, 1981).

[180] A. Devoto and D.W. Duke, *Table of Integrals and Formulae for Feynman Diagram Calculations*, Riv. Nuovo Cim. **7N6** (1984) 1–39.

[181] J. Blümlein, N. Fadeev and C. Schneider, *Computing Mellin Representations and Asymptotics of Nested Binomial Sums in a Symbolic Way: The RICA Package*, ACM Communications in Computer Algebra **57** (2023) no.2, 31–34 [arXiv:2308.06042 [hep-ph]].

[182] N. Nielsen, Handbuch der Theorie der Gammafunktion, (Teubner, Leipzig, 1906); reprinted by (Chelsea Publishing Company, Bronx, New York, 1965).

[183] E. Landau, *Über die Grundlagen der Theorie der Fakultätenreihen*, S.-Ber. math.-naturw. Kl. Bayerische Akad. Wiss. München, bf 36 (1906) 151–218.

[184] N.E. Nörlund, Vorlesungen über Differenzenrechnung, (Springer, Berlin, 1924); (Chelsea Publishing Company, New York, 1954).

[185] C.G. Raab, *Nested Integrals and Rationalizing Transformations*, in: Antidifferentiation and the Calculation of Feynman Amplitudes, Eds. J. Blümlein and C. Schneider, (Springer, Berlin, 2021), 395–422.

[186] M. Besier, D. van Straten and S. Weinzierl, *Rationalizing roots: an algorithmic approach* Commun. Num. Theor. Phys. **13** (2019) 253–297 [arXiv:1809.10983 [hep-th]].

[187] E. Catalan, *Mémoire sur la transformation des séries et sur quelques intégrales définies*, Mémoires couronnés et mémoires des savants étrangers **33** (1867) 1–50.

[188] NIST Handbook of Mathematical Functions, (Cambridge, Cambridge University Press, 2010), Eds. F.W.J Olvers, D.W. Lozier, R.F. Boisvert, and C.W. Clark.

[189] S. Klein et al., unpublished.