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The three-loop single mass polarized pure singlet operator matrix element

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Abstract

We calculate the massive polarized three-loop pure singlet operator matrix element $A_{Qq}^{(3),\rm PS}$ in the single mass case in the Larin scheme. This operator matrix element contributes to the massive polarized three-loop Wilson coefficient $H_{Qq}^{(3),\rm PS}$ in deep-inelastic scattering and constitutes a three-loop transition matrix element in the variable flavor number scheme. We provide analytic results in Mellin N and in x space and study the behaviour of this operator matrix element in the region of small and large values of the Bjorken variable x.

1. Introduction

Higher order heavy flavor corrections to deeply–inelastic structure functions are important both in the unpolarized and polarized case [1,2]. Their scaling violations are different if compared to the massless case and, therefore, influence the measurement of the strong coupling

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constant $\alpha_s(M_Z)$ from the structure functions [3–5]. Related to it, the massless parton distributions are unfolded, requiring a correct description of the heavy flavor effects. On the other hand, in order to describe the transition of massive partons becoming effectively massless, the variable flavor number scheme can be used [6–8]. This transition is described by massive operator matrix elements (OMEs), and after its application, effective calculations for scattering reactions at hadron colliders are possible, based also on heavy quark parton distributions. Several of these transition matrix elements have been already computed in the unpolarized and polarized case in the single, cf. [9–16], and two–mass case [7,8,17–20].

In this paper we calculate the massive polarized three-loop pure singlet operator matrix element $A_{Qq}^{(3),\rm PS}$ in the single mass case. The corresponding two–mass corrections, which require different computational techniques, have been computed in Ref. [20]. In the present calculation similar techniques as in Ref. [10] are used. This has become possible upon finding the correct projector in the case of external massless fermion lines in [21], which differs from the one in [22]. The main quantity to be derived is the constant part of the unrenormalized polarized massive pure singlet OME, $a_{Qq}^{\rm PS,(3)}$.

The paper is organized as follows. In Section 2 we outline the basic formalism and give an overview of the calculation. In Section 3 we present the results for $a_{Qq}^{\rm PS,(3)}$ and the massive OME $A_{Qq}^{\rm PS,(3)}$. Both quantities are given in N and x space and we discuss numerical results for $a_{Qq}^{\rm PS,(3)}(x)$. Section 4 contains the conclusions. In an ancillary file to this paper we give the massive OME in computer readable form.

2. Basic formalism and overview of the calculation

The pure singlet massive operator matrix element describes the transition between massless on-shell quark states $\langle q|$ in association with a local quark operator in the light-cone expansion [23], which in general is either located on the heavy quark line or on a massless quark loop. The latter case is denoted by $A_{qq,Q}^{\rm PS}$ and contributes to heavy quark corrections in case of massless final states only, which will be presented elsewhere because of the different context. In this paper we present the results for $A_{Qq}^{\rm PS}$. The first contribution to $A_{Qq}^{\rm PS}$ arises at two loops. Therefore, the corresponding expansion in the strong coupling constant α_s is given by, cf. [9],

$$A_{Qq}^{\rm PS} = a_s^2 A_{Qq}^{(2),\rm PS} + a_s^3 A_{Qq}^{(3),\rm PS} + O(a_s^4)\ , \tag{2.1}$$

where $a_s = g_s^2/(4\pi)^2 \equiv \alpha_s/(4\pi)$. We perform the calculations in $D = 4+\varepsilon$ dimensions, leading to the following pole structure of the unrenormalized OME at two- and three-loop order

$$\hat{A}_{Qq}^{(2),\rm PS} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon} \left(-\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{2\varepsilon^2} + \frac{\hat{\gamma}_{qq}^{(1),\rm PS}}{2\varepsilon} + a_{Qq}^{(2),\rm PS} + \varepsilon \bar{a}_{Qq}^{(2),\rm PS}\right), \tag{2.2}$$

$$\hat{A}_{Qq}^{(3),\rm PS} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2} \Bigg\{ \frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{6\varepsilon^3}\left(\gamma_{gg}^{(0)} - \gamma_{qq}^{(0)} + 6\beta_0 + 16\beta_{0,Q}\right)$$
$$+ \frac{1}{\varepsilon^2}\Bigg[-\frac{4}{3}\hat{\gamma}_{qq}^{(1),\rm PS}\left(\beta_0+\beta_{0,Q}\right) - \frac{1}{3}\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}$$
$$+ \frac{\hat{\gamma}_{qg}^{(0)}}{6}\left(2\hat{\gamma}_{gq}^{(1)} - \gamma_{gq}^{(1)}\right) + \delta m_1^{(-1)}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\Bigg]$$

$$+\frac{1}{\varepsilon}\Bigg[\frac{\hat{\gamma}_{qq}^{(2),\rm PS}}{3}-\frac{N_F}{3}\hat{\tilde{\gamma}}_{qq}^{(2),\rm PS}+\hat{\gamma}_{qg}^{(0)}a_{gq,Q}^{(2)}-\gamma_{gq}^{(0)}a_{Qg}^{(2)}$$
$$-4\big(\beta_0+\beta_{0,Q}\big)a_{Qq}^{(2),\rm PS}-\frac{\zeta_2}{16}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\big(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0\big)$$
$$+\delta m_1^{(0)}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}-\delta m_1^{(-1)}\hat{\gamma}_{qq}^{(1),\rm PS}\Bigg]+a_{Qq}^{(3),\rm PS}\Bigg\}. \tag{2.3}$$

Here $\gamma_{ij}^{(k)}$, with $k=0,1,2$, denote the polarized anomalous dimensions [21,24–35], $a_{ij}^{(k)}$, with $k=1,2,3$, is the constant part of the unrenormalized OME at $O(a_s^k)$, $\bar{a}_{ij}^{(k)}$, with $k=1,2$, denotes the $O(\varepsilon)$ contribution of the unrenormalized OME at $O(a_s^k)$, β_k and $\beta_{Q,k}$ are the expansion coefficients of the QCD β-function in the $\overline{\rm MS}$–scheme and for massive contributions, $\delta m_k^{(l)}$ are the expansion coefficients of the renormalized quark mass m, μ is the renormalization scale, N_F denotes the number of light quark flavors, and $\zeta_k=\sum_{l=1}^{\infty}(1/l^k)$, with $k\in\mathbb{N}, k\geq 2$, denotes the Riemann ζ-function at integer values. For details of the notation see Ref. [9]. The two-loop results on $a_{ij}^{(k)}$ and $\bar{a}_{ij}^{(k)}$ are given in Ref. [36,37], see also [38].

Here and in the following we use the shorthand notations

$$\hat{f}(x,N_F)\equiv f(x,N_F+1)-f(x,N_F) \tag{2.4}$$
$$\tilde{f}(x,N_F)\equiv\frac{f(x,N_F)}{N_F}\,. \tag{2.5}$$

Renormalizing the mass in the on-shell scheme and the coupling constant in the $\overline{\rm MS}$-scheme, we obtain the following expressions for the renormalized pure singlet OME at two- and three-loop order [9],

$$A_{Qq}^{(2),{\rm PS},\overline{\rm MS}}=-\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{8}\ln^2\left(\frac{m^2}{\mu^2}\right)+\frac{\hat{\gamma}_{qq}^{(1),\rm PS}}{2}\ln\left(\frac{m^2}{\mu^2}\right)+a_{Qq}^{(2),\rm PS}+\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{8}\zeta_2\,, \tag{2.6}$$

$$A_{Qq}^{(3),{\rm PS},\overline{\rm MS}}=\frac{\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}}{48}\Big(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+16\beta_{0,Q}\Big)\ln^3\left(\frac{m^2}{\mu^2}\right)$$
$$+\Bigg[-\frac{\hat{\gamma}_{qq}^{(1),\rm PS}}{2}\Big(\beta_0+\beta_{0,Q}\Big)+\frac{\hat{\gamma}_{qg}^{(0)}}{8}\Big(\hat{\gamma}_{gq}^{(1)}-\gamma_{gq}^{(1)}\Big)-\frac{1}{8}\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(1)}\Bigg]\ln^2\left(\frac{m^2}{\mu^2}\right)$$
$$+\Bigg[\frac{\hat{\gamma}_{qq}^{(2),\rm PS}}{2}-\frac{N_F}{2}\hat{\tilde{\gamma}}_{qq}^{(2),\rm PS}-2a_{Qq}^{(2),\rm PS}(\beta_0+\beta_{0,Q})+\frac{\hat{\gamma}_{qg}^{(0)}}{2}a_{gq,Q}^{(2)}$$
$$-\frac{\gamma_{gq}^{(0)}}{2}a_{Qg}^{(2)}-\frac{\zeta_2}{16}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}\Big(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0+8\beta_{0,Q}\Big)\Bigg]\ln\left(\frac{m^2}{\mu^2}\right)$$
$$+4(\beta_0+\beta_{0,Q})\overline{a}_{Qq}^{(2),\rm PS}+\gamma_{gq}^{(0)}\overline{a}_{Qg}^{(2)}-\hat{\gamma}_{qg}^{(0)}\overline{a}_{gq,Q}^{(2)}$$
$$+\frac{\zeta_3}{48}\gamma_{gq}^{(0)}\hat{\gamma}_{qg}^{(0)}\Big(\gamma_{gg}^{(0)}-\gamma_{qq}^{(0)}+6\beta_0\Big)+\frac{\zeta_2}{16}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(1)}$$
$$-\delta m_1^{(1)}\hat{\gamma}_{qg}^{(0)}\gamma_{gq}^{(0)}+\delta m_1^{(0)}\hat{\gamma}_{qq}^{(1),\rm PS}+2\delta m_1^{(-1)}a_{Qq}^{(2),\rm PS}+a_{Qq}^{(3),\rm PS}\,. \tag{2.7}$$

The connection of these OMEs to the massive Wilson coefficient in the asymptotic region has been described in Ref. [9], Eq. (2.14). The polarized two-loop result was given in [36,38]. In this paper we present the three-loop result. In particular, we calculate the constant part, $a_{Qq}^{(3),\rm PS}$, of

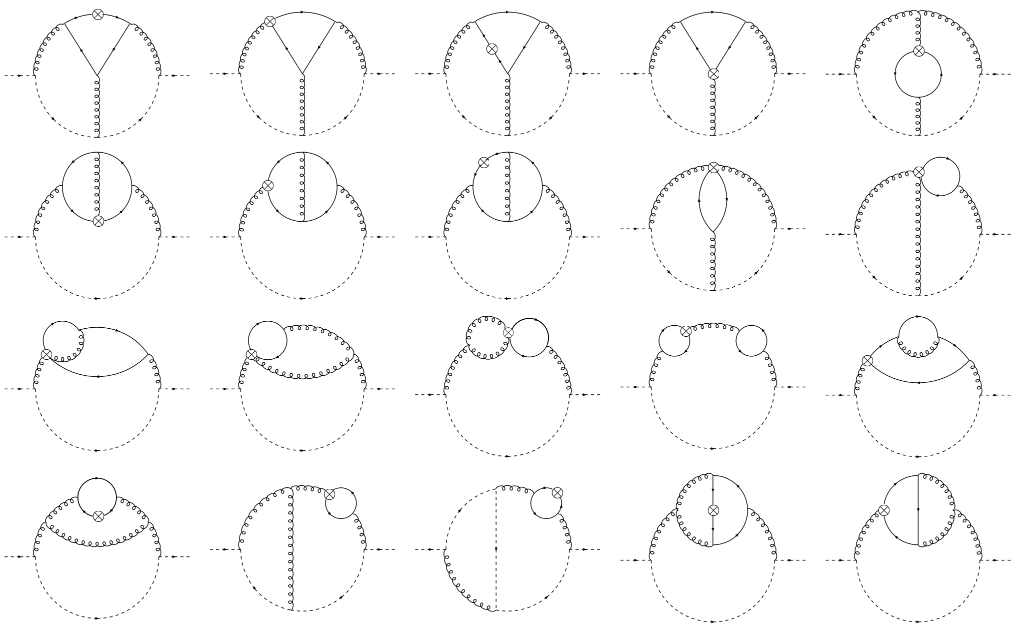

Fig. 1. Sample of diagrams for $A_{Qq}^{(3),\rm PS}$. The dashed arrow lines represent massless quarks, while the solid arrow lines represent massive quarks, and curly lines are gluons. The symbol $\otimes$ denotes the local operator insertion, see Ref. [9].

the three-loop unrenormalized pure singlet polarized OME. The calculation in the polarized case is closely related to the unpolarized one [10], since many of the required steps are common to or similar in both cases. The massive OME $A_{Qq}^{(3),\rm PS}$ consists of 125 Feynman diagrams, which we generated using QGRAF [39]. A sample of the diagrams is shown in Fig. 1. The Feynman rules for the local operator vertices can be found in Ref. [9,21]. The main difference between the polarized rules and the unpolarized ones is the presence of an additional factor of γ_5 in the former case, which requires the choice of a prescription in dimensional regularization. We performed the calculation using the Larin scheme [40],[1] where γ_5 is expressed as

$$\gamma^5 = \frac{i}{24}\varepsilon_{\mu\nu\rho\sigma}\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma, \tag{2.8}$$

$$\not{\Delta}\gamma^5 = \frac{i}{6}\varepsilon_{\mu\nu\rho\sigma}\Delta^\mu\gamma^\nu\gamma^\rho\gamma^\sigma, \tag{2.9}$$

after which the Levi-Civita symbols can be contracted in D dimensions using

$$\varepsilon_{\mu\nu\rho\sigma}\varepsilon^{\alpha\lambda\tau\gamma} = -\mathrm{Det}\left[g^\beta_\omega\right], \qquad \beta = \alpha, \lambda, \tau, \gamma; \quad \omega = \mu, \nu, \rho, \sigma. \tag{2.10}$$

In general, the calculation of OMEs requires the projection of the corresponding Green functions $\hat{G}^{ij}_l$, which is straightforward in the case of gluonic OMEs, but is more subtle in the case of quarkonic polarized OMEs. In Ref. [21], we showed that the correct projector in the Larin scheme is given by

[1] For other schemes see Ref. [41]. For a discussion of the necessary finite renormalizations see [42].

$$P_q \hat{G}_l^{ij} = -\delta_{ij} \frac{i\,(\Delta.p)^{-N-1}}{4N_c(D-2)(D-3)} \varepsilon_{\mu\nu p\Delta} \mathrm{tr}\left[\not{p} \gamma^\mu \gamma^\nu \hat{G}_l^{ij} \right], \tag{2.11}$$

where N_c is the number of QCD colours, p is the momentum of the external massless quark, N is the Mellin variable, and Δ is a D-dimensional light-like vector. Using this projector, we were able to extract the corresponding anomalous dimensions from the poles of the OMEs in [21], and after performing a finite renormalization, we found the results to agree with those presented in [35] in the so called M-scheme [43]. The full finite renormalization required to transform also the constant term $a_{Qq}^{(3),\mathrm{PS}}$ to the M-scheme is at present unknown, so in this paper we stick to the Larin scheme.

The propagators, vertices and operator insertions from the output of QGRAF were replaced by the corresponding Feynman rules using a FORM [44] program [9], which also allowed us to introduce the projector (2.11) and to perform the Dirac algebra in the numerator of the Feynman integrals. After this, we ended up with a linear combination of a large number of scalar integrals,

$$A_{Qq}^{(3),\mathrm{PS}}(N) = \sum_i c_i J_i(N) \ , \tag{2.12}$$

where the functions $J_i(N)$ are the scalar integrals and the c_i's are factors containing scalar products not involving the loop momenta. As we have done in the past for the calculation of unpolarized OMEs, we multiplied the result by an auxiliary variable t raised to the power of the Mellin moment N, and summed up to $N = \infty$, that is, we computed

$$\sum_{N=0}^{\infty} t^N \sum_i c_i J_i(N) \ . \tag{2.13}$$

This allowed us to rewrite all operator insertions in terms of artificial propagators, after which it became possible to reduce the scalar integrals to master integrals using integration by parts identities. For this we used the C++ package Reduze 2 [45].[2] We ended up with a linear combination of master integrals,

$$A_{Qq}^{(3),\mathrm{PS}}(t) = \sum_{N=0}^{\infty} t^N A_{Qq}^{(3),\mathrm{PS}}(N) = \sum_i r_i(t, D) \sum_{N=0}^{\infty} t^N M_i(N), \tag{2.14}$$

where the functions $M_i(N)$ are the master integrals and $r_i(t, D)$ are rational functions in t and the dimension D. What remained was the calculation of the master integrals and the extraction of the Nth coefficient of the expansion in t of $A_{Qq}^{(3),\mathrm{PS}}(t)$ as a function of N. The master integrals turn out to be the same ones needed in the unpolarized case. Details on their calculation can be found in Ref. [10]. In their computation we use difference field and ring techniques as implemented in the packages Sigma [48,49], EvaluateMultiSums and SumProduction [50], which also make use of the package HarmonicSums [51–57].[3] We have checked our results comparing the moments for fixed values of N with corresponding results obtained by using MATAD [59] for $N = 3, 5, 7$.

[2] The package Reduze 2 uses the packages FERMAT [46] and Ginac [47].

[3] For a recent survey on the different calculation techniques see Ref. [58].

3. Results

We now present the result for the $O(\varepsilon^0)$ term of the unrenormalized pure singlet polarized OME, namely, $a_{Qq}^{(3),\mathrm{PS}}$. In N space, this term is given by harmonic sums [51,52]

$$S_{i_n,i_{n-1},\cdots,i_2,i_1}(N) = \sum_{k=1}^{N} \frac{\mathrm{sign}(i_n)^k}{k^{|i_n|}} S_{i_{n-1},\cdots i_2,i_1}(k), \quad S_\emptyset = 1, \tag{3.1}$$

and generalized harmonic sums, cf. [55], at rational weights $a_i \in \mathbb{Q}$

$$S_{i_n i_{n-1}\cdots i_2 i_1}(a_n, a_{n-1}, \cdots, a_2, a_1; N) = \sum_{k=1}^{N} \frac{a_n^k}{k^{i_n}} S_{i_{n-1},\cdots i_2,i_1}(a_{n-1}, \cdots, a_2, a_1; k), \tag{3.2}$$

with $i_k \in \mathbb{N}\backslash\{0\}$. In the following, we will use the shorthand notation

$$S_{i_n,\cdots,i_1} \equiv S_{i_n,\cdots,i_1}(N) \quad \text{and} \quad S_{i_n,\cdots,i_1}(a_n\cdots,a_1) \equiv S_{i_n,\cdots,i_1}(a_n\cdots,a_1;N). \tag{3.3}$$

One obtains

$$\begin{aligned}
&a_{Qq}^{(3),\mathrm{PS}}(N) = \\
&C_F T_F (C_A - 2C_F) \Biggl\{ \frac{2^{4-N} P_2}{N^3(N+1)^2}\bigl[-S_{2,1}(2,1) + S_{1,1,1}(2,1,1) + 7\zeta_3\bigr] \\
&+\frac{32}{N^3}(5N-2)\Biggl\{ \frac{2^{-N}}{(N-1)(N+1)^2}\bigl[-S_2 S_1(2) + S_{2,1}(1,2)\bigr] + \frac{2^N}{N}\Biggl[S_{1,1}\left(\frac{1}{2},1\right) \\
&+S_{1,1}\left(1,\frac{1}{2}\right) - S_1 S_1\left(\frac{1}{2}\right) - S_2\left(\frac{1}{2}\right)\Biggr] + 2^N\Biggl[\frac{1}{2}S_1^2 S_1\left(\frac{1}{2}\right) + \frac{1}{2}S_2 S_1\left(\frac{1}{2}\right) \\
&+S_1 S_2\left(\frac{1}{2}\right) + S_3\left(\frac{1}{2}\right) - S_{1,1,1}\left(\frac{1}{2},1,1\right) - S_{1,1,1}\left(1,\frac{1}{2},1\right) - S_{1,1,1}\left(1,1,\frac{1}{2}\right)\Biggr]\Biggr\} \\
&+\frac{2^{4-N}(N^2+N+2)}{(N-1)N(N+1)}\bigl[S_{1,2}(2,1) - S_3(2)\bigr] + \frac{2^{5-N}(2N-1)}{(N-1)N(N+1)^2}\bigl[S_{2,1}(1,2) - S_2 S_1(2)\bigr] \\
&+32F_1\Biggl\{\Biggl[S_{1,1}\left(2,\frac{1}{2}\right) - S_1\left(\frac{1}{2}\right)S_1(2)\Biggr]S_2 - S_1(2)S_3\left(\frac{1}{2}\right) - S_2\left(\frac{1}{2}\right)S_{1,1}(2,1) \\
&+\bigl[S_{2,1}(1,2) + S_{2,1}(2,1) - S_{1,1,1}(2,1,1) - 7\zeta_3\bigr]S_1\left(\frac{1}{2}\right) + S_{2,2}\left(2,\frac{1}{2}\right) + S_{3,1}\left(\frac{1}{2},2\right) \\
&+S_{2,1,1}\left(\frac{1}{2},2,1\right) - S_{2,1,1}\left(1,2,\frac{1}{2}\right) - S_{2,1,1}\left(2,\frac{1}{2},1\right) - S_{2,1,1}\left(2,1,\frac{1}{2}\right) \\
&+S_{1,1,1,1}\left(2,\frac{1}{2},1,1\right) + S_{1,1,1,1}\left(2,1,\frac{1}{2},1\right) + S_{1,1,1,1}\left(2,1,1,\frac{1}{2}\right) - \frac{B_4}{2}\Biggr\}\Biggr\} \\
&+C_F T_F^2 N_F \Biggl\{ -\frac{32(N+2)P_{22}}{243 N^5 (N+1)^5} - \frac{(N+2)}{N^3(N+1)^3}\left[\frac{16}{27}S_1^2 + \frac{208}{27}S_2 + \frac{16}{9}\zeta_2\right]P_1 \\
&+\frac{16}{3}F_1\left[\left(\frac{13}{3}S_2 + \zeta_2\right)S_1 + \frac{1}{9}S_1^3 + \frac{110}{9}S_3 - \frac{14}{3}\zeta_3\right] + \frac{32(N+2)P_9 S_1}{81 N^4 (N+1)^4}\Biggr\}
\end{aligned}$$

$$
\begin{aligned}
&+C_F T_F^2\Biggl\{\frac{32}{3}F_1\Biggl[\Bigl(\frac{5}{3}S_2-\zeta_2\Bigr)S_1-\frac{1}{9}S_1^3+\frac{16}{9}S_3-4S_{2,1}+\frac{32\zeta_3}{3}\Biggr]+\frac{32}{9}\zeta_2 F_2\\
&+\frac{32}{27N^3(N+3)(N+4)}\Biggl[\frac{P_{11}S_1^2}{(N+1)^3}-\frac{P_{10}S_2}{(N+1)^2}+\frac{2P_{27}-6NP_{25}S_1}{9N^2(N+1)^4}\Biggr]\Biggr\}\\
&+C_A C_F T_F\Biggl\{\frac{4P_{20}S_1^2+4P_{23}S_2}{27N^4(N+1)^4(N+2)}+\frac{8P_{30}}{243(N-1)N^6(N+1)^6(N+2)}\\
&+32F_1\Biggl[\frac{9}{2}\zeta_4-S_1^2\Bigl(\frac{17}{24}S_2+\frac{\zeta_2}{8}\Bigr)-\frac{S_1^4}{144}-\Bigl(\frac{7}{6}S_1^2+\frac{3}{4}\zeta_2\Bigr)S_{-2}+\frac{5}{6}S_{2,1,1}-\frac{3}{8}\zeta_2 S_2\Biggr]\\
&+\Biggl[-\frac{8P_{28}}{81N^5(N+1)^5(N+2)}-\frac{4P_7S_2+12\zeta_2P_4}{9N^3(N+1)^3}-\frac{8(137N^2+137N-334)}{9N^2(N+1)^2}S_3\\
&+\frac{16(35N^2+35N-18)}{3N^2(N+1)^2}S_{-2,1}+\frac{8(11N^2+11N-10)\zeta_3}{3N^2(N+1)^2}\Biggr]S_1-\frac{4P_4S_1^3}{27N^3(N+1)^3}\\
&-\frac{2(29N^2+29N-74)}{3N^2(N+1)^2}S_2^2-\frac{8P_{18}S_3}{27N^3(N+1)^3}-\frac{4(167N^2+167N-358)}{3N^2(N+1)^2}S_4\\
&+\Biggl[\frac{32(N+2)}{3N^3(N+1)^3}(N^3-9N^2+16N+4)S_1+\frac{16P_{24}}{3(N-1)N^4(N+1)^4(N+2)}\\
&-\frac{64(7N^2+7N-13)}{3N^2(N+1)^2}S_2\Biggr]S_{-2}+\frac{16(3N^2+3N+2)}{3N^2(N+1)^2}S_{-2}^2+\frac{8\zeta_3P_{14}-48P_{13}S_{-2,1}}{9N^3(N+1)^3}\\
&-\Biggl[\frac{8P_{12}}{3N^3(N+1)^3}+\frac{8(69N^2+69N-94)}{3N^2(N+1)^2}S_1\Biggr]S_{-3}-\frac{16(31N^2+31N-50)}{3N^2(N+1)^2}S_{-4}\\
&+\frac{8(N-1)P_3S_{2,1}}{3N^3(N+1)^3}+\frac{24(N-2)(N+3)}{N^2(N+1)^2}S_{3,1}+\frac{64(3N^2+3N-2)}{N^2(N+1)^2}S_{-2,2}\\
&+\frac{32(23N^2+23N-22)}{3N^2(N+1)^2}S_{-3,1}-\frac{64(13N^2+13N-2)}{3N^2(N+1)^2}S_{-2,1,1}+\frac{4P_{19}\zeta_2}{9N^4(N+1)^4}\Biggr\}\\
&+C_F^2T_F\Biggl\{-\frac{4P_{29}}{3N^6(N+1)^6(N+2)}+\frac{4P_{17}S_1^2-4P_{21}S_2}{3N^4(N+1)^4(N+2)}+\frac{16P_{15}S_3}{9N^3(N+1)^3}\\
&+\Biggl(\frac{8P_{26}}{3N^5(N+1)^5(N+2)}+\frac{4P_6S_2}{3N^3(N+1)^3}\Biggr)S_1+64F_1\Biggl[-\frac{9}{4}\zeta_4-\frac{P_5\zeta_2}{32N^2(N+1)^2}\\
&+\frac{3N^2-3N-4}{16N(N+1)}\Bigl(\frac{1}{9}S_1^3+\zeta_2S_1\Bigr)+\Bigl(S_{2,1}-\frac{5}{36}S_3-\frac{7}{12}\zeta_3\Bigr)S_1+\Bigl(\frac{5}{48}S_2+\frac{\zeta_2}{16}\Bigr)S_1^2\\
&+\frac{1}{288}S_1^4-\frac{23}{96}S_2^2+\frac{17}{48}S_4+S_{3,1}-\frac{13}{6}S_{2,1,1}-\frac{3}{16}\zeta_2S_2\Biggr]-\frac{32P_8S_{2,1}+4P_{16}\zeta_3}{3N^3(N+1)^3}\Biggr\},
\end{aligned}
\tag{3.4}
$$

with the functions

$$
F_1=\frac{(N-1)(N+2)}{N^2(N+1)^2}\,, \tag{3.5}
$$

$$
F_2=\frac{(N-3)(N+2)(2N+1)}{N^3(N+1)^2}\,. \tag{3.6}
$$

The constants B_4 and B_5 are defined as

$$B_4 = 16\text{Li}_4\left(\frac{1}{2}\right) + \frac{2}{3}\ln^4(2) - 4\ln^2(2)\zeta_2 - \frac{13}{2}\zeta_4 \tag{3.7}$$

$$B_5 = 16\text{Li}_5\left(\frac{1}{2}\right) + 8\ln(2)\text{Li}_4\left(\frac{1}{2}\right) + \frac{101}{48}\zeta_2\zeta_3 - \frac{443}{32}\zeta_5 + \frac{1}{5}\ln^5(2) - \frac{2}{3}\ln^3(2)\zeta_2 - \frac{35}{4}\ln(2)\zeta_3 + \frac{61}{16}\ln(2)\zeta_4. \tag{3.8}$$

They are linear combinations of multiple zeta values [60] and $\text{Li}_n(x) = \sum_{k=1}^{\infty} x^k/k^n$, $x \in [-1, 1]$ denotes the classical polylogarithm. The polynomials P_i are given by

$$P_1 = 11N^3 - 3N^2 + 10N + 6, \tag{3.9}$$
$$P_2 = N^4 + 3N^3 + 2N^2 + 6N - 4, \tag{3.10}$$
$$P_3 = 6N^4 + 38N^3 + 52N^2 + 81N + 42, \tag{3.11}$$
$$P_4 = 11N^4 + 22N^3 - 23N^2 - 70N - 12, \tag{3.12}$$
$$P_5 = 35N^4 + 64N^3 + 28N^2 - 13N - 6, \tag{3.13}$$
$$P_6 = 71N^4 + 8N^3 - 121N^2 + 66N + 72, \tag{3.14}$$
$$P_7 = 203N^4 + 394N^3 - 125N^2 - 928N - 192, \tag{3.15}$$
$$P_8 = 6N^5 + 21N^4 - 26N^3 - 48N^2 - 39N - 22, \tag{3.16}$$
$$P_9 = 58N^5 + 25N^4 + 167N^3 - 94N^2 - 96N - 36, \tag{3.17}$$
$$P_{10} = 64N^5 + 497N^4 + 614N^3 - 545N^2 - 126N - 360, \tag{3.18}$$
$$P_{11} = 2N^6 + 15N^5 + 179N^4 + 471N^3 + 503N^2 + 774N + 360, \tag{3.19}$$
$$P_{12} = 6N^6 + 15N^5 - 24N^4 + 29N^2 - 138N - 12, \tag{3.20}$$
$$P_{13} = 6N^6 + 15N^5 + 24N^4 - 8N^3 - 3N^2 + 78N + 20, \tag{3.21}$$
$$P_{14} = 9N^6 + 54N^5 - 148N^4 - 377N^3 - 1421N^2 - 679N + 330, \tag{3.22}$$
$$P_{15} = 36N^6 + 108N^5 - 63N^4 - 531N^3 - 1001N^2 - 623N - 14, \tag{3.23}$$
$$P_{16} = 48N^6 + 48N^5 - 501N^4 - 378N^3 - 881N^2 - 524N + 268, \tag{3.24}$$
$$P_{17} = 117N^6 + 566N^5 + 1137N^4 + 1348N^3 + 944N^2 + 208N - 48, \tag{3.25}$$
$$P_{18} = 135N^6 + 540N^5 + 875N^4 + 49N^3 - 3686N^2 - 3715N + 1086, \tag{3.26}$$
$$P_{19} = 160N^6 + 447N^5 + 211N^4 + 159N^3 + 475N^2 - 192N - 108, \tag{3.27}$$
$$P_{20} = 79N^7 - 52N^6 - 1379N^5 - 2938N^4 - 1781N^3 + 947N^2 + 1308N + 468, \tag{3.28}$$
$$P_{21} = 158N^7 + 381N^6 - 566N^5 - 2683N^4 - 3502N^3 - 1860N^2 + 312N + 416, \tag{3.29}$$
$$P_{22} = 332N^7 + 490N^6 + 1167N^5 - 1555N^4 + 754N^3 + 1140N^2 + 792N + 216, \tag{3.30}$$
$$P_{23} = 2125N^7 + 8792N^6 + 9505N^5 + 632N^4 + 3487N^3 + 4535N^2 - 7188N - 2556, \tag{3.31}$$
$$P_{24} = 3N^8 + 26N^7 + 28N^6 - 41N^5 + 82N^4 + 111N^3 - 257N^2 - 20N - 4, \tag{3.32}$$
$$P_{25} = 13N^8 - 146N^7 - 1061N^6 - 2606N^5 - 2516N^4 + 502N^3 + 1746N^2 + 1620N + 432, \tag{3.33}$$

$$P_{26} = 12N^9 + 32N^8 - 5N^7 - 194N^6 - 493N^5 + 76N^4 + 1568N^3 + 1596N^2 \\ +704N + 112, \tag{3.34}$$

$$P_{27} = 80N^9 - 859N^8 - 6334N^7 - 16687N^6 - 22150N^5 - 15142N^4 - 15840N^3 \\ -15228N^2 - 9720N - 2592, \tag{3.35}$$

$$P_{28} = 968N^9 + 5625N^8 + 13824N^7 + 19941N^6 + 15627N^5 - 5448N^4 - 22490N^3 \\ -12963N^2 - 2772N - 108, \tag{3.36}$$

$$P_{29} = 184N^{11} + 1168N^{10} + 3055N^9 + 4058N^8 + 2015N^7 - 1489N^6 - 2103N^5 \\ +75N^4 + 2179N^3 + 2158N^2 + 1060N + 216, \tag{3.37}$$

$$P_{30} = 6472N^{12} + 35280N^{11} + 76634N^{10} + 67296N^9 - 65784N^8 - 151947N^7 \\ +81392N^6 + 112464N^5 - 171758N^4 - 51321N^3 - 11844N^2 \\ +18684N + 7776\,. \tag{3.38}$$

The Mellin inversion of (3.4) leads to generalized harmonic polylogarithms (HPLs) of argument x [55]. These can be transformed to standard harmonic polylogarithms [61] over the alphabet $\{-1, 0, 1\}$ evaluated at different arguments, which can be done with the help of the Mathematica package `HarmonicSums`. The harmonic polylogarithms are given by

$$H_{b,\vec{a}}(x) = \int_0^x dy f_b(y) H_{\vec{a}}(y), \quad a_i, b \in \{-1, 0, 1\}, \quad H_\emptyset = 1, \tag{3.39}$$

with $f_0 = 1/y$, $f_{-1} = 1/(1+y)$, $f_1 = 1/(1-y)$.

In the case of $a_{Qq}^{(3),\mathrm{PS}}$, we obtain the usual harmonic polylogarithms at argument x and a set of harmonic polylogarithms at argument $(1-2x)$. This representation is of advantage for later numerical representations.[4] The presence of the argument $(1-2x)$ in the OME will require a modification of the Mellin convolution. In intermediate steps we observed the supports $[0, 1/2]$ and $[1/2, 1]$. The corresponding Mellin convolutions with parton distribution functions of support $[0, 1]$ are given by, cf. [10],

$$\left[A_1(x)\theta\left(\tfrac{1}{2} - x\right)\right] \otimes f(x) = \theta\left(\tfrac{1}{2} - x\right) \int_{2x}^1 \frac{dy}{y} A_1\left(\frac{x}{y}\right) f(y) \tag{3.40}$$

$$\left[A_2(x)\theta\left(x - \tfrac{1}{2}\right)\right] \otimes f(x) = \int_x^1 \frac{dy}{y} A_2\left(\frac{x}{y}\right) f(y) - \theta\left(\tfrac{1}{2} - x\right) \int_{2x}^1 \frac{dy}{y} A_2\left(\frac{x}{y}\right) f(y)\,. \tag{3.41}$$

We will split $a_{Qq}^{(3),\mathrm{PS}}(x)$ into a part represented by the harmonic polylogarithms of only the argument x and a part containing also harmonic polylogarithms with the argument $(1-2x)$. In what follows, we use the shorthand notation

$$H_{i_n,\cdots,i_1} = H_{i_n,\cdots,i_1}(x) \quad \text{and} \quad \tilde{H}_{i_n,\cdots,i_1} = H_{i_n,\cdots,i_1}(1-2x). \tag{3.42}$$

[4] Note that using the harmonic polylogarithms at a different continuous argument implies in general a new class of functions with only exceptional relations.

One obtains

$$
\begin{aligned}
&a_{Qq}^{(3),\mathrm{PS}}(x) = \\
&C_F T_F^2 N_F \Biggl\{ \frac{32}{3}(1-x)\Bigl[\frac{2276}{81} - \Bigl(\frac{4}{3}H_1 + 5H_1^2\Bigr)H_0 + \Bigl(\frac{536}{27} + \frac{25}{2}\zeta_2\Bigr)H_1 + 10H_0^2 H_1 + \frac{1}{9}H_1^2 \\
&+ \frac{5}{18}H_1^3\Bigr] - \frac{128}{9}\Bigl[\frac{2}{27}(104-229x) + (10-11x)H_{0,1}\Bigr]H_0 - \frac{32}{27}(5-4x)\Bigl(\frac{4}{3}H_0^3 + 7\zeta_2 H_0\Bigr) \\
&+ \frac{64}{9}(x+1)\Biggl[\bigl(15\zeta_3 - 12H_{0,0,1} - 6H_{0,1,1}\bigr)H_0 + \Bigl(6H_{0,1} - \frac{7}{2}\zeta_2\Bigr)H_0^2 - \frac{1}{3}H_0^4 + 4H_{0,0,0,1} \\
&+ 10H_{0,0,1,1} + H_{0,1,1,1} + \frac{15}{2}\zeta_2 H_{0,1} - \frac{21}{2}\zeta_2^2\Biggr] - \frac{128}{81}(95x+23)H_0^2 + \frac{256}{81}(43x+16)H_{0,1} \\
&+ \frac{640}{27}(4-5x)H_{0,0,1} + \frac{64}{27}(40-41x)H_{0,1,1} - \frac{32}{81}(389x+83)\zeta_2 + \frac{32}{27}(17x+5)\zeta_3 \Biggr\} \\
&+ C_F T_F^2 \Biggl\{ \frac{64}{81}\bigl(12x^4 - 15x^3 - x - 46\bigr)H_0^2 - \frac{128}{81}\bigl(24x^4 - 30x^3 + 214x - 65\bigr)H_{0,1} \\
&+ \frac{32}{3}(1-x)\Biggl[\frac{8}{81}\bigl(36x^2 + 9x - 20\bigr) + \frac{1}{9}\bigl(8x^3 - 2x^2 - 2x + 51\bigr)H_1^2 - \frac{5}{9}H_1^3 \\
&- \Bigl(\frac{4}{9}(4x^3 - x^2 - x + 25)H_1 + 5H_1^2\Bigr)H_0 + \Bigl(20H_{0,1} - \frac{4}{27}(12x^2 + 3x + 52) - 15\zeta_2\Bigr)H_1\Biggr] \\
&+ \frac{32}{9}\Biggl[-\frac{4}{27}\bigl(36x^3 - 27x^2 - 281x + 61\bigr) - 4(5x+2)H_{0,1} - \frac{1}{3}(17-73x)\zeta_2\Biggr]H_0 \\
&+ \frac{64}{3}(x+1)\Biggl[2\bigl(-H_{0,1,1} + 3\zeta_3\bigr)H_0 - \frac{1}{9}H_0^4 + 2H_{0,1}^2 + \frac{4}{3}H_{0,0,0,1} - \frac{2}{3}H_{0,0,1,1} \\
&- \frac{2}{3}H_{0,1,1,1} - \frac{7}{6}\zeta_2 H_0^2 - 3\zeta_2 H_{0,1} + \frac{4}{5}\zeta_2^2\Biggr] - \frac{128}{81}(5-4x)H_0^3 + \frac{128}{27}(26x+17)H_{0,0,1} \\
&- \frac{256}{27}(23-40x)H_{0,1,1} + \frac{32}{81}\bigl(48x^4 - 60x^3 + 481x + 103\bigr)\zeta_2 - \frac{64}{27}(317x - 163)\zeta_3 \Biggr\} \\
&+ C_F^2 T_F \Biggl\{ -32B_4(5x+13) - \frac{2}{x-1}\bigl(4x^3 - 297x^2 + 134x + 143\bigr)H_0^2 \\
&+ \frac{32}{3}(1-x)\Biggl\{\frac{29}{24}H_1^3 + \frac{5}{48}H_1^4 + \Biggl[\frac{3x}{2} - \frac{319}{4} - 70H_{0,1} + \frac{35}{2}\zeta_2 - \frac{21}{4}H_1 - \frac{5}{6}H_1^2\Biggr]H_1 H_0 \\
&+ \Biggl(\frac{471}{8}H_1 - \frac{5}{2}H_1^2\Biggr)H_0^2 + \Biggl(\frac{25}{2}\zeta_3 - \frac{405}{4} + 140H_{0,0,1} + 95H_{0,1,1}\Biggr)H_1 - \frac{25}{6}H_0^3 H_1 - 74 \\
&+ \Biggl[\frac{451}{8} - \frac{3x}{4} - 15H_{0,1} + \frac{155}{8}\zeta_2\Biggr]H_1^2\Biggr\} + \frac{32}{3}(x+1)\Biggl[-24B_5 - \Biggl(\frac{5}{3}H_{0,1} + \frac{47}{24}\zeta_2\Biggr)H_0^3 \\
&+ \bigl(-14H_{0,1}^2 - 20H_{0,0,0,1} + 56H_{0,0,1,1} - 2H_{0,1,1,1} + 7\zeta_2 H_{0,1} - 17\zeta_2^2\bigr)H_0 + \frac{9}{80}H_0^5 \\
&+ \Biggl(\frac{9}{2}H_{0,0,1} - 2H_{0,1,1} - \frac{31}{4}\zeta_3\Biggr)H_0^2 + \bigl(56H_{0,0,1} - 12H_{0,1,1} + 5\zeta_3\bigr)H_{0,1} + 80H_{0,0,0,0,1} \\
&- 318H_{0,0,0,1,1} - 134H_{0,0,1,0,1} + 78H_{0,0,1,1,1} + 50H_{0,1,0,1,1} + H_{0,1,1,1,1} + 19\zeta_2 H_{0,0,1}
\end{aligned}
$$

$$+\frac{31}{2}\zeta_2 H_{0,1,1}\Big] + \frac{2}{3}\big[4(50x+151) + 8(493x-392)H_{0,1} - 32(67x+127)H_{0,0,1}$$
$$-16(131x-134)H_{0,1,1} - (709x-471)\zeta_2 + 8(97x-112)\zeta_3\big]H_0 + \frac{2}{9}(253-15x)H_0^3$$
$$+\Big[\frac{16}{3}(61x+104)H_{0,1} + \frac{20}{3}(7x+13)\zeta_2\Big]H_0^2 + \frac{2}{9}(43-39x)H_0^4 + \frac{16}{3}(55x-97)H_{0,1}^2$$
$$+\big[32(23x-21)H_{0,1} - 4(241x-225)\zeta_2\big]H_1 - \frac{8}{3}(1425x-953)H_{0,0,1} - 7168\ln(2)\zeta_3$$
$$-\frac{32}{3}(255x-209)H_{0,1,1} + \Big[\frac{8}{3}\big(12x^2-1007x+133\big) + 120(x+3)\zeta_2\Big]H_{0,1}$$
$$+\frac{32}{3}(183x+464)H_{0,0,0,1} - \frac{32}{3}(11-180x)H_{0,0,1,1} - \frac{16}{3}(369-377x)H_{0,1,1,1}$$
$$-\frac{2}{3}\big(24x^2-3169x-303\big)\zeta_2 - \frac{8}{15}(897x+2213)\zeta_2^2 - \frac{4}{3}(1995-1291x)\zeta_3\Big\}$$
$$+C_A C_F T_F\Big\{16B_4(5x+13) - \frac{8}{81(x+1)}\big(162x^3-29126x^2-4171x+24793\big)H_{0,1}$$
$$-\frac{4}{81(1-x^2)}\big(108x^4+58694x^3+2948x^2-59261x-3299\big)H_0^2$$
$$+\frac{32}{3}(43x+41)\big(H_{0,-1,1}+H_{0,1,-1}\big)H_0 - \frac{8}{3}\Big[\frac{1}{9}(14221-2825x) + 2(3x+7)\zeta_2\Big]H_{0,0,1}$$
$$-16(63-79x)\Big[H_{0,0,0,-1,1} + H_{0,0,0,1,-1} + \frac{1}{3}H_{0,0,1,0,-1}\Big] - \frac{16}{3}(197x+411)H_{0,0,0,0,1}$$
$$+\frac{32}{3}(1-x)\Big\{\Big(\frac{19}{4}H_{0,-1,-1} - \frac{185}{16}H_1^2\Big)H_0^2 - \Big[\frac{1}{72}(1123-27x) + \frac{25}{8}\zeta_2\Big]H_1^2 - \frac{128383}{81}$$
$$+\Big[\Big(\frac{1}{12}(2996-9x) + H_{0,-1} + \frac{239}{4}H_{0,1} - 3\zeta_2\Big)H_1 + 29H_1^2 + \frac{10}{3}H_1^3 + \frac{19}{4}H_{0,-1}^2$$
$$+14H_{0,-1,-1,-1} - 30H_{0,0,-1,-1} - \frac{73}{2}H_{0,0,0,-1} + \frac{19}{2}\zeta_2 H_{0,-1}\Big]H_0 - \frac{115}{72}H_1^3$$
$$+\Big(\frac{169}{24}H_1 - \frac{35}{12}H_{0,-1}\Big)H_0^3 + \Big(\frac{77}{108} - 2H_{0,0,-1} - \frac{361}{4}H_{0,0,1} - \frac{55}{2}H_{0,1,1} - \frac{73}{4}\zeta_3\Big)H_1$$
$$+\Big(H_{0,1} - 14H_{0,-1,-1} - \frac{57}{2}H_{0,0,-1} + \frac{71}{2}H_{0,0,1} - 19\zeta_3\Big)H_{0,-1} - 5H_{0,-1,-1,0,1} - \frac{5}{48}H_1^4$$
$$+28H_{0,-1,0,-1,-1} + 56H_{0,0,-1,-1,-1} + \frac{117}{2}H_{0,0,-1,0,-1} + \frac{351}{2}H_{0,0,0,-1,-1}$$
$$+12\zeta_2 H_{0,-1,-1} - 17\zeta_2 H_{0,0,-1}\Big\}$$
$$+\frac{32}{3}(x+1)\Big\{12B_5 + \frac{1}{4x}\big(x^2-908x+3\big)\big(H_{0,-1} - H_{-1}H_0\big) + \frac{35}{6}H_{-1}^3 H_0 + \frac{31}{12}H_0^3 H_{0,1}$$
$$-\Big(4H_{0,0,-1} + \frac{71}{2}H_{0,0,1} + \frac{11}{2}\zeta_3\Big)H_{0,1} + \Big[\Big(\frac{77}{4}H_{0,-1} - 42H_{0,1} + \frac{131}{4}\zeta_2\Big)H_0 - \frac{63}{8}H_0^3$$

$$
\begin{aligned}
&+62H_{0,-1}+35H_{0,-1,-1}-\frac{1}{2}H_{0,-1,1}-\frac{271}{4}H_{0,0,-1}+\frac{345}{4}H_{0,0,1}-\frac{1}{2}H_{0,1,-1}-2H_{0,1,1}\\
&-\frac{75}{2}\zeta_3\Bigg]H_{-1}+\Bigg(-31H_0+\frac{117}{16}H_0^2-\frac{35}{2}H_{0,-1}+\frac{1}{4}H_{0,1}+\frac{17}{2}\zeta_2\Bigg)H_{-1}^2+\Bigg(2H_{0,-1}H_{0,1}\\
&+\frac{49}{4}H_{0,1}^2-4H_{0,0,-1,1}-4H_{0,0,1,-1}+8H_{0,1,1,1}-\zeta_2H_{0,1}\Bigg)H_0-62H_{0,-1,-1}\\
&-35H_{0,-1,-1,-1}+\frac{1}{2}H_{0,-1,-1,1}+\frac{1}{2}H_{0,-1,1,-1}+2H_{0,-1,1,1}+\frac{271}{4}H_{0,0,-1,-1}\\
&-\frac{345}{4}H_{0,0,-1,1}-\frac{345}{4}H_{0,0,1,-1}-\frac{39}{4}H_0^2H_{0,1,1}-\frac{5}{2}\zeta_2H_{0,1,1}\\
&+\frac{1}{2}H_{0,1,-1,-1}+2H_{0,1,-1,1}+2H_{0,1,1,-1}-15H_{0,0,1,1,1}-11H_{0,1,0,1,1}\\
&-H_{0,1,1,1,1}\Bigg\}+\frac{4}{3}\Bigg[(173x+135)H_{0,-1}-(247x+887)H_{0,1}+\frac{\zeta_2}{3}(241x+223)\\
&-3(436-431x)H_1+8(15-17x)H_{0,0,-1}-4(25x+69)H_{0,0,1}+4(3x-41)\zeta_3\Bigg]H_0^2\\
&+\frac{8}{3}\Bigg[23(15-14x)H_{0,-1}+\frac{1}{3}(4322-2473x)H_{0,1}-(207x+319)H_{0,-1,-1}\\
&-(59x+87)H_{0,0,-1}+7(59x+209)H_{0,0,1}+120(3x-2)H_{0,1,1}-8(9-7x)H_{0,-1,0,1}\\
&+186(x+3)H_{0,0,0,1}-2(37x+35)H_{0,0,1,1}+\frac{1}{18}(3629-2707x)\zeta_2+\frac{1}{5}(377-231x)\zeta_2^2\\
&-2(179x+66)\zeta_3-\frac{1}{81}(433786x+86449)\Bigg]H_0+\frac{4}{15}(4-5x)H_0^5+32(x+73)\zeta_5\\
&+\Bigg[-4(42x+41)H_0^2+\frac{16}{3}(10x+7)H_{0,1}-16(24x+23)\zeta_2\Bigg]H_{-1}+\frac{2}{27}(292x+223)H_0^4\\
&+\Bigg[\frac{4}{81}(1733-1669x)-\frac{16}{9}(4x-5)\zeta_2\Bigg]H_0^3+4\Bigg[\frac{4}{3}(53-56x)H_{0,1}-(181-185x)\zeta_2\Bigg]H_1\\
&+\frac{8}{3}(65x+121)H_{0,-1}^2+\frac{4}{3}(209-83x)H_{0,1}^2-\frac{16}{3}(10x+7)\big(H_{0,-1,1}+H_{0,1,-1}\big)\\
&-\frac{56}{3}(81-110x)H_{0,0,-1}+\frac{8}{27}(6155x-4393)H_{0,1,1}-\frac{8}{3}(157x+169)H_{0,-1,0,1}\\
&+24(5-17x)H_{0,0,0,-1}-\frac{16}{9}(491x+2906)H_{0,0,0,1}-\frac{16}{9}(851x+47)H_{0,0,1,1}\\
&+\frac{16}{9}(358-395x)H_{0,1,1,1}-\frac{32}{3}(33-41x)H_{0,0,-1,0,1}-128(x-3)H_{0,0,0,0,-1}\\
&+\frac{16}{3}(347x+341)H_{0,0,0,1,1}+\frac{32}{3}(67x+68)H_{0,0,1,0,1}-\frac{8}{3}(115x+167)\zeta_2H_{0,-1}\\
&-\frac{8}{3}(106x+121)\zeta_2H_{0,1}+\frac{4}{15}(3163x+7429)\zeta_2^2+\Bigg[3584\ln(2)+\frac{136}{27}(100x+697)\Bigg]\zeta_3\\
&-\frac{16}{3}(45-34x)\zeta_2\zeta_3+\frac{4\zeta_2}{81(x+1)}\big(108x^3+9131x^2+40690x+31019\big)\Bigg\}+\tilde{a}_{Qq}^{(3),\mathrm{PS}},
\end{aligned}
\tag{3.43}
$$

where

$$
\begin{aligned}
&\tilde{a}_{Qq}^{(3),\rm PS}(x) = \\
&C_F T_F (C_A - 2C_F)\Biggl\{-32(11-23x)\bigl[2\ln(2)\bigl(\tilde{H}_{0,-1}+\tilde{H}_{0,1}\bigr)-\tilde{H}_{0,-1,-1}+\tilde{H}_{0,-1,1} \\
&-\tilde{H}_{0,1,-1}+\tilde{H}_{0,1,1}\bigr]+160(1-x)\bigl[-4\ln(2)\tilde{H}_{0,-1,-1}+3\tilde{H}_{0,-1,-1,-1}-\tilde{H}_{0,1,-1,1}\bigr] \\
&+32(5x+7)\bigl[-4\ln(2)\tilde{H}_{0,1,1}+\tilde{H}_{0,-1,1,-1}-3\tilde{H}_{0,1,1,1}\bigr]+96(5x+3)\tilde{H}_{0,1,1,-1} \\
&+64(x+1)\Biggl\{\ln(2)\Biggl[\bigl(-2\tilde{H}_{-1}\tilde{H}_1-\tilde{H}_1^2+2\tilde{H}_{-1,1}\bigr)\bigl(\tilde{H}_{0,-1}+\tilde{H}_{0,1}\bigr)-4\tilde{H}_{0,-1,-1,1} \\
&+4\Biggl(\tilde{H}_{0,-1,-1}+\tilde{H}_{0,-1,1}+\tilde{H}_{0,1,-1}+\tilde{H}_{0,1,1}-\frac{7}{2}\zeta_3\Biggr)\tilde{H}_1-2\tilde{H}_{0,-1,1,-1}-6\tilde{H}_{0,-1,1,1} \\
&-4\tilde{H}_{0,1,-1,1}-2\tilde{H}_{0,1,1,-1}-6\tilde{H}_{0,1,1,1}\Biggr]+2\tilde{H}_{0,1,-1,1,-1}-3\tilde{H}_{0,1,-1,1,1}+\tilde{H}_{0,1,1,-1,-1} \\
&+\Biggl(\tilde{H}_{-1}\tilde{H}_1+\frac{1}{2}\tilde{H}_1^2-\tilde{H}_{-1,1}\Biggr)\Biggl(\tilde{H}_{0,-1,-1}-\tilde{H}_{0,-1,1}+\tilde{H}_{0,1,-1}-\tilde{H}_{0,1,1}+\frac{7}{2}\zeta_3\Biggr) \\
&+\Biggl(-B_4-3\tilde{H}_{0,-1,-1,-1}+\tilde{H}_{0,-1,-1,1}-\tilde{H}_{0,-1,1,-1}+3\tilde{H}_{0,-1,1,1}-3\tilde{H}_{0,1,-1,-1} \\
&+\tilde{H}_{0,1,-1,1}-\tilde{H}_{0,1,1,-1}+3\tilde{H}_{0,1,1,1}+\frac{9}{20}\zeta_2^2\Biggr)\tilde{H}_1+3\tilde{H}_{0,-1,-1,-1,1}+2\tilde{H}_{0,-1,-1,1,-1} \\
&-3\tilde{H}_{0,-1,-1,1,1}+\tilde{H}_{0,-1,1,-1,-1}+3\tilde{H}_{0,-1,1,1,-1}-6\tilde{H}_{0,-1,1,1,1}+3\tilde{H}_{0,1,-1,-1,1} \\
&+3\tilde{H}_{0,1,1,1,-1}-6\tilde{H}_{0,1,1,1,1}\Biggr\}-32(5x+19)\tilde{H}_{0,-1,1,1}-32(5x-17)\tilde{H}_{0,1,-1,-1} \\
&+32\bigl(5(1-x)\tilde{H}_{-1}+(5x+7)\tilde{H}_1\bigr)\Biggl[2\ln(2)\bigl(\tilde{H}_{0,-1}+\tilde{H}_{0,1}\bigr)-\tilde{H}_{0,-1,-1}+\tilde{H}_{0,-1,1} \\
&-\tilde{H}_{0,1,-1}+\tilde{H}_{0,1,1}-\frac{7}{2}\zeta_3\Biggr]-768\ln(2)\bigl(\tilde{H}_{0,-1,1}+\tilde{H}_{0,1,-1}\bigr)+96(5x-1)\tilde{H}_{0,-1,-1,1}\Biggr\}.
\end{aligned}
\tag{3.44}
$$

Let us now derive expansions in the small and large x regions for $a_{Qq}^{\rm PS,(3)}(x)$. For small values of x the following approximation holds

$$
\begin{aligned}
a_{Qq}^{\rm PS,(3)}(x) \simeq{}& C_F T_F^2\Biggl\{-\frac{64}{27}\ln^4(x)-\frac{640}{81}\ln^3(x)-\frac{32}{81}(92+63\zeta_2)\ln^2(x) \\
&-\frac{32}{243}(244+153\zeta_2-972\zeta_3)\ln(x)+\frac{32}{1215}\Bigl(-800+1545\zeta_2+648\zeta_2^2+14670\zeta_3\Bigr) \\
&+N_F\Biggl[-\frac{64}{27}\ln^4(x)-\frac{640}{81}\ln^3(x)-\frac{32}{81}(92+63\zeta_2)\ln^2(x) \\
&-\frac{32}{243}(832+315\zeta_2-810\zeta_3)\ln(x)-\frac{32}{243}\Bigl(-2276+249\zeta_2+567\zeta_2^2-45\zeta_3\Bigr)\Biggr]\Biggr\}
\end{aligned}
$$

$$
\begin{aligned}
&+C_F C_A T_F \Biggl\{ \frac{16}{15} \ln^5(x) + \frac{446}{27} \ln^4(x) + \frac{4}{81}\bigl(1733 + 180\zeta_2\bigr)\ln^3(x) \\
&+\frac{4}{81}\bigl(3299 + 2007\zeta_2 - 4428\zeta_3\bigr)\ln^2(x) + \frac{4}{1215}\bigl(-866920 + 163305\zeta_2 \\
&+61074\zeta_2^2 - 106920\zeta_3\bigr)\ln(x) + 32B_4 + \frac{4}{1215}\bigl(-5132890 + 465285\zeta_2 \\
&+593001\zeta_2^2 + 692190\zeta_3 - 93150\zeta_2\zeta_3 + 660960\zeta_5\bigr)\Biggr\} \\
&+C_F^2 T_F \Biggl\{ \frac{6}{5}\ln^5(x) + \frac{86}{9}\ln^4(x) + \frac{2}{9}\bigl(253 - 94\zeta_2\bigr)\ln^3(x) \\
&+\frac{2}{3}\bigl(429 + 130\zeta_2 - 124\zeta_3\bigr)\ln^2(x) + \frac{2}{3}\bigl(604 + 471\zeta_2 - 272\zeta_2^2 - 896\zeta_3\bigr)\ln(x) \\
&-64B_4 - \frac{2}{3}\bigl(1184 - 303\zeta_2 + 1684\zeta_2^2 + 294\zeta_3 - 200\zeta_2\zeta_3 - 480\zeta_5\bigr)\Biggr\}. \qquad (3.45)
\end{aligned}
$$

Here the leading term is

$$
a_{Qq}^{\mathrm{PS},(3)}(x) \simeq \frac{2}{15} C_F T_F \left[8C_A + 9C_F\right]\ln^5(x). \qquad (3.46)
$$

For large values of x one obtains

$$
\begin{aligned}
a_{Qq}^{\mathrm{PS},(3)}(x) \simeq (1-x)\Biggl\{ & C_F T_F^2 N_F \Biggl[-\frac{16}{27}\ln^3(1-x) - \frac{128}{27}\ln^2(1-x) \\
&-\frac{16}{81}\bigl(68 + 135\zeta_2\bigr)\ln(1-x) - \frac{32}{243}\bigl(230 + 540\zeta_2 - 297\zeta_3\bigr)\Biggr] \\
&+C_F T_F^2 \Biggl[\frac{32}{27}\ln^3(1-x) - \frac{32}{27}\ln^2(1-x) - \frac{32}{81}\bigl(-32 + 27\zeta_2\bigr)\ln(1-x) \\
&-\frac{32}{243}\bigl(-64 + 459\zeta_2 - 378\zeta_3\bigr)\Biggr] \\
&+C_A C_F T_F \Biggl[-\frac{2}{9}\ln^4(1-x) + \frac{68}{27}\ln^3(1-x) - \frac{4}{27}\bigl(-136 + 45\zeta_2\bigr)\ln^2(1-x) \\
&+\frac{4}{81}\bigl(1120 + 2403\zeta_2 + 1404\zeta_3\bigr)\ln(1-x) + \frac{4}{1215}\bigl(49135 + 84915\zeta_2 \\
&+7128\zeta_2^2 - 77220\zeta_3\bigr)\Biggr] + C_F^2 T_F \Biggl[\frac{2}{9}\ln^4(1-x) - \frac{20}{9}\ln^3(1-x) \\
&+\frac{4}{3}\bigl(-19 + 7\zeta_2\bigr)\ln^2(1-x) - \frac{4}{3}\bigl(34 + 91\zeta_2 + 60\zeta_3\bigr)\ln(1-x) \\
&-\frac{2}{3}\bigl(252 + 335\zeta_2 + 168\zeta_2^2 - 278\zeta_3\bigr)\Biggr]\Biggr\}. \qquad (3.47)
\end{aligned}
$$

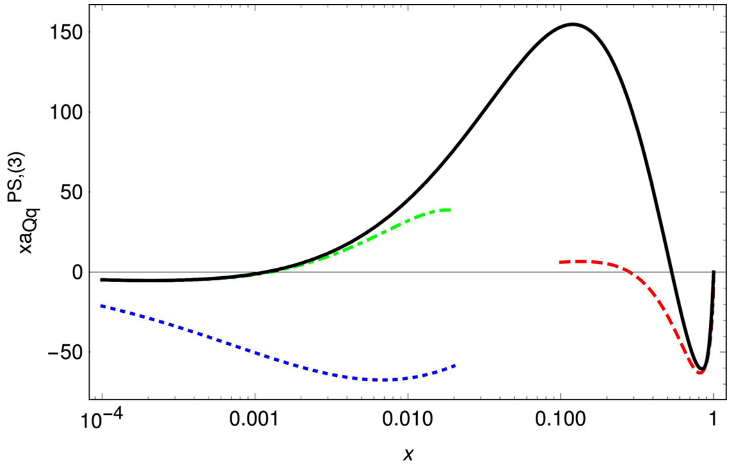

Fig. 2. The constant part of the polarized unrenormalized OME $A_{Qq}^{\rm PS,(3)}$, $xa_{Qq}^{\rm PS,(3)}$, as a function of x. Full line: complete expression; dotted line: leading small x term (3.46); dash-dotted line: small x approximation (3.45); dashed line: large x approximation (3.47) for $N_F = 3$.

In Fig. 2 we illustrate the function $xa_{Qq}^{\rm PS,(3)}$ setting $N_F = 3$. The leading small x term is phenomenologically not dominant, as has also been observed for a large number of other quantities, cf. [62–64]. A series of sub-leading terms is necessary to describe $xa_{Qq}^{\rm PS,(3)}$ at least for some region in the small x domain. The same is true in the large x region. In both cases the complete logarithmic approximations either in $\ln^k(x)$ or $\ln^k(1-x)$ down to the constant term have a limited range of validity only and the complete function mainly depends on other structures.

To our knowledge neither predictions on the small x nor the large x behaviour of the constant part $a_{Qq}^{\rm PS,(3)}(x)$ of the polarized massive three-loop OME have been given in the literature. As well-known, a stronger singular behaviour occurs in the case of the unpolarized OME $a_{Qq}^{\rm PS,(3)}(x)$ [10] at small x. Also the large x singularity is stronger as in the unpolarized case.

Let us now turn to the complete OME $A_{Qq}^{(3),\rm PS}$. From Eq. (2.7), we obtain the following renormalized result in N space,

$$
\begin{aligned}
A_{Qq}^{(3),\rm PS} = C_F^2 T_F \Biggl\{ & \frac{4}{3} F_1 \bigl(F_3 - 4S_1\bigr) L^3 + 8L^2 \Biggl[-\frac{(N-1)^2(N+2)(3N+2)}{N^3(N+1)^3} S_1 \\
& + F_1 \Biggl(\frac{P_{40}}{N^2(N+1)^2} + 2S_2 \Biggr) \Biggr] + L \Biggl[-\frac{4P_{61}}{N^5(N+1)^5} + 32 F_1 \Biggl(-\frac{1}{12} S_1^3 - \frac{1}{6} S_3 \\
& - \frac{1}{4} S_1 S_2 - S_{1,2} + S_{1,1,1} + 3\zeta_3 \Biggr) + \frac{8 P_{54} S_1}{N^4(N+1)^4} + \frac{8P_{46} S_{1,1} - 8P_{42} S_1^2}{N^3(N+1)^3} \\
& - \frac{8(N-1)P_{37} S_2}{N^3(N+1)^3} \Biggr] - \frac{4P_{64}}{N^6(N+1)^6} + F_1 \Biggl[32 \Biggl(\frac{1}{6} S_3 + \frac{3N^2-3N-4}{8N(N+1)} \zeta_2 \\
& + S_{2,1} + \frac{\zeta_3}{6} \Biggr) S_1 + 4\bigl(S_2 + 2\zeta_2\bigr) S_1^2 + \frac{2}{3} S_1^4 + 2S_2^2 - 12 S_4 + 32 S_{3,1} - 8\zeta_2 S_2 \\
& - 8\zeta_2 S_{1,1} - 64 S_{2,1,1} - \frac{2P_{47}\zeta_2}{N^2(N+1)^2} - \frac{4}{3}\zeta_3 F_3 \Biggr] - F_4 \Biggl(\frac{8}{3} S_1^3 + 8 S_1 S_2 \Biggr)
\end{aligned}
$$

$$
+\frac{24P_{39}S_1-8P_{41}S_3}{3N^3(N+1)^3}-\frac{4P_{31}S_1^2}{N^3(N+1)^2}-\frac{4P_{55}S_2}{N^4(N+1)^4}+\frac{32(N+2)S_{2,1}}{N^3(N+1)}\Bigg\}
$$

$$
+C_FT_F^2\Bigg\{-\frac{128}{9}F_1L^3+\frac{32}{3}L^2\left(-\frac{F_2}{3}+F_1S_1\right)+\frac{32}{3}L\Bigg[-\frac{2(N+2)P_{52}}{9N^4(N+1)^4}
$$

$$
-F_1\left(\frac{1}{2}S_1^2+\frac{5}{2}S_2+S_{1,1}\right)+\frac{2(N+2)P_{34}S_1}{3N^3(N+1)^3}\Bigg]+\frac{32(N+2)P_{60}}{81N^5(N+1)^5}+\frac{32}{9}\zeta_2F_2
$$

$$
+\frac{32}{9}F_1\Bigg[\left(-\frac{28N^2+41N+22}{3(N+1)^2}-\frac{3}{2}S_2-3\zeta_2\right)S_1+\frac{(5N+2)S_1^2}{2(N+1)}-\frac{1}{2}S_1^3
$$

$$
+5S_3+4\zeta_3\Bigg]-\frac{16(N+2)P_{33}S_2}{9N^3(N+1)^3}\Bigg\}+C_FT_F^2N_F\Bigg\{-\frac{32}{9}F_1L^3+\frac{32}{3}L^2\Bigg(-F_1S_1
$$

$$
+\frac{(N+2)P_{34}}{3N^3(N+1)^3}\Bigg)+\frac{32}{3}L\Bigg[-\frac{(N+2)P_{53}}{9N^4(N+1)^4}+F_1\left(\frac{1}{2}S_1^2-\frac{3}{2}S_2-2S_{1,1}\right)
$$

$$
+\frac{(N+2)P_{36}S_1}{3N^3(N+1)^3}\Bigg]-\frac{32(N+2)P_{50}}{3N^5(N+1)^5}+\frac{32}{3}F_1\left(2S_3+\frac{1}{2}\zeta_2S_1+\frac{\zeta_3}{3}\right)
$$

$$
-\frac{64(N+2)\left(N^3+2N+1\right)}{3N^3(N+1)^3}S_2-\frac{16(N+2)\zeta_2P_{36}}{9N^3(N+1)^3}\Bigg\}
$$

$$
+C_AC_FT_F\Bigg\{\frac{16}{3}F_1\left(\frac{11N^2+11N-12}{6N(N+1)}+S_1\right)L^3+8L^2\Bigg[-\frac{P_{57}}{9N^4(N+1)^4}
$$

$$
+2F_1\left(S_2+2S_{-2}\right)+\frac{P_{45}S_1}{3N^3(N+1)^3}\Bigg]+8L\Bigg[\frac{P_{62}}{27N^5(N+1)^5}+4F_1\Bigg(S_{-2}S_1
$$

$$
+\frac{1}{12}S_1^3+\frac{3}{4}S_1S_2+S_{1,2}+S_{1,-2}-S_{1,1,1}-3\zeta_3\Bigg)-\frac{P_{59}S_1}{9N^4(N+1)^4}
$$

$$
+\frac{P_{35}S_1^2}{N^2(N+1)^3}+\frac{23N^2+23N-58}{3N^2(N+1)^2}S_3+\frac{4\left(3N^2+3N-4\right)}{N^2(N+1)^2}S_{-3}
$$

$$
-\frac{2(N-2)P_{32}S_{-2}}{N^3(N+1)^3}+\frac{P_{49}S_2}{3N^3(N+1)^3}-\frac{P_{48}S_{1,1}}{3N^3(N+1)^3}-4NF_4S_{-2,1}\Bigg]
$$

$$
+32F_1\Bigg[-S_1^2\left(\frac{5}{8}S_2+\frac{\zeta_2}{4}\right)-S_{-2}\left(\frac{2S_1}{N+1}+S_1^2+S_2+\frac{3\zeta_2}{4}\right)-\frac{1}{48}S_1^4
$$

$$
-\frac{1}{16}S_2^2+\left(-\frac{5}{3}S_3+2S_{-2,1}-\frac{\zeta_3}{6}\right)S_1-\frac{9}{8}S_4-\left(\frac{1}{N+1}+S_1\right)S_{-3}
$$

$$
-\frac{1}{2}S_{-4}+\frac{1}{2}S_{3,1}+\frac{2S_{-2,1}}{N+1}+S_{-2,2}+S_{-3,1}+\frac{1}{2}S_{2,1,1}-2S_{-2,1,1}-\frac{1}{2}\zeta_2S_2
$$

$$
+\frac{1}{4}\zeta_2S_{1,1}-\frac{\left(11N^2+11N-12\right)\zeta_3}{36N(N+1)}\Bigg]+\frac{16P_{63}}{3N^6(N+1)^6}-\Bigg(\frac{8P_{51}}{N^2(N+1)^5}
$$

$$
+\frac{8\left(3N^2-13\right)S_2}{N^2(N+1)^3}+\frac{4P_{44}\zeta_2}{3N^3(N+1)^3}\Bigg)S_1+\frac{4P_{38}S_1^2}{N^2(N+1)^4}+\frac{4P_{56}S_2}{3N^4(N+1)^4}
$$

$$+\frac{8(N^2+4N+5)}{3N^2(N+1)^3}S_1^3-\frac{16P_{43}S_3}{3N^3(N+1)^3}+\frac{32(N+2)(N^2+3)S_{-2}}{N^2(N+1)^4}$$
$$+\frac{4P_{58}\zeta_2}{9N^4(N+1)^4}\Bigg\}+a_{Qq}^{(3),\mathrm{PS}}(N). \quad (3.48)$$

Here $L=\ln(m^2/\mu^2)$. F_1 and F_2 were given in Eqs. (3.5) and (3.6), and

$$F_3=\frac{3N^2+3N+2}{N(N+1)}, \quad (3.49)$$
$$F_4=\frac{3N^2+3N-2}{N^3(N+1)^2}. \quad (3.50)$$

The polynomials P_i are

$$P_{31}=N^3-6N^2-22N-36, \quad (3.51)$$
$$P_{32}=N^3-2N^2-10N-1, \quad (3.52)$$
$$P_{33}=7N^3+3N^2+26N+12, \quad (3.53)$$
$$P_{34}=8N^3-3N^2+4N+3, \quad (3.54)$$
$$P_{35}=10N^3+13N^2-4N-5, \quad (3.55)$$
$$P_{36}=11N^3-3N^2+10N+6, \quad (3.56)$$
$$P_{37}=13N^3+18N^2-13N-14, \quad (3.57)$$
$$P_{38}=N^4+2N^3-5N^2-12N+2, \quad (3.58)$$
$$P_{39}=2N^4-4N^3-3N^2+20N+12, \quad (3.59)$$
$$P_{40}=2N^4+N^3-3N-2, \quad (3.60)$$
$$P_{41}=3N^4+48N^3+123N^2+98N+8, \quad (3.61)$$
$$P_{42}=10N^4+11N^3-6N^2-N+2, \quad (3.62)$$
$$P_{43}=11N^4+18N^3-39N^2-54N+24, \quad (3.63)$$
$$P_{44}=11N^4+22N^3-23N^2-70N-12, \quad (3.64)$$
$$P_{45}=11N^4+22N^3-11N^2-46N-12, \quad (3.65)$$
$$P_{46}=17N^4+22N^3+N^2+4N+4, \quad (3.66)$$
$$P_{47}=35N^4+64N^3+28N^2-13N-6, \quad (3.67)$$
$$P_{48}=49N^4+62N^3-13N^2-2N+12, \quad (3.68)$$
$$P_{49}=52N^4+71N^3-100N^2-125N+48, \quad (3.69)$$
$$P_{50}=N^5-7N^4+6N^3+7N^2+4N+1, \quad (3.70)$$
$$P_{51}=2N^5+10N^4+29N^3+64N^2+67N+8, \quad (3.71)$$
$$P_{52}=43N^5+19N^4+38N^3-22N^2-21N-9, \quad (3.72)$$
$$P_{53}=58N^5+25N^4+95N^3-22N^2-42N-18, \quad (3.73)$$
$$P_{54}=22N^6+51N^5+6N^4-69N^3-142N^2-92N-24, \quad (3.74)$$
$$P_{55}=27N^6+102N^5+131N^4+52N^3+20N+8, \quad (3.75)$$

$$P_{56} = 47N^6 + 186N^5 + 365N^4 + 560N^3 + 398N^2 - 104N - 48, \tag{3.76}$$
$$P_{57} = 118N^6 + 321N^5 + 97N^4 - 27N^3 + 253N^2 - 114N - 72, \tag{3.77}$$
$$P_{58} = 160N^6 + 447N^5 + 211N^4 + 159N^3 + 475N^2 - 192N - 108, \tag{3.78}$$
$$P_{59} = 169N^6 + 474N^5 + 355N^4 + 240N^3 + 547N^2 + 321N + 18, \tag{3.79}$$
$$P_{60} = 164N^7 + 244N^6 - 66N^5 - 82N^4 - 260N^3 - 189N^2 - 108N - 27, \tag{3.80}$$
$$P_{61} = 36N^8 + 110N^7 + 98N^6 - 4N^5 - 149N^4 - 188N^3 - 187N^2 - 128N - 36, \tag{3.81}$$
$$P_{62} = 968N^8 + 3473N^7 + 4952N^6 + 6113N^5 + 3887N^4 - 2512N^3 + 705N^2 + 1062N + 432, \tag{3.82}$$
$$P_{63} = 6N^{10} + 33N^9 + 73N^8 + 32N^7 - 88N^6 + 38N^5 + 241N^4 + 87N^3 + 29N^2 - 13N - 6, \tag{3.83}$$
$$P_{64} = 24N^{10} + 104N^9 + 213N^8 + 272N^7 + 101N^6 - 207N^5 - 259N^4 - 107N^3 - 13N^2 + 12N + 4. \tag{3.84}$$

The corresponding result in x space is given by

$$\begin{aligned}
A_{Qq}^{(3),\mathrm{PS}} = {} & C_F T_F^2 \Biggl\{ -\frac{256}{9} L^3 \Biggl[\frac{5}{2}(1-x) + (x+1) H_0 \Biggr] + \frac{32}{3} L^2 \Biggl[(1-x)\Biggl(5H_1 - \frac{7}{3}\Biggr) \\
& + 2(x+1)\Biggl(\frac{1}{2}H_0^2 + H_{0,1} - \zeta_2\Biggr) - \frac{1}{3}(19x+1)H_0 \Biggr] + \frac{32}{3} L \Biggl\{ (1-x)\Biggl[-\frac{328}{9} \\
& + \Biggl(\frac{2}{3} + 10H_0\Biggr) H_1 - 5H_1^2 - 10H_{0,1} \Biggr] + (x+1)\Biggl[4\bigl(H_{0,1} - \zeta_2\bigr) H_0 - \frac{2}{3}H_0^3 \\
& - 4H_{0,0,1} - 4H_{0,1,1} + 8\zeta_3 \Biggr] - \frac{x+7}{3}\bigl(H_0^2 - 2H_{0,1} + 2\zeta_2\bigr) - \frac{2}{9}(83x+41)H_0 \Biggr\} \\
& + \frac{32}{3}(1-x)\Biggl[\frac{556}{27} + \Biggl(-\frac{116}{9} - 2H_0 + 5H_0^2 - 5\zeta_2 \Biggr) H_1 + \frac{2}{3}H_1^2 - 10H_0H_{0,1} \\
& - \frac{5}{6}H_1^3 + 2H_{0,1} + 10H_{0,0,1} \Biggr] + \frac{32}{9} H_0 \Biggl[\frac{2}{9}(353x+17) - 6(3x-1)H_{0,1} \\
& + (19x+1)\zeta_2 \Biggr] + \frac{32}{3}(x+1)\Biggl[4\Biggl(-H_{0,0,1} + \frac{8}{3}\zeta_3 \Biggr) H_0 + \bigl(2H_{0,1} - \zeta_2\bigr) H_0^2 \\
& - \frac{1}{12}H_0^4 - 2H_{0,1,1,1} - 2H_{0,1}\zeta_2 + \frac{14}{5}\zeta_2^2 \Biggr] - 16(5x+1)H_0^2 + \frac{16}{9}(3x-1)H_0^3 \\
& - \frac{128}{27}(14x+11)H_{0,1} + \frac{128}{3}(3x-1)H_{0,0,1} + \frac{64}{9}(5x+2)H_{0,1,1} \\
& + \frac{160}{27}(7x+13)\zeta_2 - \frac{64}{9}(33x-14)\zeta_3 \Biggr\} + C_F T_F^2 N_F \Biggl\{ -\frac{32}{9} L^3 \bigl[5(1-x) \\
& + 2(x+1)H_0 \bigr] + \frac{32}{3} L^2 \Biggl[(1-x)\Biggl(\frac{1}{3} - 5H_1 \Biggr) + (x+1)\bigl(H_0^2 - 2H_{0,1} + 2\zeta_2\bigr) \\
& + \frac{x+7}{3} H_0 \Biggr] + \frac{32}{3} L \Biggl\{ (1-x)\Biggl[\Biggl(10H_0 - \frac{2}{3} \Biggr) H_1 - \frac{212}{9} - \frac{5}{2}H_1^2 - 10H_{0,1} \Biggr]
\end{aligned}$$

$$+(x+1)\Big[\big(4H_{0,1}-4\zeta_2\big)H_0-\frac{2}{3}H_0^3-4H_{0,0,1}-2H_{0,1,1}+6\zeta_3\Big]$$
$$-\frac{2}{9}(55x+19)H_0-\frac{x+7}{3}H_0^2+\frac{2}{3}(4x-5)\big(\zeta_2-H_{0,1}\big)\Big\}-16(5x+1)H_0^2$$
$$+\frac{32}{3}(1-x)\Big[8+\Big(-2H_0+5H_0^2+\frac{5\zeta_2}{2}\Big)H_1+2H_{0,1}-10H_0H_{0,1}+\frac{\zeta_2}{3}$$
$$+10H_{0,0,1}\Big]+\frac{64}{3}\Big[-3+7x+(1-3x)H_{0,1}+\frac{1}{6}(4x-5)\zeta_2\Big]H_0$$
$$+\frac{32}{3}(x+1)\Big[\Big(-4H_{0,0,1}+\frac{26}{3}\zeta_3\Big)H_0+\Big(2H_{0,1}-\zeta_2\Big)H_0^2-\frac{1}{12}H_0^4$$
$$+\zeta_2H_{0,1}-\zeta_2^2\Big]+\frac{16}{9}(3x-1)H_0^3+\frac{128}{3}(3x-1)H_{0,0,1}-\frac{32}{9}(41x-17)\zeta_3\Big\}$$
$$+C_F^2T_F\Big\{\frac{32}{3}L^3\Big[-(1-x)\Big(\frac{13}{8}+\frac{5}{2}H_1\Big)+(x+1)\Big(-\frac{1}{4}H_0^2-H_{0,1}+\zeta_2\Big)$$
$$+\frac{1}{2}(3x-2)H_0\Big]+32L^2\Big\{\frac{5}{2}(1-x)\Big(H_{0,1}-\frac{5}{2}-\frac{3}{2}H_1-H_0H_1\Big)-3H_{0,1}$$
$$+(x+1)\Big[\big(\zeta_2-H_{0,1}\big)H_0-\frac{1}{6}H_0^3+H_{0,0,1}-\zeta_3\Big]+\frac{1}{4}(7x-19)H_0+3\zeta_2$$
$$+\frac{1}{2}(2x-3)H_0^2\Big\}+32L\Big\{(1-x)\Big[\frac{27}{4}+\Big(\frac{47}{4}H_1+\frac{5}{2}H_1^2\Big)H_0+\frac{13}{12}H_0^3$$
$$+\Big(\frac{59}{4}-5H_{0,1}\Big)H_1-\frac{5}{8}H_1^2+\frac{5}{12}H_1^3-\frac{47}{4}H_{0,1}+5H_{0,1,1}\Big]-17H_{0,0,1}$$
$$+(x+1)\Big[\big(3H_{0,0,1}+2H_{0,1,1}+6\zeta_3\big)H_0+\frac{3}{16}H_0^4-H_{0,1}^2-\frac{3}{2}H_{0,1,1}-3\zeta_2H_0^2$$
$$-3H_{0,0,0,1}+H_{0,1,1,1}+\frac{9}{5}\zeta_2^2\Big]+\frac{7}{2}(2x+1)\big(H_{0,1}-\zeta_2\big)+\Big[\frac{1}{8}(87-115x)$$
$$-3(x-3)H_{0,1}+(6x-1)\zeta_2\Big]H_0+\frac{1}{16}(87-17x)H_0^2+\frac{1}{2}(67-27x)\zeta_3\Big\}$$
$$+32(1-x)\Big\{\Big(\frac{5}{2}H_{0,0,1}-\frac{35}{4}H_{0,1}+10H_{0,1,1}\Big)H_0-\frac{5}{4}H_0^2H_{0,1}-\frac{5}{2}H_{0,1}^2$$
$$+\Big[\frac{35}{8}H_0^2+\frac{5}{12}H_0^3+\frac{9}{4}-H_{0,1}+\Big(\frac{81}{4}-5H_{0,1}+\frac{5}{2}\zeta_2\Big)H_0+10H_{0,0,1}$$
$$+10H_{0,1,1}+\frac{37}{8}\zeta_2-\frac{55}{6}\zeta_3\Big]H_1-\frac{83}{2}+\Big(\frac{35}{4}-\frac{5}{2}H_{0,1}+\frac{25}{8}\zeta_2\Big)H_1^2+\frac{3}{4}H_1^3$$
$$+\frac{5}{48}H_1^4-\Big(\frac{81}{4}+\frac{5}{2}\zeta_2\Big)H_{0,1}+\frac{35}{4}H_{0,0,1}+2H_{0,1,1}-\frac{5}{2}H_{0,0,0,1}-10H_{0,0,1,1}$$
$$-15H_{0,1,1,1}\Big\}+8\Big[-29-134x+(43x+25)H_{0,1}-\frac{1}{4}(255x+83)\zeta_2$$
$$-28(x+1)H_{0,0,1}+\frac{2}{3}(3x-16)\zeta_3\Big]H_0+8\big[16-79x-(23x-15)\zeta_2\big]H_{0,1}$$

$$
\begin{aligned}
&+2\big[1+27x+8(4x+5)H_{0,1}-2(3x-7)\zeta_2\big]H_0^2-\frac{2}{3}(83x+1)H_0^3\\
&+32(x+1)\Bigg[\Bigg(5H_{0,0,0,1}-H_{0,1}^2+4H_{0,0,1,1}+\zeta_2 H_{0,1}-\frac{14}{5}\zeta_2^2\Bigg)H_0+\frac{1}{240}H_0^5\\
&-\Bigg(\frac{3}{2}H_{0,0,1}+\frac{11}{12}\zeta_3\Bigg)H_0^2+\Bigg(\frac{1}{6}H_{0,1}+\frac{\zeta_2}{8}\Bigg)H_0^3-6H_{0,0,0,0,1}-24H_{0,0,0,1,1}\\
&+\Bigg(4H_{0,0,1}-2H_{0,1,1}-\frac{11}{3}\zeta_3\Bigg)H_{0,1}-10H_{0,0,1,0,1}+13H_{0,0,1,1,1}+\zeta_2 H_{0,0,1}\\
&+6H_{0,1,0,1,1}+H_{0,1,1,1,1}+\frac{5}{2}\zeta_2 H_{0,1,1}-\frac{5}{6}\zeta_2\zeta_3+5\zeta_5\Bigg]-\frac{2}{3}(x-3)H_0^4\\
&+16(5x-1)H_{0,1}^2-16(28x+19)H_{0,0,1}+8(3x+50)H_{0,1,1}\\
&+96(3x+2)H_{0,0,0,1}-32(9x-11)H_{0,0,1,1}-16(3x-7)H_{0,1,1,1}\\
&+(926x-422)\zeta_2+\frac{8}{5}(23x-163)\zeta_2^2+\frac{4}{3}(305x-59)\zeta_3\Bigg\}\\
&+C_AC_FT_F\Bigg\{\frac{32}{3}L^3\Bigg[(1-x)\Bigg(\frac{223}{12}+\frac{5}{2}H_1\Bigg)+(x+1)\big(H_{0,1}-\zeta_2\big)\\
&+\frac{1}{6}(38x+53)H_0+\frac{1}{2}(2-x)H_0^2\Bigg]+32L^2\Bigg\{(1-x)\Bigg[-\frac{1}{3}H_0^3+\frac{55}{12}H_1\\
&+\frac{739}{36}-H_0\Bigg(\frac{5}{2}H_1+2H_{0,-1}+\zeta_2\Bigg)+\frac{5}{2}H_{0,1}+4H_{0,0,-1}\Bigg]+2(x-2)\zeta_3\\
&+(x+1)\Bigg[-\big(5H_{-1}+H_{0,1}\big)H_0+5H_{0,-1}+H_{0,0,1}\Bigg]+\frac{1}{36}(703x-11)H_0\\
&-\frac{1}{12}(50x+29)H_0^2+\frac{1}{6}(17x+5)H_{0,1}-\frac{1}{6}(17x+35)\zeta_2\Bigg\}\\
&+32L\Bigg\{(1-x)\Bigg[\Bigg(4H_{0,-1,-1}-4H_{0,0,-1}-\frac{265}{6}H_1-\frac{15}{4}H_1^2-\frac{33}{4}H_{0,1}\Bigg)H_0\\
&+\frac{5023}{27}+\Bigg(\frac{33}{8}H_1+H_{0,-1}+\frac{\zeta_2}{4}\Bigg)H_0^2+\Bigg(-\frac{451}{18}+5H_{0,1}-\frac{5}{2}\zeta_2\Bigg)H_1\\
&+\frac{1}{24}H_1^2-\frac{5}{12}H_1^3-2H_{0,-1}^2+\frac{265}{6}H_{0,1}+\frac{33}{4}H_{0,0,1}-\frac{5}{2}H_{0,1,1}+6H_{0,0,0,-1}\\
&+2\zeta_2 H_{0,-1}\Bigg]+(x+1)\Bigg[\Bigg(-\frac{51}{2}H_0+3H_0^2-10H_{0,-1}+2H_{0,1}+3\zeta_2\Bigg)H_{-1}\\
&-\big[6H_{0,-1}+7H_{0,0,1}+3H_{0,1,1}\big]H_0+5H_{-1}^2H_0+\frac{51}{2}H_{0,-1}+\frac{7}{4}H_0^2H_{0,1}\\
&+H_{0,1}^2+10H_{0,-1,-1}-2H_{0,-1,1}+6H_{0,0,-1}-2H_{0,1,-1}+11H_{0,0,0,1}\\
&+H_{0,0,1,1}-H_{0,1,1,1}-\zeta_2 H_{0,1}\Bigg]+\Bigg[\frac{1}{2}(19x-13)H_{0,-1}-\frac{1}{6}(82x+127)H_{0,1}\\
&+(1-5x)H_{0,0,-1}+2(x-2)H_{0,0,1}+\frac{1}{12}(29x+5)\zeta_2-(9x+16)\zeta_3
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{108}(16603x+5227)\Big]H_0+\frac{1}{72}(625-1316x)H_0^2+\frac{1}{36}(100x+61)H_0^3\\
&-\frac{1}{36}(179x+557)H_{0,1}+\frac{1}{36}(179x-361)\zeta_2+\frac{1}{12}(299x+425)H_{0,0,1}\\
&+(13-19x)H_{0,0,-1}+3(5x-1)H_{0,0,0,-1}-\frac{1}{20}(87x+209)\zeta_2^2\\
&+\frac{1}{3}(7x-2)H_{0,1,1}-6(x-2)H_{0,0,0,1}+\frac{1}{24}(4-5x)H_0^4+\frac{1}{2}(4x-137)\zeta_3\Big\}\\
&+8\Big(8-13x-\frac{1}{3}(20x+17)\zeta_2\Big)H_{0,1}+32(1-x)\Big\{\Big[\frac{7}{2}H_1^2+\frac{5}{6}H_1^3+H_{0,-1}^2\\
&+\frac{107}{3}H_{0,1}-\frac{25}{2}H_{0,1,1}+\Big(\frac{263}{6}+\frac{15}{2}H_{0,1}+\frac{5\zeta_2}{4}\Big)H_1+4H_{0,-1,-1,-1}\\
&-2H_{0,-1,0,1}-3H_{0,0,0,-1}-2H_{0,0,0,1}+\frac{3}{2}\zeta_2H_{0,-1}\Big]H_0+\frac{1}{120}H_0^5-\frac{1331}{6}\\
&+\Big(-\frac{107}{6}H_1-\frac{5}{8}H_1^2-H_{0,-1,-1}+H_{0,0,-1}\Big)H_0^2+\Big(-\frac{1}{6}H_{0,-1}+\frac{\zeta_2}{4}\Big)H_0^3\\
&+\Big(-\frac{27}{4}-\frac{25}{2}H_{0,0,1}-\frac{5}{2}H_{0,1,1}-\frac{115}{24}\zeta_2+\frac{25}{6}\zeta_3\Big)H_1-\Big(\frac{5}{2}+\frac{5}{8}\zeta_2\Big)H_1^2\\
&-\frac{11}{12}H_1^3-\frac{5}{48}H_1^4+\big(4H_{0,0,1}-4H_{0,-1,-1}-2H_{0,0,-1}-3\zeta_3\big)H_{0,-1}+\frac{5}{2}H_{0,1}^2\\
&-\Big(\frac{263}{6}+\frac{5}{4}\zeta_2\Big)H_{0,1}-\frac{107}{3}H_{0,0,1}-7H_{0,1,1}+\frac{25}{2}H_{0,0,1,1}+8H_{0,-1,0,-1,-1}\\
&+\frac{5}{2}H_{0,1,1,1}+16H_{0,0,-1,-1,-1}+2H_{0,0,-1,0,-1}-4H_{0,0,-1,0,1}+6H_{0,0,0,-1,-1}\\
&-12H_{0,0,0,-1,1}+4H_{0,0,0,0,-1}+8H_{0,0,0,0,1}-12H_{0,0,0,1,-1}-4H_{0,0,1,0,-1}\\
&+2H_{0,-1,-1}\zeta_2-3H_{0,0,-1}\zeta_2\Big\}+32(x+1)\Big\{\Big[\frac{7}{2}H_0^2-\frac{5}{12}H_0^3+10H_{0,-1,-1}\\
&-5H_{0,0,-1}+10H_{0,0,1}+14H_{0,-1}+\Big(21+5H_{0,-1}-5H_{0,1}+\frac{15}{4}\zeta_2\Big)H_0\\
&-7\zeta_2-\frac{15}{2}\zeta_3\Big]H_{-1}+\Big(-7H_0-\frac{5}{4}H_0^2-5H_{0,-1}+\frac{5}{2}\zeta_2\Big)H_{-1}^2+\frac{5}{3}H_{-1}^3H_0\\
&+\Big(-7H_{0,-1}+5H_{0,-1,1}+\frac{3}{2}H_{0,1}^2-5H_{0,-1,-1}-\frac{5}{2}H_{0,0,-1}+5H_{0,1,-1}\\
&-4H_{0,0,1,1}+2H_{0,1,1,1}+\frac{1}{2}\zeta_2H_{0,1}\Big)H_0+\Big(-\frac{1}{2}H_{0,1,1}+\frac{5}{4}H_{0,-1}\Big)H_0^2\\
&-\Big(21+\frac{15}{4}\zeta_2\Big)H_{0,-1}+\Big(\frac{5}{3}\zeta_3-5H_{0,0,1}\Big)H_{0,1}-14H_{0,-1,-1}+7H_{0,0,-1}\\
&-10H_{0,-1,-1,-1}-5H_{0,-1,0,1}+5H_{0,0,-1,-1}-10H_{0,0,-1,1}+27H_{0,0,0,1,1}\\
&+\frac{5}{2}H_{0,0,0,-1}-10H_{0,0,1,-1}+9H_{0,0,1,0,1}-4H_{0,0,1,1,1}-H_{0,1,0,1,1}-\frac{\zeta_2}{2}H_{0,0,1}\\
&-\frac{\zeta_2}{2}H_{0,1,1}-H_{0,1,1,1,1}\Big\}+\frac{32}{3}\Big[(75x+41)H_{0,1}-12H_{0,-1,-1}-12H_{0,0,-1}
\end{aligned}
$$

$$
\begin{aligned}
&-3(x-6)H_{0,-1}+2(22x+49)H_{0,0,1}+6H_{0,1,1}-18(x-2)H_{0,0,0,1}\\
&+\frac{1}{24}(269-1009x)\zeta_2-\frac{1}{6}(431x+221)\zeta_3-\frac{1}{4}(1993x+600)\\
&-\frac{3}{10}(5x-38)\zeta_2^2\Bigg]H_0+32\Bigg[\frac{1}{8}(217x-16)+H_{0,-1}-\frac{1}{12}(79x+109)H_{0,1}\\
&+(x-2)H_{0,0,1}+\frac{1}{12}(41x+20)\zeta_2+\frac{1}{6}(13x-14)\zeta_3\Bigg]H_0^2+64H_{0,-1}^2\\
&+8(3x-2)H_{0,1,1}+64(x-6)H_{0,0,-1}-\frac{4}{9}(39x-38)H_0^3+192H_{0,0,0,-1}\\
&+\frac{2}{9}(26x+23)H_0^4-\frac{64}{3}(78x+41)H_{0,0,1}-48(3x+29)H_{0,0,0,1}\\
&-16(3x+8)H_{0,0,1,1}-16(x+5)H_{0,1,1,1}+384(x-2)H_{0,0,0,0,1}\\
&+\frac{4}{9}(1735x-133)\zeta_2+\frac{8}{3}(37x+43)\zeta_2\zeta_3+\frac{8}{15}(229x+1402)\zeta_2^2\\
&-64\zeta_2H_{0,-1}+\frac{8}{9}(2014x+851)\zeta_3-80(3x-7)\zeta_5\Bigg\}+a_{Qq}^{(3),\mathrm{PS}}(x)\,. \qquad (3.85)
\end{aligned}
$$

4. Conclusions

We have calculated the polarized three-loop massive OME $A_{Qq}^{\mathrm{PS},(3)}$ in the single mass case. For the treatment of the Dirac matrix γ_5 we applied the Larin scheme. It is then convenient to use this scheme also in the calculation of the associated massless Wilson coefficient. After this, an expression for the pure singlet contribution to the structure function can be obtained, also referring to parton distribution functions in the Larin scheme, which are obtained in fits describing the evolution in the Larin scheme [21,35]. More work is needed in the future to construct the transition to the $\overline{\mathsf{MS}}$ scheme. In this calculation the central quantity is the constant part of the unrenormalized polarized pure singlet OME, $a_{Qq}^{\mathrm{PS},(3)}$, since the other contributions to the OME are coming from lower order calculations or are known from massless calculations to three-loop order. The present massive OME is given by the usual and generalized harmonic sums at rational weights in Mellin N space and by harmonic polylogarithms in x space, allowing besides the argument x also for the argument $y = 1 - 2x \in [-1, 1]$. The latter functions are obtained from generalized harmonic polylogarithms. Their numerical representation can be obtained by using the packages of Refs. [65]. We have calculated the expressions of $a_{Qq}^{\mathrm{PS},(3)}$ in the small and large x regions. It is in principle possible to calculate the leading contributions of these expressions in the small and large x region by applying other techniques. To our knowledge that has not been done in the present case. These terms are not of phenomenological importance, since they receive large corrections form sub-leading contributions, which is also known from various other analyses. Therefore, the complete quantity has to be calculated. The OME $A_{Qq}^{\mathrm{PS},(3)}$ forms one contribution in the polarized variable flavor number scheme at three-loop order.

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.

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Appendix A. Supplementary material

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.nuclphysb.2020.114945.

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