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The 3-loop non-singlet heavy flavor contributions to the structure function $g_1(x, Q^2)$ at large momentum transfer

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Abstract

We calculate the massive flavor non-singlet Wilson coefficient for the heavy flavor contributions to the polarized structure function $g_1(x, Q^2)$ in the asymptotic region $Q^2 \gg m^2$ to 3-loop order in Quantum Chromodynamics at general values of the Mellin variable N and the momentum fraction x , and derive heavy flavor corrections to the Bjorken sum-rule. Numerical results are presented for the charm quark contribution. Results on the structure function $g_2(x, Q^2)$ in the twist-2 approximation are also given.

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1. Introduction

Massless and massive contributions to the unpolarized and polarized structure functions in deep-inelastic scattering exhibit different scaling violations. For a precise determination of the QCD scale Λ_{QCD} or the strong coupling constant $\alpha_s(M_Z^2)$ their precise knowledge is therefore

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of importance [1]. In the case of the polarized structure function $g_1(x, Q^2)$ the complete heavy flavor corrections are only available at 1-loop order [2,3].¹ At higher orders in the coupling constant, the heavy flavor contributions were calculated in the asymptotic region $Q^2 \gg m^2$ based on the factorization derived in Ref. [5]. Here Q^2 denotes the virtuality of the exchanged gauge boson and m the heavy quark mass. The $O(\alpha_s^2)$ corrections in the polarized case were calculated in Refs. [6,7]. In the case of the structure function $g_1(x, Q^2)$, the 1-loop heavy flavor corrections have been accounted for at next-to-leading order (NLO) QCD analysis [8]. The corresponding flavor non-singlet corrections in the unpolarized case were calculated for pure photon exchange to $O(\alpha_s^2)$ in [5,9] and in Ref. [10] to $O(\alpha_s^3)$.

In the present paper we calculate the $O(\alpha_s^3)$ massive flavor non-singlet Wilson coefficient for the inclusive structure function $g_1(x, Q^2)$ in the asymptotic region $Q^2 \gg m^2$, and also present the corresponding $O(\alpha_s^2)$ result, extending Refs. [6,7], in which the results in the non-inclusive tagged-flavor case were given.

The differential cross section for polarized deep-inelastic scattering [11–13] is given by

$$\frac{d^2\sigma_B}{dxdy} = \frac{2\pi\alpha^2}{Q^4} \lambda_N^p f^p S \left[S_1^p(x, y) g_1(x, Q^2) + S_2^p(x, y) g_2(x, Q^2) \right], \quad (1.1)$$

with

$$\begin{aligned} f^L &= 1, & f^T &= \cos(\beta - \varphi) \frac{d\varphi}{2\pi} \sqrt{\frac{4M^2x}{Sy}} \left[1 - y - \frac{M^2xy}{S} \right], \\ S_1^L &= 2xy \left[(2-y) - 2\frac{M^2}{S}xy \right], & S_1^T &= 2xy^2, \\ S_2^L &= -8x^2y \frac{M^2}{S}, & S_2^T &= 4xy. \end{aligned} \quad (1.2)$$

Here $\alpha = e^2/(4\pi)$ denotes the fine structure constant, M is the nucleon mass, $S = (p+l)^2$ is the center of mass energy of the lepton–nucleon system, with p and l the nucleon and lepton 4-momenta, respectively, $q = l - l'$ is the 4-momentum transfer and $Q^2 = -q^2$. $x = Q^2/(2p.q)$ and $y = p.q/p.l$ are the Bjorken variables. λ_N^p denotes the degree of the nucleon polarization. The spin 4-vectors in the longitudinal and transverse cases are given by

$$S_L = M(0, 0, 0; 1) \quad (1.3)$$

$$S_T = M(0, \cos(\beta), \sin(\beta); 0), \quad (1.4)$$

and φ denotes the angle between the vectors of the spin and the outgoing lepton. It contributes in a non-trivial way in the case of transverse polarization.

The polarized structure functions are denoted by $g_1(x, Q^2)$ and $g_2(x, Q^2)$. In the leading twist approximation, the heavy flavor contributions to the structure function $g_1(x, Q^2)$ is given by, cf. [14],

$$\begin{aligned} g_1(x, Q^2) &= \frac{1}{2} \left\{ \sum_{k=1}^{N_F} e_i^k \left\{ L_{q,g_1}^{\text{NS}} \left(x, N_F + 1, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) \right. \right. \\ &\quad \left. \left. \otimes \left[\Delta f_k(x, \mu^2, N_F) + \Delta f_{\bar{k}}(x, \mu^2, N_F) \right] \right\} \right\} \end{aligned}$$

¹ For an implementation in Mellin space, see [4].

$$\begin{aligned}
& + \frac{1}{N_F} L_{q,g_1}^{\text{PS}} \left(x, N_F + 1, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) \otimes \Delta \Sigma(x, \mu^2, N_F) \\
& + \frac{1}{N_F} L_{g,g_1}^{\text{S}} \left(x, N_F + 1, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) \otimes \Delta G(x, \mu^2, N_F) \Bigg\} \\
& + e_Q^2 \left[H_{q,g_1}^{\text{PS}} \left(x, N_F + 1, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) \otimes \Delta \Sigma(x, \mu^2, N_F) \right. \\
& \left. + H_{g,g_1}^{\text{PS}} \left(x, N_F + 1, \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) \otimes \Delta G(x, \mu^2, N_F) \right] \Bigg\}, \tag{1.5}
\end{aligned}$$

with $\Delta f_{k(\bar{k})}$ the N_F light flavor polarized (anti)quark densities, ΔG and $\Delta \Sigma = \sum_{l=1}^{N_F} [\Delta f_k + \Delta f_{\bar{k}}]$ the polarized gluon and singlet distributions, and e_i and e_Q the electric charges of the light quarks and the heavy quark Q , respectively. μ denotes the factorization scale and \otimes the Mellin convolution

$$A(x) \otimes B(x) = \int_0^1 dx_1 \int_0^1 dx_2 \delta(x - x_1 x_2) A(x_1) B(x_2). \tag{1.6}$$

The actual flavor non-singlet distribution is defined by

$$\Delta^{\text{NS}}(x, Q^2) = \sum_{k=1}^{N_F} e_k^2 \left[\Delta f_k(x, \mu^2, N_F) + \Delta f_{\bar{k}}(x, \mu^2, N_F) - \frac{1}{N_F} \Delta \Sigma(x, \mu^2, N_F) \right]. \tag{1.7}$$

However, according to the representation (1.5), we will consider its whole first term, depending on $L_{q,1}^{\text{NS}}$ as the non-singlet contribution in what follows. The structure function $g_2(x, Q^2)$ can be obtained from $g_1(x, Q^2)$ using the Wandzura–Wilson relation [15].

The paper is organized as follows. In Section 2 we calculate the heavy flavor contributions to the non-singlet Wilson coefficient in the asymptotic region $Q^2 \gg m^2$ to the structure function $g_1(x, Q^2)$ to 3-loop order in the strong coupling constant. We present the results both in Mellin N and x -space. Numerical results are given in Section 3. Consequences for the polarized Bjorken sum rule are discussed in Section 4, and Section 5 contains the conclusions.

2. The Wilson coefficient

The heavy flavor non-singlet Wilson coefficient contributing to the structure function $g_1(x, Q^2)$ in the asymptotic region $Q^2 \gg m^2$ receives its first contributions at $O(\alpha_s^2)$. In previous analyses [6,7] the tagged flavor case at $O(\alpha_s^2)$ has been considered. In what follows we will refer to the inclusive case, i.e. the complete contribution to the structure function $g_1(x, Q^2)$, and consider the terms due a single heavy quark.

The non-singlet heavy flavor Wilson coefficient contributing to the structure function $g_1(x, Q^2)$ in the asymptotic region $Q^2 \gg m^2$ is given by [16]

$$\begin{aligned}
L_{q,g_1}^{\text{h,NS}}(N_F + 1) \\
= \alpha_s^2 \left[A_{qq,Q}^{(2),\text{NS}}(N_F + 1) + \hat{C}_{q,g_1}^{(2),\text{NS}}(N_F) \right]
\end{aligned}$$

$$+ a_s^3 \left[A_{qq,Q}^{(3),\text{NS}}(N_F + 1) + A_{qq,Q}^{(2),\text{NS}}(N_F + 1) C_{q,g_1}^{(1),\text{NS}}(N_F + 1) + \hat{C}_{q,g_1}^{(3),\text{NS}}(N_F) \right]. \quad (2.1)$$

Here $A_{qq,Q}^{\text{NS}}$ is the massive non-singlet operator matrix element (OME) and the label ‘ $N_F + 1$ ’ symbolically denotes that the OME is calculated at N_F massless and one massive flavor, $a_s = \alpha_s/(4\pi) \equiv g_s^2/(4\pi)^2$ parameterizes the strong coupling constant, and we use the convention

$$\hat{f}(N_F) = f(N_F + 1) - f(N_F). \quad (2.2)$$

The calculation of the different contributions to the Wilson coefficient is performed in $D = 4 + \varepsilon$ dimensions to regulate the Feynman integrals. In the present polarized case the treatment of γ_5 has to be considered. In the flavor non-singlet case, both for the massive OMEs and the massless Wilson coefficients, γ_5 always appears in traces along one massless line and there is a Ward–Takahashi identity which implies the use of anti-commuting γ_5 . Usually the argument of the Ward–Takahashi identity is applied to relate the momentum derivative of the self-energy to the vertex function at zero-momentum insertion. Here we relate the latter to the former instead, isolating the γ_5 -effect on the vertex. In this way, it can be seen that the calculation is in the flavor non-singlet case the same as in the unpolarized case, leading effectively to anti-commuting γ_5 , see also Ref. [18].

The inclusive massive OME $A_{qq,Q}^{\text{NS}}$ to 3-loop order for even and odd moments N has been calculated in Ref. [10]. The corresponding diagrams have been reduced using integration-by-parts relations [17] applying an extension of the package `Reduze 2` [19].² The master integrals have been calculated using hypergeometric, Mellin–Barnes and differential equation techniques, mapping them to recurrences, which have been solved by modern summation technologies using extensively the packages `Sigma` [22,23], `EvaluateMultiSums`, `SumProduction` [24], `ρsum` [25], and `HarmonicSums` [26].

The massless Wilson coefficients $C_{q,g_1}(x, Q^2)$ from 1- to 3-loop order were calculated in Refs. [27–30]. At 3-loop order those of the structure function g_1 are obtained by that of F_3 [30], setting the d_{abc} terms in $\hat{C}_{q,g_1}^{(3),\text{NS}}(N_F)$ to zero, cf. also [31,32]. The non-singlet OMEs $A_{qq,Q}^{(k),\text{NS}}$ at 2- and 3-loop order were calculated in [5,9] and [10], respectively.

For comparison, the massless flavor non-singlet Wilson coefficient in Mellin space is given by [29,30]

$$L_{q,g_1}^{1,\text{NS}}(N_F) = 1 + \sum_{k=1}^3 a_s^k C_{q,g_1}^{(k),\text{NS}}(N_F). \quad (2.3)$$

In Mellin N space the Wilson coefficient can be expressed by nested harmonic sums $S_{\vec{a}}(N)$ [33] which are defined by

$$S_{b,\vec{a}}(N) = \sum_{k=1}^N \frac{(\text{sign}(b))^k}{k^{|b|}} S_{\vec{a}}(k), \quad S_\emptyset = 1, \quad b, a_i \in \mathbb{Z}, \quad b, a_i \neq 0, \quad N > 0, \quad N \in \mathbb{N}. \quad (2.4)$$

In the following, we drop the argument N of the harmonic sums and use the short-hand notation $S_{\vec{a}}(N) \equiv S_{\vec{a}}$. The Wilson coefficients depend on the logarithms

$$L_Q = \ln \left(\frac{Q^2}{\mu^2} \right) \quad \text{and} \quad L_M = \ln \left(\frac{m^2}{\mu^2} \right), \quad (2.5)$$

² The package `Reduze 2` uses the packages `Fermat` [20] and `Ginac` [21].

where the renormalization scale has been set equal to the factorization scale $\mu = \mu_R = \mu_F$.

As a short-hand notation we define the leading order splitting function $\Delta\gamma_{qq}^{(0)}$ up to its color factor

$$\Delta\gamma_{qq}^{(0)} = 4 \left[2S_1 - \frac{3N^2 + 3N + 2}{2N(N+1)} \right]. \quad (2.6)$$

The massive Wilson coefficient for the structure function $g_1(x, Q^2)$ in the asymptotic region in Mellin space in the on-shell scheme is given by

$$\begin{aligned} L_{q,g_1}^{\text{h,NS}}(N) = & \frac{1}{2} \left[1 - (-1)^N \right] \left\{ a_s^2 \mathbf{C}_F \mathbf{T}_F \left\{ -\frac{1}{3} [L_M^2 + L_Q^2] \Delta\gamma_{qq}^{(0)} \right. \right. \\ & + L_M \left[-\frac{2P_1}{9N^2(N+1)^2} - \frac{80}{9} S_1 + \frac{16}{3} S_2 \right] \\ & + L_Q \left[-\frac{2P_6}{9N^2(N+1)^2} + \frac{4(29N^2 + 29N - 6)}{9N(N+1)} S_1 + \frac{8}{3} S_1^2 - 8S_2 \right] + \frac{16}{3} S_{2,1} \\ & + \frac{P_{34}}{27N^3(N+1)^3} + \left(-\frac{2P_{11}}{27N^2(N+1)^2} + \frac{8}{3} S_2 \right) S_1 \\ & - \frac{2(29N^2 + 29N - 6)}{9N(N+1)} S_1^2 - \frac{8}{9} S_1^3 + \frac{2(35N^2 + 35N - 2)}{3N(N+1)} S_2 - \frac{112}{9} S_3 \Big\} \\ & + a_s^3 \left\{ \mathbf{C}_F^2 \mathbf{T}_F \left[\frac{1}{6} [L_Q^3 + L_M^2 L_Q] \Delta\gamma_{qq}^{(0)2} + L_M^2 \left[-\frac{2P_{28}}{3N^3(N+1)^3} - \frac{16}{3} S_1^3 \right. \right. \right. \\ & + \frac{2P_5}{3N^2(N+1)^2} S_1 - \frac{4(N-1)(N+2)}{N(N+1)} S_1^2 + \frac{64}{3} S_3 + \frac{64}{3} S_{-3} - \frac{128}{3} S_{-2,1} \\ & + \left(-\frac{64}{3N(N+1)} + \frac{128}{3} S_1 \right) S_{-2} + \frac{10}{3} \Delta\gamma_{qq}^{(0)} S_2 \Big] + L_Q^2 \left[-\frac{2P_{30}}{9N^3(N+1)^3} \right. \\ & + \frac{2P_{12}}{9N^2(N+1)^2} S_1 - \frac{4(107N^2 + 107N - 54)}{9N(N+1)} S_1^2 - 16S_1^3 + \frac{64}{3} [S_3 + S_{-3}] \\ & + \left(-\frac{64}{3N(N+1)} + \frac{128}{3} S_1 \right) S_{-2} - \frac{128}{3} S_{-2,1} + \frac{22}{3} \Delta\gamma_{qq}^{(0)} S_2 \Big] \\ & + L_M L_Q \Delta\gamma_{qq}^{(0)} \left[\frac{P_1}{9N^2(N+1)^2} + \frac{40}{9} S_1 - \frac{8}{3} S_2 \right] + L_M \left[\frac{P_{40}}{9N^4(N+1)^4} \right. \\ & + \left(\frac{2P_{31}}{9N^3(N+1)^3} + \frac{16(59N^2 + 59N - 6)}{9N(N+1)} S_2 - \frac{256}{3} S_3 - \frac{256}{3} S_{-2,1} \right) S_1 \\ & + \left(-\frac{4P_3}{3N^2(N+1)^2} + \frac{32}{3} S_2 \right) S_1^2 - \frac{160}{9} S_1^3 - \frac{4P_8}{9N^2(N+1)^2} S_2 - 32S_2^2 \\ & + \frac{32(29N^2 + 29N + 12)}{9N(N+1)} S_3 - \frac{256}{3} S_4 \\ & + \left(-\frac{64(16N^2 + 10N - 3)}{9N^2(N+1)^2} - \frac{128}{3} S_2 + \frac{1280}{9} S_1 \right) S_{-2} \Big\} \end{aligned}$$

$$\begin{aligned}
& + \left(\frac{64(10N^2 + 10N + 3)}{9N(N+1)} - \frac{128}{3}S_1 \right) S_{-3} - \frac{128}{3}S_{-4} \\
& + \frac{128}{3}S_{3,1} - \frac{128(10N^2 + 10N - 3)}{9N(N+1)}S_{-2,1} - \frac{128}{3}S_{-2,2} \\
& + \frac{512}{3}S_{-2,1,1} + 8\Delta\gamma_{qq}^{(0)}\zeta_3 \Big] \\
& + L_Q \left[\frac{4P_{48}}{27N^4(N+1)^4(N+2)^3} + \left(-\frac{4P_{36}}{27N^3(N+1)^3} + \frac{640}{9}S_3 \right. \right. \\
& - \frac{32(67N^2 + 67N - 21)}{9N(N+1)}S_2 + \frac{64}{3}S_{2,1} + \frac{512}{3}S_{-2,1} \Big) S_1 \\
& + \left(\frac{2P_{15}}{27N^2(N+1)^2} - \frac{224}{3}S_2 \right) S_1^2 \\
& + \frac{32(4N-1)(4N+5)}{9N(N+1)}S_1^3 + \frac{80}{9}S_1^4 + \frac{2P_{14}}{9N^2(N+1)^2}S_2 + 48S_2^2 \\
& - \frac{32(53N^2 + 53N + 16)}{9N(N+1)}S_3 + \frac{352}{3}S_4 + \left(-\frac{64P_{27}}{9(N-1)N^2(N+1)^2(N+2)} \right. \\
& - \frac{128(10N^2 + 10N - 3)}{9N(N+1)}S_1 - \frac{256}{3}S_1^2 + \frac{256}{3}S_2 \Big) S_{-2} + 64S_{-2}^2 + \frac{448}{3}S_{-4} \\
& + \left(-\frac{64(10N^2 + 10N + 9)}{9N(N+1)} + \frac{256}{3}S_1 \right) S_{-3} + \frac{16(9N^2 + 9N - 2)}{3N(N+1)}S_{2,1} \\
& + 64S_{3,1} + \frac{128(10N^2 + 10N - 3)}{9N(N+1)}S_{-2,1} - \frac{256}{3}S_{-3,1} - 64S_{2,1,1} \\
& - \frac{512}{3}S_{-2,1,1} + \left(-\frac{16(9N^2 + 9N - 2)}{N(N+1)} + 64S_1 \right) \zeta_3 \Big] + \frac{P_{46}}{162N^5(N+1)^5} \\
& - \frac{128(112N^3 + 112N^2 - 39N + 18)}{81N^2(N+1)}S_{-2,1} + \left(\frac{P_{45}}{162N^4(N+1)^4} - \frac{64}{9}S_2^2 \right. \\
& + \frac{8P_{16}}{81N^2(N+1)^2}S_2 - \frac{8(347N^2 + 347N + 54)}{27N(N+1)}S_3 + \frac{128}{9N(N+1)}S_{2,1} \\
& + \frac{704}{9}S_4 - \frac{320}{9}S_{3,1} - \frac{256(10N^2 + 10N - 3)}{27N(N+1)}S_{-2,1} + \frac{1024}{9}S_{-2,1,1} \\
& - \frac{256}{9}S_{-2,2} \Big) S_1 + \left(\frac{P_{25}}{9N^3(N+1)^3} + \frac{16(5N^2 + 5N - 4)}{9N(N+1)}S_2 - \frac{128}{9}S_{2,1} \right. \\
& + 16S_3 - \frac{256}{9}S_{-2,1} \Big) S_1^2 + \left(-\frac{16P_4}{27N^2(N+1)^2} + \frac{128}{27}S_2 \right) S_1^3 + \left(\frac{400}{27}S_3 \right. \\
& + \frac{P_{24}}{81N^3(N+1)^3} + \frac{256}{3}S_{-2,1} \Big) S_2 - \frac{32(23N^2 + 23N - 3)}{27N(N+1)}S_2^2 + \frac{512}{9}S_5 \\
& + \frac{8P_{17}}{81N^2(N+1)^2}S_3 - \frac{176(17N^2 + 17N + 6)}{27N(N+1)}S_4 + \left(-\frac{64P_9}{81N^3(N+1)^3} \right.
\end{aligned}$$

$$\begin{aligned}
& + \frac{128P_7}{81N^2(N+1)^2}S_1 - \frac{128}{9N(N+1)}S_1^2 + \frac{256}{27}S_1^3 - \frac{1280}{27}S_2 + \frac{512}{27}S_3 \\
& - \frac{512}{9}S_{2,1}\Big)S_{-2} + \left(\frac{64(112N^3 + 224N^2 + 169N + 39)}{81N(N+1)^2} + \frac{128}{9}S_1^2\right. \\
& + \frac{128}{9}S_2 - \frac{128(10N^2 + 10N + 3)}{27N(N+1)}S_1\Big)S_{-3} + \left(-\frac{128(10N^2 + 10N + 3)}{27N(N+1)}\right. \\
& + \frac{256}{9}S_1\Big)S_{-4} + \frac{256}{9}S_{-5} + \frac{16P_2}{9N^2(N+1)^2}S_{2,1} + \frac{256}{9}S_{2,3} - \frac{512}{9}S_{2,-3} \\
& + \frac{16(89N^2 + 89N + 30)}{27N(N+1)}S_{3,1} - \frac{512}{9}S_{4,1} - \frac{128(10N^2 + 10N - 3)}{27N(N+1)}S_{-2,2,2} \\
& + \frac{512}{9}S_{-2,3} + \frac{512}{9}S_{2,1,-2} + \frac{256}{9}S_{3,1,1} + \frac{512(10N^2 + 10N - 3)}{27N(N+1)}S_{-2,1,1} \\
& + \frac{512}{9}S_{-2,2,1} - \frac{2048}{9}S_{-2,1,1,1} + \frac{16(2N^3 + 2N^2 + 2N + 1)}{3N^3(N+1)^3}\zeta_2 \\
& + \left(-\frac{64}{3}S_2 + \frac{2P_{13}}{9N^2(N+1)^2} - \frac{1208}{9}S_1\right)\zeta_3 \\
& + \left(\frac{8}{3}S_{2,1,1} - \frac{8}{3}B_4 + 12\zeta_4\right)\Delta\gamma_{qq}^{(0)} \\
& + (-1)^N \left(-L_M^2 \frac{64}{3(N+1)^3} - L_Q^2 \frac{64}{3(N+1)^3} + L_M \left[-\frac{256(4N+1)}{9(N+1)^4} \right. \right. \\
& \left. \left. + \frac{128}{3(N+1)^3}S_1 \right] + L_Q \frac{64P_{39}}{9(N-1)N^2(N+1)^4(N+2)^3} + \frac{16P_{41}}{81N^5(N+1)^5} \right. \\
& \left. - \frac{32P_{26}}{27N^4(N+1)^4}S_1 + \frac{64(2N^2 + 2N + 1)}{9N^3(N+1)^3}S_1^2 + \frac{64(2N^2 + 2N + 1)}{9N^3(N+1)^3}S_2 \right. \\
& \left. + \frac{16(2N^3 + 2N^2 + 2N + 1)}{3N^3(N+1)^3}\zeta_2 \right) \\
& + \textcolor{blue}{C_A C_F T_F} \left[L_M^3 \frac{22}{27} \Delta\gamma_{qq}^{(0)} + L_Q^3 \frac{44}{27} \Delta\gamma_{qq}^{(0)} \right. \\
& + L_M^2 \left[\frac{2P_{21}}{9N^3(N+1)^2} - \frac{184}{9}S_1 \right. \\
& \left. + \left(\frac{32}{3N(N+1)} - \frac{64}{3}S_1 \right)S_{-2} - \frac{32}{3}[S_3 + S_{-3}] \right. \\
& \left. + \frac{64}{3}S_{-2,1} \right] + L_Q^2 \left[\frac{2P_{23}}{27N^3(N+1)^2} - \frac{16(194N^2 + 194N - 33)}{27N(N+1)}S_1 \right. \\
& \left. - \frac{176}{9}S_1^2 + \frac{176}{3}S_2 - \frac{32}{3}S_3 \right. \\
& \left. + \left(\frac{32}{3N(N+1)} - \frac{64}{3}S_1 \right)S_{-2} - \frac{32}{3}S_{-3} + \frac{64}{3}S_{-2,1} \right]
\end{aligned}$$

$$\begin{aligned}
& + L_M \left[\frac{P_{38}}{81N^4(N+1)^3} + \left(-\frac{8P_{29}}{81N^3(N+1)^3} + 32S_3 + \frac{128}{3}S_{-2,1} \right) S_1 \right. \\
& + \frac{1792}{27}S_2 - \frac{16(31N^2 + 31N + 9)}{9N(N+1)}S_3 + \frac{160}{3}S_4 + \left(\frac{32(16N^2 + 10N - 3)}{9N^2(N+1)^2} \right. \\
& \left. - \frac{640}{9}S_1 + \frac{64}{3}S_2 \right) S_{-2} + \left(-\frac{32(10N^2 + 10N + 3)}{9N(N+1)} + \frac{64}{3}S_1 \right) S_{-3} \\
& + \frac{64}{3}S_{-4} - \frac{128}{3}S_{3,1} + \frac{64(10N^2 + 10N - 3)}{9N(N+1)}S_{-2,1} \\
& \left. + \frac{64}{3}S_{-2,2} - \frac{256}{3}S_{-2,1,1} - 8\Delta\gamma_{qq}^{(0)}\zeta_3 \right] \\
& + L_Q \left[-\frac{16(230N^3 + 460N^2 + 213N - 11)}{9N(N+1)^2}S_2 - \frac{4P_{49}}{81N^4(N+1)^4(N+2)^3} \right. \\
& + \left(\frac{4P_{37}}{81N^3(N+1)^3} - \frac{32(11N^2 + 11N + 3)}{9N(N+1)}S_2 - \frac{128}{3}S_{2,1} - \frac{256}{3}S_{-2,1} \right. \\
& \left. + 32S_3 \right) S_1 + \left(\frac{16(194N^2 + 194N - 33)}{27N(N+1)} + \frac{32}{3}S_2 \right) S_1^2 + \frac{352}{27}S_1^3 - \frac{32}{3}S_2^2 \\
& + \frac{16(368N^2 + 368N - 9)}{27N(N+1)}S_3 - \frac{224}{3}S_4 + \left(\frac{32P_{27}}{9(N-1)N^2(N+1)^2(N+2)} \right. \\
& \left. + \frac{64(10N^2 + 10N - 3)}{9N(N+1)}S_1 + \frac{128}{3}S_1^2 - \frac{128}{3}S_2 \right) S_{-2} - 32S_{-2}^2 \\
& + \left(-\frac{128}{3}S_1 + \frac{32(10N^2 + 10N + 9)}{9N(N+1)} \right) S_{-3} - \frac{224}{3}S_{-4} \\
& - \frac{64(11N^2 + 11N - 3)}{9N(N+1)}S_{2,1} - \frac{64}{3}S_{3,1} - \frac{64(10N^2 + 10N - 3)}{9N(N+1)}S_{-2,1} \\
& + \frac{128}{3}S_{-3,1} + 64S_{2,1,1} + \frac{256}{3}S_{-2,1,1} \\
& \left. + \left(96 - 64S_1 \right) \zeta_3 \right] + \frac{64(112N^3 + 112N^2 - 39N + 18)}{81N^2(N+1)}S_{-2,1} \\
& + \frac{P_{47}}{729N^5(N+1)^5} + \left(-\frac{16(N-1)(2N^3 - N^2 - N - 2)}{9N^2(N+1)^2}S_2 + \frac{112}{9}S_2^2 \right. \\
& - \frac{4P_{44}}{729N^4(N+1)^4} + \frac{80(2N+1)^2}{9N(N+1)}S_3 - \frac{208}{9}S_4 - \frac{8(9N^2 + 9N + 16)}{9N(N+1)}S_{2,1} \\
& + \frac{64}{3}S_{3,1} + \frac{128(10N^2 + 10N - 3)}{27N(N+1)}S_{-2,1} + \frac{128}{9}S_{-2,2} - \frac{512}{9}S_{-2,1,1} \Big) S_1 \\
& + \left(\frac{4P_{18}}{9N^3(N+1)^3} + \frac{32}{9N(N+1)}S_2 - \frac{80}{9}S_3 + \frac{128}{9}S_{2,1} + \frac{128}{9}S_{-2,1} \right) S_1^2 \\
& + \left(\frac{4P_{35}}{81N^3(N+1)^3} + \frac{496}{27}S_3 - \frac{64}{3}S_{2,1} - \frac{128}{3}S_{-2,1} \right) S_2 - \frac{64}{27}S_1^3 S_2
\end{aligned}$$

$$\begin{aligned}
& - \frac{4(15N^2 + 15N + 14)}{9N(N+1)} S_2^2 - \frac{8P_{20}}{81N^2(N+1)^2} S_3 \\
& + \frac{4(443N^2 + 443N + 78)}{27N(N+1)} S_4 - \frac{224}{9} S_5 \\
& + \left(\frac{32P_9}{81N^3(N+1)^3} - \frac{64P_7}{81N^2(N+1)^2} S_1 + \frac{64}{9N(N+1)} S_1^2 - \frac{128}{27} S_1^3 \right. \\
& + \frac{640}{27} S_2 - \frac{256}{27} S_3 + \frac{256}{9} S_{2,1} \Big) S_{-2} \\
& + \left(-\frac{32(112N^3 + 224N^2 + 169N + 39)}{81N(N+1)^2} \right. \\
& + \frac{64(10N^2 + 10N + 3)}{27N(N+1)} S_1 - \frac{64}{9} S_1^2 - \frac{64}{9} S_2 \Big) S_{-3} \\
& + \left(\frac{64(10N^2 + 10N + 3)}{27N(N+1)} - \frac{128}{9} S_1 \right) S_{-4} \\
& - \frac{128}{9} S_{-5} - \frac{8P_{19}}{9N^2(N+1)^2} S_{2,1} - \frac{8(13N+4)(13N+9)}{27N(N+1)} S_{3,1} \\
& + \frac{256}{9} [S_{2,-3} + S_{4,1} - S_{-2,3} - S_{2,1,-2} - S_{3,1,1} - S_{-2,2,1}] - \frac{128}{3} S_{2,3} \\
& + \frac{64}{3} S_{2,2,1} + \frac{64(10N^2 + 10N - 3)}{27N(N+1)} S_{-2,2} - \frac{256(10N^2 + 10N - 3)}{27N(N+1)} S_{-2,1,1} \\
& + \frac{224}{9} S_{2,1,1,1} + \frac{1024}{9} S_{-2,1,1,1} - \frac{8(2N^3 + 2N^2 + 2N + 1)}{3N^3(N+1)^3} \zeta_2 \\
& + \left(\frac{P_{22}}{27N^2(N+1)^2} + \frac{4(593N^2 + 593N + 108)}{27N(N+1)} S_1 - 16S_1^2 + 16S_2 \right) \zeta_3 \\
& + \left(\frac{4B_4}{3} - 4S_{2,1,1} - 12\zeta_4 \right) \Delta\gamma_{qq}^{(0)} \\
& + (-1)^N \left(L_M^2 \frac{32}{3(N+1)^3} + L_Q^2 \frac{32}{3(N+1)^3} \right. \\
& + L_M \left[\frac{128(4N+1)}{9(N+1)^4} - \frac{64}{3(N+1)^3} S_1 \right] \\
& - L_Q \frac{32P_{39}}{9(N-1)N^2(N+1)^4(N+2)^3} \\
& - \frac{8P_{41}}{81N^5(N+1)^5} + \frac{16P_{26}}{27N^4(N+1)^4} S_1 - \frac{32(2N^2 + 2N + 1)}{9N^3(N+1)^3} [S_1^2 + S_2] \\
& \left. - \frac{8(2N^3 + 2N^2 + 2N + 1)}{3N^3(N+1)^3} \zeta_2 \right) \\
& + \textcolor{blue}{C_F T_F^2} \left[-L_M^3 \frac{16}{27} \Delta\gamma_{qq}^{(0)} - L_Q^3 \frac{8}{27} \Delta\gamma_{qq}^{(0)} \right]
\end{aligned}$$

$$\begin{aligned}
& + L_M^2 \left[-\frac{8P_1}{27N^2(N+1)^2} - \frac{320}{27}S_1 + \frac{64}{9}S_2 \right] \\
& + L_Q^2 \left[\frac{16(29N^2 + 29N - 6)}{27N(N+1)} S_1 \right. \\
& \quad \left. - \frac{8P_6}{27N^2(N+1)^2} + \frac{32}{9}S_1^2 - \frac{32}{3}S_2 \right] - L_M \frac{248}{81} \Delta \gamma_{qq}^{(0)} \\
& + L_Q \left[\frac{8P_{33}}{81N^3(N+1)^3} \right. \\
& \quad \left. + \left(-\frac{16P_{10}}{81N^2(N+1)^2} + \frac{64}{9}S_2 \right) S_1 - \frac{16(29N^2 + 29N - 6)}{27N(N+1)} S_1^2 - \frac{64}{27}S_1^3 \right. \\
& \quad \left. + \frac{16(35N^2 + 35N - 2)}{9N(N+1)} S_2 - \frac{896}{27}S_3 + \frac{128}{9}S_{2,1} \right] \\
& - \frac{2P_{43}}{729N^4(N+1)^4} + \frac{64}{81}S_2 + \frac{12064}{729}S_1 + \frac{320}{81}S_3 \\
& \quad \left. - \frac{64}{27}S_4 - \frac{112}{27} \Delta \gamma_{qq}^{(0)} \zeta_3 \right] + \textcolor{blue}{C_F} \textcolor{blue}{N_F} \textcolor{blue}{T_F^2} \left[-L_M^3 \frac{8}{27} \Delta \gamma_{qq}^{(0)} \right. \\
& \quad \left. - L_Q^3 \frac{16}{27} \Delta \gamma_{qq}^{(0)} + L_M \left[\frac{4P_{32}}{81N^3(N+1)^3} - \frac{2176}{81}S_1 - \frac{320}{27}S_2 + \frac{64}{9}S_3 \right] \right. \\
& \quad \left. + L_Q^2 \left[-\frac{16P_6}{27N^2(N+1)^2} + \frac{32(29N^2 + 29N - 6)}{27N(N+1)} S_1 + \frac{64}{9}S_1^2 - \frac{64}{3}S_2 \right] \right. \\
& \quad \left. + L_Q \left[\left(-\frac{32P_{10}}{81N^2(N+1)^2} + \frac{128}{9}S_2 \right) S_1 \right. \right. \\
& \quad \left. \left. - \frac{32(29N^2 + 29N - 6)}{27N(N+1)} S_1^2 - \frac{128}{27}S_1^3 \right. \right. \\
& \quad \left. \left. + \frac{16P_{33}}{81N^3(N+1)^3} + \frac{32(35N^2 + 35N - 2)}{9N(N+1)} S_2 - \frac{1792}{27}S_3 + \frac{256}{9}S_{2,1} \right] \right. \\
& \quad \left. + \frac{4P_{42}}{729N^4(N+1)^4} - \frac{24064}{729}S_1 + \frac{128}{81}S_2 + \frac{640}{81}S_3 - \frac{128}{27}S_4 + \frac{64}{27} \Delta \gamma_{qq}^{(0)} \zeta_3 \right] \\
& \quad \left. + \hat{C}_{q,g_1}^{\text{NS},(3)}(N_F) \right\} . \tag{2.7}
\end{aligned}$$

Here the color factors are given by $C_A = N_c$, $C_F = (N_c^2 - 1)/(2N_c)$, $T_F = 1/2$ in $SU(N_c)$, and $N_c = 3$ in the case of Quantum Chromodynamics. $\hat{C}_{q,g_1}^{\text{NS},(3)}(N_F)$ denotes the massless Wilson coefficient at 3-loop order, cf. (2.2), and the polynomials P_i are given by

$$P_1 = -3N^4 - 6N^3 - 47N^2 - 20N + 12 \tag{2.8}$$

$$P_2 = 7N^4 + 14N^3 + 3N^2 - 4N - 4 \tag{2.9}$$

$$P_3 = 19N^4 + 38N^3 - 9N^2 - 20N + 4 \tag{2.10}$$

$$P_4 = 28N^4 + 56N^3 + 28N^2 + 2N + 1 \tag{2.11}$$

$$P_5 = 33N^4 + 54N^3 + 9N^2 - 52N - 28 \quad (2.12)$$

$$P_6 = 57N^4 + 96N^3 + 65N^2 - 10N - 24 \quad (2.13)$$

$$P_7 = 112N^4 + 224N^3 + 121N^2 + 9N + 9 \quad (2.14)$$

$$P_8 = 141N^4 + 246N^3 + 241N^2 - 8N - 84 \quad (2.15)$$

$$P_9 = 181N^4 + 266N^3 + 82N^2 - 3N + 18 \quad (2.16)$$

$$P_{10} = 235N^4 + 524N^3 + 211N^2 + 30N + 72 \quad (2.17)$$

$$P_{11} = 359N^4 + 772N^3 + 335N^2 + 30N + 72 \quad (2.18)$$

$$P_{12} = 501N^4 + 894N^3 + 541N^2 - 116N - 204 \quad (2.19)$$

$$P_{13} = 561N^4 + 1122N^3 + 767N^2 + 302N + 48 \quad (2.20)$$

$$P_{14} = 1131N^4 + 2118N^3 + 1307N^2 + 32N - 276 \quad (2.21)$$

$$P_{15} = 1139N^4 + 2710N^3 + 635N^2 + 216N + 828 \quad (2.22)$$

$$P_{16} = 1199N^4 + 2398N^3 + 1181N^2 + 18N + 90 \quad (2.23)$$

$$P_{17} = 1220N^4 + 2359N^3 + 1934N^2 + 357N - 138 \quad (2.24)$$

$$P_{18} = 3N^5 + 11N^4 + 10N^3 + 3N^2 + 7N + 8 \quad (2.25)$$

$$P_{19} = 12N^5 + 16N^4 + 18N^3 - 15N^2 - 5N - 8 \quad (2.26)$$

$$P_{20} = 27N^5 + 863N^4 + 1573N^3 + 1151N^2 + 144N - 36 \quad (2.27)$$

$$P_{21} = 51N^5 + 102N^4 + 121N^3 + 118N^2 + 48N + 48 \quad (2.28)$$

$$P_{22} = 648N^5 - 2103N^4 - 4278N^3 - 3505N^2 - 682N - 432 \quad (2.29)$$

$$P_{23} = 1407N^5 + 2418N^4 + 1793N^3 + 134N^2 - 384N + 144 \quad (2.30)$$

$$P_{24} = -11\,145N^6 - 32\,355N^5 - 37\,523N^4 - 14\,329N^3 + 2392N^2 + 120N - 1512 \quad (2.31)$$

$$P_{25} = -151N^6 - 469N^5 - 181N^4 + 305N^3 + 208N^2 + 40N + 8 \quad (2.32)$$

$$P_{26} = 3N^6 + 9N^5 + 70N^4 + 77N^3 + 39N^2 - 10N - 12 \quad (2.33)$$

$$P_{27} = 6N^6 + 18N^5 - N^4 - 20N^3 + 46N^2 + 29N - 6 \quad (2.34)$$

$$P_{28} = 15N^6 + 36N^5 + 30N^4 + 8N^3 + 3N^2 + 16N + 20 \quad (2.35)$$

$$P_{29} = 155N^6 + 465N^5 + 465N^4 + 371N^3 + 108N^2 + 108N + 54 \quad (2.36)$$

$$P_{30} = 216N^6 + 567N^5 + 687N^4 + 381N^3 + 37N^2 - 44N + 12 \quad (2.37)$$

$$P_{31} = 309N^6 + 807N^5 + 693N^4 - 271N^3 - 638N^2 + 68N + 216 \quad (2.38)$$

$$P_{32} = 525N^6 + 1575N^5 + 1535N^4 + 973N^3 + 536N^2 + 48N - 72 \quad (2.39)$$

$$P_{33} = 609N^6 + 1485N^5 + 1393N^4 + 83N^3 - 422N^2 + 156N + 216 \quad (2.40)$$

$$P_{34} = 795N^6 + 2043N^5 + 2075N^4 + 517N^3 - 298N^2 + 156N + 216 \quad (2.41)$$

$$P_{35} = 868N^6 + 2469N^5 + 2487N^4 + 940N^3 + 27N^2 + 63N + 72 \quad (2.42)$$

$$P_{36} = 1770N^6 + 4671N^5 + 4765N^4 + 1205N^3 - 227N^2 + 1044N + 756 \quad (2.43)$$

$$P_{37} = 7531N^6 + 23\,673N^5 + 23\,055N^4 + 7375N^3 + 1614N^2 + 936N - 324 \quad (2.44)$$

$$\begin{aligned} P_{38} = & -4785N^7 - 14355N^6 - 4399N^5 + 10327N^4 + 3548N^3 + 3000N^2 \\ & + 1080N - 1728 \end{aligned} \quad (2.45)$$

$$P_{39} = 25N^7 + 138N^6 + 311N^5 + 464N^4 + 672N^3 + 670N^2 + 264N + 48 \quad (2.46)$$

$$\begin{aligned} P_{40} = & -45N^8 - 162N^7 - 858N^6 - 1960N^5 - 1885N^4 - 1094N^3 - 804N^2 \\ & - 40N + 192 \end{aligned} \quad (2.47)$$

$$\begin{aligned} P_{41} = & 39N^8 + 138N^7 + 847N^6 + 1371N^5 + 1283N^4 + 485N^3 + 101N^2 \\ & + 132N + 72 \end{aligned} \quad (2.48)$$

$$\begin{aligned} P_{42} = & 3549N^8 + 14196N^7 + 23870N^6 + 25380N^5 + 15165N^4 + 1712N^3 - 2016N^2 \\ & + 144N + 432 \end{aligned} \quad (2.49)$$

$$\begin{aligned} P_{43} = & 5487N^8 + 21948N^7 + 36370N^6 + 28836N^5 + 11943N^4 + 4312N^3 + 2016N^2 \\ & - 144N - 432 \end{aligned} \quad (2.50)$$

$$\begin{aligned} P_{44} = & 10807N^8 + 43228N^7 + 62898N^6 + 39178N^5 + 7027N^4 + 702N^3 + 3240N^2 \\ & + 3456N + 1620 \end{aligned} \quad (2.51)$$

$$\begin{aligned} P_{45} = & 42591N^8 + 166764N^7 + 245088N^6 + 128254N^5 - 26735N^4 - 40762N^3 \\ & - 3928N^2 - 1272N - 2160 \end{aligned} \quad (2.52)$$

$$\begin{aligned} P_{46} = & -18351N^{10} - 89784N^9 - 208773N^8 - 267222N^7 - 192265N^6 - 46700N^5 \\ & + 14565N^4 + 7730N^3 + 1240N^2 + 1464N + 144 \end{aligned} \quad (2.53)$$

$$\begin{aligned} P_{47} = & 165N^{10} + 825N^9 + 106856N^8 + 321746N^7 + 396657N^6 + 247433N^5 \\ & + 126914N^4 + 51804N^3 + 6336N^2 + 4752N + 5184 \end{aligned} \quad (2.54)$$

$$\begin{aligned} P_{48} = & 828N^{11} + 7632N^{10} + 29217N^9 + 59592N^8 + 66844N^7 + 35738N^6 + 7405N^5 \\ & + 16688N^4 + 27880N^3 + 11552N^2 - 3312N - 2304 \end{aligned} \quad (2.55)$$

$$\begin{aligned} P_{49} = & 8274N^{11} + 78519N^{10} + 313841N^9 + 686295N^8 + 881001N^7 + 638778N^6 \\ & + 204948N^5 + 7992N^4 + 32296N^3 + 26544N^2 - 10656N - 8640. \end{aligned} \quad (2.56)$$

We would like to note that we disagree with the $O(a_s^2 \ln(Q^2/\mu^2))$ terms given in [29], but agree with the representation in [30,52].

One obtains the analytic continuation of the harmonic sums to complex values of N by performing their asymptotic expansion analytically, cf. [34,35].³ Furthermore, the nested harmonic sums obey the shift relations

$$S_{b,\vec{a}}(N) = S_{b,\vec{a}}(N-1) + \frac{\text{sign}(b)^N}{N^{|b|}} S_{\vec{a}}(N), \quad (2.57)$$

through which any regular point in the complex plane can be reached using the analytic asymptotic representation as input. The poles of the nested harmonic sums $S_{\vec{a}}(N)$ are located at the non-positive integers. In data analyses, one may thus encode the QCD evolution [36] together with the Wilson coefficient for complex values of N analytically and finally perform one numerical contour integral around the singularities of the problem.⁴

³ These expansions can now be obtained automatically using the package `HarmonicSums` [26].

⁴ For precise numerical implementations of the analytic continuation of harmonic sums see [37].

In x -space the Wilson coefficient is represented in terms of harmonic polylogarithms [38] over the alphabet $\{f_0, f_1, f_{-1}\}$, which were again reduced applying the shuffle relations [39]. They are defined by

$$H_{b,\tilde{a}}(x) = \int_0^x dy f_b(y) H_{\tilde{a}}(y), \quad \underbrace{H_{0,\dots,0}}_k(x) = \frac{1}{k!} \ln^k(x), \quad H_\emptyset = 1, \quad (2.58)$$

$$f_0(x) = \frac{1}{x}, \quad f_1(x) = \frac{1}{1-x}, \quad f_{-1}(x) = \frac{1}{1+x}. \quad (2.59)$$

The Wilson coefficient is represented by three contributions, the $(\dots)_+$ -function term, the $\delta(1-x)$ -term, and the regular term. Here the $+$ -distribution is defined by

$$\int_0^1 dy [F(y)]_+ g(y) = \int_0^1 dy F(y) [g(y) - g(1)]. \quad (2.60)$$

One obtains

$$\begin{aligned} L_{q,g_1}^{\text{NS}}(x) = & a_s^2 \left\{ \left(\frac{1}{1-x} \mathcal{C}_F \mathcal{T}_F \left[\frac{8}{3} \left[L_Q^2 + L_M^2 \right] + L_M \left[\frac{80}{9} + \frac{16}{3} H_0 \right] \right. \right. \right. \\ & + L_Q \left[-\frac{116}{9} - \frac{32}{3} H_0 - \frac{16}{3} H_1 \right] + \frac{718}{27} + \frac{268}{9} H_0 + 8 H_0^2 \\ & \left. \left. \left. + \left(\frac{116}{9} + \frac{16}{3} H_0 \right) H_1 + \frac{8}{3} H_1^2 + \frac{16}{3} H_{0,1} - \frac{32}{3} \zeta_2 \right] \right) \right)_+ \\ & + \delta(1-x) \left(\mathcal{C}_F \mathcal{T}_F \left[2 \left[L_M^2 + L_Q^2 \right] + L_M \frac{2}{3} - L_Q \frac{38}{3} + \frac{265}{9} \right] \right) \\ & + \mathcal{C}_F \mathcal{T}_F \left[-\frac{4}{3} (x+1) \left[L_Q^2 + L_M^2 \right] + L_M \left[-\frac{8}{9} (11x-1) - \frac{8}{3} (x+1) H_0 \right] \right. \\ & + L_Q \left[\frac{8}{9} (14x+5) + \frac{16}{3} (x+1) H_0 + \frac{8}{3} (x+1) H_1 \right] - \frac{4}{27} (218x+47) \\ & - \frac{8}{9} (28x+13) H_0 - 4(x+1) H_0^2 + \left(-\frac{8}{9} (14x+5) - \frac{8}{3} (x+1) H_0 \right) H_1 \\ & \left. \left. - \frac{4}{3} (x+1) H_1^2 - \frac{8}{3} (x+1) H_{0,1} + \frac{16}{3} (x+1) \zeta_2 \right] \right\} \\ & + a_s^3 \left\{ \left(\frac{1}{(1-x)^2} \mathcal{C}_A \mathcal{C}_F \mathcal{T}_F \left[-\frac{4}{81} (800x-773) H_0^2 + \frac{32}{81} (94x-121) \zeta_2 \right. \right. \right. \\ & + \frac{32}{9} (x+2) H_{0,1} \left. \right] + \frac{1}{1-x} \left(\mathcal{C}_A \mathcal{C}_F \mathcal{T}_F \left[-L_M^3 \frac{176}{27} - L_Q^3 \frac{352}{27} \right. \right. \\ & \left. \left. + L_M^2 \left[\frac{184}{9} + \frac{16}{3} H_0^2 - \frac{32}{3} \zeta_2 \right] \right] \right) \right\} \end{aligned}$$

$$\begin{aligned}
& + L_Q^2 \left[\frac{3104}{27} + \frac{704}{9} H_0 + \frac{16}{3} H_0^2 + \frac{352}{9} H_1 - \frac{32}{3} \zeta_2 \right] \\
& + L_M \left[\frac{1240}{81} + \frac{1792}{27} H_0 + \frac{248}{9} H_0^2 + \frac{32}{9} H_0^3 \right. \\
& \quad \left. - 16 H_0^2 H_1 + 32 H_0 H_{0,1} - \frac{64}{3} H_{0,0,1} \right. \\
& \quad \left. + \left(-\frac{320}{9} - \frac{64}{3} H_0 \right) \zeta_2 + 96 \zeta_3 \right] \\
& + L_Q \left[-\frac{80}{9} H_0^3 - \frac{30124}{81} - \frac{14144}{27} H_0 - \frac{1216}{9} H_0^2 \right. \\
& \quad \left. + \left(-\frac{6208}{27} - \frac{704}{9} H_0 - \frac{16}{3} H_0^2 \right) H_1 \right. \\
& \quad \left. + \left(-\frac{352}{9} + \frac{32}{3} H_0 \right) H_1^2 - 64 H_0 H_{0,-1} \right. \\
& \quad \left. + \left(-\frac{704}{9} + \frac{32}{3} H_0 - \frac{128}{3} H_1 \right) H_{0,1} - \frac{128}{3} H_{0,0,1} + 128 H_{0,0,-1} + 64 H_{0,1,1} \right. \\
& \quad \left. + \left(192 + \frac{128}{3} H_0 + 64 H_1 \right) \zeta_2 - \frac{256}{3} \zeta_3 \right] \\
& + \frac{43228}{729} + \frac{3256}{81} H_0 + \frac{496}{81} H_0^3 + \frac{16}{27} H_0^4 \\
& + \left(\frac{32}{3} - \frac{32}{9} H_0 - \frac{160}{9} H_0^2 - \frac{112}{27} H_0^3 \right) H_1 \\
& + \frac{8}{9} H_0^2 H_1^2 - \frac{64}{27} H_0 H_1^3 \\
& + \left(\frac{368}{9} H_0 + \frac{16}{3} H_0^2 + \left(-8 - \frac{128}{9} H_0 \right) H_1 + \frac{128}{9} H_1^2 \right) H_{0,1} \\
& - \frac{32}{9} H_{0,1}^2 + \left(-\frac{1072}{27} + \frac{32}{9} H_0 + \frac{320}{9} H_1 \right) H_{0,0,1} \\
& + \frac{224}{9} [H_{0,1,1,1} - H_{0,0,1,1}] + \left(\frac{160}{9} H_0 - 32 H_1 + 24 \right) H_{0,1,1} \\
& + \left(-\frac{496}{27} H_0 - \frac{112}{9} H_0^2 + \left(8 - \frac{160}{9} H_0 \right) H_1 - \frac{128}{9} H_1^2 + \frac{32}{9} H_{0,1} \right) \zeta_2 \\
& + \left(-\frac{1196}{27} + \frac{160}{9} H_0 - \frac{32}{9} H_1 \right) \zeta_3 + \frac{296}{3} \zeta_4 - \frac{32}{3} B_4 \\
& + \textcolor{blue}{C_F^2 T_F} \left[L_Q^3 \left[16 - \frac{32}{3} H_0 - \frac{64}{3} H_1 \right] \right. \\
& + L_M^2 L_Q \left[16 - \frac{32}{3} H_0 - \frac{64}{3} H_1 \right] + L_M^2 \left[-22 - 16 H_0 + \left(8 + \frac{128}{3} H_0 \right) H_1 \right. \\
& \quad \left. + \frac{16}{3} H_0^2 + 16 H_1^2 - \frac{64}{3} \zeta_2 \right] + L_Q^2 \left[-\frac{334}{3} + \frac{32}{9} H_0 + \left(\frac{856}{9} + \frac{320}{3} H_0 \right) H_1 \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{80}{3}H_0^2 + 48H_1^2 - \frac{256}{3}\zeta_2 \Big] + L_M L_Q \left[\frac{88}{3} - \frac{176}{9}H_0 \right. \\
& + \left(-\frac{640}{9} - \frac{64}{3}H_0 \right) H_1 - \frac{32}{3}H_0^2 + \frac{64}{3}\zeta_2 \Big] \\
& + L_M \left[-\frac{206}{3} - \frac{112}{3}H_0 + \frac{88}{9}H_0^2 + \left(\frac{160}{3} + \frac{32}{3}H_0 \right) H_1^2 \right. \\
& + \frac{64}{9}H_0^3 + \left(\frac{152}{3} + \frac{1424}{9}H_0 + \frac{160}{3}H_0^2 \right) H_1 - \frac{64}{3}H_0 H_{0,1} \\
& + \left(-\frac{784}{9} - \frac{128}{3}H_0 - \frac{64}{3}H_1 \right) \zeta_2 - 64\zeta_3 \Big] \\
& + L_Q \left[\frac{2360}{9} + \frac{4508}{27}H_0 - \frac{160}{3}H_0^2 - \frac{224}{9}H_0^3 - \frac{320}{9}H_1^3 \right. \\
& + \left(-\frac{4556}{27} - \frac{3680}{9}H_0 - 128H_0^2 \right) H_1 \\
& + \left(-\frac{512}{3} - 128H_0 \right) H_1^2 + 128H_0 H_{0,-1} \\
& + \left(48 - \frac{64}{3}H_0 + \frac{64}{3}H_1 \right) H_{0,1} - 256H_{0,0,-1} - 64H_{0,1,1} \\
& + \left(\frac{2608}{9} + \frac{832}{3}H_0 + \frac{448}{3}H_1 \right) \zeta_2 + 320\zeta_3 \Big] \\
& - \frac{14197}{54} - \frac{3262}{27}H_0 + \frac{4}{3}H_0^4 + \frac{196}{27}H_0^2 + \frac{380}{81}H_0^3 \\
& + \left(\frac{302}{9} + \frac{13624}{81}H_0 + \frac{1628}{27}H_0^2 + \frac{304}{27}H_0^3 \right) H_1 \\
& + \left(\frac{448}{9} + \frac{80}{9}H_0 - \frac{8}{9}H_0^2 \right) H_1^2 \\
& + \frac{128}{27}H_0 H_1^3 + \left(\frac{112}{9} - \frac{1304}{27}H_0 - \frac{32}{3}H_0^2 + \frac{160}{9}H_0 H_1 - \frac{128}{9}H_1^2 \right) H_{0,1} \\
& + \left(\frac{1184}{27} + \frac{128}{9}H_0 - \frac{256}{9}H_1 \right) H_{0,0,1} + \left(-16 - \frac{32}{3}H_0 + \frac{64}{3}H_1 \right) H_{0,1,1} \\
& - \frac{16}{9}H_{0,1}^2 - \frac{128}{9}H_{0,0,0,1} + \frac{64}{3}H_{0,0,1,1} + \left(-\frac{2488}{27} - \frac{1192}{27}H_0 - \frac{80}{9}H_0^2 \right. \\
& + \left(-\frac{160}{9} + \frac{32}{3}H_0 \right) H_1 + \frac{128}{9}H_1^2 - \frac{32}{9}H_{0,1} \Big) \zeta_2 \\
& + \left(\frac{3088}{27} - \frac{128}{9}H_0 + \frac{160}{9}H_1 \right) \zeta_3 + \frac{64}{3}B_4 - \frac{664}{9}\zeta_4 \Big] \\
& + \textcolor{blue}{C_F T_F^2} \left[L_M^3 \frac{128}{27} + L_Q^3 \frac{64}{27} + L_M^2 \left[\frac{320}{27} + \frac{64}{9}H_0 \right] \right. \\
& \left. + L_Q^2 \left[-\frac{464}{27} - \frac{128}{9}H_0 - \frac{64}{9}H_1 \right] + L_M \frac{1984}{81} \right]
\end{aligned}$$

$$\begin{aligned}
& + L_Q \left[\frac{3760}{81} + \frac{2144}{27} H_0 + \left(\frac{928}{27} + \frac{128}{9} H_0 \right) H_1 \right. \\
& + \frac{64}{3} H_0^2 + \frac{64}{9} H_1^2 + \frac{128}{9} H_{0,1} - \frac{256}{9} \zeta_2 \Big] \\
& - \frac{12064}{729} + \frac{64}{81} H_0 - \frac{160}{81} H_0^2 - \frac{32}{81} H_0^3 + \frac{896}{27} \zeta_3 \Big] \\
& + \textcolor{blue}{C_F N_F T_F^2} \left[L_M^3 \frac{64}{27} + L_Q^3 \frac{128}{27} + L_Q^2 \left[-\frac{928}{27} - \frac{256}{9} H_0 - \frac{128}{9} H_1 \right] \right. \\
& + L_M \left[\frac{2176}{81} - \frac{320}{27} H_0 - \frac{32}{9} H_0^2 \right] + L_Q \left[\frac{7520}{81} + \frac{4288}{27} H_0 + \frac{128}{3} H_0^2 \right. \\
& + \left(\frac{1856}{27} + \frac{256}{9} H_0 \right) H_1 + \frac{128}{9} H_1^2 + \frac{256}{9} H_{0,1} - \frac{512}{9} \zeta_2 \Big] \\
& + \left. \left. \frac{24064}{729} + \frac{128}{81} H_0 - \frac{320}{81} H_0^2 - \frac{64}{81} H_0^3 - \frac{512}{27} \zeta_3 \right] \right) \Big)_+ \\
& + \delta(1-x) \left(\textcolor{blue}{C_A C_F T_F} \left[-L_M^3 \frac{44}{9} - L_Q^3 \frac{88}{9} + L_M^2 \left[\frac{34}{3} - \frac{16}{3} \zeta_3 \right] \right. \right. \\
& + L_Q^2 \left[\frac{938}{9} - \frac{16}{3} \zeta_3 \right] + L_M \left[-\frac{1595}{27} + \frac{272}{9} \zeta_3 + \frac{68}{3} \zeta_4 \right] \\
& + L_Q \left[-\frac{11032}{27} - \frac{32}{3} \zeta_2 + \frac{1024}{9} \zeta_3 - \frac{196}{3} \zeta_4 \right] \\
& + \frac{55}{243} - \frac{10045}{81} \zeta_3 - \frac{16}{9} \zeta_2 \zeta_3 + \frac{2624}{27} \zeta_4 - \frac{176}{9} \zeta_5 - 8B_4 \Big] \\
& + \textcolor{blue}{C_F^2 T_F} \left[L_Q^3 6 + L_M^2 L_Q 6 + L_M^2 \left[-10 + \frac{32}{3} \zeta_3 \right] \right. \\
& + L_Q^2 \left[-48 + \frac{32}{3} \zeta_3 \right] + L_M L_Q 2 \\
& + L_M \left[-5 - \frac{112}{9} \zeta_3 - \frac{136}{3} \zeta_4 \right] + L_Q \left[\frac{368}{3} + \frac{64}{3} \zeta_2 - \frac{1616}{9} \zeta_3 \right. \\
& + \frac{392}{3} \zeta_4 \Big] - \frac{2039}{18} + \frac{13682}{81} \zeta_3 + \frac{32}{9} \zeta_2 \zeta_3 - \frac{3304}{27} \zeta_4 + 16B_4 + \frac{352}{9} \zeta_5 \Big] \\
& + \textcolor{blue}{C_F T_F^2} \left[L_M^3 \frac{32}{9} + L_Q^3 \frac{16}{9} + L_M^2 \frac{8}{9} - L_Q^2 \frac{152}{9} \right. \\
& + L_M \frac{496}{27} + L_Q \frac{1624}{27} - \frac{3658}{243} + \frac{224}{9} \zeta_3 \Big] \\
& + \textcolor{blue}{C_F N_F T_F^2} \left[L_M^3 \frac{16}{9} + L_Q^3 \frac{32}{9} - L_Q^2 \frac{304}{9} + L_M \frac{700}{27} \right]
\end{aligned}$$

$$\begin{aligned}
& + L_Q \left[\frac{3248}{27} + \frac{4732}{243} - \frac{128}{9} \zeta_3 \right] \Bigg) \\
& + \textcolor{blue}{C_A} \textcolor{blue}{C_F} \textcolor{blue}{T_F} \left[L_M^3 \frac{88}{27} (x+1) + L_Q^3 \frac{176}{27} (x+1) + L_M^2 \left[-\frac{4}{9} (83x - 37) \right. \right. \\
& \left. \left. + \frac{32}{3} (x+1) H_0 + \frac{32}{3} \frac{x^2+1}{x+1} [H_{0,-1} - H_{-1} H_0] + \frac{16}{3} \frac{x}{x+1} [2\zeta_2 - H_0^2] \right] \right. \\
& \left. + L_Q^2 \left[-\frac{4}{27} (865x + 109) - \frac{256}{9} (x+1) H_0 + \frac{32}{3} \frac{x^2+1}{x+1} [H_{0,-1} - H_{-1} H_0] \right. \right. \\
& \left. \left. - \frac{176}{9} (x+1) H_1 + \frac{16}{3} \frac{x}{x+1} [2\zeta_2 - H_0^2] \right] + L_M \left[-\frac{4}{81} (4577x - 4267) \right. \right. \\
& \left. \left. - \frac{16}{27} (29x - 109) H_0 + \frac{4}{9} \frac{19x^2 + 4x + 25}{x+1} H_0^2 - \frac{32}{9} \frac{x}{x+1} H_0^3 \right. \right. \\
& \left. \left. + \left(\frac{32}{3} (x-1) + 8(x+1) H_0^2 \right) H_1 + \frac{128}{9} \frac{4x^2 + 3x + 4}{x+1} H_{0,-1} \right. \right. \\
& \left. \left. + \left(-\frac{16}{3} - 16H_0 \right) (x+1) H_{0,1} \right. \right. \\
& \left. \left. + \left(-\frac{128}{9} \frac{4x^2 + 3x + 4}{x+1} H_0 + \frac{16}{3} \frac{x^2+1}{x+1} [4H_{0,1} - H_0^2] \right) H_{-1} \right. \right. \\
& \left. \left. + \frac{64}{3} \frac{x}{x+1} H_{0,0,1} + \frac{32}{3} \frac{x^2+1}{x+1} [H_{0,0,-1} - 2H_{0,-1,1} - 2H_{0,1,-1}] \right. \right. \\
& \left. \left. + \left(\frac{16}{9} \frac{3x^2 + 14x - 9}{x+1} - \frac{64}{3} \frac{x^2+1}{x+1} H_{-1} + \frac{16}{3} \frac{3x^2 + 4x + 3}{x+1} H_0 \right) \zeta_2 \right. \right. \\
& \left. \left. - 32 \frac{x^2 + 3x + 1}{x+1} \zeta_3 \right] + L_Q \left[\frac{4}{81} (12329x - 577) \right. \right. \\
& \left. \left. + \left(\frac{64}{27} \frac{181x^2 + 239x + 49}{x+1} - \frac{32}{3} \frac{(x-1)^2}{x+1} H_{-1}^2 \right. \right. \right. \\
& \left. \left. \left. + \frac{32}{9} \frac{6x^4 + 25x^3 + 18x^2 + 25x + 6}{(x+1)x} H_{-1} \right) H_0 \right. \right. \\
& \left. \left. + \left(-\frac{8}{9} \frac{12x^3 - 21x^2 - 77x - 24}{x+1} + \frac{16}{3} \frac{5x^2 - 2x + 5}{x+1} H_{-1} \right) H_0^2 \right. \right. \\
& \left. \left. + \frac{80}{9} \frac{x}{x+1} H_0^3 + \left(\frac{8}{27} (703x + 253) - \frac{8}{3} (x-3) H_0^2 + \frac{352}{9} (x+1) H_0 \right) H_1 \right. \right. \\
& \left. \left. + \left(\frac{176}{9} (x+1) - \frac{16}{3} (x+1) H_0 \right) H_1^2 + \left(\frac{64}{3} \frac{3x+1}{x+1} H_0 \right. \right. \right. \\
& \left. \left. \left. - \frac{32}{9} \frac{6x^4 + 25x^3 + 18x^2 + 25x + 6}{(x+1)x} + \frac{64}{3} \frac{(x-1)^2}{x+1} H_{-1} \right) H_{0,-1} \right. \right. \\
& \left. \left. + \left(\frac{208}{9} (x+1) + \frac{16}{3} (x-3) H_0 + \frac{64}{3} (x+1) H_1 \right) H_{0,1} \right]
\end{aligned}$$

$$\begin{aligned}
& + \frac{32}{3}(x+3)H_{0,0,1} - 32(x+1)H_{0,1,1} \\
& - \frac{64}{3} \frac{(x-1)^2}{x+1} H_{0,-1,-1} \\
& - \frac{32}{3} \frac{5x^2 + 10x + 9}{x+1} H_{0,0,-1} + \left(-\frac{64}{3}(x+2)H_1 \right. \\
& + \frac{16}{9} \frac{12x^3 - 23x^2 - 72x - 17}{x+1} - \frac{32}{3} \frac{(x-1)^2}{x+1} H_{-1} \\
& \left. - \frac{16}{3} \frac{3x^2 + 8x + 3}{x+1} H_0 \right) \zeta_2 + \frac{64}{3} \frac{3x^2 + 3x + 2}{x+1} \zeta_3 \\
& - \frac{2}{729} (108295x - 86681) + \left(-\frac{4}{81}(995x - 2807) \right. \\
& - \frac{32}{81} \frac{199x^2 + 174x + 199}{x+1} H_{-1} + \frac{32}{9}(x+1)H_{-1}^2 - \frac{64}{27} \frac{x^2 + 1}{x+1} H_{-1}^3 \\
& \left. + \left(\frac{4}{81} \frac{253x^2 + 391x + 586}{x+1} - \frac{16}{27} \frac{19x^2 + 18x + 19}{x+1} H_{-1} \right. \right. \\
& \left. \left. + \frac{16}{9} \frac{x^2 + 1}{x+1} H_0^2 \right) H_0^2 \right. \\
& \left. + \left(\frac{8}{81} \frac{22x^2 + 7x + 25}{x+1} - \frac{32}{27} \frac{x^2 + 1}{x+1} H_{-1} \right) H_0^3 \right. \\
& \left. - \frac{16}{27} \frac{x}{x+1} H_0^4 + \left(\frac{8}{9}(9x+4)H_0 \right. \right. \\
& \left. \left. - \frac{8}{27}(65x-29) + \frac{8}{9}(14x+3)H_0^2 + \frac{56}{27}(x+1)H_0^3 \right) H_1 \right. \\
& \left. + \left(-\frac{4}{9}(43x-46) - \frac{8}{9}(2x+5)H_0 - \frac{4}{9}(x+1)H_0^2 \right) H_1^2 \right. \\
& \left. + \frac{32}{27}(x+1)H_0H_1^3 + \left(-\frac{64}{9}(x+1)H_{-1} \right. \right. \\
& \left. \left. + \frac{32}{81} \frac{199x^2 + 174x + 199}{x+1} + \frac{64}{9} \frac{x^2 + 1}{x+1} H_{-1}^2 \right) H_{0,-1} \right. \\
& \left. + \left(\frac{256}{27} \frac{4x^2 + 3x + 4}{x+1} H_{-1} - \frac{8}{27}(143x+2) \right. \right. \\
& \left. \left. - \frac{16}{9}(13x+6)H_0 - \frac{8}{3}(x+1)H_0^2 + \left(\frac{8}{9}(11x+20) \right. \right. \right. \\
& \left. \left. \left. + \frac{64}{9}(x+1)H_0 \right) H_1 - \frac{64}{9}(x+1)H_1^2 \right) H_{0,1} \right. \\
& \left. + \frac{16}{9}(7x+1)H_{0,1}^2 + \left(\frac{64}{9}(x+1) - \frac{128}{9} \frac{x^2 + 1}{x+1} H_{-1} \right) H_{0,-1,-1} \right)
\end{aligned}$$

$$\begin{aligned}
& - \frac{256}{27} \frac{4x^2 + 3x + 4}{x+1} H_{0,-1,1} + \left(-\frac{64}{9} \frac{x^2 + 1}{x+1} H_{-1} \right. \\
& + \frac{32}{27} \frac{19x^2 + 18x + 19}{x+1} \Big) H_{0,0,-1} + \left(\frac{8}{27} \frac{9x^2 + 101x + 12}{x+1} + \frac{64}{9} \frac{x^2 + 1}{x+1} H_{-1} \right. \\
& - \frac{16}{9} (7x+1) H_0 - \frac{160}{9} (x+1) H_1 \Big) H_{0,0,1} - \frac{256}{27} \frac{4x^2 + 3x + 4}{x+1} H_{0,1,-1} \\
& + \left(-\frac{16}{9} (x+7) - \frac{128}{9} \frac{x^2 + 1}{x+1} H_{-1} \right. \\
& - \frac{16}{9} (11x+5) H_0 + 16(x+1) H_1 \Big) H_{0,1,1} \\
& + \frac{64}{9} \frac{x^2 + 1}{x+1} [2H_{0,-1,-1,-1} + 2H_{0,-1,1,1} \\
& + H_{0,0,-1,-1} - H_{0,0,-1,1} + H_{0,0,0,-1} \\
& - H_{0,0,1,-1} + 2H_{0,1,-1,1} + 2H_{0,1,1,-1}] + \frac{64}{9} \frac{5x^2 + 6x - 1}{x+1} H_{0,0,0,1} \\
& - \frac{16}{9} \frac{x^2 - 2x - 11}{x+1} H_{0,0,1,1} - \frac{112}{9} (x+1) H_{0,1,1,1} \\
& + \left(\frac{16}{81} \frac{174x^2 + 209x - 189}{x+1} - \frac{32}{27} \frac{29x^2 + 18x + 29}{x+1} H_{-1} \right. \\
& + \left(-\frac{8}{9} (3x+14) + \frac{80}{9} (x+1) H_0 \right) H_1 \\
& + \left(\frac{8}{27} \frac{63x^2 + 29x + 6}{x+1} - \frac{32}{9} \frac{x^2 + 1}{x+1} H_{-1} \right) H_0 \\
& - \frac{32}{9} \frac{x^2 + 1}{x+1} H_{-1}^2 + \frac{64}{9} (x+1) H_1^2 \\
& + \frac{8}{9} \frac{3x^2 + 8x + 9}{x+1} H_0^2 - \frac{16}{9} (7x+1) H_{0,1} \Big) \zeta_2 \\
& + \left(\frac{2}{27} \frac{497x^2 + 1102x + 1085}{x+1} \right. \\
& + \frac{128}{9} \frac{x^2 + 1}{x+1} H_{-1} + \frac{32}{9} \frac{6x^2 + 4x - 3}{x+1} H_0 + \frac{16}{9} (x+1) H_1 \Big) \zeta_3 \\
& + \frac{16}{3} (x+1) B_4 - \frac{8}{3} \frac{36x^2 + 51x + 22}{x+1} \zeta_4 \Big] \\
& + \textcolor{blue}{C_F^2 T_F} \left[[L_Q^3 + L_M^2 L_Q] \left[-\frac{8}{3} (x+5) + \frac{32}{3} (x+1) H_1 \right. \right. \\
& + 8(x+1) H_0 \Big] + L_M^2 \left[28(2x-1) + \left(-\frac{8}{3} (11x+5) + \frac{64}{3} \frac{x^2 + 1}{x+1} H_{-1} \right) H_0 \right. \\
& - \frac{4}{3} \frac{9x^2 + 10x + 9}{x+1} H_0^2 + \left(-\frac{16}{3} (2x+1) - \frac{64}{3} (x+1) H_0 \right) H_1
\end{aligned}$$

$$\begin{aligned}
& -\frac{8}{3}(x+1)H_{0,1} - 8(x+1)H_1^2 \\
& - \frac{64}{3}\frac{x^2+1}{x+1}H_{0,-1} + \frac{8}{3}\frac{9x^2+10x+9}{x+1}\zeta_2 \Big] \\
& + L_Q^2 \left[\frac{4}{9}(161x+130) \right. \\
& + \left(-\frac{16}{3}(15x+4) + \frac{64}{3}\frac{x^2+1}{x+1}H_{-1} \right) H_0 \\
& - 24(x+1)H_1^2 + \left(-\frac{16}{9}(50x+17) \right. \\
& - \frac{160}{3}(x+1)H_0 \Big) H_1 - \frac{4}{3}\frac{21x^2+34x+21}{x+1}H_0^2 + \frac{8}{3}\frac{23x^2+38x+23}{x+1}\zeta_2 \\
& \left. - \frac{64}{3}\frac{x^2+1}{x+1}H_{0,-1} - 8(x+1)H_{0,1} \right] \\
& + L_M L_Q \left[\frac{4}{9}(19x-85) + \frac{8}{3}(13x+1)H_0 \right. \\
& + 8(x+1)H_0^2 + \left(\frac{128}{9}(4x+1) + \frac{32}{3}(x+1)H_0 \right) H_1 - \frac{32}{3}(x+1)\zeta_2 \Big] \\
& + L_M \left[-\frac{4}{9}(337x+235)H_0 - \frac{4}{9}\frac{195x^2+238x+123}{x+1}H_0^2 \right. \\
& - \frac{32}{9}\frac{3x^2+4x+3}{x+1}H_0^3 + \left(-\frac{4}{9}(287x-113) - \frac{224}{9}(5x+2)H_0 \right. \\
& - \frac{80}{3}(x+1)H_0^2 \Big) H_1 + \frac{4}{3}(178x-125) \\
& + \left(-\frac{16}{3}(7x+3) - \frac{16}{3}(x+1)H_0 \right) H_1^2 \\
& + \left(\frac{184}{9}(x+1) + \frac{32}{3}(x+1)H_0 \right) H_{0,1} \\
& - \frac{256}{9}\frac{4x^2+3x+4}{x+1}H_{0,-1} + \frac{16}{3}\frac{3x^2-2x+3}{x+1}H_{0,0,1} \\
& + \left(\frac{256}{9}\frac{4x^2+3x+4}{x+1}H_0 + \frac{32}{3}\frac{x^2+1}{x+1}[H_0^2 - 4H_{0,1}] \right) H_{-1} \\
& + \frac{64}{3}\frac{x^2+1}{x+1}[2H_{0,-1,1} - H_{0,0,-1} + 2H_{0,1,-1}] \\
& + \left(\frac{8}{9}\frac{117x^2+118x+81}{x+1} + \frac{128}{3}\frac{x^2+1}{x+1}H_{-1} + \frac{16}{3}\frac{(x+3)(3x+1)}{x+1}H_0 \right. \\
& + \frac{32}{3}(x+1)H_1 \Big) \zeta_2 + \frac{16}{3}\frac{x^2+14x+1}{x+1}\zeta_3 \Big] + L_Q \left[-\frac{8}{27}(557x+652) \right. \\
& + \left(\frac{8}{9}\frac{115x^2+99x+32}{x+1} - \frac{64}{9}\frac{6x^4+25x^3+18x^2+25x+6}{(x+1)x}H_{-1} \right)
\end{aligned}$$

$$\begin{aligned}
& + \frac{64}{3} \frac{(x-1)^2}{x+1} H_{-1}^2 \Big) H_0 + \frac{32}{9} \frac{9x^2 + 13x + 9}{x+1} H_0^3 \\
& + \left(-\frac{32}{3} \frac{5x^2 - 2x + 5}{x+1} H_{-1} + \frac{4}{9} \frac{48x^3 + 519x^2 + 706x + 315}{x+1} \right) H_0^2 \\
& + \left(\frac{8}{27} (908x - 19) + \frac{16}{9} (169x + 97) H_0 \right. \\
& \left. + \frac{32}{3} (7x + 5) H_0^2 \right) H_1 + \left(\frac{32}{3} (13x + 6) + 64(x + 1) H_0 \right) H_1^2 \\
& + \frac{160}{9} (x + 1) H_1^3 + \left(\frac{64}{9} (13x + 1) + \frac{16}{3} (x + 9) H_0 - \frac{32}{3} (x + 1) H_1 \right) H_{0,1} \\
& + \left(-\frac{128}{3} \frac{3x + 1}{x+1} H_0 + \frac{64}{9} \frac{6x^4 + 25x^3 + 18x^2 + 25x + 6}{(x+1)x} \right. \\
& \left. - \frac{128}{3} \frac{(x-1)^2}{x+1} H_{-1} \right) H_{0,-1} \\
& + \frac{128}{3} \frac{(x-1)^2}{x+1} H_{0,-1,-1} + \frac{64}{3} \frac{5x^2 + 10x + 9}{x+1} H_{0,0,-1} + \frac{16}{3} (5x - 3) H_{0,0,1} \\
& + 48(x + 1) H_{0,1,1} + \left(-\frac{16}{9} \frac{24x^3 + 245x^2 + 318x + 137}{x+1} \right. \\
& \left. + \frac{64}{3} \frac{(x-1)^2}{x+1} H_{-1} - \frac{16}{3} \frac{35x^2 + 66x + 35}{x+1} H_0 \right. \\
& \left. - \frac{32}{3} (9x + 5) H_1 \right) \zeta_2 - \frac{32}{3} \frac{21x^2 + 30x + 17}{x+1} \zeta_3 \\
& + \frac{1}{27} (12332x - 4905) + \left(-\frac{64}{9} (x + 1) H_{-1}^2 + \frac{64}{81} \frac{199x^2 + 174x + 199}{x+1} H_{-1} \right. \\
& \left. + \frac{1}{81} (-10999x - 8399) + \frac{128}{27} \frac{x^2 + 1}{x+1} H_{-1}^3 \right) H_0 \\
& + \left(\frac{32}{27} \frac{19x^2 + 18x + 19}{x+1} H_{-1} - \frac{32}{9} \frac{x^2 + 1}{x+1} H_{-1}^2 \right. \\
& \left. - \frac{2}{81} \frac{4179x^2 + 5255x + 2868}{x+1} \right) H_0^2 \\
& + \left(\frac{64}{27} \frac{x^2 + 1}{x+1} H_{-1} - \frac{10}{81} \frac{177x^2 + 218x + 105}{x+1} \right) H_0^3 \\
& - \frac{1}{27} \frac{51x^2 + 70x + 51}{x+1} H_0^4 + \left(-\frac{152}{27} (x + 1) H_0^3 \right. \\
& \left. + \frac{1}{27} (-3457x + 1951) - \frac{16}{81} (593x + 335) H_0 - \frac{8}{27} (146x + 71) H_0^2 \right) H_1 \\
& + \left(-\frac{8}{9} (3x + 55) - \frac{8}{9} (9x + 1) H_0 + \frac{4}{9} (x + 1) H_0^2 \right) H_1^2 - \frac{64}{27} (x + 1) H_0 H_1^3
\end{aligned}$$

$$\begin{aligned}
& + \left(-\frac{64}{81} \frac{199x^2 + 174x + 199}{x+1} + \frac{128}{9}(x+1)H_{-1} - \frac{128}{9} \frac{x^2 + 1}{x+1} H_{-1}^2 \right) H_{0,-1} \\
& + \left(\frac{4}{27}(251x + 407) + \frac{16}{27}(10x + 43)H_0 + \frac{16}{3}(x+1)H_0^2 + \left(\frac{64}{9}(x-1) \right. \right. \\
& \left. \left. - \frac{80}{9}(x+1)H_0 \right) H_1 - \frac{512}{27} \frac{4x^2 + 3x + 4}{x+1} H_{-1} + \frac{64}{9}(x+1)H_1^2 \right) H_{0,1} \\
& + \frac{8}{9}(x+1)H_{0,1}^2 + \frac{512}{27} \frac{4x^2 + 3x + 4}{x+1} H_{0,-1,1} \\
& + \left(\frac{256}{9} \frac{x^2 + 1}{x+1} H_{-1} - \frac{128}{9}(x+1) \right) H_{0,-1,-1} \\
& + \left(-\frac{64}{27} \frac{19x^2 + 18x + 19}{x+1} + \frac{128}{9} \frac{x^2 + 1}{x+1} H_{-1} \right) H_{0,0,-1} \\
& + \left(\frac{4}{27} \frac{357x^2 + 130x + 93}{x+1} - \frac{128}{9} \frac{x^2 + 1}{x+1} H_{-1} \right. \\
& \left. + \frac{64}{9}(x+1)[2H_1 - H_0] \right) H_{0,0,1} \\
& + \frac{512}{27} \frac{4x^2 + 3x + 4}{x+1} H_{0,1,-1} + \left(-\frac{32}{9}(13x+1) + \frac{16}{3}(x+1)[H_0 - 2H_1] \right. \\
& \left. + \frac{256}{9} \frac{x^2 + 1}{x+1} H_{-1} \right) H_{0,1,1} \\
& + \frac{128}{9} \frac{x^2 + 1}{x+1} [H_{0,0,-1,1} - 2H_{0,-1,-1,-1} - 2H_{0,-1,1,1} \\
& - H_{0,0,-1,-1} - H_{0,0,0,-1} + H_{0,0,1,-1} - 2H_{0,1,-1,1} - 2H_{0,1,1,-1}] \\
& + \frac{8}{9} \frac{21x^2 + 10x + 21}{x+1} H_{0,0,0,1} - \frac{32}{9} \frac{7x^2 + 6x + 7}{x+1} H_{0,0,1,1} \\
& + \left(\frac{64}{9} \frac{x^2 + 1}{x+1} H_{-1}^2 + \frac{4}{81} \frac{1619x^2 + 1338x + 1511}{x+1} \right. \\
& \left. + \left(\frac{4}{27} \frac{147x^2 + 298x - 9}{x+1} + \frac{64}{9} \frac{x^2 + 1}{x+1} H_{-1} \right) H_0 \right. \\
& \left. + \frac{64}{27} \frac{29x^2 + 18x + 29}{x+1} H_{-1} + \frac{4}{9} \frac{(x+5)(5x+1)}{x+1} H_0^2 - \frac{64}{9}(x+1)H_1^2 \right. \\
& \left. + \left(\frac{16}{9}(x+9) - \frac{16}{3}(x+1)H_0 \right) H_1 + \frac{16}{9}(x+1)H_{0,1} \right) \xi_2 \\
& + \left(-\frac{80}{9}(x+1)H_1 - \frac{8}{27} \frac{235x^2 + 404x + 409}{x+1} \right. \\
& \left. - \frac{256}{9} \frac{x^2 + 1}{x+1} H_{-1} + \frac{8}{9} \frac{15x^2 + 22x + 15}{x+1} H_0 \right) \xi_3 \\
& + \left. \frac{4}{9} \frac{131x^2 + 178x + 131}{x+1} \xi_4 - \frac{32}{3}(x+1)B_4 \right] + \textcolor{blue}{C_F T_F^2} \left[-L_M^3 \frac{64}{27}(x+1) \right]
\end{aligned}$$

$$\begin{aligned}
& -L_Q^3 \frac{32}{27}(x+1) + L_M^2 \left[-\frac{32}{27}(11x-1) - \frac{32}{9}(x+1)H_0 \right] \\
& + L_Q^2 \left[\frac{32}{27}(14x+5) + \frac{64}{9}(x+1)H_0 + \frac{32}{9}(x+1)H_1 \right] \\
& - L_M \frac{992}{81}(x+1) + L_Q \left[-\frac{32}{81}(187x+16) \right. \\
& \quad \left. - \frac{64}{27}(28x+13)H_0 - \frac{32}{3}(x+1)H_0^2 \right. \\
& \quad \left. + \left(-\frac{64}{27}(14x+5) - \frac{64}{9}(x+1)H_0 \right)H_1 \right. \\
& \quad \left. - \frac{32}{9}(x+1)H_1^2 - \frac{64}{9}(x+1)H_{0,1} + \frac{128}{9}(x+1)\xi_2 \right] \\
& + \frac{16}{729}(431x+323) + \frac{64}{81}(6x-7)H_0 + \frac{16}{81}(11x-1)H_0^2 \\
& \quad \left. + \frac{16}{81}(x+1)H_0^3 - \frac{448}{27}(x+1)\xi_3 \right] \\
& + \textcolor{blue}{C_F N_F T_F^2} \left[-[L_M^3 + 2L_Q^3] \frac{32}{27}(x+1) \right. \\
& \quad \left. + L_Q^2 \left[\frac{64}{27}(14x+5) + \frac{128}{9}(x+1)H_0 \right. \right. \\
& \quad \left. \left. + \frac{64}{9}(x+1)H_1 \right] + L_M \left[\frac{32}{81}(5x-73) + \frac{32}{27}(11x-1)H_0 + \frac{16}{9}(x+1)H_0^2 \right] \right. \\
& \quad \left. + L_Q \left[-\frac{64}{81}(187x+16) - \frac{128}{27}(28x+13)H_0 \right. \right. \\
& \quad \left. \left. + \frac{64}{9}(x+1)[4\xi_2 - 2H_{0,1} - H_1^2] \right. \right. \\
& \quad \left. \left. - \frac{64}{3}(x+1)H_0^2 + \left(-\frac{128}{9}(x+1)H_0 - \frac{128}{27}(14x+5) \right)H_1 \right] \right. \\
& \quad \left. + \frac{32}{81}(x+1)H_0^3 - \frac{64}{729}(161x+215) + \frac{128}{81}(6x-7)H_0 \right. \\
& \quad \left. + \frac{32}{81}(11x-1)H_0^2 + \frac{256}{27}(x+1)\xi_3 \right] \\
& \quad \left. + \hat{C}_{q,g_1}^{\text{NS},(3)}(N_F) \right\}. \tag{2.61}
\end{aligned}$$

Again, we used the short hand notation $H_{\vec{a}}(x) \equiv H_{\vec{a}}$ also here. The transformation of the Wilson coefficient to the $\overline{\text{MS}}$ scheme for the heavy quark mass affects the massive OME at 3-loops and was given in Ref. [10]; the terms are the same in the unpolarized and polarized case.

The non-singlet contributions to the structure function $g_2(x, Q^2)$ can be obtained via the Wandzura–Wilczek relation [15]

$$g_2(x, Q^2) = -g_1(x, Q^2) + \int_x^1 \frac{dy}{y} g_1(y, Q^2), \quad (2.62)$$

where both structure functions refer to the twist-2 contributions. This relation is implied by a relation of the OMEs in the light-cone expansion, cf. [40]. The relation has also been proven in the covariant parton model in Refs. [41–43]. For gluonic initial states, it was derived in [44]. Eq. (2.62) also holds including target mass corrections [45,46] and finite light quark contributions [46]. Furthermore, it holds in non-forward [47] and diffractive scattering, including target mass corrections [49,48].

3. Numerical results

In what follows, we will choose the factorization and renormalization scale $\mu^2 = Q^2$. We first study the behavior of the massive and massless Wilson coefficients in the small and large x region and then give numerical illustrations in the whole x -region.

At small x , the pure massive Wilson coefficient behaves like

$$\begin{aligned} L_{q,g_1}^{h,NS}(N_F + 1) - \hat{C}_{q,g_1}^{NS,(3)}(N_F) &\propto a_s^2 4 C_F T_F \ln^2(x) \\ &+ a_s^3 \left[\frac{16}{27} C_A C_F T_F - \frac{5}{9} C_F^2 T_F \right] \ln^4(x), \end{aligned} \quad (3.1)$$

while in the region $x \rightarrow 1$ one obtains

$$\begin{aligned} L_{q,g_1}^{h,NS}(N_F + 1) - \hat{C}_{q,g_1}^{NS,(3)}(N_F) &\propto a_s^2 C_F T_F \frac{8}{3} \left(\frac{\ln^2(1-x)}{1-x} \right)_+ + a_s^3 C_F^2 T_F \left[16 \ln^2 \left(\frac{Q^2}{m^2} \right) \right. \\ &\left. + \frac{160}{3} \ln^2 \left(\frac{Q^2}{m^2} \right) + \frac{448}{9} \right] \left(\frac{\ln^2(1-x)}{1-x} \right)_+. \end{aligned} \quad (3.2)$$

There is a term $\propto \ln^3(1-x)/(1-x)$ at $O(\ln(Q^2/\mu^2))$, being of relevance for different choices of the factorization scale.

The above results can be compared with the case of the massless Wilson coefficient

$$\hat{C}_{q,g_1}^{NS,(2)}(N_F) \propto a_s^2 \frac{10}{3} C_F T_F \ln^2(x) \quad (3.3)$$

$$\hat{C}_{q,g_1}^{NS,(3)}(N_F) \propto a_s^3 \left[\frac{92}{27} C_F C_A T_F - \frac{31}{9} C_F^2 T_F \right] \ln^4(x) \quad (3.4)$$

$$\hat{C}_{q,g_1}^{NS,(2)}(N_F) \propto a_s^2 \frac{8}{3} C_F T_F \left(\frac{\ln^2(1-x)}{1-x} \right)_+ \quad (3.5)$$

$$\hat{C}_{q,g_1}^{NS,(3)}(N_F) \propto a_s^3 \frac{80}{9} C_F^2 T_F \left(\frac{\ln^4(1-x)}{1-x} \right)_+. \quad (3.6)$$

The small x behavior can be compared with leading order predictions for the non-singlet evolution kernel in Refs. [50,51]. Indeed both the massive and massless contributions follow the principle pattern $\sim c_k a_s^{k+1} \ln^{2k}(x)$. However, as is well known [50], less singular terms widely

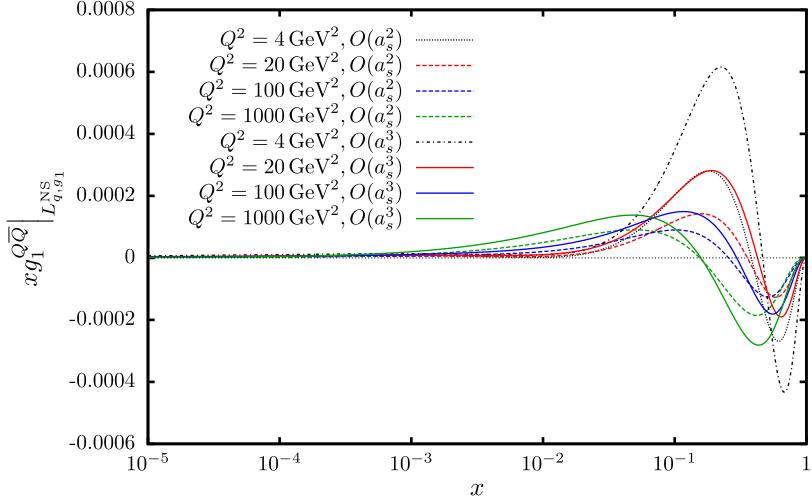


Fig. 1. The 2- and 3-loop non-singlet charm contributions to the structure function $xg_1(x, Q^2)$ by the asymptotic heavy flavor Wilson coefficients in the on-shell scheme for $m_c = 1.59$ GeV. Here we used the value of $\alpha_s(M_Z^2) = 0.1132$ and the NLO parton distribution [8] as reference. Figs. 2–8 below are calculated using the same setting.

cancel the numerical effect of these leading terms. For the large x terms the massless terms exhibit a stronger soft singularity than the massive ones.

In the following numerical illustrations we use the polarized parton distributions of Ref. [8], which are of next-to-leading order (NLO), since no next-to-next-to-leading order (NNLO) data analysis based on the anomalous dimensions calculated in Ref. [52] has been performed yet. The values of α_s correspond to those of the unpolarized NNLO analysis [53]. The heavy and light flavor Wilson coefficients being discussed in the following are given in Eqs. (2.1) and (2.3).

In Fig. 1, the 2- and 3-loop heavy flavor corrections to the non-singlet term of the structure function $xg_1(x, Q^2)$ are calculated in the case of charm, assuming $m_c = 1.59$ GeV [54], using the formula for the Wilson coefficient Eq. (2.61), and setting $\mu^2 = Q^2$. With growing Q^2 , the distribution diminishes at larger values of x and grows towards medium values. The $O(\alpha_s^3)$ corrections lead to stronger effects if compared to those at $O(\alpha_s^2)$. We have applied the asymptotic Wilson coefficients for all the Q^2 values given here, which only holds for values $Q^2/m^2 \gtrsim 10$. For the heavy quark distributions we formally show also the result at $Q^2 = 4$ GeV 2 , outside this region, indicated by dotted ($O(a_s^2)$) and dash-dotted lines ($O(a_s^3)$).

Fig. 2 shows the effect of the Wilson coefficients comparing the contributions from $O(\alpha_s^0)$ to $O(\alpha_s^3)$ at $Q^2 = 4$ GeV 2 as an example, where a depletion is obtained with growing order. The 3-loop light flavor contributions to $xg_1(x, Q^2)$ ($N_F = 3$) are illustrated in Fig. 3. Here the evolution is strengthened by growing Q^2 in the large x region and depleted for lower values of Q^2 , considering only the effects due to the Wilson coefficient.

In Figs. 4 and 5 we illustrate the ratio of the flavor non-singlet charm corrections to those by the light quarks given in Eq. (2.3) up to $O(\alpha_s^2)$ and $O(\alpha_s^3)$, respectively. At $O(\alpha_s^2)$ the effect is of $O(1\%)$ and below, for the lower scales Q^2 , but higher values are obtained for very large scales as $Q^2 \simeq 1000$ GeV 2 in the region $x \sim 0.003$. A qualitatively similar picture is obtained including the $O(\alpha_s^3)$ corrections. The effect on the ratio $g_1^{\text{heavy}}/g_1^{\text{light}}|_{\text{NS}}$ is about doubled. To resolve relative effects of $O(2\%)$ requires higher luminosities than available in present day experiments. They may become available in the planned experiments at a future EIC [55].

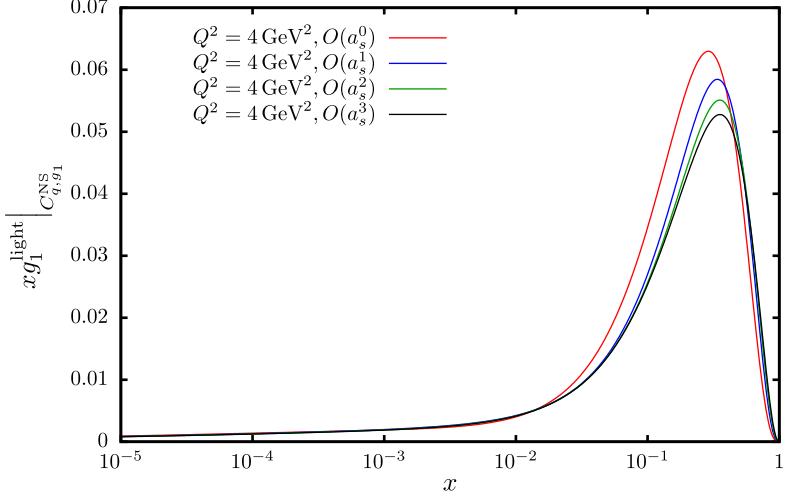


Fig. 2. The light flavor contributions ($N_F = 3$) to the non-singlet charm contributions to the structure function $xg_1(x, Q^2)$ at $Q^2 = 4 \text{ GeV}^2$ illustrating the contributions for the different orders in a_s .

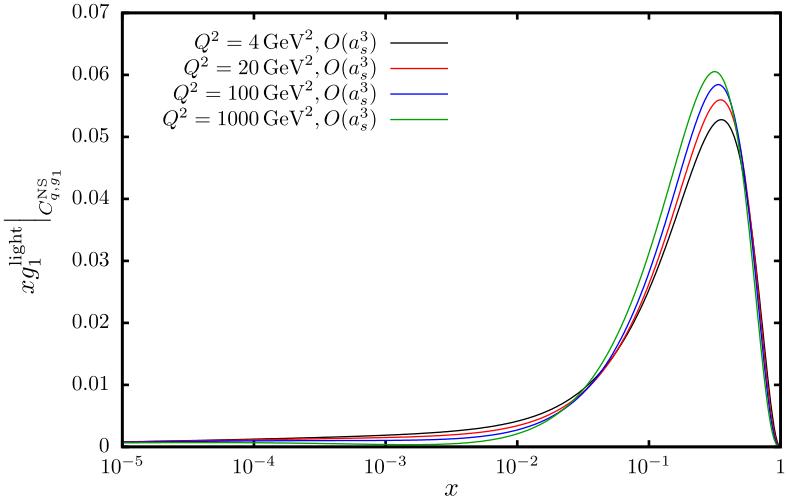


Fig. 3. The light flavor contributions ($N_F = 3$) to the non-singlet charm contributions to the structure function $xg_1(x, Q^2)$ at $O(a_s^3)$ for different values of Q^2 .

In Fig. 6 we illustrate the scale dependence in μ^2 , normalizing the structure function $g_1^{\text{NS}}(x, Q^2)$, including both the light and heavy flavor effects accounting for charm, to the case $Q^2 = \mu^2$. The yellow band illustrates the variation of $\mu^2 \in [Q^2/4, 4Q^2]$ for $Q^2 = 100 \text{ GeV}^2$ at 3-loop order. We checked that very similar results are obtained for $Q^2 = 20 \text{ GeV}$. In Fig. 7 we show the ratio of $g_1^{\text{NS}}(x, Q^2)$ calculated up to $O(a_s^3)$ to the result obtained taking only the contributions up to $O(a_s^2)$ and illustrate the scale dependence varying μ^2 in the same range as for $Q^2 = 100 \text{ GeV}^2$. In the low x region this ratio is slightly below one and it grows towards large values of x to values ~ 1.4 as an effect of the 3-loop corrections.

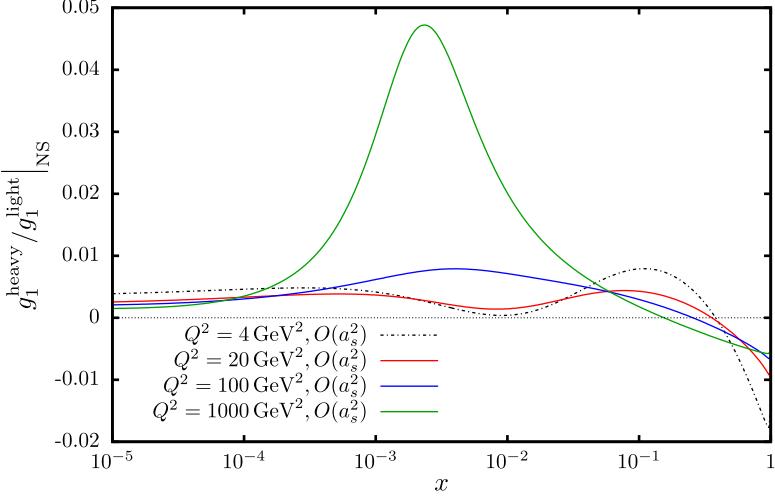


Fig. 4. The ratio $g_1^{\text{charm}}/g_1^{\text{light}}|_{\text{NS}}$ in the non-singlet case at $O(a_s^2)$ for different values of Q^2 .

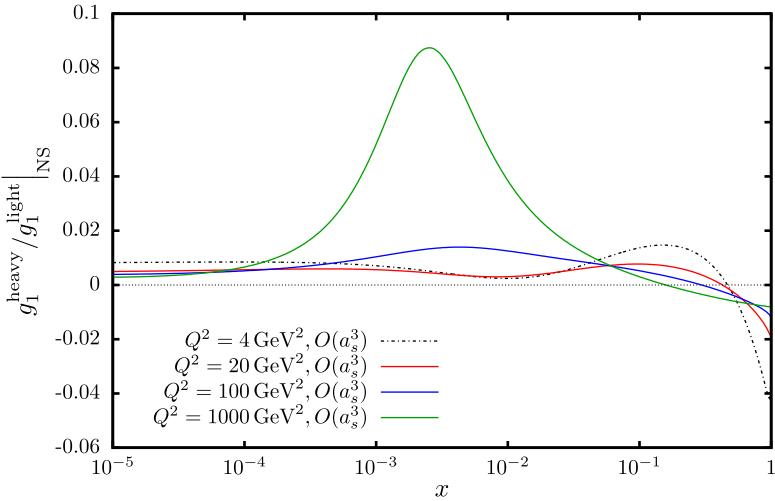


Fig. 5. The ratio $g_1^{\text{charm}}/g_1^{\text{light}}|_{\text{NS}}$ in the non-singlet case at $O(a_s^3)$ for different values of Q^2 .

If the parton distributions are properly evolved in Mellin N space to $O(a_s^3)$ analytically [36, 56], unlike the case for x -space programs, cf. e.g. [57], the μ -dependence exactly cancels. Ideally this is the preferred way of solving the evolution equations, cf. Ref. [8]. Therefore, a remaining μ -dependence stems from higher order terms in the parton distribution functions only starting with $O(a_s^4)$. One should note, however, that at present only NLO polarized parton distributions are available. Therefore, the 3-loop scale matching is not yet perfect. One thus expects to obtain smaller error bands for the scale variation upon using fitted NNLO parton distributions from future analyses. Yet the scale variation errors are below the present experimental accuracy, cf. e.g. [8].

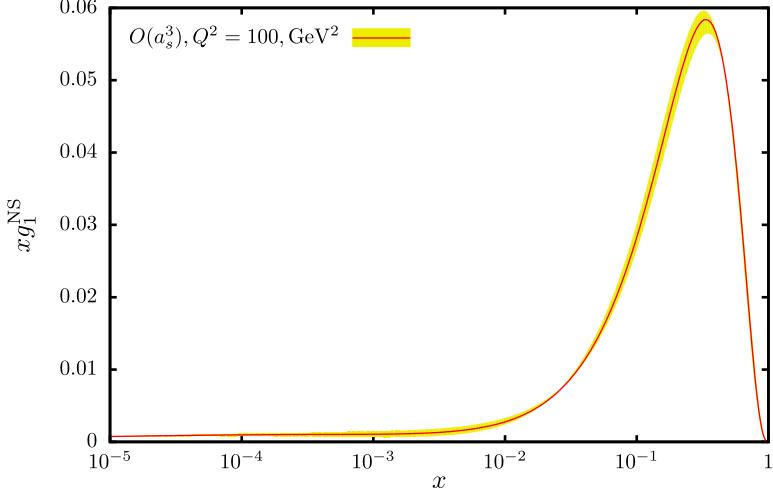


Fig. 6. The structure function $g_1^{\text{NS}}(x)$ to 3-loop order containing both the massless terms and the charm contribution at $Q^2 = 100 \text{ GeV}^2$. The yellow band illustrates the variation of the factorization and renormalization scale $\mu_R^2 = \mu_F^2 = \mu^2$ in the range $Q^2/4$ to $4Q^2$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

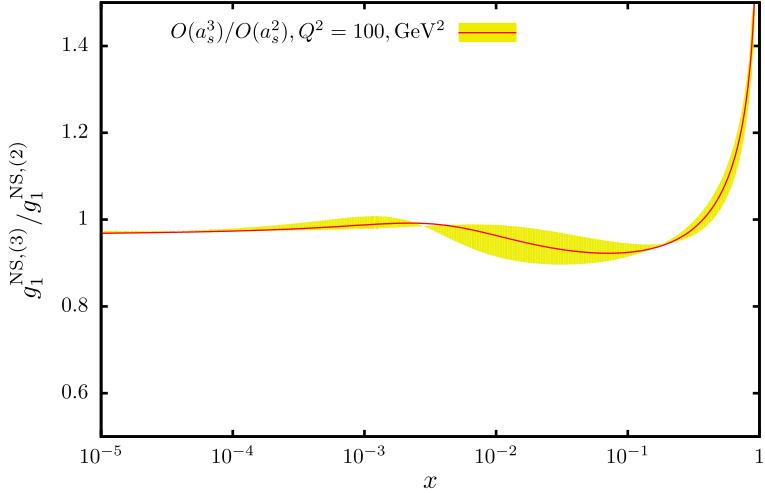


Fig. 7. The ratio of the structure function $g_1^{\text{NS}}(x)$ evaluated up to 3-loop and 2-loop order, respectively, containing both the massless terms and the charm contribution at $Q^2 = 100 \text{ GeV}^2$. The yellow band illustrates the variation of the factorization and renormalization scale $\mu_R^2 = \mu_F^2 = \mu^2$ in the range $Q^2/4$ to $4Q^2$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 8 shows the 2- and 3-loop charm flavor non-singlet contributions to the structure function $xg_2(x, Q^2)$ according to the Wandzura–Wilczek relation (2.62) implying the oscillatory behavior. In size these effects are comparable to those of the structure function $xg_1(x, Q^2)$ shown in Fig. 1. With growing Q^2 the effects become somewhat smaller. In Fig. 9 we show the corresponding massless contributions to the structure function $g_2(x, Q^2)$ at $Q^2 = 4 \text{ GeV}^2$ for the different

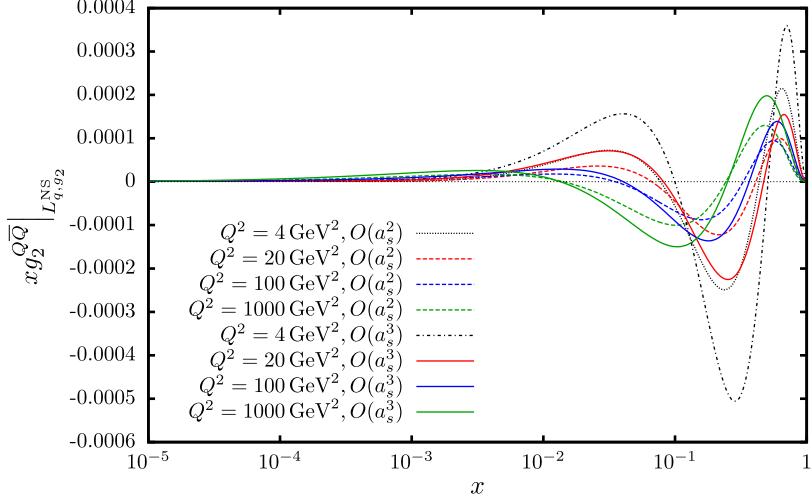


Fig. 8. The 2- and 3-loop non-singlet charm contributions to the twist 2 contributions of the structure function $xg_2(x, Q^2)$ by the asymptotic heavy flavor Wilson coefficients in the on-shell scheme.

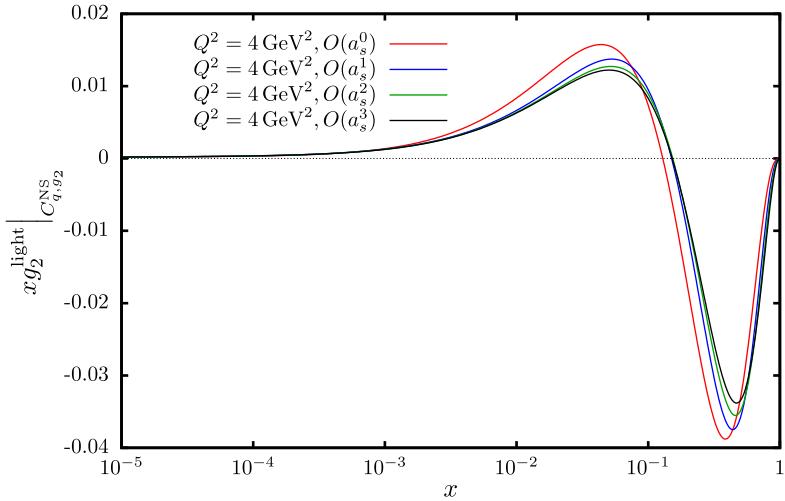


Fig. 9. The light flavor contributions ($N_F = 3$) to the non-singlet charm contributions to the structure function $xg_2(x, Q^2)$ at $Q^2 = 4 \text{ GeV}^2$ illustrating the contributions for the different orders in a_s .

orders in a_s , which slightly diminish adding higher order contributions. Taking into account the $O(a_s^3)$ corrections, the light flavor corrections to $g_2(x, Q^2)$ (1.5), (2.62) grow somewhat in size with larger values of Q^2 , see Fig. 10. Similar to the case of the structure function xg_1 the $O(a_s^3)$ charm flavor non-singlet corrections to the structure function $xg_2(x, Q^2)$ amount to $O(1\%)$.

4. The Bjorken sum rule

The polarized Bjorken sum rule [58] refers to the first moment of the flavor non-singlet combination

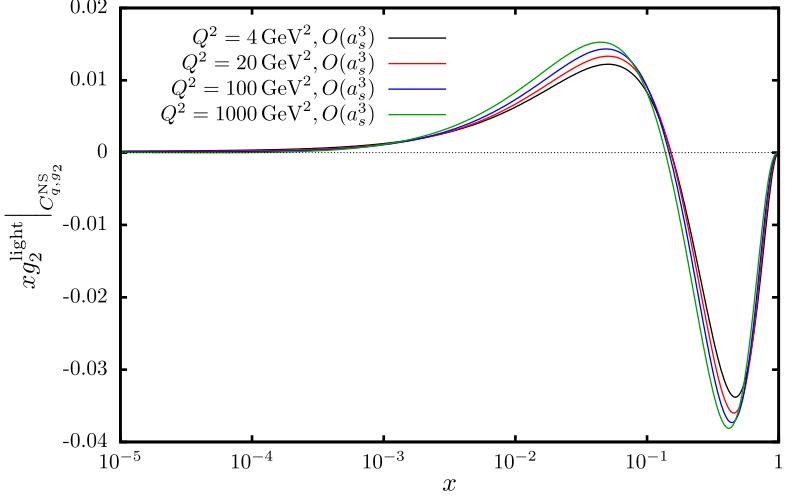


Fig. 10. The light flavor contributions ($N_F = 3$) to the non-singlet charm contributions to the structure function $xg_2(x, Q^2)$ at $O(\alpha_s^3)$ for different values of Q^2 .

$$\int_0^1 dx \left[g_1^{ep}(x, Q^2) - g_1^{en}(x, Q^2) \right] = \frac{1}{6} \left| \frac{g_A}{g_V} \right| C_{\text{BJ}}(\hat{\alpha}_s), \quad (4.1)$$

with $g_{A,V}$ the neutron decay constants, $g_A/g_V \approx -1.2767 \pm 0.0016$ [59] and $\hat{\alpha}_s = \alpha_s/\pi$. The 1- [60], 2- [61], 3- [31] and 4-loop QCD corrections [32] in the massless case are given by

$$\begin{aligned} C_{\text{BJ}}(\hat{\alpha}_s) = & 1 - \hat{\alpha}_s + \hat{\alpha}_s^2 (-4.58333 + 0.33333 N_F) \\ & + \hat{\alpha}_s^3 (-41.4399 + 7.60729 N_F - 0.17747 N_F^2) \\ & + \hat{\alpha}_s^4 (-479.448 + 123.472 N_F - 7.69747 N_F^2 + 0.10374 N_F^3), \end{aligned} \quad (4.2)$$

choosing the renormalization scale $\mu^2 = Q^2$, cf. [29] for $SU(3)_c$. Here N_F denotes the number of active light flavors. The expression for general color factors was given in Ref. [32].

For the asymptotic massive corrections (2.1) only the first moments of the massless Wilson coefficients $\hat{C}_{q,g1}^{(2,3),\text{NS}}(N_F)$ contribute, since the first moments of the massive non-singlet OMEs vanish due to fermion number conservation, a property holding even at higher order. Therefore, any new heavy quark changes Eq. (4.2) by a shift in $N_F \rightarrow N_F + 1$ only, for the asymptotic corrections. Different results are obtained in the tagged flavor case [5,7] at $O(\alpha_s^2)$, where no inclusive structure functions are considered. Corresponding power corrections were derived in [62,63].

5. Conclusions

We calculated the heavy flavor non-singlet Wilson coefficients of the polarized inclusive structure function $g_1(x, Q^2)$ to $O(\alpha_s^3)$ in the asymptotic region $Q^2 \gg m^2$. The first contributions of this kind are of $O(\alpha_s^2)$. In the case of twist-2 operators the corresponding contributions to the structure function $g_2(x, Q^2)$ can be obtained using the Wandzura–Wilczek relation (2.62) [15], cf. [40–43,46]. The asymptotic Wilson coefficient is obtained by using the factorization

formula [5], Eq. (2.2), based on the massive OME [10] and the massless Wilson coefficient [30] to 3-loop order. The heavy flavor Wilson coefficient can be thoroughly represented by nested harmonic sums in Mellin- N space and by harmonic polylogarithms in x -space. We presented numerical results corresponding to the charge weighted polarized parton contributions $\propto \Delta f(x, Q^2) + \Delta \bar{f}(x, Q^2)$, cf. (1.5), referring to the polarized parton distribution functions at NLO [8] for an illustration. Comparing with the corresponding massless cases the heavy flavor corrections in case of charm are of $O(1\text{--}2\%)$, requiring high luminosity experiments to be resolved, which are planned for the future electron-ion collider EIC [55]. We also considered the contribution of the asymptotic Wilson coefficient to the polarized Bjorken sum-rule. Due to fermion number conservation for the massive flavor non-singlet OME in all orders in α_s , only the first moment of the massless Wilson coefficient contributes and the effect of each heavy flavor results in a shift of N_F by one unit in the expression for the massless polarized Bjorken sum-rule. The results of the present calculation could be easily applied to derive the asymptotic heavy flavor corrections to the neutral current structure function xG_3 , [64]. However, the corresponding massless Wilson coefficient to 3-loop order has not been calculated yet.

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References

- [1] S. Bethke, et al., Workshop on precision measurements of α_s , arXiv:1110.0016 [hep-ph];
S. Moch, S. Weinzierl, et al., High precision fundamental constants at the TeV scale, arXiv:1405.4781 [hep-ph].
- [2] A.D. Watson, Z. Phys. C 12 (1982) 123.
- [3] W. Vogelsang, Z. Phys. C 50 (1991) 275.
- [4] S.I. Alekhin, J. Blümlein, Phys. Lett. B 594 (2004) 299, arXiv:hep-ph/0404034.
- [5] M. Buza, Y. Matiounine, J. Smith, R. Migneron, W.L. van Neerven, Nucl. Phys. B 472 (1996) 611, arXiv:hep-ph/9601302.
- [6] M. Buza, Y. Matiounine, J. Smith, W.L. van Neerven, Nucl. Phys. B 485 (1997) 420, arXiv:hep-ph/9608342.
- [7] I. Bierenbaum, J. Blümlein, S. Klein, arXiv:0706.2738 [hep-ph];
J. Blümlein, et al., in preparation.
- [8] J. Blümlein, H. Böttcher, Nucl. Phys. B 841 (2010) 205, arXiv:1005.3113 [hep-ph].
- [9] I. Bierenbaum, J. Blümlein, S. Klein, Nucl. Phys. B 780 (2007) 40, arXiv:hep-ph/0703285.
- [10] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider, F. Wißbrock, Nucl. Phys. B 886 (2014) 733, arXiv:1406.4654 [hep-ph].
- [11] D.Y. Bardin, J. Blümlein, P. Christova, L. Kalinovskaya, Nucl. Phys. B 506 (1997) 295, arXiv:hep-ph/9612435.
- [12] B. Lampe, E. Reya, Phys. Rep. 332 (2000) 1, arXiv:hep-ph/9810270.
- [13] J. Blümlein, Prog. Part. Nucl. Phys. 69 (2013) 28, arXiv:1208.6087 [hep-ph].
- [14] M. Buza, Y. Matiounine, J. Smith, W.L. van Neerven, Eur. Phys. J. C 1 (1998) 301, arXiv:hep-ph/9612398.
- [15] S. Wandzura, F. Wilczek, Phys. Lett. B 72 (1977) 195.
- [16] I. Bierenbaum, J. Blümlein, S. Klein, Nucl. Phys. B 820 (2009) 417, arXiv:0904.3563 [hep-ph].
- [17] J. Lagrange, Nouvelles recherches sur la nature et la propagation du son, *Miscellanea Taurinensis*, t. II, 1760–61; *Oeuvres t. I*, p. 263;
C.F. Gauss, *Theoria attractionis corporum sphaeroidicorum ellipticorum homogeneorum methodo novo tractate*, in: *Commentationes societas scientiarum Gottingensis recentiores*, Vol III, 1813, *Werke Bd. V*, pp. 5–7;
G. Green, *Essay on the Mathematical Theory of Electricity and Magnetism*, Nottingham, 1828 [*Green Papers*, pp. 1–115];

- M. Ostrogradski, Mem. Ac. Sci. St. Peters. 6 (1831) 39;
 K.G. Chetyrkin, A.L. Kataev, F.V. Tkachov, Nucl. Phys. B 174 (1980) 345.
- [18] Y. Matiounine, J. Smith, W.L. van Neerven, Phys. Rev. D 58 (1998) 076002, arXiv:hep-ph/9803439.
- [19] A. von Manteuffel, C. Studerus, arXiv:1201.4330 [hep-ph];
 C. Studerus, Comput. Phys. Commun. 181 (2010) 1293, arXiv:0912.2546 [physics.comp-ph].
- [20] R.H. Lewis, Computer algebra system *Fermat*, <http://home.bway.net/lewis>.
- [21] C.W. Bauer, A. Frink, R. Kreckel, Symb. Comput. 33 (2002) 1, cs/0004015 [cs.sc].
- [22] C. Schneider, Sémin. Lothar. Comb. 56 (2007) 1, article B56b.
- [23] C. Schneider, Computer algebra in quantum field theory: integration, summation and special functions, in: C. Schneider, J. Blümlein (Eds.), Texts and Monographs in Symbolic Computation, Springer, Wien, 2013, p. 325, arXiv:1304.4134 [cs.SC], 2013.
- [24] J. Ablinger, J. Blümlein, S. Klein, C. Schneider, Nucl. Phys. Proc. Suppl. 205–206 (2010) 110, arXiv:1006.4797 [math-ph];
 J. Blümlein, A. Hasselhuhn, C. Schneider, PoS RADCOR 2011 (2011) 032, arXiv:1202.4303 [math-ph];
 C. Schneider, Proc. of ACAT 2013, J. Phys. Conf. Ser. 523 (012037) (2014) 1, arXiv:1310.0160 [cs.SC].
- [25] C. Schneider, in: D. Bressoud (Ed.), Adv. Appl. Math. 34 (4) (2005) 740;
 J. Ablinger, J. Blümlein, M. Round, C. Schneider, PoS LL 2012 (2012) 050, arXiv:1210.1685 [cs.SC];
 M. Round, et al., in preparation.
- [26] J. Ablinger, PoS LL 2014 (2014) 019;
 J. Ablinger, Computer algebra algorithms for special functions, Ph.D. thesis, J. Kepler University, Linz, 2012, arXiv:1305.0687 [math-ph];
 J. Ablinger, A computer algebra toolbox for harmonic sums related to particle physics, Diploma thesis, J. Kepler University, Linz, 2009, arXiv:1011.1176 [math-ph];
 J. Ablinger, J. Blümlein, C. Schneider, J. Math. Phys. 52 (2011) 102301, arXiv:1105.6063 [math-ph];
 J. Ablinger, J. Blümlein, C. Schneider, J. Math. Phys. 54 (2013) 082301, arXiv:1302.0378 [math-ph].
- [27] W. Furmanski, R. Petronzio, Z. Phys. C 11 (1982) 293, and references therein.
- [28] W.L. van Neerven, E.B. Zijlstra, Phys. Lett. B 272 (1991) 127.
- [29] E.B. Zijlstra, W.L. van Neerven, Nucl. Phys. B 417 (1994) 61;
 E.B. Zijlstra, W.L. van Neerven, Nucl. Phys. B 426 (1994) 245 (Erratum);
 E.B. Zijlstra, W.L. van Neerven, Nucl. Phys. B 773 (2007) 105 (Erratum).
- [30] S. Moch, J.A.M. Vermaseren, A. Vogt, Nucl. Phys. B 813 (2009) 220, arXiv:0812.4168 [hep-ph].
- [31] S.A. Larin, J.A.M. Vermaseren, Phys. Lett. B 259 (1991) 345.
- [32] P.A. Baikov, K.G. Chetyrkin, J.H. Kühn, Phys. Rev. Lett. 104 (2010) 132004, arXiv:1001.3606 [hep-ph].
- [33] J.A.M. Vermaseren, Int. J. Mod. Phys. A 14 (1999) 2037, arXiv:hep-ph/9806280;
 J. Blümlein, S. Kurth, Phys. Rev. D 60 (1999) 014018, arXiv:hep-ph/9810241.
- [34] J. Blümlein, Comput. Phys. Commun. 180 (2009) 2218, arXiv:0901.3106 [hep-ph].
- [35] J. Blümlein, in: A. Carey, D. Ellwood, S. Paycha, S. Rosenberg (Eds.), Proceedings of the Workshop Motives, Quantum Field Theory, and Pseudodifferential Operators, Clay Mathematics Institute, Boston University, 2–13 June 2008, in: Clay Mathematics Proceedings, vol. 12, 2010, pp. 167–186, arXiv:0901.0837 [math-ph].
- [36] J. Blümlein, A. Vogt, Phys. Rev. D 58 (1998) 014020, arXiv:hep-ph/9712546.
- [37] J. Blümlein, Comput. Phys. Commun. 133 (2000) 76, arXiv:hep-ph/0003100;
 J. Blümlein, S.O. Moch, Phys. Lett. B 614 (2005) 53, arXiv:hep-ph/0503188.
- [38] E. Remiddi, J.A.M. Vermaseren, Int. J. Mod. Phys. A 15 (2000) 725, arXiv:hep-ph/9905237.
- [39] J. Blümlein, Comput. Phys. Commun. 159 (2004) 19, arXiv:hep-ph/0311046.
- [40] J. Blümlein, N. Kochelev, Nucl. Phys. B 498 (1997) 285, arXiv:hep-ph/9612318.
- [41] J.D. Jackson, G.G. Ross, R.G. Roberts, Phys. Lett. B 226 (1989) 159.
- [42] R.G. Roberts, G.G. Ross, Phys. Lett. B 373 (1996) 235, arXiv:hep-ph/9601235.
- [43] J. Blümlein, N. Kochelev, Phys. Lett. B 381 (1996) 296, arXiv:hep-ph/9603397.
- [44] J. Blümlein, V. Ravindran, W.L. van Neerven, Phys. Rev. D 68 (2003) 114004, arXiv:hep-ph/0304292.
- [45] A. Piccione, G. Ridolfi, Nucl. Phys. B 513 (1998) 301, arXiv:hep-ph/9707478.
- [46] J. Blümlein, A. Tkabladze, Nucl. Phys. B 553 (1999) 427, arXiv:hep-ph/9812478.
- [47] J. Blümlein, D. Robaschik, Nucl. Phys. B 581 (2000) 449, arXiv:hep-ph/0002071.
- [48] J. Blümlein, D. Robaschik, B. Geyer, Eur. Phys. J. C 61 (2009) 279, arXiv:0812.1899 [hep-ph].
- [49] J. Blümlein, D. Robaschik, Phys. Rev. D 65 (2002) 096002, arXiv:hep-ph/0202077.
- [50] R. Kirschner, L.N. Lipatov, Nucl. Phys. B 213 (1983) 122;
 J. Blümlein, A. Vogt, Phys. Lett. B 370 (1996) 149, arXiv:hep-ph/9510410;
 J. Blümlein, A. Vogt, Acta Phys. Pol. B 27 (1996) 1309, arXiv:hep-ph/9603450.

- [51] Y. Kiyo, J. Kodaira, H. Tochimura, *Z. Phys. C* 74 (1997) 631, arXiv:hep-ph/9701365.
- [52] S. Moch, J.A.M. Vermaasen, A. Vogt, *Nucl. Phys. B* 889 (2014) 351, arXiv:1409.5131 [hep-ph].
- [53] S. Alekhin, J. Blümlein, S. Moch, *Phys. Rev. D* 89 (5) (2014) 054028, arXiv:1310.3059 [hep-ph].
- [54] S. Alekhin, J. Blümlein, K. Daum, K. Lipka, S. Moch, *Phys. Lett. B* 720 (2013) 172, arXiv:1212.2355 [hep-ph].
- [55] D. Boer, M. Diehl, R. Milner, R. Venugopalan, W. Vogelsang, D. Kaplan, H. Montgomery, S. Vigdor, et al., arXiv:1108.1713 [nucl-th];
A. Accardi, J.L. Albacete, M. Anselmino, N. Armesto, E.C. Aschenauer, A. Bacchetta, D. Boer, W. Brooks, et al., arXiv:1212.1701 [nucl-ex].
- [56] J. Blümlein, H. Böttcher, A. Guffanti, *Nucl. Phys. B* 774 (2007) 182, arXiv:hep-ph/0607200.
- [57] J. Blümlein, S. Riemersma, M. Botje, C. Pascaud, F. Zomer, W.L. van Neerven, A. Vogt, in: *Proceedings Future Physics at HERA*, Hamburg, 1995/96, p. 23, arXiv:hep-ph/9609400;
J. Blümlein, S. Riemersma, W.L. van Neerven, A. Vogt, *Nucl. Phys. Proc. Suppl.* 51C (1996) 97, arXiv:hep-ph/9609217.
- [58] J.D. Bjorken, *Phys. Rev. D* 1 (1970) 1376.
- [59] D. Mund, B. Märkisch, M. Deissenroth, J. Krempel, M. Schumann, H. Abele, A. Petoukhov, T. Soldner, *Phys. Rev. Lett.* 110 (2013) 172502, arXiv:1204.0013 [hep-ex].
- [60] J. Kodaira, S. Matsuda, T. Muta, K. Sasaki, T. Uematsu, *Phys. Rev. D* 20 (1979) 627.
- [61] S.G. Gorishnii, S.A. Larin, *Phys. Lett. B* 172 (1986) 109.
- [62] J. Blümlein, W.L. van Neerven, *Phys. Lett. B* 450 (1999) 417, arXiv:hep-ph/9811351.
- [63] W.L. van Neerven, in: A.H. Blin, B. Hiller, M.C. Ruivo, C.A. de Sousa, E. van Beveren (Eds.), *Proceedings of the Workshop Hadron Physics: Effective Theories of Low-Energy QCD*, Coimbra, Portugal, 1999, in: *AIP Conf. Proc.*, vol. 508, 2000, p. 162, arXiv:hep-ph/9910356.
- [64] A. Arbuzov, D.Y. Bardin, J. Blümlein, L. Kalinovskaya, T. Riemann, *Comput. Phys. Commun.* 94 (1996) 128, arXiv:hep-ph/9511434;
J. Blümlein, M. Klein, T. Naumann, T. Riemann, *Structure Functions, Quark Distributions and Λ_{QCD} at Hera*, PHE-88-01.