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The three-loop polarized pure singlet operator matrix element with two different masses

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Abstract

We present the two-mass QCD contributions to the polarized pure singlet operator matrix element at three loop order in x-space. These terms are relevant for calculating the polarized structure function $g_1(x, Q^2)$ at $O(\alpha_s^3)$ as well as for the matching relations in the variable flavor number scheme and the polarized heavy quark distribution functions at the same order. The result for the operator matrix element is given in terms of generalized iterated integrals. These integrals depend on the mass ratio through the main argument, and the alphabet includes square–root valued letters.

1. Introduction

Massive operator matrix elements (OMEs) are essential building blocks for the massive Wilson coefficients in deep–inelastic scattering in the limit $Q^2 \gg m^2$, and they are the transition matrix elements in the variable flavor number scheme (VFNS) [1,2]. Here Q^2 denotes the virtuality of the deep-inelastic process and m is the heavy quark mass. From 2–loop order onward

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these matrix elements A_{ij} receive two–mass corrections, aside of the single mass corrections, i.e. contributions of two closed fermion lines with different heavy quark flavors, cf. [3,4]. In the unpolarized case the two–mass corrections have been calculated for all OMEs to three–loop order in Refs. [3–7]. For the OME $A_{Qg}^{(3),\rm tm}$ a large set of Mellin moments for even values of the Mellin variable $N \in \mathbb{N}$ has been derived, expanding in the mass ratio

$$\eta = \frac{m_c^2}{m_b^2}, \tag{1.1}$$

to a finite power, where $m_{c(b)}$ denote the charm and bottom quark mass, respectively.

In the polarized case, the flavor non–singlet three loop OME $A_{qq,Q}^{(3),\rm NS,tm}$ [4] and $A_{gq,Q}^{(3),\rm tm}$ [7] have been calculated. In the present paper we compute the two mass contributions to the pure singlet massive OME $A_{Qq}^{(3),\rm PS,tm}$. As in the unpolarized case, the calculation cannot be performed in N space, transforming to momentum fraction x space later, because the associated recurrences do not factorize to first order. This, however, is the case for the corresponding differential equations in x space. In the result we obtain iterative integrals, partly with limited support in $x \in [0, 1]$. This has also been observed in the single mass pure singlet case [8].

Since we will use dimensional regularization in the calculation, a consistent description of the Dirac matrix γ_5 is necessary. For this we use the Larin scheme [9]. The polarized massive OME $A_{Qq}^{(3),\rm PS,tm}$ contributes to the polarized three-loop massive Wilson coefficient $H_{Qq}^{(3)}(z, Q^2)$ and is one of the contributions of the two–mass variable flavor number scheme [4,10] in the polarized case, describing the respective transitions of the polarized parton densities in the case the heavy quarks become light. They contribute in particular also to the charm- and bottom quark distributions. In the formalism we will as widely as possible follow earlier work in Ref. [5].[1]

The paper is organized as follows. In Section 2 we present details of the calculation. Section 3 contains the analytic results and numerical results are discussed in Section 4 before concluding in Section 5. In the appendix we provide complete analytic expressions for a number of Mellin moments $N \in \mathbb{N}$.

2. Details of the calculation

The generic pole structure of the unrenormalized polarized PS three–loop two–mass contribution to the massive OME has been given in [5], Eq. (2.1). As often the case considering the massive corrections, one applies the symbols $\hat{}$ and $\hat{\hat{}}$ to some quantities. This has been defined in [5], Eqs. (2.2, 2.3). The dimensional parameter is $\varepsilon = D - 4$, with D the dimension of space–time. The corresponding expressions given in terms of the expansion coefficients of the β-function in QCD (massless and massive), the anomalous dimensions [11–14], and the constant parts and higher parts in the ε expansion of the massive OME, a_{ij}^k and $\bar{a}_{ij}^k$, cf. Refs. [7,15–18]. Here and in what follows, ζ_k, $k \in \mathbb{N}$, $k \geq 2$ denotes the Riemann ζ-function at integer argument. The OMEs depend on two the two logarithms

$$L_1 = \ln\left(\frac{m_1^2}{\mu^2}\right), \quad L_2 = \ln\left(\frac{m_2^2}{\mu^2}\right), \tag{2.1}$$

[1] We follow the suggestion of the referee and do not repeat any of the equations given in [5] in the unpolarized case already, which can be re-used schematically, i.e. considering now the polarized case instead. As it is easily understood, we refrain from using the symbol $'\Delta'$ sometimes applied to mark the polarized case.

where m_1 and m_2 are the masses of the heavy quarks, and μ is the renormalization scale.

There are sixteen irreducible diagrams for $\tilde{A}_{Qq}^{(3),\rm PS,tm}$, which are shown in Figure 1 of Ref. [5]. Here the unpolarized insertion has to be replaced by the polarized one. The unrenormalized operator matrix element is obtained by adding all the diagrams and applying the quarkonic projector P_q to the corresponding Green function $\hat{G}_Q^{ij}$, cf. [14],

$$P_q \hat{G}_l^{ij} = -\delta_{ij} \frac{i(\Delta.p)^{-N-1}}{4N_c(D-2)(D-3)} \varepsilon_{\mu\nu p\Delta} {\rm tr}\left[\not p \gamma^\mu \gamma^\nu \hat{G}_l^{ij}\right], \tag{2.2}$$

where p is the momentum of the on-shell external massless quark ($p^2 = 0$), Δ is a light-like D-vector, with $D = 4 + \varepsilon$, the dimension of space-time in which we work, i and j are the color indices of each external leg, and N_c is the number of colors. Note that the projector (2.2) is different from that in the unpolarized case [5]. The diagrams, $D_1, \ldots, D_{16}$, are calculated directly within dimensional regularization. The Dirac algebra is performed using `FORM` [19]. Diagrams 1–8 turn out to vanish. Diagrams 9–12 and 13–16 can be mapped by symmetry relations to each other. These two classes are furthermore related by exchanging $\eta \Leftrightarrow 1/\eta$.

One therefore obtains

$$A_{Qq}^{(3),\rm PS,tm}(N) = 2\left[1 + (-1)^{N-1}\right] D_9(m_1, m_2, N) + 2\left[1 + (-1)^{N-1}\right] D_9(m_2, m_1, N), \tag{2.3}$$

where N is the Mellin variable appearing in the Feynman rules for the operator insertions, cf. [11, 14]. In the following we use the variable

$$\eta = \frac{m_2^2}{m_1^2}, \tag{2.4}$$

with $m_2 < m_1$, i.e. $\eta < 1$, which we will assume in what follows.

While in other calculations one could derive the results working either in Mellin N or x–space, cf. e.g. [5,6], this is not the case here, see also [5]. We will, therefore, present our result only in x-space, which is anyway all we need in order to obtain the corresponding contribution to the structure function $g_1(x, Q^2)$ for large values of Q^2, as well as the contribution to the variable flavor number scheme. In most of the applications one finally works in x-space.

All the diagrams contain a massive fermion loop with an operator insertion (Figure 2 [5], b_1 and b_2) and a massive bubble without the operator (Figure 2 [5], a_1). The latter can be rendered effectively massless by using a Mellin–Barnes integral [20–24]. One obtains

$$I_{a_1}^{\mu\nu,ab}(k) = -\frac{8iT_F g_s^2}{(4\pi)^{D/2}} \delta_{ab}(k^2 g^{\mu\nu} - k^\mu k^\nu) \int_0^1 dx \frac{\Gamma(2-D/2)(x(1-x))^{D/2-1}}{\left(-k^2 + \frac{m^2}{x(1-x)}\right)^{2-D/2}}, \tag{2.5}$$

$$\begin{aligned} I_{b_2}^{\mu\nu,ab}(k) = {} & \alpha_s T_F i e^{-\gamma_E \varepsilon/2} (k \cdot \Delta)^{N-1} (\mu^2)^{-\varepsilon/2} S_\varepsilon \varepsilon^{\Delta k \mu\nu} \int_0^1 dx\, x^{N+D/2-1}(1-x)^{D/2-1} \\ & \times \left\{ \left(-k^2 + \frac{m^2}{x(1-x)}\right)^{-2+D/2} 2\Gamma(2-D/2) \right. \\ & \times \left[(D-6)x^{-2} + (D+2N)x^{-1}\right] \end{aligned} \tag{2.6}$$

$$+\left(-k^2+\frac{m^2}{x(1-x)}\right)^{-3+D/2} 4\Gamma(3-D/2)(1-x)^{-1}\Big[m^2(x^{-3}+x^{-2}) + (-k^2)(1-x^{-1})\Big]\Bigg\}, \tag{2.7}$$

where μ and ν are the respective Lorentz indices of the external legs, a and b are the color indices, k is the external momentum, m is the mass of the fermion, which can be either m_1 or m_2, $g_s = \sqrt{4\pi\alpha_s}$ is the strong coupling constant, and $T_F = 1/2$ in $SU(N_c)$, with N_c the number of colors. The other color factors are $C_F = (N_c^2-1)/(2N_c)$ and $C_A = N_c$. The term $I_{b_1}^{\mu\nu,ab}(k)$ only appears in diagrams which vanish and is not displayed here.

For diagram 9 we obtain the representation

$$\begin{aligned} D_9(m_1,m_2,N) = C_F T_F^2 \alpha_s^3 S_\varepsilon^3 \frac{16}{2+\varepsilon}\Bigg\{ & 4(2-\varepsilon)J_1 - 8\eta J_2 - 8(N+3)J_3 \\ & + 8J_4 + 8\left(2+\frac{\varepsilon}{2}+N\right)J_5 - 8J_6 - (\varepsilon-2)^2 J_7 + 2(2-\varepsilon)\eta J_8 \\ & + 2(2-\varepsilon)(3+N)J_9 - 2(2-\varepsilon)J_{10} - 2(2-\varepsilon)\left(2+\frac{\varepsilon}{2}+N\right)J_{11} \\ & + 2(2-\varepsilon)J_{12} - 8\eta J_{13} + 2(2-\varepsilon)\eta J_{14}\Bigg\}, \end{aligned} \tag{2.8}$$

with[2]

$$J_1 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{-1+\frac{\varepsilon}{2}+N} B_1\left(\frac{\eta}{x(1-x)}\right), \tag{2.9}$$

$$J_2 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{-1+\frac{\varepsilon}{2}+N} B_3\left(\frac{\eta}{x(1-x)}\right), \tag{2.10}$$

$$J_3 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{\frac{\varepsilon}{2}+N} B_1\left(\frac{\eta}{x(1-x)}\right), \tag{2.11}$$

$$J_4 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{\frac{\varepsilon}{2}+N} B_2\left(\frac{\eta}{x(1-x)}\right), \tag{2.12}$$

$$J_5 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{1+\frac{\varepsilon}{2}+N} B_1\left(\frac{\eta}{x(1-x)}\right), \tag{2.13}$$

$$J_6 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{1+\frac{\varepsilon}{2}+N} B_2\left(\frac{\eta}{x(1-x)}\right), \tag{2.14}$$

[2] The functions J_k are structurally different from the functions with the same name in Ref. [5].

$$J_7 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{-1+\frac{\varepsilon}{2}+N} B_1\left(\frac{\eta}{x(1-x)}\right), \tag{2.15}$$

$$J_8 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{-1+\frac{\varepsilon}{2}+N} B_3\left(\frac{\eta}{x(1-x)}\right), \tag{2.16}$$

$$J_9 = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{\frac{\varepsilon}{2}+N} B_1\left(\frac{\eta}{x(1-x)}\right), \tag{2.17}$$

$$J_{10} = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{\frac{\varepsilon}{2}+N} B_2\left(\frac{\eta}{x(1-x)}\right), \tag{2.18}$$

$$J_{11} = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{1+\frac{\varepsilon}{2}+N} B_1\left(\frac{\eta}{x(1-x)}\right), \tag{2.19}$$

$$J_{12} = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{1+\frac{\varepsilon}{2}+N} B_2\left(\frac{\eta}{x(1-x)}\right), \tag{2.20}$$

$$J_{13} = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N)}{\Gamma\left(1+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{-2+\frac{\varepsilon}{2}+N} B_3\left(\frac{\eta}{x(1-x)}\right), \tag{2.21}$$

$$J_{14} = \left(\frac{m_1^2}{\mu^2}\right)^{\frac{3}{2}\varepsilon} \frac{\Gamma(N+1)}{\Gamma\left(2+\frac{\varepsilon}{2}+N\right)} \int_0^1 dx\,(1-x)^{\frac{\varepsilon}{2}} x^{-2+\frac{\varepsilon}{2}+N} B_3\left(\frac{\eta}{x(1-x)}\right). \tag{2.22}$$

The functions B_i are given by Eqs. (3.18, 3.28) and (3.29) of Ref. [5]. Expanding in the dimensional parameter ε the pre-factors of the functions J_i reduce to the following denominators

$$\frac{1}{N+l}, \quad \text{with} \quad l \in \{0, 1\}, \tag{2.23}$$

after partial fractioning. These factors have still to be absorbed under the integral, which can be achieved by applying Eq. (3.32) Ref. [5].

One has still to perform the contour integral in the functions B_i. To do this, the range in x is split into the intervals

$$[0, \eta_-], \quad [\eta_-, \eta_+], \quad [\eta_+, 1], \quad \text{with } \eta_\pm = \frac{1}{2}\left(1 \pm \sqrt{1-\eta}\right). \tag{2.24}$$

For the second region the integral contour is closed to the right, and for the two other regions to the left. One obtains then the functions B_i for both regions in terms of infinite sum representations, cf. [5], over rational expressions and harmonic sums [25,26]. In the expressions ratios of Γ-functions are related to special binomial coefficients. All of the above sums can be performed using the Mathematica packages `Sigma` [27,28], `HarmonicSums` [29–31], `EvaluateMultiSums` and `SumProduction` [32]. We have performed numerical checks on these steps using the packages `MB` and `MBresolve` [33,34].

The results can be expressed in terms of the generalized iterated integrals, Eqs. (3.31, 3.32) of Ref. [5], a subset of which are harmonic polylogarithms [35], see the appendix of Ref. [5] for details. Square-root valued letters usually play a role in two mass OMEs but also for some single mass OMEs starting from three–loop order and related quantities [5,6,10,36–39].

3. The massive operator matrix element

We obtain the following expression for the $O(\varepsilon^0)$ term of the unrenormalized 3-loop two-mass pure singlet operator matrix element

$$\begin{aligned}\tilde{a}_{Qq}^{(3),\mathrm{PS}}(x) = C_F T_F^2 \Bigg\{ & R_0(m_1, m_2, x) + \big(\theta(\eta_- - x) + \theta(x - \eta_+)\big) x\, g_0(\eta, x) \\ & + \theta(\eta_+ - x)\theta(x - \eta_-)\left[x\, f_0(\eta, x) - \int_{\eta_-}^{x} dy \left(f_1(\eta, y) + \frac{x}{y} f_3(\eta, y)\right)\right] \\ & + \theta(\eta_- - x) \int_{x}^{\eta_-} dy \left(g_1(\eta, y) + \frac{x}{y} g_3(\eta, y)\right) \\ & - \theta(x - \eta_+) \int_{\eta_+}^{x} dy \left(g_1(\eta, y) + \frac{x}{y} g_3(\eta, y)\right) \\ & + x\, h_0(\eta, x) + \int_{x}^{1} dy \left(h_1(\eta, y) + \frac{x}{y} h_3(\eta, y)\right) \\ & + \theta(\eta_+ - x) \int_{\eta_-}^{\eta_+} dy \left(f_1(\eta, y) + \frac{x}{y} f_3(\eta, y)\right) \\ & + \int_{\eta_+}^{1} dy \left(g_1(\eta, y) + \frac{x}{y} g_3(\eta, y)\right) \Bigg\}. \end{aligned} \tag{3.1}$$

Here we follow the notation used in Ref. [5]. In the present case no functions carrying the index 2 occur. The functions $g_i(\eta, x)$ in Eq. (3.1) shall not be confounded with polarized structure functions, also often denoted by g_i. Here $\theta(z)$ denotes the Heaviside function

$$\theta(z) = \begin{cases} 1 & z \geq 0 \\ 0 & z < 0. \end{cases} \tag{3.2}$$

The pole terms are obtained in analytic form in terms of harmonic polylogarithms. For convenience we define the auxiliary functions u and v as

$$u = \frac{x(1-x)}{\eta}, \quad v = \frac{\eta}{x(1-x)}. \tag{3.3}$$

If in the following expressions the harmonic polylogarithms $H_{\vec{a}}$ are given without argument it is understood that their argument is x. The functions appearing in Eq. (3.1) are given by

$$
\begin{aligned}
R_0(m_1, m_2, x) = {} & 32\Big(L_1^3 + L_1 L_2 (L_1 + L_2) + L_2^3\Big)\Big[5(-1+x) - 2(1+x)H_0\Big] \\
& + 128 L_1 L_2 \Big[(x+1)\Big(\frac{2}{3}H_{0,1} - \frac{10}{9}H_0 - \frac{2}{3}\zeta_2\Big) + (x-1)\Big(\frac{10}{9} - \frac{5}{3}H_1\Big)\Big] \\
& + 32\big(L_1^2 + L_2^2\big)\Big[(x+1)\Big(\frac{2}{3}H_{0,1} + H_0^2 - \frac{2}{3}\zeta_2\Big) + (x-1)\Big(\frac{1}{9} - \frac{5}{3}H_1\Big) \\
& + \frac{1}{9}(17 - 37x)H_0\Big] \\
& + 64(L_1 + L_2)\Big[(1+x)\Big(\Big(2H_{0,1} - \frac{8\zeta_2}{3}\Big)H_0 - \frac{2}{9}H_0^3 - \frac{10}{3}H_{0,0,1} \\
& - \frac{4}{3}H_{0,1,1} + \frac{14}{3}\zeta_3\Big) + (x-1)\Big(\frac{442}{27} + \frac{5}{3}H_1^2 - \frac{5}{9}H_1\Big(1 + 9H_0\Big)\Big) \\
& - \frac{2}{27}(56 + 137x)H_0 + \frac{1}{9}(-5 + 4x)H_0^2 + \frac{2}{9}(-17 + 28x)H_{0,1} \\
& + \frac{2}{9}(-28 + 17x)\zeta_2\Big] + \frac{64}{1215}\Big[(1+x)\Big(\Big(3240 H_{0,0,1} + 1620 H_{0,1,1}\Big)H_0 \\
& + \Big(-1620 H_{0,1} + 945\zeta_2\Big)H_0^2 + 90 H_0^4 - 1080 H_{0,0,0,1} \\
& - 2700 H_{0,0,1,1} + 540 H_{0,1,1,1} + 1296\zeta_2^2\Big) + (-1+x)\Big(20(437 + 54x) \\
& + \Big(1080 H_0 + 4050 H_0^2 + 2025\zeta_2\Big)H_1 - 225 H_1^3 \\
& - 45 H_1^2\Big(11 + 45 H_0\Big)\Big) + \Big(-10\big(-842 + 1111x + 81x^2\big) \\
& - 540(-7 + 11x)H_{0,1} - 45(-53 + 73x)\zeta_2 - 4860(1+x)\zeta_3\Big)H_0 \\
& + 165(19 + 37x)H_0^2 - 30(-19 + 8x)H_0^3 + 30(-1+x)(157 + 27x)H_1 \\
& + \Big(-30(61 + 169x) - 810(1+x)\zeta_2\Big)H_{0,1} + 180(-11 + 25x)H_{0,0,1} \\
& + 180(-14 + 13x)H_{0,1,1} + 15(131 + 329x)\zeta_2 + 90(-55 + 29x)\zeta_3\Big],
\end{aligned}
\tag{3.4}
$$

$$
\begin{aligned}
g_0(\eta, x) = {} & -\frac{32(1-x)}{9}\Big[-\frac{16(-1+x)x}{\eta} \\
& + 18\Big(-\frac{2(\eta - 4(-1+x)x)^2}{9\eta^2} + \frac{1}{3}\zeta_2\Big)H_0\big(u\big) \\
& + 5H_0^2\big(u\big) + 2\Big(-1 + \frac{(\eta - 4(1-x)x)^{3/2}}{\eta^{3/2}}\Big)\zeta_2 + H_0^3\big(u\big)\Big] \\
& - \frac{64(1-x)}{9}\Big[\Big(2\frac{(\eta - 4(1-x)x)^{3/2}}{\eta^{3/2}} - 3\zeta_2\Big)G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\}, u\right)\Big]
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{64(1-x)}{3}\Biggl[G^2\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\},u\right)\\
&+G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau},\frac{\sqrt{1-4\tau}}{\tau},\frac{1}{\tau}\right\},u\right)\Biggr]\\
&-\frac{64(1-x)}{9}G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau},\frac{1}{\tau}\right\},u\right)\frac{(\eta-4(1-x)x)^{3/2}}{\eta^{3/2}},
\end{aligned}
\tag{3.5}
$$

$$
\begin{aligned}
g_1(\eta,x)=&\frac{64}{27\eta^2x}\Biggl[-6(1-x)H_0\bigl(u\bigr)P_2-8\eta(-1+x)(1+x)(7\eta+24(1-x)x)\\
&+3\eta^2(-1+x)(-5+13x)H_0^2\bigl(u\bigr)-3\eta^2(1-x)(-1+2x)H_0^3\bigl(u\bigr)\\
&-(6(1-x))\Bigl((1+x)\eta^{3/2}-4\eta(1+x)\sqrt{\eta-4(1-x)x}\\
&+2(-1+x)x(1+10x)\sqrt{\eta-4(1-x)x}\Bigr)\sqrt{\eta}\zeta_2\Biggr]\\
&+\frac{128(-1+x)}{9x}\Biggl[\Bigl(-4\frac{\sqrt{\eta-4(1-x)x}}{\eta^{3/2}}P_1\\
&-3(-1+2x)\zeta_2\Bigr)G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\},u\right)\Biggr]\\
&-\frac{128(-1+x)(-1+2x)}{3x}G^2\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\},u\right)\\
&-\frac{128(-1+x)(-1+2x)}{3x}G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau},\frac{\sqrt{1-4\tau}}{\tau},\frac{1}{\tau}\right\},u\right)\\
&-\frac{256(-1+x)P_1}{9x}G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau},\frac{1}{\tau}\right\},u\right)\frac{\sqrt{\eta-4(1-x)x}}{\eta^{3/2}},
\end{aligned}
\tag{3.6}
$$

$$
\begin{aligned}
g_3(\eta,x)=&-\frac{32}{27\eta^2x}\Biggl[8\eta(1-x)P_4-6(1-x)H_0\bigl(u\bigr)P_5+3\eta^2(-1+x)(-5+8x)\\
&\times H_0^2\bigl(u\bigr)+3\eta^2(-1+x)^2H_0^3\bigl(u\bigr)-(6(1-x))\\
&\times\Bigl((1+2x)\eta^{3/2}-\eta(4+5x)\sqrt{\eta-4(1-x)x}\\
&+2(-1+x)x(1+8x)\sqrt{\eta-4(1-x)x}\Bigr)\sqrt{\eta}\zeta_2\Biggr]-\frac{64(1-x)}{9x}\\
&\times\Biggl[\Bigl(2\frac{\sqrt{\eta-4(1-x)x}}{\eta^{3/2}}P_3+3(-1+x)\zeta_2\Bigr)G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\},u\right)\Biggr]\\
&+\frac{64(-1+x)^2}{3x}G^2\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\},u\right)\\
&+\frac{64(-1+x)^2}{3x}G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau},\frac{\sqrt{1-4\tau}}{\tau},\frac{1}{\tau}\right\},u\right)
\end{aligned}
$$

$$
- \frac{64(1-x)P_3}{9x} G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}\right\}, u\right) \frac{\sqrt{\eta - 4(1-x)x}}{\eta^{3/2}}, \tag{3.7}
$$

with the polynomials

$$
P_1 = 2\eta(x+1) - 10x^3 + 9x^2 + x, \tag{3.8}
$$

$$
P_2 = 3\eta^2(2x\zeta_2 + x - \zeta_2 + 1) + 8\eta x\left(10x^2 - 9x - 1\right) - 16(1-x)^2x^2(10x+1), \tag{3.9}
$$

$$
P_3 = \eta(5x+4) + 2x\left(-8x^2 + 7x + 1\right), \tag{3.10}
$$

$$
P_4 = 7\eta(x+1) + 6x\left(-5x^2 + x + 4\right), \tag{3.11}
$$

$$
P_5 = \eta^2(x(3\zeta_2+5) - 3\zeta_2 + 3) + 8\eta x\left(8x^2 - 7x - 1\right) - 16(x-1)^2x^2(8x+1), \tag{3.12}
$$

and

$$
\begin{aligned}
f_0(\eta, x) = \Bigg[& -\frac{16(1-x)}{3} G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, v\right) - \frac{4P_6}{9(-1+x)x^2}\Big[-1 + 2H_0(v)\Big] \\
& \times \frac{(-\eta + 4(1-x)x)^{3/2}}{\eta^{3/2}}\Bigg] G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\}, v\right) \\
& + \frac{4(1-x)}{3}\Bigg[\Big[-1 + 2H_0(v)\Big] G^2\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\}, v\right)\Bigg] \\
& + \frac{16(1-x)}{3} G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, v\right) \\
& + \frac{1}{18}\Bigg[-1536(1-x) - \frac{9\eta^4}{(-1+x)^3x^4} - \frac{80\eta^3}{(-1+x)^2x^3} - \frac{104\eta^2}{(-1+x)x^2} \\
& + \frac{576\eta}{x} + \frac{4P_7}{(-1+x)^3x^4} H_0(v) - 320(1-x)H_0^2(v) + 64(1-x)H_0^3(v) \\
& - \Big(128(1-x)\Big)\Big(5 - 3H_0(v)\Big)\zeta_2 + 768(1-x)\zeta_3\Bigg] \\
& - \frac{8P_6}{9(1-x)x^2} G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, v\right) \frac{(-\eta + 4(1-x)x)^{3/2}}{\eta^{3/2}},
\end{aligned} \tag{3.13}
$$

$$
\begin{aligned}
f_1(\eta, x) = \frac{1}{27x^5}\Bigg[& -\frac{1}{(1-x)^3}\Big[6912\eta(-1+x)^3x^4 - 27\eta^4(-1+2x) - 240\eta^3(-1+x)x \\
& \times(-1+2x) + 512(-1+x)^4x^4(-16+11x) + 12H_0(v)P_9 \\
& - 24\eta^2(-1+x)^2x^2(-25+2x) + 192(-1+x)^4x^4(-5+13x)H_0^2(v) \\
& - 192(-1+x)^4x^4(-1+2x)H_0^3(v)\Big] + 384(1-x)x^4\Big(5 - 13x \\
& + 3(-1+2x)H_0(v)\Big)\zeta_2 - 2304(-1+x)x^4(-1+2x)\zeta_3\Bigg] + \\
& \Bigg[\frac{32(-1+x)(-1+2x)}{3x} G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, v\right)
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{8P_8}{9(1-x)x^3}\Big(-1+2H_0(v)\Big)\frac{\sqrt{-\eta+4(1-x)x}}{\eta^{3/2}}\Bigg] \\
&\times G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\},v\right) - \frac{8(-1+x)(-1+2x)}{3x}\Bigg[\Big(-1+2H_0(v)\Big) \\
&\times G^2\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\},v\right)\Bigg] + \frac{32(1-x)(-1+2x)}{3x} \\
&\times G\left(\left\{\frac{1}{\tau},\sqrt{4-\tau}\sqrt{\tau},\sqrt{4-\tau}\sqrt{\tau}\right\},v\right) - \frac{16P_8}{9(-1+x)x^3} \\
&\times G\left(\left\{\frac{1}{\tau},\sqrt{4-\tau}\sqrt{\tau}\right\},v\right)\frac{\sqrt{-\eta+4(1-x)x}}{\eta^{3/2}},
\end{aligned} \tag{3.14}
$$

$$
\begin{aligned}
f_3(\eta,x) = {} & \frac{1}{54(-1+x)^2x^5}\Bigg[27\eta^4 - 240\eta^3(1-x)x - 5184\eta(-1+x)^2x^4 \\
&- 1024(-8+x)(-1+x)^3x^4 - 12H_0(v)P_{10} - 24\eta^2(-1+x)x^2(25+11x) \\
&- 192(-1+x)^3x^4(-5+8x)H_0^2(v) + 192(-1+x)^4x^4H_0^3(v) \\
&+ 384(-1+x)^3x^4\Big(5-8x-3(1-x)H_0(v)\Big)\zeta_2 + 2304(-1+x)^4x^4\zeta_3\Bigg] \\
&+ \Bigg[-\frac{16(-1+x)^2}{3x}G\left(\left\{\frac{1}{\tau},\sqrt{4-\tau}\sqrt{\tau}\right\},v\right) - \frac{4P_{11}}{9x^3}\Big(-1 \\
&+ 2H_0(v)\Big)\frac{\sqrt{-\eta+4(1-x)x}}{\eta^{3/2}}\Bigg]G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\},v\right) \\
&+ \frac{4(-1+x)^2}{3x}\Bigg[\Big(-1+2H_0(v)\Big)G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\},v\right)^2\Bigg] \\
&+ \frac{16(-1+x)^2}{3x}G\left(\left\{\frac{1}{\tau},\sqrt{4-\tau}\sqrt{\tau},\sqrt{4-\tau}\sqrt{\tau}\right\},v\right) + \frac{8P_{11}}{9x^3} \\
&\times G\left(\left\{\frac{1}{\tau},\sqrt{4-\tau}\sqrt{\tau}\right\},v\right)\frac{\sqrt{-\eta+4(1-x)x}}{\eta^{3/2}},
\end{aligned} \tag{3.15}
$$

with

$$P_6 = 3\eta^2 + 6\eta(1-x)x + 4(x-1)^2x^2, \tag{3.16}$$

$$
\begin{aligned}
P_7 = {} & 3\eta^4 - 24\eta^3(1-x)x + 20\eta^2(x-1)^2x^2 - 160\eta\,(x-1)^3x^3 \\
&- 128(x-1)^4x^4,
\end{aligned} \tag{3.17}
$$

$$
\begin{aligned}
P_8 = {} & \eta^3(6x-3) + 6\eta^2x\left(2x^2-3x+1\right) - 8\eta\,(x-1)^2x^2(8x-1) \\
&+ 8(x-1)^3x^3(10x+1),
\end{aligned} \tag{3.18}
$$

$$
\begin{aligned}
P_9 = {} & \eta^4(6x-3) + 24\eta^3x\left(2x^2-3x+1\right) - 4\eta^2(x-1)^2x^2(2x+11) \\
&- 64\eta(x-1)^3x^3(8x-1) + 96(x-1)^4x^4(x+4),
\end{aligned} \tag{3.19}
$$

$$
\begin{aligned}
P_{10} = {} & 3\eta^4 - 24\eta^3(1-x)x - 4\eta^2x^2\left(7x^2+4x-11\right) - 32\eta(x-1)^2x^3(11x-2) \\
&+ 32(x-1)^3x^4(7x+12),
\end{aligned} \tag{3.20}
$$

$$P_{11} = 3\eta^3 - 6\eta^2(1-x)x - 4\eta x^2\left(11x^2-13x+2\right) + 8(1-x)^2x^3(8x+1). \tag{3.21}$$

The functions h_i are defined as follows

$$h_i(\eta, x) = g_i\left(\frac{1}{\eta}, x\right), \quad i = 0, 1, 3. \tag{3.22}$$

In deriving the expressions given above, we have used shuffle algebra relations wherever possible, cf. [40]. The function $R_0(m_1, m_2, x)$ arises from the residues taken in order to resolve the singularities in ε of the contour integrals in the functions B_i. The functions $f_i(\eta, x)$, $g_i(\eta, x)$, with $i = 0, 1, 3$, arise from the sum of residues of the contour integrals that remain after the ε expansion, as described in the previous section. The functions with $i = 0$ are those where no additional factor depending on N occurs. The functions with $i = 1$ and $i = 3$ are those where a factor of $1/N$ and $1/(N+1)$ was absorbed, respectivly. The different Heaviside functions restrict the corresponding values of x to the appropriate regions.

Since no contour integral needs to be performed in the case $R_0(m_1, m_2, x)$, the easiest way to compute this function is to integrate in x and then perform the Mellin inversion using `HarmonicSums`. The expressions of the G-functions in the above equations can all be given in terms of harmonic polylogarithms, cf. Appendix of Ref. [5], containing square-root valued arguments.

We see that iterated integrals of up to weight three appear in our result. The alphabet of these integrals is given in terms of just three letters:

$$\frac{1}{\tau}, \quad \sqrt{4-\tau}\sqrt{\tau}, \quad \frac{\sqrt{1-4\tau}}{\tau}. \tag{3.23}$$

One may try to integrate the remaining integrals in Eq. (3.1) over y into iterated integrals of higher weight. However, the numerical representation needs to be done in addition, unlike the case of harmonic polylogarithms [41,42].

In order to compute the corresponding contribution to the structure function $g_1(x, Q^2)$ or for the transition rate in the VFNS, we have to perform the convolution with parton distribution functions, which can be obtained straightforwardly.

4. Numerical results

We compare the polarized pure singlet 2-mass contributions to the complete $O(T_F^2 C_F)$ term as a function of x and μ^2 in Fig. 1. The single mass three–loop polarized pure singlet OME has been calculated in [43]. Typical virtualities are $\mu^2 \in [30, 1000]$ GeV^2. The ratio of the 2-mass contributions to the complete term of $O(T_F^2 C_F)$ has a singularity around $x \sim 0.1$. At lower virtualities the corrections are nearly constant in the small x region and grow with μ^2 rising from negative to positive values. In the large x region the ratio falls and rises once again towards $x \to 1$. At $\mu^2 = 1000$ GeV^2 the corrections are comparatively large and positive due to the large logarithms, except in the pole region. In size the corrections are comparable to those found in the unpolarized case and do majorly range between -0.1 to 0.4.

5. Conclusions

We have calculated the two-mass 3-loop contributions to the polarized massive OME $A_{Qq}^{\mathrm{PS},(3)}$ in analytic form in x-space for a general mass-ratio η in the Larin scheme. It contributes to the massive 3-loop Wilson coefficient of the deep-inelastic structure function $g_1(x, Q^2)$ in the region $m^2 \ll Q^2$ and is, as well, one of the polarized OMEs in the two–mass 3-loop VFNS, needed to describe the process of heavy quarks becoming massless at large virtualities. As a function of x,

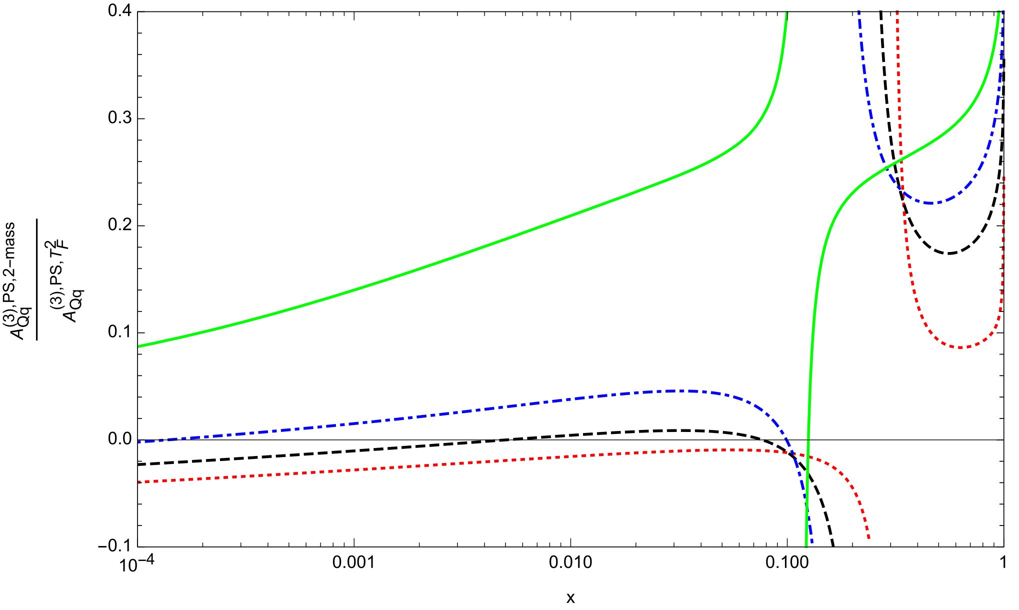

Fig. 1. The ratio of the 2-mass (tm) contributions to the massive OME $A_{Qq}^{\mathrm{PS},(3)}$ to all contributions to $A_{Qq}^{\mathrm{PS},(3)}$ of $O(T_F^2)$ as a function of x and μ^2. Dotted line (red): $\mu^2 = 30$ GeV^2. Dashed line (black): $\mu^2 = 50$ GeV^2. Dash-dotted line (blue): $\mu^2 = 100$ GeV^2. Full line (green): $\mu^2 = 1000$ GeV^2. Here the on-shell heavy quark masses $m_c = 1.59$ GeV and $m_b = 4.78$ GeV [44,45] have been used.

its relative contribution to the $O(T_F^2 C_{A,F})$ terms of the whole matrix element $A_{Qq}^{\mathrm{PS,TF^2},(3)}$ lay in the region of about $[-0.1, 0.4]$ and exhibit a pole at $x \sim 0.1$. The two-mass contribution is not negligible against the single mass contributions.

We applied Mellin-Barnes techniques to obtain the x-space result by factoring out the N-dependence in terms of the kernel x^N, and used integration by parts to absorb the N-dependent polynomial pre-factors. The result can be written as single limited integrals within the range $x \in [0, 1]$ over iterated integrals containing also square-root valued letters. These integrals can be turned into polylogarithms of involved root-valued arguments, depending on the real parameter η. This technique has been applied in the calculation of the corresponding unpolarized OME already. The odd Mellin moments of the OME exhibit a growing number of polynomial terms in η with growing values of N. Due to this structural property and the arbitrariness of η, which enters the ground field, the method of arbitrarily large moments [46] cannot be used to find the result in the present case. The set of necessary integrals for these representations has already been derived in the unpolarized case in Ref. [5]. The concept of square root-valued iterated integrals turned out to be of central importance in deriving the present results. Moreover, their weights are such that one can still relate them to harmonic polylogarithms of more complicated arguments.[3]

The Larin scheme is one of the valid schemes to perform calculations in the polarized case. At present the massless polarized three-loop Wilson coefficients are not yet available [49]. They will also be calculated in the Larin scheme first. Together with parton distribution functions, evolved

[3] This has been a principle also in early Mellin-representations of harmonic sums [26] and [47], limiting the alphabet to that of Nielsen integrals [48].

in the Larin scheme, one can then form observables like $g_1(x, Q^2)$ and related quantities [50]. The anomalous dimensions for the Larin scheme are available to three–loop order [13,14].

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Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Fixed moments of $\tilde{A}_{Qq}^{\mathrm{PS,\,tm,}(3)}$

For fixed values of $N = 2k + 1, k \in \mathbb{N}$, the difference equations describing the moments of the massive OMEs factorize to first order and we find the following moments, unexpanded in the mass ratio η. In the following we will use the notation

$$H_{\vec{w}}(\sqrt{\eta}) \equiv H_{\vec{w}}. \tag{A.1}$$

The fixed moments are given by

$$\begin{aligned}
&\hat{\tilde{A}}_{Qq}^{\mathrm{PS,\,tm,}(3)}(N=1) = \\
&C_F T_F^2 \Biggl\{ \frac{256}{3\varepsilon^2} + \frac{1}{\varepsilon}\left[\frac{320}{9} + 64\bigl(L_1 + L_2\bigr)\right] - \frac{3}{2\eta^{3/2}}\Bigl[-2Q_1 + Q_2\bigl(H_1 + H_{-1}\bigr)\Bigr] \\
&\times \left(L_1^2 + L_2^2\right) + \frac{3}{\eta^{3/2}} L_1 L_2 \Bigl[-2Q_3 + Q_2\bigl(H_1 + H_{-1}\bigr)\Bigr] \\
&- \frac{2}{3\eta^{3/2}}\Bigl[2Q_4 + 9Q_2\bigl(H_{0,1} + H_{0,-1}\bigr)\Bigr] L_1 \\
&+ \frac{2}{3\eta^{3/2}}\Bigl[2Q_5 + 9Q_2\bigl(H_{0,1} + H_{0,-1}\bigr)\Bigr] L_2 \\
&- \frac{4}{27\eta^{3/2}}\Bigl[-2Q_6 + 81Q_2\bigl(H_{0,0,1} + H_{0,0,-1}\bigr)\Bigr] + 32\zeta_2,
\end{aligned} \tag{A.2}$$

$$Q_1 = \sqrt{\eta}\bigl(1 + 10\eta + \eta^2\bigr), \tag{A.3}$$

$$Q_2 = (1 - \eta)^2(1 + \eta), \tag{A.4}$$

$$Q_3 = \sqrt{\eta}\bigl(1 - 6\eta + \eta^2\bigr), \tag{A.5}$$

$$Q_4 = \sqrt{\eta}\bigl(-9 - 20\eta + 9\eta^2\bigr), \tag{A.6}$$

$$Q_5 = \sqrt{\eta}\bigl(-9 + 20\eta + 9\eta^2\bigr), \tag{A.7}$$

$$Q_6 = \sqrt{\eta}\bigl(81 + 284\eta + 81\eta^2\bigr), \tag{A.8}$$

$$
\begin{aligned}
&\hat{\hat{A}}_{Qq}^{\mathrm{PS,\,tm},(3)}(N=3) = \\
&C_F T_F^2 \Biggl\{ -\frac{1280}{81\varepsilon^3} + \frac{1}{\varepsilon^2}\Biggl[\frac{1760}{243} - \frac{320}{27}\bigl(L_1+L_2\bigr)\Biggr] + \frac{1}{\varepsilon}\Biggl[-\frac{12820}{729} \\
&- \frac{160}{27}\bigl(L_1^2+L_1L_2+L_2^2\bigr) + \frac{440}{81}\bigl(L_1+L_2\bigr) - \frac{160}{27}\zeta_2\Biggr] \\
&- \frac{200}{81}L_1^3 - \frac{160}{81}L_2^3 - \frac{80}{27}L_1L_2^2 - \frac{40}{27}L_2L_1^2 + (L_1^2+L_2^2)\Biggl[\frac{5Q_7}{324\eta} \\
&- \frac{5Q_{12}}{216}\frac{H_1}{\eta^{3/2}} - \frac{5Q_{13}}{216}\frac{H_{-1}}{\eta^{3/2}}\Biggr] + L_1L_2\Biggl[-\frac{5Q_8}{162\eta} \\
&+ \frac{5Q_{12}}{108}\frac{H_1}{\eta^{3/2}} + \frac{5Q_{13}}{108}\frac{H_{-1}}{\eta^{3/2}}\Biggr] + L_1\Biggl[-\frac{5Q_9}{243\eta} \\
&- \frac{5Q_{12}}{54}\frac{H_{0,1}}{\eta^{3/2}} - \frac{5Q_{13}}{54}\frac{H_{0,-1}}{\eta^{3/2}} - \frac{40}{9}\zeta_2\Biggr] + \frac{5Q_{10}}{4374\eta} \\
&+ L_2\Biggl[\frac{5Q_{11}}{243\eta} + \frac{5Q_{12}}{54}\frac{H_{0,1}}{\eta^{3/2}} + \frac{5Q_{13}}{54}\frac{H_{0,-1}}{\eta^{3/2}} - \frac{40}{9}\zeta_2\Biggr] \\
&- \frac{5Q_{12}}{27}\frac{H_{0,0,1}}{\eta^{3/2}} - \frac{5Q_{13}}{27}\frac{H_{0,0,-1}}{\eta^{3/2}} + \frac{220}{81}\zeta_2 + \frac{160}{81}\zeta_3\Biggr\}
\end{aligned}
\tag{A.9}
$$

$$Q_7 = 15 + 262\eta + 15\eta^2, \tag{A.10}$$

$$Q_8 = 15 - 2\eta + 15\eta^2, \tag{A.11}$$

$$Q_9 = -45 + 641\eta + 45\eta^2, \tag{A.12}$$

$$Q_{10} = 1620 + 5659\eta + 1620\eta^2, \tag{A.13}$$

$$Q_{11} = -45 - 641\eta + 45\eta^2, \tag{A.14}$$

$$Q_{12} = 5 + 27\eta + 27\eta^2 + 5\eta^3 - 64\eta^{3/2}, \tag{A.15}$$

$$Q_{13} = 5 + 27\eta + 27\eta^2 + 5\eta^3 + 64\eta^{3/2}, \tag{A.16}$$

$$
\begin{aligned}
&\hat{\hat{A}}_{Qq}^{\mathrm{PS,\,tm},(3)}(N=5) = \\
&C_F T_F^2 \Biggl\{ -\frac{14336}{2025\varepsilon^3} + \frac{1}{\varepsilon^2}\Biggl[\frac{20608}{6075} - \frac{3584}{675}\bigl(L_1+L_2\bigr)\Biggr] + \frac{1}{\varepsilon}\Biggl[-\frac{3724784}{455625} \\
&- \frac{1792}{675}\bigl(L_1^2+L_1L_2+L_2^2\bigr) + \frac{5152}{2025}\bigl(L_1+L_2\bigr) - \frac{1792}{675}\zeta_2\Biggr] - \frac{448}{405}L_1^3 \\
&- \frac{1792}{2025}L_2^3 - \frac{896}{675}L_1L_2^2 - \frac{448}{675}L_1^2L_2 + \frac{7Q_{16}}{583200\eta^2} \\
&+ (L_1^2+L_2^2)\Biggl[\frac{7Q_{17}}{864000\eta^2} - \frac{7Q_{14}}{345600\eta^{5/2}}H_1 - \frac{7Q_{15}}{345600\eta^{5/2}}H_{-1}\Biggr] \\
&+ L_1L_2\Biggl[-\frac{7Q_{18}}{432000\eta^2} + \frac{7Q_{14}}{172800\eta^{5/2}}H_1 + \frac{7Q_{15}}{172800\eta^{5/2}}H_{-1}\Biggr] \\
&+ L_1\Biggl[-\frac{7Q_{19}}{9720000\eta^2} - \frac{7Q_{14}}{86400\eta^{5/2}}H_{0,1} - \frac{7Q_{15}}{86400\eta^{5/2}}H_{0,-1} - \frac{448}{225}\zeta_2\Biggr]
\end{aligned}
$$

$$+ L_2\left[\frac{7Q_{20}}{9720000\eta^2} + \frac{7Q_{14}}{86400\eta^{5/2}} H_{0,1} + \frac{7Q_{15}}{86400\eta^{5/2}} H_{0,-1} - \frac{448}{225}\zeta_2\right]$$

$$- \frac{7Q_{14}}{43200\eta^{5/2}} H_{0,0,1} - \frac{7Q_{15}}{43200\eta^{5/2}} H_{0,0,-1} + \frac{2576\zeta_2}{2025} + \frac{1792\zeta_3}{2025}\Bigg\}, \quad (A.17)$$

$$Q_{14} = 189 + 2425\eta + 13770\eta^2 + 13770\eta^3 + 2425\eta^4 + 189\eta^5 - 32768\eta^{5/2}, \quad (A.18)$$

$$Q_{15} = 189 + 2425\eta + 13770\eta^2 + 13770\eta^3 + 2425\eta^4 + 189\eta^5 + 32768\eta^{5/2}, \quad (A.19)$$

$$Q_{16} = 5103 + 65664\eta + 260834\eta^2 + 65664\eta^3 + 5103\eta^4, \quad (A.20)$$

$$Q_{17} = 945 + 12440\eta + 230094\eta^2 + 12440\eta^3 + 945\eta^4, \quad (A.21)$$

$$Q_{18} = 945 + 12440\eta - 5426\eta^2 + 12440\eta^3 + 945\eta^4, \quad (A.22)$$

$$Q_{19} = -42525 - 550350\eta + 8513792\eta^2 + 550350\eta^3 + 42525\eta^4, \quad (A.23)$$

$$Q_{20} = -42525 - 550350\eta - 8513792\eta^2 + 550350\eta^3 + 42525\eta^4, \quad (A.24)$$

$$\hat{\hat{A}}_{Qq}^{\mathrm{PS,\,tm},(3)}(N=7) =$$

$$C_F T_F^2 \Bigg\{ -\frac{192}{49\varepsilon^3} + \frac{1}{\varepsilon^2}\left[\frac{508}{245} - \frac{144}{49}\big(L_1 + L_2\big)\right] + \frac{1}{\varepsilon}\Bigg[-\frac{45155}{9604}$$

$$- \frac{72}{49}\big(L_1^2 + L_1 L_2 + L_2^2\big) + \frac{381}{245}\big(L_1 + L_2\big) - \frac{72}{49}\zeta_2\Bigg] - \frac{30}{49} L_1^3 - \frac{24}{49} L_2^3$$

$$- \frac{Q_{21}}{2765952000\eta^3} - \frac{36}{49} L_1 L_2^2 - \frac{18}{49} L_1^2 L_2 + (L_1^2 + L_2^2)\Bigg[-\frac{3Q_{22}}{14049280\eta^3}$$

$$+ \frac{9Q_{23}}{802816\eta^{7/2}} H_1 + \frac{9Q_{24}}{802816\eta^{7/2}} H_{-1}\Bigg] + L_1 L_2\Bigg[\frac{3Q_{27}}{1404928\eta^3}$$

$$- \frac{9Q_{23}}{401408\eta^{7/2}} H_1 - \frac{9Q_{24}}{401408\eta^{7/2}} H_{-1}\Bigg] + L_2\Bigg[\frac{Q_{25}}{24586240\eta^3}$$

$$- \frac{9Q_{23}}{200704\eta^{7/2}} H_{0,1} - \frac{9Q_{24}}{200704\eta^{7/2}} H_{0,-1} - \frac{54}{49}\zeta_2\Bigg]$$

$$+ L_1\left[-\frac{Q_{26}}{24586240\eta^3} + \frac{9Q_{23}}{200704\eta^{7/2}} H_{0,1} + \frac{9Q_{24}}{200704\eta^{7/2}} H_{0,-1} - \frac{54}{49}\zeta_2\right]$$

$$+ \frac{9Q_{23}}{100352\eta^{7/2}} H_{0,0,1} + \frac{9Q_{24}}{100352\eta^{7/2}} H_{0,0,-1} + \frac{381}{490}\zeta_2 + \frac{24}{49}\zeta_3\Bigg\}, \quad (A.25)$$

$$Q_{21} = 22325625 + 170997750\eta - 1400033145\eta^2 - 5593159388\eta^3 - 1400033145\eta^4 + 170997750\eta^5 + 22325625\eta^6, \quad (A.26)$$

$$Q_{22} = 4725 + 37590\eta - 284725\eta^2 - 5196076\eta^3 - 284725\eta^4 + 37590\eta^5 + 4725\eta^6, \quad (A.27)$$

$$Q_{23} = 45 + 343\eta - 2835\eta^2 - 13937\eta^3 - 13937\eta^4 - 2835\eta^5 + 343\eta^6 + 45\eta^7 + 32768\eta^{7/2}, \quad (A.28)$$

$$Q_{24} = 45 + 343\eta - 2835\eta^2 - 13937\eta^3 - 13937\eta^4 - 2835\eta^5 + 343\eta^6 + 45\eta^7 - 32768\eta^{7/2}, \quad (A.29)$$

$$Q_{25} = 99225 + 767340\eta - 6163171\eta^2 - 86697600\eta^3 + 6163171\eta^4$$

$$- 767340\eta^5 - 99225\eta^6, \tag{A.30}$$

$$Q_{26} = 99225 + 767340\eta - 6163171\eta^2 + 86697600\eta^3 + 6163171\eta^4 - 767340\eta^5 - 99225\eta^6, \tag{A.31}$$

$$Q_{27} = 945 + 7518\eta - 56945\eta^2 + 53188\eta^3 - 56945\eta^4 + 7518\eta^5 + 945\eta^6, \tag{A.32}$$

$$\begin{aligned}
&\hat{\hat{A}}_{Qq}^{\rm PS,\,tm,(3)}(N=9) = \\
&C_F T_F^2 \Biggl\{ -\frac{45056}{18225\varepsilon^3} + \frac{1}{\varepsilon^2}\Biggl[\frac{2721664}{1913625} - \frac{11264}{6075}\bigl(L_1+L_2\bigr)\Biggr] \\
&+ \frac{1}{\varepsilon}\Biggl[-\frac{5568605768}{1808375625} - \frac{5632}{6075}\bigl(L_1^2+L_1L_2+L_2^2\bigr) + \frac{680416}{637875}\bigl(L_1+L_2\bigr) \\
&- \frac{5632\zeta_2}{6075}\Biggr] - \frac{1408}{3645}L_1^3 - \frac{5632}{18225}L_2^3 - \frac{2816}{6075}L_1L_2^2 - \frac{1408}{6075}L_1^2L_2 \\
&+ \frac{11Q_{28}}{777746188800000\eta^4} + (L_1^2+L_2^2)\Biggl[\frac{11Q_{29}}{62705664000\eta^4} - \frac{11Q_{30}}{398131200\eta^{9/2}}H_1 \\
&- \frac{11Q_{31}}{398131200\eta^{9/2}}H_{-1}\Biggr] + L_1L_2\Biggl[-\frac{11Q_{32}}{4478976000\eta^4} + \frac{11Q_{30}}{199065600\eta^{9/2}}H_1 \\
&+ \frac{11Q_{31}}{199065600\eta^{9/2}}H_{-1}\Biggr] + L_1\Biggl[-\frac{11Q_{33}}{4938071040000\eta^4} - \frac{11Q_{30}}{99532800\eta^{9/2}}H_{0,1} \\
&- \frac{11Q_{31}}{99532800\eta^{9/2}}H_{0,-1} - \frac{1408\zeta_2}{2025}\Biggr] + L_2\Biggl[\frac{11Q_{34}}{4938071040000\eta^4} + \frac{11Q_{30}}{99532800\eta^{9/2}}H_{0,1} \\
&+ \frac{11Q_{31}}{99532800\eta^{9/2}}H_{0,-1} - \frac{1408\zeta_2}{2025}\Biggr] - \frac{11Q_{30}}{49766400\eta^{9/2}}H_{0,0,1} \\
&- \frac{11Q_{31}}{49766400\eta^{9/2}}H_{0,0,-1} + \frac{340208\zeta_2}{637875} + \frac{5632\zeta_3}{18225}\Biggr\},
\end{aligned} \tag{A.33}$$

$$Q_{28} = 84234583125 + 1142396443125\eta - 12238532911710\eta^2 + 27996557899275\eta^3 + 103736391394322\eta^4 + 27996557899275\eta^5 - 12238532911710\eta^6 + 1142396443125\eta^7 + 84234583125\eta^8, \tag{A.34}$$

$$Q_{29} = 848925 + 11764725\eta - 119776230\eta^2 + 247801995\eta^3 + 4258879634\eta^4 + 247801995\eta^5 - 119776230\eta^6 + 11764725\eta^7 + 848925\eta^8, \tag{A.35}$$

$$Q_{30} = 2695 + 36450\eta - 392931\eta^2 + 909975\eta^3 + 3638115\eta^4 + 3638115\eta^5 + 909975\eta^6 - 392931\eta^7 + 36450\eta^8 + 2695\eta^9 - 8388608\eta^{9/2}, \tag{A.36}$$

$$Q_{31} = 2695 + 36450\eta - 392931\eta^2 + 909975\eta^3 + 3638115\eta^4 + 3638115\eta^5 + 909975\eta^6 - 392931\eta^7 + 36450\eta^8 + 2695\eta^9 + 8388608\eta^{9/2}, \tag{A.37}$$

$$Q_{32} = 121275 + 1680675\eta - 17110890\eta^2 + 35400285\eta^3 - 43091362\eta^4 + 35400285\eta^5 - 17110890\eta^6 + 1680675\eta^7 + 121275\eta^8, \tag{A.38}$$

$$Q_{33} = -267411375 - 3646463625\eta + 38576020770\eta^2 - 86110332525\eta^3 + 1036773146624\eta^4 + 86110332525\eta^5 - 38576020770\eta^6$$

$$+ 3646463625\eta^7 + 267411375\eta^8, \tag{A.39}$$

$$Q_{34} = -267411375 - 3646463625\eta + 38576020770\eta^2 - 86110332525\eta^3 - 1036773146624\eta^4 + 86110332525\eta^5 - 38576020770\eta^6 + 3646463625\eta^7 + 267411375\eta^8. \tag{A.40}$$

The above expressions depend on η only, but not on $\sqrt{\eta}$, and they are symmetric under $\eta \leftrightarrow \eta^{-1}$. The expansions of the $O(\varepsilon^0)$ terms for $N = 1, 3, 5$ up to $O(\eta^3 \ln^3(\eta))$ for $\eta < 1$ agree with the results we have found in an independent calculation using `Q2e` [51,52]. With growing values of N, these expressions exhibit a growing degree of the polynomials in η. We have found that the general N formula cannot be expressed as a sum–product solution by means of difference field theory. This means that the corresponding solution will be given by a higher transcendental function depending on N and η. Forming the corresponding numerical Mellin moments for the complete x-space expressions, we agree with the analytic Mellin moments given in this appendix.

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