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The transition matrix element $A_{gq}(N)$ of the variable flavor number scheme at $O(\alpha_s^3)$

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Abstract

We calculate the massive unpolarized operator matrix element $A_{gq}^{(3)}(N)$ to 3-loop order in Quantum Chromodynamics at general values of the Mellin variable N. This is the first complete transition function needed in the variable flavor number scheme obtained at $O(\alpha_s^3)$. A first independent recalculation is performed for the contributions $\propto N_F$ of the 3-loop anomalous dimension $\gamma_{gq}^{(2)}(N)$.

1. Introduction

The variable flavor number scheme (VFNS) allows, in a process independent manner, the transition of the twist-2 parton distributions for N_f light flavors to $N_f + 1$ light flavors at a scale μ^2, i.e. making one single heavy flavor Q light at the time. This has been worked out to 2-loop order in [1] and to 3-loop order in [2]. The new $(N_f + 1)$-flavor massless parton densities for the different flavor combinations are given by:

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$$
\begin{aligned}
&f_k(N_f+1,\mu^2)+f_{\bar{k}}(N_f+1,\mu^2)\\
&\quad= A_{qq,Q}^{\rm NS}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes\left[f_k(N_f,\mu^2)+f_{\bar{k}}(N_f,\mu^2)\right]\\
&\qquad+\tilde{A}_{qq,Q}^{\rm PS}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes\Sigma(N_f,\mu^2)+\tilde{A}_{qg,Q}^{\rm S}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes G(N_f,\mu^2),\\
&f_{Q+\bar{Q}}(N_f+1,\mu^2)=\tilde{A}_{Qq}^{\rm PS}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes\Sigma(N_f,\mu^2)+\tilde{A}_{Qg}^{\rm S}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes G(N_f,\mu^2),\\
&G(N_f+1,\mu^2)=A_{gq,Q}^{\rm S}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes\Sigma(N_f,\mu^2)+A_{gg,Q}^{S}\left(N_f,\frac{\mu^2}{m^2}\right)\otimes G(N_f,\mu^2),\\
&\Sigma(N_f+1,\mu^2)=\sum_{k=1}^{N_f+1}\left[f_k(N_f+1,\mu^2)+f_{\bar{k}}(N_f+1,\mu^2)\right]\\
&\qquad=\left[A_{qq,Q}^{\rm NS}\left(N_f,\frac{\mu^2}{m^2}\right)+N_f\tilde{A}_{qq,Q}^{\rm PS}\left(N_f,\frac{\mu^2}{m^2}\right)\right.\\
&\qquad\quad\left.+\tilde{A}_{Qq}^{\rm PS}\left(N_f,\frac{\mu^2}{m^2}\right)\right]\otimes\Sigma(N_f,\mu^2)\\
&\qquad\quad+\left[N_f\tilde{A}_{qg,Q}^{\rm S}\left(N_f,\frac{\mu^2}{m^2}\right)+\tilde{A}_{Qg}^{\rm S}\left(N_f,\frac{\mu^2}{m^2}\right)\right]\otimes G(N_f,\mu^2).
\end{aligned}
\tag{1.1}
$$

Here, f_k and $f_{\bar{k}}$ denote the quark and antiquark densities, $\Sigma(N_f,\mu^2)=\sum_{k=1}^{N_f}[f_k+f_{\bar{k}}]$ is the singlet-quark density and $G(N_f,\mu^2)$ the gluon density. The mass m of the decoupling heavy quark Q, enters the massive operator matrix elements (OMEs) $A_{ij}(N_F,m^2/\mu^2)$, which are process independent quantities, in terms of logarithms, and μ denotes the decoupling scale. In total seven OMEs contribute. Here we use the shorthand notation $\tilde{f}=f/N_F$, $\hat{f}=f(N_F+1)-f(N_F)$. Representations of parton distribution functions in the VFNS are important at very large virtualities, as e.g. for scattering processes at the Tevatron or the Large Hadron Collider (LHC), in particular in the context of precision measurements of different observables in Quantum Chromodynamics (QCD) and the determination of the strong coupling constant $\alpha_s(M_Z)$ [3]. At 1-loop order only the OME $\tilde{A}_{Qg}^{\rm S}$ contributes. At 2-loop order $\tilde{A}_{Qq}^{\rm PS}$, $A_{qq,Q}^{\rm NS}$, $A_{gg,Q}^{S}$, $A_{gq,Q}^{\rm S}$ emerge, and from 3-loop order onward also $\tilde{A}_{qq,Q}^{\rm PS}$ and $\tilde{A}_{qg,Q}^{\rm S}$ contribute. The 2-loop corrections to all the matrix elements have been calculated in Refs. [4,1,5,6] in complete form. At 3-loop order, Mellin moments ranging for $N=2\ldots10(14)$, depending on the process, were calculated in [2] and for transversity $A_{qq,Q}^{\rm NS,TR}$ in [7].

The OMEs $\tilde{A}_{qq,Q}^{\rm PS}(N)$ and $\tilde{A}_{qg,Q}^{\rm S}(N)$ have been computed in [8]. There also the 3-loop $O(N_f T_F^2 C_{A,F})$ corrections to the OMEs to $\tilde{A}_{Qg}^{\rm S}$, $\tilde{A}_{Qq}^{\rm PS}$, $A_{qq,Q}^{\rm NS}$ and $A_{qq,Q}^{\rm NS,TR}$ were calculated, with $T_F=1/2, C_A=N_c, C_F=(N_c^2-1)/(2N_c)$ for the gauge group $SU(N_c)$. The corresponding contributions to $A_{gg,Q}^{S}$ and $A_{gq,Q}^{\rm S}$ were calculated in [9].

In the present paper we compute the complete matrix element $A_{gq,Q}^{\rm S(3)}(N)$ for general values of N. As a by-product of the calculation we also obtain the two-loop anomalous dimension $\gamma_{gq}^{(1)}(N)$ and the term $\propto T_F$ of the three-loop anomalous dimension, $\bar{\gamma}_{gq}^{(2)}(N)$. The paper is organized as follows. We first describe technical details of the calculation and then present the constant part of the massive 3-loop operator matrix element $A_{gq,Q}^{(3)\rm S}$ in Mellin-N space as well as

$\bar{\gamma}_{gq}^{(2)}(N)$ which is obtained in an independent calculation. In Appendix A we present the matrix element $A_{gq,Q}^{\rm S}$ in Mellin and momentum fraction space.

2. The formalism

The massive operator matrix element $A_{gq,Q}^{(3),\overline{\rm MS}}$ in the $\overline{\rm MS}$-scheme is given by [2]:

$$\begin{aligned}
A_{gq,Q}^{(3),\overline{\rm MS}} = &-\frac{\gamma_{gq}^{(0)}}{24}\left\{\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \left(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 10\beta_0 + 24\beta_{0,Q}\right)\beta_{0,Q}\right\}\ln^3\left(\frac{m^2}{\mu^2}\right)\\
&+\frac{1}{8}\left\{6\gamma_{gq}^{(1)}\beta_{0,Q} + \hat{\gamma}_{gq}^{(1)}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} - 4\beta_0 - 6\beta_{0,Q}\right)\right.\\
&\left.+\gamma_{gq}^{(0)}\left(\hat{\gamma}_{qq}^{(1),\rm NS} + \hat{\gamma}_{qq}^{(1),\rm PS} - \hat{\gamma}_{gg}^{(1)} + 2\beta_{1,Q}\right)\right\}\ln^2\left(\frac{m^2}{\mu^2}\right)\\
&+\frac{1}{8}\left\{4\hat{\gamma}_{gq}^{(2)} + 4a_{gq,Q}^{(2)}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} - 4\beta_0 - 6\beta_{0,Q}\right)\right.\\
&+4\gamma_{gq}^{(0)}\left(a_{qq,Q}^{(2),\rm NS} + a_{Qq}^{(2),\rm PS} - a_{gg,Q}^{(2)}\right.\\
&\left.\left.+\beta_{1,Q}^{(1)}\right) + \gamma_{gq}^{(0)}\zeta_2\left(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \left[\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 12\beta_{0,Q} + 10\beta_0\right]\beta_{0,Q}\right)\right\}\ln\left(\frac{m^2}{\mu^2}\right)\\
&+\bar{a}_{gq,Q}^{(2)}\left(\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 4\beta_0 + 6\beta_{0,Q}\right)\\
&+\gamma_{gq}^{(0)}\left(\bar{a}_{gg,Q}^{(2)} - \bar{a}_{Qq}^{(2),\rm PS} - \bar{a}_{qq,Q}^{(2),\rm NS}\right) - \gamma_{gq}^{(0)}\beta_{1,Q}^{(2)}\\
&-\frac{\gamma_{gq}^{(0)}\zeta_3}{24}\left(\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)} + \left[\gamma_{qq}^{(0)} - \gamma_{gg}^{(0)} + 10\beta_0\right]\beta_{0,Q}\right)\\
&-\frac{3\gamma_{gq}^{(1)}\beta_{0,Q}\zeta_2}{8} + 2\delta m_1^{(-1)}a_{gq,Q}^{(2)}\\
&+\delta m_1^{(0)}\hat{\gamma}_{gq}^{(1)} + 4\delta m_1^{(1)}\beta_{0,Q}\gamma_{gq}^{(0)} + a_{gq,Q}^{(3)},
\end{aligned} \tag{2.1}$$

where $\zeta_k = \sum_{l=1}^{\infty}(1/l^k), k \in \mathbb{N}, k \geqslant 2$ are the values of the Riemann ζ-function. The different logarithmic terms $\propto \ln^n(m^2/\mu^2)$, from highest to lowest power $n = 3\ldots 0$, depend on anomalous dimensions $\gamma_{ij}^{(k)}(N)$ $(k = 0\ldots 2)$, the expansion coefficients of the QCD β-function, the heavy quark mass, and of the constant parts of the unrenormalized massive OMEs $a_{ij}^{(k)}$ [1,4–6,10] from 1- to 3-loop order. Calculating the OMEs order by order in α_s delivers all these quantities. Moreover, one obtains from the $\ln^2(m^2/\mu^2)$ term the complete 2-loop anomalous dimension $\gamma_{gq}^{(1)}(N)$ and from the contribution $\ln(m^2/\mu^2)$ the term $\propto T_F$ of the 3-loop anomalous dimension $\gamma_{gq}^{(2)}(N)$.

The 86 Feynman diagrams contributing to $A_{gq,Q}^{(3)}$ were generated with an extension of QGRAF [11] allowing for local operator insertions [2]. The diagrams are calculated using TFORM [12]. With respect to the latter the corresponding diagrams are mapped into generating functions in a subsidiary variable x, cf. [13]. The resulting Feynman integrals contain not only the usual propagator-denominators, but also denominator factors in which the loop momenta enter linearly. The latter stem from the local operator insertions which have been resummed in terms of a generating function representation. We then use integration-by-parts relations [14] as encoded in Reduze2 [15], which has been adapted to this extension. Furthermore we used FERMAT [16] and GINAC [17]. The master integrals are calculated using hypergeometric function techniques [5,13,18–21] and Mellin–Barnes [22] representations applying the codes MB [23] and `MBresolve` [24]. One obtains multiple nested sums over hypergeometric expressions still containing the dimensional parameter $\varepsilon = D - 4$. After expanding in ε, these sums are performed applying modern summation technologies [25–33] encoded in the packages `Sigma` [34,35], `HarmonicSums` [36,37], `EvaluateMultiSums`, `SumProduction` [38], and ρ-`Sum` [39]. All but one master integral could be calculated in this way. For the missing case we have applied the multivariate Almkvist–Zeilberger algorithm [40] in Mellin-space, which allowed us to find a difference equation using the package `MultiIntegrate` [37]. This equation could then be solved applying the summation packages quoted before. Both the master integrals as well as the final results for individual diagrams were checked comparing to a finite number of moments calculated using `MATAD` [41].

Finally it turns out that the OME $A_{gq,Q}^{(3)}$ can be expressed by harmonic sums $S_{\vec{a}}(N)$ and ζ-values [42] only. The harmonic sums are defined by [43]

$$S_{b,\vec{a}}(N) = \sum_{k=1}^{N} \frac{\mathrm{sign}(b)^k}{k^{|b|}} S_{\vec{a}}(k), \quad S_{\emptyset}(N) = 1; \quad a_i, b \in \mathbb{Z} \setminus \{0\}, \quad N \in \mathbb{N} \setminus \{0\}. \tag{2.2}$$

The renormalization and factorization of $A_{gq,Q}^{(3)}$ has been worked out in Ref. [2]. It consists of mass, coupling constant and operator renormalization, and the factorization of the collinear singularities. Unlike the case of massless OMEs, the Z-factors for the renormalization of the ultraviolet singularities of the operators are not the inverse of those for the collinear singularities. For the renormalization of the coupling constant, one first refers to a MOM-scheme, using the background-field method [44] and then translates to the $\overline{\mathsf{MS}}$-scheme afterwards.

3. Anomalous dimensions

The anomalous dimension may be obtained from the logarithmic contributions in Eq. (2.1). In the following we drop the argument N of the harmonic sums and use the short-hand notation $S_{\vec{a}}(N) \equiv S_{\vec{a}}$. Here and in the following we simplify the result applying the algebraic relations of the harmonic sums [45]. In the present calculation the complete 2-loop anomalous dimension $\gamma_{gq}^{(1)}(N)$ and the T_F-part of the 3-loop anomalous dimension $\bar{\gamma}_{gq}^{(2)}(N)$ are calculated in an independent way and may be compared to the result obtained previously in Ref. [46].

Let us define the leading order splitting function $\bar{p}_{gq}(N)$ without color factor,

$$\bar{p}_{gq}(N) = \frac{N^2 + N + 2}{(N-1)N(N+1)}. \tag{3.1}$$

The 2-loop anomalous dimension $\gamma_{gq}^{(1)}$ is then given by

$$\begin{aligned}
\gamma_{gq}^{(1)}(N) = \frac{1}{2}\left[1 + (-1)^N\right]\Bigg\{ & C_A C_F \Bigg[8\bar{p}_{gq}\left[S_2 - S_1^2 + 2S_{-2}\right] \\
& + \frac{8(17N^4 + 41N^2 - 22N - 12)}{3(N-1)^2 N^2 (N+1)} S_1 - (-1)^N \frac{16(3N^3 + 5N^2 + 6N + 2)}{(N-1)N^2(N+1)^3} \\
& - \frac{8Q_1}{9(N-1)^2 N^3 (N+1)^2 (N+2)^2} \Bigg] \\
& + C_F^2 \Bigg[8\bar{p}_{gq}\left[S_1^2 + S_2\right] - \frac{8(5N^3 + 8N^2 + 17N + 10)}{(N-1)N(N+1)^2} S_1
\end{aligned}$$

$$+\frac{4Q_2}{(N-1)N^3(N+1)^3}\Bigg]$$
$$+C_F T_F N_F\Bigg[\frac{32(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2}-\frac{32}{3}\bar{p}_{gq}S_1\Bigg]\Bigg\}, \tag{3.2}$$

where Q_1 and Q_2 are the polynomials

$$Q_1 = 109N^8+512N^7+834N^6+592N^5$$
$$-275N^4-900N^3-152N^2+432N+144, \tag{3.3}$$
$$Q_2 = 12N^6+30N^5+43N^4+28N^3-N^2-12N-4. \tag{3.4}$$

The contribution to the 3-loop anomalous dimension is given by

$$\bar{\gamma}_{gq}^{(2)}(N) = \frac{1}{2}\big[1+(-1)^N\big]\Bigg\{C_F^2 T_F N_F\Bigg\{\frac{80}{9}\bar{p}_{gq}S_1^3$$
$$-\frac{16(58N^4+95N^3+192N^2+113N-6)}{9(N-1)N^2(N+1)^2}S_1^2$$
$$+\Bigg[\frac{64Q_3}{27(N-1)N^3(N+1)^3}+\frac{208}{3}\bar{p}_{gq}S_2\Bigg]S_1$$
$$-(-1)^N\frac{64Q_4}{9(N-1)^2N^2(N+1)^4(N+2)^3}$$
$$+\frac{2Q_5}{27(N-1)^2N^5(N+1)^5(N+2)^3}$$
$$-\frac{16(88N^4+155N^3+294N^2+185N+18)}{9(N-1)N^2(N+1)^2}S_2$$
$$+\frac{256}{9}\bar{p}_{gq}S_3-\frac{256}{(N-1)N(N+1)(N+2)}\bar{p}_{gq}S_{-2}-\frac{64}{3}\bar{p}_{gq}[S_{2,1}+6\zeta_3]\Bigg\}$$
$$+C_F T_F^2 N_F^2\Bigg\{-\frac{32}{3}\bar{p}_{gq}\big[S_1^2+S_2\big]+\frac{64(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2}S_1$$
$$-\frac{64(4N^4+4N^3+23N^2+25N+8)}{9(N-1)N(N+1)^3}\Bigg\}$$
$$+C_F C_A T_F N_F\Bigg\{-\frac{80}{9}\bar{p}_{gq}S_1^3+\frac{32Q_6}{9(N-1)^2N^2(N+1)^2(N+2)}S_1^2$$
$$+\Bigg[-\frac{16Q_7}{27(N-1)^2N^3(N+1)^3(N+2)^2}+\frac{80}{3}\bar{p}_{gq}S_2\Bigg]S_1$$
$$+\frac{8Q_8}{27(N-1)^2N^4(N+1)^4(N+2)^3}$$
$$+\Bigg[-\frac{32Q_9}{3(N-1)^2N^2(N+1)^2(N+2)}+\frac{256}{3}\bar{p}_{gq}S_1\Bigg]S_{-2}$$
$$+(-1)^N\Bigg[\frac{32Q_{10}}{9(N-1)^2N^3(N+1)^4(N+2)^3}-\frac{128(3N^3+5N^2+6N+2)}{3(N-1)N^2(N+1)^3}S_1\Bigg]$$
$$-\frac{32(N^6-N^4-7N^3-20N^2+5N+10)}{3(N-1)^2N^2(N+1)^2(N+2)}S_2$$

$$+\frac{128}{3}\bar{p}_{gq}\left[\frac{4}{3}S_3+S_{-3}-S_{-2,1}+3\zeta_3\right]\Bigg]\Bigg\}, \tag{3.5}$$

and the polynomials Q_i are

$$Q_3=88N^6+171N^5+374N^4+320N^3+23N^2-78N-18, \tag{3.6}$$

$$\begin{aligned}Q_4=\;&4N^8+106N^7+653N^6+1411N^5+453N^4\\&-2429N^3-3394N^2-1644N-344,\end{aligned} \tag{3.7}$$

$$\begin{aligned}Q_5=\;&129N^{14}+3522N^{13}+27\,035N^{12}+113\,832N^{11}+320\,915N^{10}+585\,194N^9\\&+526\,437N^8-136\,068N^7-910\,532N^6-1\,191\,312N^5-976\,400N^4\\&-562\,880N^3-276\,672N^2-122\,112N-27\,648,\end{aligned} \tag{3.8}$$

$$Q_6=32N^6+96N^5+132N^4+167N^3-26N^2-167N-54, \tag{3.9}$$

$$\begin{aligned}Q_7=\;&736N^9+4233N^8+10\,139N^7+15\,625N^6+15\,401N^5+2050N^4-10\,784N^3\\&-7400N^2-336N+576,\end{aligned} \tag{3.10}$$

$$\begin{aligned}Q_8=\;&1485N^{12}+12\,021N^{11}+40\,816N^{10}+77\,198N^9+77\,813N^8+6809N^7\\&-58\,634N^6+5012N^5+124\,920N^4+145\,680N^3\\&+77\,984N^2+18\,240N+1152,\end{aligned} \tag{3.11}$$

$$Q_9=13N^6+37N^5+51N^4+39N^3-76N^2-72N-40, \tag{3.12}$$

$$\begin{aligned}Q_{10}=\;&73N^9+655N^8+2495N^7+4747N^6+3420N^5-2846N^4-7048N^3\\&-4872N^2-1616N-192.\end{aligned} \tag{3.13}$$

Both quantities agree with the results in the literature for individual moments [47,2] and the result for general values of N [48]. In the 3-loop case the results given in [46] are confirmed for the first time for general values of N.

4. The operator matrix element

The renormalized operator matrix element (2.1) is represented by known lower order terms and the newly evaluated constant part $a_{gq}^{(3)}(N)$ of the unrenormalized OME:

$$\begin{aligned}a_{gq}^{(3)}(N)=\;&\frac{1}{2}\left[1+(-1)^N\right]\Bigg\{C_F^2T_F\Bigg\{\bar{p}_{gq}\left(\frac{64}{3}B_4-96\zeta_4\right)-2\Bigg[-\frac{29}{27}\bar{p}_{gq}S_1^4\\&+\frac{2(275N^4+472N^3+951N^2+598N+96)}{81(N-1)N^2(N+1)^2}S_1^3\\&+\left[-\frac{2P_1}{81(N-1)N^3(N+1)^3}+\frac{14}{9}\bar{p}_{gq}S_2\right]S_1^2\\&+\Bigg[-\frac{2(209N^3+376N^2+669N+418)}{27(N-1)N(N+1)^2}S_2\\&-\frac{4P_0}{243(N-1)N^4(N+1)^4}+\frac{104}{27}\bar{p}_{gq}S_3-\frac{16}{9}\bar{p}_{gq}S_{2,1}\Bigg]S_1+\frac{1}{3}\bar{p}_{gq}S_2^2\\&+\frac{2P_2}{243(N-2)(N-1)^2N^5(N+1)^5(N+2)^4}\end{aligned}$$

$$
\begin{aligned}
&+ \frac{2P_3}{81(N-2)(N-1)^2N^4(N+1)^4(N+2)^2} S_2 \\
&- \frac{64\bar{p}_{gq}}{(N-1)N(N+1)(N+2)} S_{-1}S_2 \\
&- \frac{4P_4}{81(N-1)^2N^3(N+1)^3(N+2)} S_3 + \frac{110}{9}\bar{p}_{gq}S_4 \\
&+ \biggl[\frac{64\bar{p}_{gq}}{(N-1)N(N+1)(N+2)} S_{-1} \\
&+ \frac{16P_5}{3(N-2)(N-1)^2N^3(N+1)^3(N+2)^2}\biggr] S_{-2} \\
&- \frac{64\bar{p}_{gq}}{3(N-1)N(N+1)(N+2)}[S_{-3} - 3S_{2,-1} + 3S_{-2,-1}] \\
&+ \frac{8(35N^3+64N^2+111N+70)}{27(N-1)N(N+1)^2} S_{2,1} - \frac{16}{9}\bar{p}_{gq}[3S_{3,1} - S_{2,1,1}]\biggr] \\
&- 2\biggl[\frac{2(17N^4+28N^3+69N^2+46N+24)}{9(N-1)N^2(N+1)^2} S_1 \\
&+ \frac{P_6}{9(N-1)^2N^3(N+1)^3(N+2)^2} - \frac{1}{3}\bar{p}_{gq}\bigl(10S_1^2 - 14S_2\bigr)\biggr]\zeta_2 \\
&+ 2\biggl[\frac{2P_7}{9(N-1)^2N^3(N+1)^3(N+2)} + \frac{152}{9}\bar{p}_{gq}S_1\biggr]\zeta_3\biggr\} \\
&+ C_F T_F^2 \biggl\{-2N_F\biggl[\frac{8}{27}\bar{p}_{gq}S_1^3 - \frac{8(8N^3+13N^2+27N+16)}{27(N-1)N(N+1)^2}\bigl[S_1^2 + S_2\bigr] \\
&+ \biggl[\frac{16(35N^4+97N^3+178N^2+180N+70)}{27(N-1)N(N+1)^3} + \frac{8}{9}\bar{p}_{gq}S_2\biggr]S_1 \\
&- \frac{16(1138N^5+4237N^4+8861N^3+11\,668N^2+8236N+2276)}{243(N-1)N(N+1)^4} \\
&+ \frac{16}{27}\bar{p}_{gq}S_3\biggr] \\
&- 2\biggl[3\biggl[\frac{16(39N^4+101N^3+201N^2+205N+78)}{81(N-1)N(N+1)^3} + \frac{16}{27}\bar{p}_{gq}S_2\biggr]S_1 \\
&- \frac{16(8N^3+13N^2+27N+16)}{27(N-1)N(N+1)^2}\bigl[S_1^2 + S_2\bigr] + \frac{16}{27}\bar{p}_{gq}\bigl[S_1^3 + 2S_3\bigr] \\
&- \frac{8(1129N^5+3814N^4+8618N^3+11\,884N^2+8425N+2258)}{243(N-1)N(N+1)^4}\biggr] \\
&- 2(2+N_F)\biggl[\frac{8}{3}\bar{p}_{gq}S_1 - \frac{8(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2}\biggr]\zeta_2 \\
&+ \bar{p}_{gq}\biggl[\frac{512}{9} - \frac{224}{9}N_F\biggr]\zeta_3\biggr\} \\
&+ C_A C_F T_F \biggl\{\bar{p}_{gq}\biggl(96\zeta_4 - \frac{32}{3}B_4\biggr) - 2\biggl[\frac{29}{27}\bar{p}_{gq}S_1^4
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{2P_8}{81(N-1)^2N^2(N+1)^2(N+2)} S_1^3 \\
&+ \left[\frac{2P_9}{81(N-1)^2N^3(N+1)^3(N+2)^2} + \frac{58}{9}\bar{p}_{gq}S_2\right]S_1^2 \\
&+ \left[\frac{32}{9}\bar{p}_{gq}\left[\frac{53}{12}S_3 + S_{2,1}\right] - \frac{4P_{10}}{243(N-1)^2N^4(N+1)^4(N+2)^3}\right. \\
&\left. - \frac{2P_{11}}{27(N-1)^2N^2(N+1)^2(N+2)}S_2 - 16\bar{p}_{gq}S_{-2,1}\right]S_1 \\
&+ \frac{2P_{12}}{243(N-2)(N-1)^2N^5(N+1)^5(N+2)^4} + \frac{61}{9}\bar{p}_{gq}S_2^2 + \frac{16}{9}\bar{p}_{gq}S_{-2}^2 \\
&+ \left[\frac{152}{9}\bar{p}_{gq}S_1 - \frac{8P_{13}}{27(N-1)^2N^2(N+1)^2(N+2)}\right]S_{-3} \\
&+ \frac{32\bar{p}_{gq}}{(N-1)N(N+1)(N+2)}S_{-1}S_2 \\
&+ \frac{2P_{14}}{27(N-2)(N-1)^2N^3(N+1)^3(N+2)^2}S_2 \\
&- \frac{8P_{15}}{81(N-1)^2N^2(N+1)^2(N+2)}S_3 + \frac{178}{9}\bar{p}_{gq}S_4 \\
&+ \left[\frac{88}{9}\bar{p}_{gq}\left[S_1^2 + S_2\right] - \frac{16(52N^4+95N^3+210N^2+137N+36)}{27(N-1)N^2(N+1)^2}S_1\right. \\
&- \frac{32\bar{p}_{gq}}{(N-1)N(N+1)(N+2)}S_{-1} \\
&\left. + \frac{8P_{16}}{27(N-2)(N-1)^2N^3(N+1)^3(N+2)^2}\right]S_{-2} \\
&- \frac{8(14N^5+15N^4+4N^3+81N^2-10N+88)}{9(N-1)^2N^2(N+1)^2(N+2)}S_{2,1} \\
&- \frac{32\bar{p}_{gq}}{(N-1)N(N+1)(N+2)}S_{2,-1} - \frac{16}{3}S_{3,1} + \frac{160}{9}\bar{p}_{gq}S_{-4} \\
&+ \frac{16(26N^4+49N^3+126N^2+85N+36)}{27(N-1)N^2(N+1)^2}S_{-2,1} - \frac{112}{9}\bar{p}_{gq}S_{-2,2} \\
&+ \frac{32\bar{p}_{gq}}{(N-1)N(N+1)(N+2)}S_{-2,-1} - \frac{136}{9}S_{-3,1} - 8\bar{p}_{gq}S_{2,1,1} \\
&\left. + \frac{176}{9}\bar{p}_{gq}S_{-2,1,1}\right] - \frac{16}{9}\frac{(-2-2N-N^2+N^3)}{(N-1)N(N+1)}[17S_{-3,1}+6S_{3,1}] \\
&- 2\left[\bar{p}_{gq}\left(\frac{10}{3}S_1^2 + 2S_2 + 4S_{-2}\right)\right. \\
&- \frac{2(59N^5+94N^4+59N^3-84N^2-224N+168)}{9(N-1)^2N^2(N+1)(N+2)}S_1 \\
&\left. + \frac{2P_{17}}{9(N-1)N^3(N+1)^3(N+2)^2}\right]\zeta_2
\end{aligned}
$$

$$-2\left[\frac{2P_{18}}{9(N-1)^2N^2(N+1)^2(N+2)}+\frac{56}{9}\bar{p}_{gq}S_1\right]\zeta_3\Bigg\}\Bigg\}, \tag{4.1}$$

with the polynomials P_i given by

$$P_0 = 205N^8+268N^7-3541N^6-11\,258N^5-19\,844N^4-19\,936N^3-9870N^2 -2016N-216 \tag{4.2}$$

$$P_1 = 916N^6+2547N^5+5666N^4+6683N^3+4028N^2+1200N+144 \tag{4.3}$$

$$P_2 = 17\,223N^{16}+165\,192N^{15}+598\,459N^{14}+791\,304N^{13}-970\,086N^{12} -5\,283\,698N^{11}-8\,410\,804N^{10}-5\,109\,721N^9+3\,632\,942N^8+8\,912\,043N^7 +3\,490\,278N^6-6\,793\,396N^5-9\,096\,296N^4-3\,512\,432N^3+179\,232N^2 +131\,904N+24\,192 \tag{4.4}$$

$$P_3 = 2708N^{12}+12\,913N^{11}+15\,444N^{10}-20\,600N^9-94\,758N^8-142\,761N^7 -38\,594N^6+131\,744N^5+139\,824N^4+30\,368N^3-5184N-10\,368 \tag{4.5}$$

$$P_4 = 613N^8+2350N^7+3726N^6+3208N^5-1179N^4-4742N^3-2080N^2 +264N+1296 \tag{4.6}$$

$$P_5 = N^8+3N^7+3N^6+3N^5-2N^3-16N^2+120N+64 \tag{4.7}$$

$$P_6 = 195N^9+1152N^8+2431N^7+1949N^6-1038N^5-4577N^4-4568N^3 -2376N^2-320N-912 \tag{4.8}$$

$$P_7 = 233N^8+980N^7+1492N^6+926N^5+39N^4-426N^3 +1068N^2+1352N+480 \tag{4.9}$$

$$P_8 = 371N^6+945N^5+945N^4-N^3-2132N^2-728N+744 \tag{4.10}$$

$$P_9 = 1540N^9+8277N^8+18\,725N^7+20\,707N^6-1501N^5-31\,700N^4-20\,384N^3 +9664N^2+7056N-1152 \tag{4.11}$$

$$P_{10} = 5042N^{12}+42\,402N^{11}+155\,879N^{10}+312\,989N^9+312\,249N^8 -24\,387N^7-415\,670N^6-329\,640N^5+53\,392N^4+118\,912N^3-17\,472N^2 -33\,984N-3456 \tag{4.12}$$

$$P_{11} = 319N^6+765N^5+945N^4+523N^3-1696N^2-592N-120 \tag{4.13}$$

$$P_{12} = 10\,393N^{16}+100\,762N^{15}+401\,681N^{14}+757\,324N^{13}+161\,109N^{12} -2\,974\,044N^{11}-8\,597\,809N^{10}-11\,649\,324N^9-5\,136\,842N^8+7\,823\,954N^7 +15\,364\,644N^6+13\,824\,600N^5+8\,495\,280N^4+3\,677\,408N^3+943\,296N^2 +153\,216+34560 \tag{4.14}$$

$$P_{13} = 52N^6+159N^5+291N^4+253N^3-373N^2-334N-192 \tag{4.15}$$

$$P_{14} = 324N^{10}+975N^9+347N^8-2523N^7-7715N^6-7672N^5+8128N^4 +14168N^3+2480N^2+4448N+4608 \tag{4.16}$$

$$P_{15} = 184N^6+432N^5+675N^4+484N^3-1087N^2-268N+84 \tag{4.17}$$

$$P_{16} = 136N^{10}+503N^9+285N^8-1445N^7-4499N^6-5032N^5+1254N^4 +5838N^3+3640N^2-1304N-960 \tag{4.18}$$

$$P_{17} = 40N^8 + 247N^7 + 787N^6 + 1771N^5 + 2775N^4 + 2564N^3 + 1384N^2 + 704N + 240 \quad (4.19)$$

$$P_{18} = 41N^6 + 315N^5 + 139N^4 - 215N^3 + 1028N^2 - 236N + 1136. \quad (4.20)$$

$a_{qg}^{(3)}(N)$ contains contributions up to weight w = 4, including the constant

$$B_4 = -4\zeta_2 \ln^2(2) + \frac{2}{3}\ln^4(2) - \frac{13}{2}\zeta_4 + 16\,\mathrm{Li}_4\left(\frac{1}{2}\right) = -8S_{-3,-1}(\infty) + \frac{11}{2}\zeta_4. \quad (4.21)$$

After algebraic reduction [45] the result is represented in terms of the basis:

$$S_1,\ S_2,\ S_3,\ S_4,\ S_{-1},\ S_{-2},\ S_{-3},\ S_{-4},\ S_{2,1},\ S_{2,-1},\ S_{-2,-1},\ S_{-2,1},\ S_{-2,2},\ S_{3,1},\ S_{-3,1},\ S_{2,1,1},\ S_{-2,1,1}. \quad (4.22)$$

Due to structural relations, such as differentiation and multiple argument relations, [49], only the representatives

$$S_1, S_{2,1}, S_{-2,1}, S_{-3,1}, S_{2,1,1}, S_{-2,1,1} \quad (4.23)$$

remain as basic sums. The function $a_{gq}^{(3)}(N)$ contains a removable singularity at $N = 2$ yielding

$$a_{gq}^{(3)}(N \to 2) = -C_F C_A T_F \left[\frac{414817}{2187} + \frac{296}{9}\zeta_3\right] - C_F^2 T_F \left[\frac{1098203}{2187} + 16\zeta_3\right] \quad (4.24)$$

for the evanescent pole term. This is in accordance with the expectation that the gluonic OMEs have their rightmost singularity at $N = 1$. In massive OMEs, removable singularities can in general also occur at rational values of $N > 1$, cf. [50]. $A_{gq}(N)$ can be represented by harmonic sums [43] over $\mathbb{Q}(N)$ with rational weights whose denominators factorize into terms $(N-k)^l$, $k \in \mathbb{Z}$, $l \in \mathbb{N}$. It is therefore a meromorphic function [49]. More specifically, its poles are located at the integers $N \leqslant 1$.

Let us finally consider the behavior of $a_{gq}^{(3)}(N)$ for $N \to \infty$ and around the so-called 'leading singularity' at $N = 1$.

For large values of $N \in \mathbb{C}$ outside the singularities one obtains

$$\begin{aligned} a_{gq}^{(3)}(N \to \infty) \propto & -\frac{58}{27N}(C_A - C_F)C_F T_F L^4(N) \\ & - \frac{2C_F T_F}{81N}\left[-742C_A + 550C_F + 24T_F(N_F+2)\right]L^3(N) \\ & + \frac{C_F T_F}{N}\left[C_A\left(-\frac{88}{9}\zeta_2 - \frac{6160}{81}\right) + C_F\left(\frac{32}{9}\zeta_2 + \frac{3664}{81}\right)\right. \\ & \left. + \frac{128}{27}(N_F+2)T_F\right]L^2(N) + O\left(\frac{L(N)}{N}\right) \end{aligned} \quad (4.25)$$

as the first terms in the asymptotic representation, with $L(N) = \ln(N) + \gamma_E$ and γ_E denotes the Euler–Mascheroni constant. In x-space the leading singular term is $\propto \alpha_s^3 \ln^4(1-x)$ for $x \to 1$.

Analyzing the anomalous dimensions for different scattering processes in fixed order perturbation theory one finds that so-called 'leading-poles' are situated at $N = 1$ for massless vector operators [51], $N = 0$ in case of massless quark operators [52,53], and $N = -1$ for massless scalar operators [54]. Expanding $a_{gq}^{(3)}(N)$ around $N = 1$ the leading term is given by

$$a_{gq}^{(3)}(N \to 1) \propto \frac{1}{(N-1)^2}\Bigg[C_A C_F T_F\left(\frac{16}{3}\zeta_2 - \frac{736}{9}\zeta_3 + \frac{20224}{81}\right) + C_F^2 T_F\left(\frac{224}{9}\zeta_2 + \frac{1024}{9}\zeta_3 - \frac{37376}{243}\right)\Bigg] + O\left(\frac{1}{N-1}\right). \tag{4.26}$$

In QCD, $C_A = 3$, $C_F = 4/3$, $T_F = 1/2$, the first expansion coefficients are given by

$$a_{gq}^{(3)}(N) \propto \frac{341.543}{(N-1)^2} - \frac{1}{N-1}(1814.73 - 66.0055 N_F) + 3222.81 - 71.4816 N_F - (5345.61 - 81.4031 N_F)(N-1) + (8454.89 - 85.7885 N_F)(N-1)^2 + O\big((N-1)^3\big). \tag{4.27}$$

In x-space the leading term is $\propto \alpha_s^3 \ln(1/x)/x$. The values of the sub-leading terms have oscillating signs and rise from term to term, which leads to a strong compensation of the leading behavior in the physical region, e.g. at HERA. This is in accordance with earlier observations in other cases, cf. Refs. [53,55,56,54]. The complete OME $A_{gq,Q}^{(2,3),\overline{\mathsf{MS}}}$ in N and x-space are given in Appendix A.

5. Conclusions

We calculated the massive operator matrix element $A_{gq}^{(3)}(N)$, which represents the first complete transition matrix element in the variable flavor number scheme at 3-loop order. The corresponding Feynman integrals have been reduced using the integration-by-parts technique to master integrals, which have been computed using different techniques in terms of generating functions. In Mellin-space the final result for the individual diagrams has been obtained using difference-field techniques. The matrix element $A_{gq}^{(3)}(N)$ can be expressed by harmonic sums up to weight $\mathsf{w} = 4$ in Mellin space and harmonic polylogarithms up to weight $\mathsf{w} = 5$ in x-space. This simple form may be due to the fact that at most four of the lines of the corresponding diagrams are massive. The contributing graphs include diagrams of the Benz-topology. Both the results for renormalizing the heavy quark mass in the on-shell and $\overline{\text{MS}}$ scheme were presented. As a by-product of the calculation also the contribution $\propto T_F$ to the 3-loop anomalous dimension $\gamma_{gq}(N)$ has been obtained and confirms the results in the literature for the first time.

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Appendix A

In the $\overline{\mathsf{MS}}$-scheme for the strong coupling and the on-shell-scheme for the heavy quark mass m the massive OME $A_{gq,Q}(N)$ up to 3-loop order is given in Mellin space by:

$$A_{gq,Q}^{\rm OMS}(N,a_s) = a_s^2 A_{gq,Q}^{(2),{\rm OMS}}(N) + a_s^3 A_{gq,Q}^{(3),{\rm OMS}}(N) \tag{A.1}$$

with $a_s = \alpha_s^{\overline{\rm MS}}(\mu^2)/(4\pi)$ and

$$\begin{aligned}
A_{gq,Q}^{(2),{\rm OMS}}(N) = {} & \frac{1}{2}\big[1+(-1)^N\big] C_F T_F \Bigg\{ \frac{8}{3}\bar{p}_{gq} \ln^2\left(\frac{m^2}{\mu^2}\right) + \Bigg[\frac{16(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2} \\
& - \frac{16}{3}\bar{p}_{gq} S_1\Bigg] \ln\left(\frac{m^2}{\mu^2}\right) + \frac{4}{3}\bar{p}_{gq}\big[S_1^2 + S_2\big] \\
& - \frac{8(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2} S_1 \\
& + \frac{8(43N^4+105N^3+224N^2+230N+86)}{27(N-1)N(N+1)^3} \Bigg\}
\end{aligned} \tag{A.2}$$

$$\begin{aligned}
A_{gq,Q}^{(3),{\rm OMS}}(N) = {} & \frac{1}{2}\big[1+(-1)^N\big] \Bigg\{ \bar{p}_{gq} \Bigg\{ C_F^2 T_F \Bigg[\frac{4P_{32}}{9(N-1)N^2(N+1)^2(N+2)} - \frac{16}{9} S_1 \Bigg] \\
& + \frac{32}{9} C_F T_F^2 (2+N_F) \\
& + C_F C_A T_F \Bigg[\frac{16}{9} S_1 - \frac{8P_{20}}{9(N-1)N(N+1)(N+2)} \Bigg] \Bigg\} \ln^3\left(\frac{m^2}{\mu^2}\right) \\
& + \Bigg\{ C_F^2 T_F \Bigg\{ -\frac{2P_{47}}{9(N-1)^2N^3(N+1)^3(N+2)^2} \\
& + \frac{16(7N^3+4N^2+17N-6)}{9(N-1)N^2(N+1)} S_1 + \frac{8}{3}\big(S_1^2 - 5S_2\big)\bar{p}_{gq} \Bigg\} \\
& + C_F T_F^2 \Bigg\{ \frac{32(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2} - \frac{32}{3}\bar{p}_{gq} S_1 \Bigg\} \\
& + C_F C_A T_F \Bigg\{ \frac{4P_{46}}{9(N-1)^2N^3(N+1)^3(N+2)^2} \\
& + \frac{32P_{26}}{9(N-1)^2N^2(N+1)(N+2)} S_1 \\
& + \Bigg[-\frac{8}{3} S_1^2 - 8S_2 - 16S_{-2} \Bigg] \bar{p}_{gq} \Bigg\} \Bigg\} \ln^2\left(\frac{m^2}{\mu^2}\right) \\
& + \Bigg\{ C_F^2 T_F \Bigg\{ -\frac{4P_{23}}{9(N-1)N^2(N+1)^2} S_1^2 + \frac{8P_{39}}{27(N-1)N^3(N+1)^3} S_1 \\
& - \frac{2P_{54}}{27(N-1)^2N^5(N+1)^4(N+2)^2} - \frac{4P_{44}}{9(N-1)^2N^3(N+1)^3(N+2)} S_2 \\
& + \Bigg[-\frac{8}{9} S_1^3 + \frac{88}{3} S_2 S_1 + \frac{176}{9} S_3 - \frac{128}{(N-1)N(N+1)(N+2)} S_{-2} \\
& - \frac{32}{3} S_{2,1} - 64\zeta_3 \Bigg] \bar{p}_{gq} \Bigg\} + C_F T_F^2 N_F \Bigg\{ \frac{32(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2} S_1 \\
& + \frac{32P_{21}}{27(N-1)N(N+1)^3} + \Bigg[-\frac{16}{3} S_1^2 - \frac{16}{3} S_2 \Bigg] \bar{p}_{gq} \Bigg\} + C_F T_F^2 \frac{992}{27} \bar{p}_{gq}
\end{aligned}$$

$$
\begin{aligned}
&+ C_F C_A T_F \Biggl\{ \frac{4 P_{29}}{9(N-1)^2 N^2 (N+1)(N+2)} S_1^2 \\
&- \frac{8 P_{49}}{27(N-1)^2 N^3 (N+1)^3 (N+2)^2} S_1 \\
&+ \frac{8 P_{53}}{27(N-1)^2 N^4 (N+1)^4 (N+2)^3} \\
&- \frac{4 P_{35}}{3(N-1)^2 N^2 (N+1)^2 (N+2)} S_2 \\
&- \frac{16 P_{34}}{3(N-1)^2 N^2 (N+1)^2 (N+2)} S_{-2} \\
&+ \biggl[\frac{8}{9} S_1^3 + \frac{56}{3} S_2 S_1 + \frac{128}{3} S_{-2} S_1 + \frac{256}{9} S_3 + \frac{64}{3} S_{-3} - \frac{64}{3} S_{-2,1} \\
&+ 64 \zeta_3 \biggr] \bar{p}_{gq} \Biggr\} \Biggr\} \ln\left(\frac{m^2}{\mu^2}\right) + C_F^2 T_F \Biggl\{ \frac{40(4N^3 + N^2 + 11N - 6)}{81(N-1)N^2(N+1)} S_1^3 \\
&- \frac{8 P_{33}}{81(N-1) N^3 (N+1)^3} S_1^2 + \biggl[\frac{16 P_{45}}{243(N-1) N^4 (N+1)^4} \\
&+ \frac{8 P_{25}}{27(N-1) N^2 (N+1)^2} S_2 \biggr] S_1 + \frac{8 P_{43}}{9(N-1)^2 N^3 (N+1)^3 (N+2)} \zeta_3 \\
&+ \frac{P_{57}}{486(N-2)(N-1)^2 N^5 (N+1)^6 (N+2)^4} \\
&- \frac{8 P_{52}}{81(N-2)(N-1)^2 N^4 (N+1)^4 (N+2)} S_2 \\
&+ \frac{16 P_{41}}{81(N-1)^2 N^2 (N+1)^2 (N+2)} S_3 \\
&- \frac{32 P_{42}}{3(N-2)(N-1)^2 N^3 (N+1)^3 (N+2)^2} S_{-2} \\
&- \frac{16(35N^3 + 64N^2 + 111N + 70)}{27(N-1)N(N+1)^2} S_{2,1} \\
&+ \biggl[\frac{10}{27} S_1^4 - \frac{76}{9} S_2 S_1^2 + \biggl[-\frac{304}{27} S_3 + \frac{32}{9} S_{2,1} + \frac{320}{9} \zeta_3 \biggr] S_1 - \frac{2}{3} S_2^2 - 96 \zeta_4 \\
&+ \frac{64}{3} B_4 + \frac{128}{(N-1)N(N+1)(N+2)} S_{-1} S_2 - \frac{172}{9} S_4 \\
&- \frac{128}{(N-1)N(N+1)(N+2)} S_{-2} S_{-1} \\
&+ \frac{128}{3(N-1)N(N+1)(N+2)} S_{-3} \\
&- \frac{128}{(N-1)N(N+1)(N+2)} S_{2,-1} + \frac{32}{3} S_{3,1} \\
&+ \frac{128}{(N-1)N(N+1)(N+2)} S_{-2,-1} - \frac{32}{9} S_{2,1,1} \biggr] \bar{p}_{gq} \Biggr\}
\end{aligned}
$$

$$+ C_F T_F^2 \Bigg\{ -\frac{16(8N^3+13N^2+27N+16)}{27(N-1)N(N+1)^2} S_1^2$$
$$+ \frac{32P_{19}}{27(N-1)N(N+1)^3} S_1 - \frac{16P_{31}}{243(N-1)N(N+1)^4}$$
$$- \frac{16(8N^3+13N^2+27N+16)}{27(N-1)N(N+1)^2} S_2$$
$$+ N_F \Bigg[-\frac{32(8N^3+13N^2+27N+16)}{27(N-1)N(N+1)^2} S_1^2$$
$$+ \frac{64P_{19}}{27(N-1)N(N+1)^3} S_1 + \frac{64P_{30}}{243(N-1)N(N+1)^4}$$
$$- \frac{32(8N^3+13N^2+27N+16)}{27(N-1)N(N+1)^2} S_2 \Bigg] + \Bigg[\frac{16}{27} S_1^3 + \frac{16}{9} S_2 S_1 + \frac{32}{27} S_3$$
$$+ N_F \Bigg[\frac{32}{27} S_1^3 + \frac{32}{9} S_2 S_1 + \frac{64}{27} S_3 - \frac{256}{9} \zeta_3 \Bigg] + \frac{448}{9} \zeta_3 \Bigg] \bar{p}_{gq} \Bigg\}$$
$$+ C_F C_A T_F \Bigg\{ -\frac{16P_{27}}{81(N-1)^2 N^2 (N+1)(N+2)} S_1^3$$
$$+ \frac{4P_{48}}{81(N-1)^2 N^3 (N+1)^3 (N+2)^2} S_1^2$$
$$+ \Bigg[\frac{16P_{37}}{27(N-1)^2 N^2 (N+1)^2 (N+2)} S_2$$
$$- \frac{8P_{55}}{243(N-1)^2 N^4 (N+1)^4 (N+2)^3} \Bigg] S_1$$
$$- \frac{4P_{36}}{9(N-1)^2 N^2 (N+1)^2 (N+2)} \zeta_3$$
$$+ \frac{8P_{56}}{243(N-2)(N-1)^2 N^5 (N+1)^5 (N+2)^4}$$
$$+ \Bigg[\frac{32P_{24}}{27(N-1)N^2(N+1)^2} S_1$$
$$- \frac{16P_{51}}{27(N-2)(N-1)^2 N^3 (N+1)^3 (N+2)^2} \Bigg] S_{-2}$$
$$- \frac{4P_{50}}{27(N-2)(N-1)^2 N^3 (N+1)^3 (N+2)^2} S_2$$
$$+ \frac{8P_{40}}{81(N-1)^2 N^2 (N+1)^2 (N+2)} S_3$$
$$+ \frac{16P_{38}}{27(N-1)^2 N^2 (N+1)^2 (N+2)} S_{-3}$$
$$+ \frac{16P_{28}}{9(N-1)^2 N^2 (N+1)^2 (N+2)} S_{2,1} - \frac{32P_{22}}{27(N-1)N^2(N+1)^2} S_{-2,1}$$
$$+ \bar{p}_{gq} \Bigg[-\frac{10}{27} S_1^4 - \frac{68}{9} S_2 S_1^2 - \frac{304}{9} S_{-3} S_1 + \Bigg[-\frac{752}{27} S_3 - \frac{64}{9} S_{2,1} + 32 S_{-2,1}$$

$$
\begin{aligned}
&- \frac{128}{9}\zeta_3\Big]S_1 - \frac{122}{9}S_2^2 - \frac{32}{9}S_{-2}^2 + 96\zeta_4 \\
&- \frac{64}{(N-1)N(N+1)(N+2)}S_{-1}S_2 \\
&- \frac{356}{9}S_4 + \Big[-\frac{176}{9}S_1^2 - \frac{176}{9}S_2 + \frac{64}{(N-1)N(N+1)(N+2)}S_{-1}\Big]S_{-2} \\
&- \frac{320}{9}S_{-4} + \frac{64}{(N-1)N(N+1)(N+2)}S_{2,-1} + \frac{32}{3}S_{3,1} + \frac{224}{9}S_{-2,2} \\
&- \frac{64}{(N-1)N(N+1)(N+2)}S_{-2,-1} + \frac{272}{9}S_{-3,1} + 16S_{2,1,1} \\
&- \frac{352}{9}S_{-2,1,1} - \frac{32}{3}B_4\Big]\Big]\Big\}\Big\}, \qquad \text{(A.3)}
\end{aligned}
$$

with the polynomials P_i

$$P_{19} = 4N^4 + 4N^3 + 23N^2 + 25N + 8 \qquad \text{(A.4)}$$

$$P_{20} = 11N^4 + 22N^3 - 7N^2 - 18N + 4 \qquad \text{(A.5)}$$

$$P_{21} = 19N^4 + 81N^3 + 86N^2 + 80N + 38 \qquad \text{(A.6)}$$

$$P_{22} = 26N^4 + 49N^3 + 126N^2 + 85N + 36 \qquad \text{(A.7)}$$

$$P_{23} = 43N^4 + 68N^3 + 135N^2 + 74N - 24 \qquad \text{(A.8)}$$

$$P_{24} = 52N^4 + 95N^3 + 210N^2 + 137N + 36 \qquad \text{(A.9)}$$

$$P_{25} = 166N^4 + 293N^3 + 546N^2 + 341N + 18 \qquad \text{(A.10)}$$

$$P_{26} = N^5 - N^4 - 8N^3 - 33N^2 - 7N + 30 \qquad \text{(A.11)}$$

$$P_{27} = 4N^5 + 23N^4 + 49N^3 + 165N^2 - N - 150 \qquad \text{(A.12)}$$

$$P_{28} = 14N^5 + 15N^4 + 4N^3 + 81N^2 - 10N + 88 \qquad \text{(A.13)}$$

$$P_{29} = 31N^5 + 86N^4 + 127N^3 + 324N^2 - 88N - 264 \qquad \text{(A.14)}$$

$$P_{30} = 197N^5 + 824N^4 + 1540N^3 + 1961N^2 + 1388N + 394 \qquad \text{(A.15)}$$

$$P_{31} = 359N^5 + 1364N^4 + 2944N^3 + 3608N^2 + 2495N + 718 \qquad \text{(A.16)}$$

$$P_{32} = 3N^6 + 9N^5 + 17N^4 + 19N^3 + 52N^2 + 44N + 48 \qquad \text{(A.17)}$$

$$P_{33} = 4N^6 - 216N^5 - 343N^4 - 694N^3 - 847N^2 - 456N - 72 \qquad \text{(A.18)}$$

$$P_{34} = 13N^6 + 37N^5 + 51N^4 + 39N^3 - 76N^2 - 72N - 40 \qquad \text{(A.19)}$$

$$P_{35} = 15N^6 + 33N^5 + 37N^4 - N^3 - 92N^2 + 56 \qquad \text{(A.20)}$$

$$P_{36} = 19N^6 + 249N^5 + 65N^4 - 253N^3 + 1084N^2 - 172N + 1120 \qquad \text{(A.21)}$$

$$P_{37} = 31N^6 + 54N^5 + 72N^4 + 19N^3 - 283N^2 - 7N - 66 \qquad \text{(A.22)}$$

$$P_{38} = 52N^6 + 159N^5 + 291N^4 + 253N^3 - 373N^2 - 334N - 192 \qquad \text{(A.23)}$$

$$P_{39} = 164N^6 + 243N^5 + 472N^4 + 175N^3 - 446N^2 - 408N - 72 \qquad \text{(A.24)}$$

$$P_{40} = 269N^6 + 567N^5 + 981N^4 + 725N^3 - 2066N^2 - 356N + 24 \qquad \text{(A.25)}$$

$$P_{41} = 275N^6 + 774N^5 + 828N^4 + 434N^3 - 1631N^2 - 1532N - 876 \qquad \text{(A.26)}$$

$$P_{42} = N^8 + 3N^7 + 3N^6 + 3N^5 - 2N^3 - 16N^2 + 120N + 64 \qquad \text{(A.27)}$$

$$P_{43} = 115N^8 + 484N^7 + 730N^6 + 436N^5 - 33N^4 - 280N^3 + 436N^2 + 608N + 192 \tag{A.28}$$

$$P_{44} = 187N^8 + 706N^7 + 1056N^6 + 802N^5 - 807N^4 - 2036N^3 - 1444N^2 - 480N - 288 \tag{A.29}$$

$$P_{45} = 1031N^8 + 3236N^7 + 5986N^6 + 5051N^5 - 1186N^4 - 6041N^3 - 4161N^2 - 1008N - 108 \tag{A.30}$$

$$P_{46} = 69N^9 + 414N^8 + 860N^7 + 694N^6 - 309N^5 - 820N^4 - 124N^3 + 528N^2 + 896N + 384 \tag{A.31}$$

$$P_{47} = 87N^9 + 450N^8 + 604N^7 - 526N^6 - 2451N^5 - 3236N^4 - 1616N^3 - 720N^2 + 112N - 768 \tag{A.32}$$

$$P_{48} = 284N^9 + 1821N^8 + 5119N^7 + 12\,689N^6 + 22\,753N^5 + 16\,190N^4 - 7888N^3 - 17\,128N^2 - 4752N + 1152 \tag{A.33}$$

$$P_{49} = 356N^9 + 2139N^8 + 5347N^7 + 9317N^6 + 11\,533N^5 + 4460N^4 - 7168N^3 - 8464N^2 - 1680N + 576 \tag{A.34}$$

$$P_{50} = 78N^{10} + 81N^9 - 265N^8 - 759N^7 - 1853N^6 + 434N^5 + 10\,204N^4 + 10\,352N^3 + 2528N^2 + 5984N + 4608 \tag{A.35}$$

$$P_{51} = 136N^{10} + 503N^9 + 285N^8 - 1445N^7 - 4499N^6 - 5032N^5 + 1254N^4 + 5838N^3 + 3640N^2 - 1304N - 960 \tag{A.36}$$

$$P_{52} = 1132N^{11} + 3042N^{10} + 297N^9 - 8170N^8 - 20\,968N^7 - 14\,788N^6 + 14\,047N^5 + 21932N^4 - 6172N^3 - 8496N^2 - 7776N - 5184 \tag{A.37}$$

$$P_{53} = 301N^{12} + 2301N^{11} + 7232N^{10} + 13\,239N^9 + 14\,891N^8 + 8033N^7 + 5814N^6 + 23\,063N^5 + 44\,966N^4 + 49\,136N^3 + 28\,928N^2 + 7440N + 288 \tag{A.38}$$

$$P_{54} = 339N^{12} + 1545N^{11} + 436N^{10} - 11\,406N^9 - 31\,663N^8 - 32\,981N^7 + 3704N^6 + 44\,386N^5 + 81\,160N^4 + 65\,344N^3 + 18\,240N^2 + 9504N + 3456 \tag{A.39}$$

$$P_{55} = 1207N^{12} + 10\,131N^{11} + 39\,379N^{10} + 120\,121N^9 + 299\,724N^8 + 482\,244N^7 + 382\,214N^6 - 15\,780N^5 - 256\,840N^4 - 118\,240N^3 + 39\,648N^2 + 33\,984N + 3456 \tag{A.40}$$

$$P_{56} = 2596N^{16} + 23\,287N^{15} + 76\,658N^{14} + 88\,963N^{13} - 121\,050N^{12} - 504\,489N^{11} - 386\,836N^{10} + 625\,443N^9 + 1\,086\,304N^8 - 574\,564N^7 - 3\,300\,816N^6 - 4\,766\,232N^5 - 3\,890\,160N^4 - 1\,844\,224N^3 - 441\,984N^2 - 47\,232N - 6912 \tag{A.41}$$

$$P_{57} = -138\,495N^{17} - 1\,469\,301N^{16} - 6\,177\,407N^{15} - 11\,396\,201N^{14} + 794\,307N^{13} + 49\,867\,573N^{12} + 113\,250\,363N^{11} + 119\,019\,157N^{10} + 23\,906\,680N^9 - 106\,346\,044N^8 - 139\,149\,336N^7 - 31\,178\,992N^6 + 90\,199\,968N^5 + 96\,114\,752N^4 + 36\,681\,856N^3 + 7\,448\,064N^2 + 3\,036\,672N + 718\,848. \tag{A.42}$$

The analytic continuation of the OMEs $A_{gq,Q}^{\mathrm{S},(2,3)}(N)$ to complex values of N are obtained as has been described in Refs. [49,57–59].

For the x-space representation it is convenient to define

$$p_{gq}(x) = \frac{1}{x}\left[1 + (1-x)^2\right]. \tag{A.43}$$

The operator matrix elements $A_{gq,Q}^{(2,3),\mathrm{OMS}}(x)$ can be expressed in terms of harmonic polylogarithms [60], for which we use the shorthand notation $H_{\vec{a}}(x) \equiv H_{\vec{a}}$. It reads:

$$A_{gq,Q}^{(2),\mathrm{OMS}}(x) = C_F T_F \left\{\frac{8}{3} p_{gq} \ln^2\left(\frac{m^2}{\mu^2}\right) + \left[\frac{32(4x^2-5x+5)}{9x} - \frac{16}{3} p_{gq} H_1\right]\ln\left(\frac{m^2}{\mu^2}\right) + \frac{4}{3} p_{gq} H_1^2 - \frac{16(4x^2-5x+5)}{9x} H_1 + \frac{8(43x^2-56x+56)}{27x}\right\} \tag{A.44}$$

$$\begin{aligned}
A_{gq,Q}^{(3),\mathrm{OMS}}(x) = &\Bigg\{C_F C_A T_F\left[\frac{32(x^2+x+1)}{9x} H_0 + \frac{16}{9} p_{gq} H_1 - \frac{8(4x^3+36x^2-42x+35)}{27x}\right] \\
&+ C_F T_F^2 (N_F+2)\frac{32}{9} p_{gq} + C_F^2 T_F\left[\frac{8(17x^2+2x-16)}{9x} H_0 - \frac{16}{9} p_{gq} H_1 - \frac{16}{3}(x-2) H_0^2 + \frac{4(32x^3-327x^2+552x-248)}{27x}\right]\Bigg\}\ln^3\left(\frac{m^2}{\mu^2}\right) \\
&+ \Bigg\{C_F C_A T_F\Bigg\{p_{gq}\left[\frac{16}{3}[H_0 H_1 - H_{0,1}] - \frac{8}{3} H_1^2\right] \\
&+ \frac{16(x^2+2x+2)}{x}[H_0 H_{-1} - H_{0,-1}] \\
&- \frac{16(x^2+10x-2)}{3x} H_{0,1} - \frac{16(8x^3-4x^2+32x+3)}{9x} H_0 \\
&+ \frac{16(4x^3+5x^2+14x-21)}{9x} H_1 + \frac{16}{3}(x+4) H_0^2 + \frac{32(2+x)(1+2x)}{3x}\zeta_2 \\
&+ \frac{4(68x^3-104x^2+296x-191)}{9x}\Bigg\} \\
&+ C_F T_F^2\left\{\frac{64(4x^2-5x+5)}{9x} - \frac{32}{3} p_{gq} H_1\right\} \\
&+ C_F^2 T_F\Bigg\{p_{gq}\left[16[H_0 H_1 - H_{0,1}] + \frac{8}{3} H_1^2\right] + \frac{16}{3}(x-2) H_{0,1} \\
&+ \frac{16(13x^2-23x+17)}{9x} H_1 - \frac{4(32x^3-191x^2-134x+56)}{9x} H_0 \\
&- \frac{8}{3}(13x-8) H_0^2 \\
&+ \frac{2(896x^3-3945x^2+3468x-680)}{27x} - \frac{16}{3}(x-2)\zeta_2\Bigg\}\Bigg\}\ln^2\left(\frac{m^2}{\mu^2}\right)
\end{aligned}$$

$$+\left\{C_F^2T_F\left\{\frac{4}{3}(x-2)H_0^4+\frac{4}{3}(7x-2)H_0^3-\frac{2}{9}(973x+640)H_0^2\right.\right.$$
$$-\frac{32(x+1)(4x^2-31x+31)}{9x}H_{-1}H_0$$
$$+\left[-\frac{4(480x^3-3656x^2-3407x-528)}{27x}\right.$$
$$\left.-\frac{32(5x^2+2x+4)\zeta_2}{3x}+64(x-2)\zeta_3\right]H_0-\frac{8}{9}p_{gq}H_1^3$$
$$+\left[-\frac{4(67x^2-110x+86)}{9x}-16p_{gq}H_0\right]H_1^2+96(x-2)\zeta_4$$
$$+\frac{2(3616x^3-15955x^2+7324x+4676)}{27x}$$
$$+\left[\frac{32(x+1)(4x^2-31x+31)}{9x}-\frac{64(3x^2-6x+2)}{3x}H_0\right]H_{0,-1}$$
$$+\left[\frac{16(8x^3-116x^2+145x-104)}{9x}-\frac{16(3x^2-4)}{x}H_0+\frac{32}{3}p_{gq}H_1\right]H_{0,1}$$
$$+\frac{128(3x^2-6x+2)}{3x}H_{0,0,-1}+\left[32(x-2)H_0-\frac{32(10-9x^2)}{3x}\right]H_{0,0,1}$$
$$+\frac{64}{3x}H_{0,1,1}-96(x-2)H_{0,0,0,1}$$
$$+\frac{16(65x^2+20x-62)}{9x}\zeta_2+\left[\frac{16(115x^2+16x-49)}{27x}\right.$$
$$\left.-\frac{16(8x^3-105x^2+165x-104)}{9x}H_0-\frac{16}{3}p_{gq}H_0^2+\frac{64}{3}p_{gq}\zeta_2\right]H_1$$
$$\left.-\frac{64(12x^2-15x+5)}{3x}\zeta_3\right\}+C_FT_F^2\frac{992}{27}p_{gq}+C_FT_F^2N_F\left\{-\frac{16}{3}p_{gq}H_1^2\right.$$
$$\left.+\frac{64(4x^2-5x+5)}{9x}H_1+\frac{32(19x^2-68x+68)}{27x}\right\}$$
$$+C_FC_AT_F\left\{-\frac{8}{9}(x+2)H_0^3\right.$$
$$+\left[\frac{4}{9}\left(8x^2+151x+292\right)-\frac{32(x^2+2x+2)}{3x}H_{-1}\right]H_0^2$$
$$+\left[\frac{64(x^2+2x+2)}{3x}H_{-1}^2+\frac{16(4x^3-9x^2+30x+82)}{9x}H_{-1}\right.$$
$$\left.-\frac{8(424x^3+136x^2+1387x+356)}{27x}+\frac{32(5x^2+4x+2)}{3x}\zeta_2\right]H_0$$
$$+\frac{8}{9}p_{gq}H_1^3+\left[-\frac{4(16x^3-19x^2+122x-150)}{9x}\right.$$

$$
\begin{aligned}
& - 8 p_{gq} H_0 \Big] H_1^2 + \frac{4(1512x^3 - 1811x^2 + 4944x - 4043)}{27x} \\
& - \frac{16(8x^3 - x^2 - 76x - 62)}{9x} \zeta_2 + \Big[- \frac{16(4x^3 - 9x^2 + 30x + 82)}{9x} \\
& - \frac{128(x^2 + 2x + 2)}{3x} H_{-1} + \frac{32(5x^2 - 6x + 6)}{3x} H_0 \Big] H_{0,-1} \\
& + \Big[\frac{16}{9} \big(8x^2 - 29x - 56\big) - \frac{64(x^2 + 2x + 2)}{3x} H_{-1} - \frac{64}{3} p_{gq} H_0 \Big] H_{0,1} \\
& + \frac{128(x^2 + 2x + 2)}{3x} H_{0,-1,-1} + \frac{64(x^2 + 2x + 2)}{3x} H_{0,-1,1} \\
& - \frac{256(x-1)^2}{3x} H_{0,0,-1} + \frac{32(x^2 - 10x + 6)}{3x} H_{0,0,1} \\
& + \frac{64(x^2 + 2x + 2)}{3x} H_{0,1,-1} + \frac{64}{3}(x+4) H_{0,1,1} \\
& + \frac{128(x^2 + 2x + 2)}{3x} \zeta_2 H_{-1} \\
& + \Big[\frac{16}{3} p_{gq} H_0^2 + \frac{16(19x^2 - 20x + 20)}{9x} H_0 - \frac{16(12x^3 + 16x^2 + x + 149)}{27x} \\
& - \frac{16}{3} p_{gq} \zeta_2 \Big] H_1 + \frac{16(19x^2 - 60x + 26)}{3x} \zeta_3 \Big\} \Big\} \ln\left(\frac{m^2}{\mu^2}\right) \\
& + C_F^2 T_F \Big\{ \frac{4}{27}(11x - 13) H_0^4 + \frac{2}{81} \big(32x^2 + 1147x - 614\big) H_0^3 \\
& + \Big[- \frac{2}{81} \big(176x^2 + 10121x + 7325\big) - \frac{16}{9}(x-2)\zeta_2 + \frac{128}{3}(x-2)\zeta_3 \Big] H_0^2 \\
& + \frac{256}{9} x^2 H_{-1,1} H_0 \\
& + \Big[- \frac{2(11\,808x^3 - 156\,125x^2 - 140\,534x - 17\,296)}{243x} + 192(x-2)\zeta_4 \\
& - \frac{16(145x^2 + 28x + 28)}{27x} \zeta_2 - \frac{32(17x^2 + 38x + 16)}{9x} \zeta_3 \Big] H_0 + \frac{10}{27} p_{gq} H_1^4 \\
& + \Big[\frac{40(10x^2 - 17x + 11)}{81x} + \frac{32}{9} p_{gq} H_0 \Big] H_1^3 + \frac{64(x^2 - 5x + 2)}{3x} B_4 \\
& + \frac{565\,568x^3 - 4\,038\,891x^2 + 2\,578\,290x + 479\,548}{1458x} \\
& - \frac{8(325x^2 - 308x + 222)}{9x} \zeta_4 \\
& - \frac{8(8x^3 + 395x^2 + 3524x - 182)}{27x} \zeta_3 + \Big[\frac{32(x+1)(4x^2 - 31x + 31)}{27x} H_0^2 \\
& - \frac{16(x+1)(161x^3 + 55x^2 + 314x + 18)}{81x^2} H_0
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{32(x-1)(4x^2+31x+31)}{9x}H_1H_0\\
&-\frac{16}{9}(x+1)\big(4x^2-31x+31\big)\frac{\zeta_2}{x}\Bigg]H_{-1}+\Bigg[\frac{64(3x^2-6x+2)}{3x}H_0\\
&-\frac{32(x-1)(4x^2+31x+31)}{9x}\Bigg]H_{0,-1,1}+\Bigg[\frac{64(8x^3+45x^2+27x+45)}{27x}\\
&-\frac{256(3x^2-9x+2)}{9x}H_0\Bigg]H_{0,0,-1}+\Bigg[\frac{16(56x^3-85x^2+1646x+52)}{27x}\\
&+\frac{16(-5x^2-2x+34)}{9x}H_0-\frac{64}{9}p_{gq}H_1\Bigg]H_{0,0,1}\\
&+\Bigg[\frac{32(x+1)(4x^2-31x+31)}{9x}\\
&+\frac{64(3x^2+6x+2)}{3x}H_0\Bigg]H_{0,1,-1}+\Bigg[-\frac{32(2x^2-49x+15)}{27x}+\frac{32}{9}p_{gq}H_1\\
&-\frac{128(x^2-2x+3)}{9x}H_0\Bigg]H_{0,1,1}+256H_{0,-1,0,1}+512H_{0,0,-1,1}\\
&+\frac{128(3x^2-12x+2)}{3x}H_{0,0,0,-1}\\
&+\Bigg[64(x-2)H_0-\frac{16(-65x^2-50x+42)}{9x}\Bigg]H_{0,0,0,1}\\
&+\frac{128(x^2-2x+3)}{9x}H_{0,0,1,1}-\frac{16(7x^2-14x+24)}{9x}H_{0,1,1,1}\\
&-256(x-2)H_{0,0,0,0,1}-\frac{16(200x^2-403x+332)}{81x}\zeta_2+\Bigg[\frac{16}{9}p_{gq}H_0^2\\
&-\frac{8(49x^2-62x+86)}{27x}H_0-\frac{8(109x^2+208x-313)}{81x}-\frac{80}{9}p_{gq}\zeta_2\Bigg]H_1^2\\
&+\Bigg[\frac{64(3x^2-6x+2)}{9x}H_0^2-\frac{32(12x^3+18x^2+27x+76)}{27x}H_0\\
&+\frac{16(x+1)(161x^3+55x^2+314x+18)}{81x^2}\\
&+\frac{32(x-1)(4x^2+31x+31)}{9x}H_1-\frac{32(3x^2-6x+2)}{3x}\zeta_2\Bigg]H_{0,-1}\\
&+\Bigg[-\frac{8(19x^2+10x+26)}{9x}H_0^2-\frac{32(16x^3-2x^2+391x+8)}{27x}H_0\\
&-\frac{16}{9}p_{gq}H_1^2-\frac{32(x+1)(4x^2-31x+31)}{9x}H_{-1}\\
&+\frac{16(117x^4-2611x^3+1838x^2-273x-54)}{81x^2}\\
&+\Bigg[\frac{16(35x^2-58x+58)}{27x}+\frac{64}{9}p_{gq}H_0\Bigg]H_1-\frac{64(3x^2+6x+2)}{3x}H_{0,-1}
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{32(11x^2+14x+14)}{9x}\zeta_2\Bigg]H_{0,1}\\
&+H_1\Bigg[\frac{8}{3}p_{gq}H_0^3+\frac{16(4x^3+39x^2-27x-10)}{27x}H_0^2\\
&+\Bigg[-\frac{16(39x^4-865x^3+747x^2-91x-18)}{27x^2}-\frac{128}{9}p_{gq}\zeta_2\Bigg]H_0\\
&+\frac{16(1646x^2-2413x+1798)}{243x}-\frac{16(12x^3+67x^2+4x-121)}{27x}\zeta_2\\
&+32p_{gq}\zeta_3\Bigg]+256(x-2)\zeta_5\Bigg\}\\
&+C_F T_F^2 N_F\Bigg\{\frac{32}{27}p_{gq}H_1^3-\frac{64(4x^2-5x+5)}{27x}H_1^2\\
&+\frac{128(x+1)(2x-1)}{27x}H_1+\frac{64(197x^2-376x+376)}{243x}-\frac{256}{9}p_{gq}\zeta_3\Bigg\}\\
&+C_F T_F^2\Bigg\{\frac{16}{27}p_{gq}H_1^3-\frac{32(4x^2-5x+5)}{27x}H_1^2+\frac{64(x+1)(2x-1)}{27x}H_1\\
&-\frac{16(359x^2-754x+754)}{243x}+\frac{448}{9}p_{gq}\zeta_3\Bigg\}+C_F C_A T_F\Bigg\{\frac{8}{27}(x+1)H_0^4\\
&+\Bigg[\frac{8(x^2+2x+2)}{27x}H_{-1}-\frac{4}{81}\big(8x^2-15x+80\big)\Bigg]H_0^3\\
&+\Bigg[-\frac{4(x^2+2x+2)}{3x}H_{-1}^2-\frac{4(16x^3-25x^2+130x+275)}{27x}H_{-1}\\
&+\frac{2}{81}\big(544x^2+1915x+8206\big)-\frac{64}{9}(2x+1)\zeta_2\Bigg]H_0^2-\frac{128}{9}x^2H_{-1,1}H_0\\
&+\Bigg[\frac{176(x^2+2x+2)}{27x}H_{-1}^3+\frac{8(41x^2+70x+133)}{27x}H_{-1}^2\\
&+\Bigg[\frac{8(161x^4+861x^3+1437x^2+1703x+150)}{81x^2}\\
&-\frac{64(x^2+2x+2)}{9x}\zeta_2\Bigg]H_{-1}-\frac{4(14\,352x^3+7072x^2+39\,319x+12\,324)}{243x}\\
&+\frac{32(4x^3+110x^2+88x+7)}{27x}\zeta_2+\frac{128(11x^2-3x+4)}{9x}\zeta_3\Bigg]H_0\\
&-\frac{10}{27}p_{gq}H_1^4+\Bigg[\frac{8(20x^3+7x^2+106x-141)}{81x}+\frac{16}{9}p_{gq}H_0\Bigg]H_1^3\\
&+\frac{64}{3}H_{0,-1}^2+\frac{40(x^2+2x+2)}{3x}\zeta_2H_{-1}^2-\frac{16(-21x^2-28x-2)}{9x}H_{0,1}^2\\
&-\frac{32(x^2-5x+2)}{3x}B_4+\frac{4(27\,864x^3-35\,544x^2+75\,811x-62\,939)}{243x}\\
&+\frac{4}{9x}\big(197x^2-1316x+558\big)\zeta_4
\end{aligned}
$$

$$
\begin{aligned}
&- \frac{8(228x^3-1645x^2-1732x-1443)}{81x}\zeta_2 \\
&+ \frac{4(88x^3-835x^2+2212x+950)}{27x}\zeta_3 \\
&+ \left[\frac{16(41x^2+70x+133)}{27x} + \frac{352(x^2+2x+2)}{9x}H_{-1} \right. \\
&\left. - \frac{16(x^2+10x+2)}{3x}H_0\right]H_{0,-1,-1} \\
&+ \left[\frac{16(12x^3+133x^2+80x-13)}{27x} + \frac{64(x^2+2x+2)}{9x}H_{-1} \right. \\
&\left. - \frac{32(9x^2-26x+6)}{9x}H_0\right]H_{0,-1,1} + \left[-\frac{8(32x^3+287x^2-34x+331)}{27x} \right. \\
&- \frac{16(x^2+2x+2)}{3x}H_{-1} + \frac{16(25x^2-94x+18)}{9x}H_0 \\
&\left. - \frac{128}{9}p_{gq}H_1\right]H_{0,0,-1} \\
&+ \left[-\frac{8(104x^3+389x^2+982x+82)}{27x} + \frac{160(x^2+2x+2)}{9x}H_{-1} \right. \\
&\left. + \frac{16(-23x^2-74x-14)}{9x}H_0 + \frac{32}{9}p_{gq}H_1\right]H_{0,0,1} \\
&+ \left[\frac{64(x^2+2x+2)}{9x}H_{-1} \right. \\
&\left. - \frac{16(12x^3-133x^2-80x+13)}{27x} - \frac{32(9x^2+10x+6)}{9x}H_0\right]H_{0,1,-1} \\
&+ \left[\frac{8(24x^3+586x^2+226x-345)}{27x} + \frac{128(x^2+2x+2)}{9x}H_{-1} \right. \\
&\left. - \frac{64}{9}(5x+9)H_0 - 16p_{gq}H_1\right]H_{0,1,1} \\
&+ \frac{(x^2+2x+2)}{9x}[-352H_{0,-1,-1,-1} - 64H_{0,-1,-1,1} - 64H_{0,-1,1,-1} \\
&- 128H_{0,-1,1,1} + 48H_{0,0,-1,-1} - 160H_{0,0,1,-1} - 64H_{0,1,-1,-1} \\
&- 128H_{0,1,-1,1} - 128H_{0,1,1,-1}] \\
&- \frac{32(5x^2+38x+10)}{9x}H_{0,-1,0,1} - \frac{32(5x^2+82x+10)}{9x}H_{0,0,-1,1} \\
&- \frac{16(37x^2-202x+26)}{9x}H_{0,0,0,-1} - \frac{16(-63x^2-178x-22)}{9x}H_{0,0,0,1} \\
&- \frac{256(3x^2+2)}{9x}H_{0,0,1,1} + \frac{64(x^2-17x+7)}{9x}H_{0,1,1,1} + \left[-\frac{32}{9}p_{gq}H_0^2 \right. \\
&+ \frac{4(16x^3+113x^2-22x-177)}{27x}H_0 - \frac{8(14x^3+191x^2-298x-49)}{81x}
\end{aligned}
$$

$$
\begin{aligned}
&+ \frac{8}{9} p_{gq} \zeta_2 \Big] H_1^2 + \Big[- \frac{176(x^2+2x+2)}{9x} H_{-1}^2 \\
&- \frac{16(41x^2+70x+133)}{27x} H_{-1} - \frac{8(13x^2-26x+10)}{9x} H_0^2 \\
&- \frac{8(161x^4+861x^3+1437x^2+1703x+150)}{81x^2} \\
&+ \Big[\frac{8(24x^3+131x^2+48x+303)}{27x} + \frac{16(x^2+2x+2)}{3x} H_{-1} \Big] H_0 \\
&+ \Big[\frac{64}{9} p_{gq} H_0 - \frac{16(x-1)(4x^2+31x+31)}{9x} \Big] H_1 \\
&+ \frac{16(13x^2-22x+14)}{9x} \zeta_2 \Big] H_{0,-1} \\
&+ H_{0,1} \Big[- \frac{32(x^2+2x+2)}{9x} H_{-1}^2 + \frac{16(12x^3-133x^2-80x+13)}{27x} H_{-1} \\
&- \frac{8(-7x^2-18x-6)}{9x} H_0^2 \\
&+ \frac{4(678x^4-3385x^3-466x^2-1293x-108)}{81x^2} + \frac{32}{9} p_{gq} H_1^2 \\
&+ \Big[\frac{16(24x^3+44x^2+149x+3)}{27x} - \frac{64(x^2+2x+2)}{9x} H_{-1} \Big] H_0 \\
&+ \Big[\frac{64}{9} p_{gq} H_0 - \frac{8(x-1)(32x^2+335x+221)}{27x} \Big] H_1 \\
&+ \frac{32(11x^2+14x+10)}{9x} H_{0,-1} - \frac{16(37x^2+38x+22)}{9x} \zeta_2 \Big] \\
&+ \Big[\frac{8}{27} p_{gq} H_0^3 - \frac{4(8x^3+71x^2-34x-70)}{27x} H_0^2 \\
&+ \Big[- \frac{4(222x^4-1817x^3+2998x^2-1813x-108)}{81x^2} \\
&+ \frac{16(x-1)(4x^2+31x+31)}{9x} H_{-1} \Big] H_0 \\
&+ \frac{8(360x^3+842x^2+980x-3389)}{243x} - \frac{224}{9} p_{gq} \zeta_3 \\
&+ \frac{16(14x^3+115x^2-11x-135)}{27x} \zeta_2 \Big] H_1 \\
&+ \Big[\frac{16(6x^3+32x^2+115x+193)}{27x} \zeta_2 \\
&- \frac{112(x^2+2x+2)}{3x} \zeta_3 \Big] H_{-1} \Big\}. \qquad \text{(A.45)}
\end{aligned}
$$

In the above expression the harmonic polylogarithms

$$H_0,\ H_{-1},\ H_1,\ H_{0,1},\ H_{0,-1},\ H_{-1,1},\ H_{0,0,1},\ H_{0,0,-1},\ H_{0,1,1},\ H_{0,-1,-1},\ H_{0,1,-1},$$
$$H_{0,-1,1,},\ H_{0,0,0,1},\ H_{0,0,0,-1},\ H_{0,0,1,1},\ H_{0,0,-1,-1},\ H_{0,0,-1,1},\ H_{0,0,1,-1},\ H_{0,-1,0,1},$$
$$H_{0,1,1,1},\ H_{0,-1,-1,-1},\ H_{0,-1,-1,1},\ H_{0,1,-1,-1},\ H_{0,-1,1,-1},\ H_{0,-1,1,1},$$
$$H_{0,1,-1,1},\ H_{0,1,1,-1},\ H_{0,0,0,0,1} \tag{A.46}$$

contribute. Since $H_{0,-1,1}$ and $H_{0,1,-1}$ only appear as a sum, the polylogarithms up to three indices can be written as Nielsen integrals of argument $\pm x, x^2$, cf. [57], with

$$H_{0,-1,1}(x) + H_{0,1,-1}(x) = 2\big[S_{1,2}(x) + S_{1,2}(-x) - S_{1,2}\big(x^2\big)\big]. \tag{A.47}$$

For harmonic polylogarithms with more than three indices of which three are different, usually a representation in terms of Nielsen integrals is not possible. Numerical representations of the harmonic polylogarithms were given in [61].

The corresponding expressions for the mass $m = \bar{m}$ in the $\overline{\mathsf{MS}}$-scheme in the 2-loop case are identical and are given at the 3-loop order by:

$$\begin{aligned} A_{gq,Q}^{(3),\overline{\mathsf{MS}}}(N) = A_{gq,Q}^{(3),\mathrm{OMS}}(N) - a_s^3 C_F^2 T_F \bigg\{ & 32\bar{p}_{gq} \ln^2\left(\frac{m^2}{\mu^2}\right) \\ & + 32\left[\frac{4N^3+5N^2+15N+8}{3(N-1)N(N+1)^2} - \bar{p}_{gq} S_1\right]\ln\left(\frac{m^2}{\mu^2}\right) \\ & - \frac{128(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2} + \frac{128}{3}\bar{p}_{gq} S_1(N)\bigg\}, \end{aligned} \tag{A.48}$$

$$\begin{aligned} A_{gq,Q}^{(3),\overline{\mathsf{MS}}}(x) = A_{gq,Q}^{(3),\mathrm{OMS}}(x) - a_s^3 C_F^2 T_F \bigg\{ & 32 p_{gq} \ln^2\left(\frac{m^2}{\mu^2}\right) \\ & + 32\left[\frac{2(2x^2-x+1)}{3x} - p_{gq} H_1\right]\ln\left(\frac{m^2}{\mu^2}\right) + \frac{128}{3}\bar{p}_{gq} H_1 \\ & - \frac{256(4x^2-5x+5)}{9x}\bigg\}. \end{aligned} \tag{A.49}$$

Here we have put the different masses both to m, to obtain a more compact expression. Since the masses in both schemes are different, the results in the OMS and $\overline{\mathsf{MS}}$ scheme differ already by terms $O(a_s^2 \ln(\bar{m}^2/m^2_{\mathrm{OMS}}) \ln(\bar{m}^2/\mu^2))$, however. The heavy quark mass in the OMS and the $\overline{\mathsf{MS}}$–scheme are related by [62]

$$\begin{aligned} \frac{\bar{m}(m)}{m} &= 1 - \frac{4}{3}\frac{\alpha_s}{\pi} + \left[-\frac{3019}{288} + \frac{\zeta_3}{6} + \frac{71}{144}N_f\left(-\frac{1}{3} - \frac{\ln(2)}{9} + \frac{n_f}{18}\right)\pi^2\right]\left(\frac{\alpha_s}{\pi}\right)^2 \\ &\quad + O\left(\left(\frac{\alpha_s}{\pi}\right)^3\right) \\ &\simeq 1.00000 - 1.33333\left(\frac{\alpha_s}{\pi}\right) + (-14.3323 + 1.04137 N_f)\left(\frac{\alpha_s}{\pi}\right)^2. \end{aligned} \tag{A.50}$$

In the presence of N_f massless and one heavy quark. The corresponding relation keeping also the scale dependence has been given e.g. in [63].

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