A calculation of the three-loop helicity-dependent splitting functions in QCD

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We have calculated the complete matrix of three-loop helicity-difference (‘polarized’) splitting functions $\Delta F^{(2)}_{ik}(x)$, $i,k = q,g$, in massless perturbative QCD. In this note we briefly discuss some properties of the polarized splitting functions and our non-standard determination of the hitherto missing lower-row quantities $\Delta F^{(2)}_{gq}$ and $\Delta F^{(2)}_{gg}$. The resulting next-to-next-to-leading order (NNLO) corrections to the evolution of polarized parton distributions are illustrated and found to be small even at rather large values of the strong coupling constant $\alpha_s$. 

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1. Introduction: Polarized PDFs, their evolution, $\alpha_s^2$ calculations, large-x limit

The unpolarized and polarized parton distributions of a longitudinally polarized hadron are given by

$$f_i(x, \mu^2) = f_i^\rightarrow(x, \mu^2) + f_i^\leftarrow(x, \mu^2)$$

and

$$\Delta f_i(x, \mu^2) = f_i^\rightarrow(x, \mu^2) - f_i^\leftarrow(x, \mu^2),$$

respectively, in terms of the quark and gluon distributions $f_i^\rightarrow$ and $f_i^\leftarrow$ for the same and opposite helicity. Here $x$ is the parton’s momentum fraction, and $\mu$ denotes the factorization scale which, in the present context, can be identified with the renormalization scale without loss of information.

Their scale dependence is governed by the renormalization-group evolution equations

$$\frac{d}{d \ln \mu^2} (\Delta) f_i(x, \mu^2) = \left[(\Delta) P_{ik}^{(s)}(\alpha_s(\mu^2)) \otimes (\Delta) f_i(x, \mu^2)\right](x),$$

where $\otimes$ represents the standard Mellin convolution. The expansion of the respective splitting functions powers of the strong coupling constant $\alpha_s(\mu^2)$ can be written as

$$(\Delta) P_{ik}^{(s)}(x, \mu^2) = \sum_{n=0} \alpha_s^{n+1}(\Delta) P_{ik}^{(n)}(x)$$

with $a_s \equiv \alpha_s(\mu^2)/(4\pi)$.

The third-order (NNLO) contributions $\Delta P_{ik}^{(2)}$ for the polarized case are the subject of this note.

The corresponding second-order order calculations were performed in the 1990s, when a lot of attention was devoted to the polarized parton distributions in the wake of the ‘spin-crisis’ set off by Ref. [1] in 1988. All these calculations were performed in the framework of dimensional regularization, and thus had to address the treatment of the Dirac matrix $\gamma_5$ in $D \neq 4$ dimensions.

The splitting functions $\Delta P_{qg}^{(1)}$ and $\Delta P_{qg}^{(1)}$ were obtained, together with the second-order coefficient functions for the structure function $g_1$ in polarized deep-inelastic scattering (DIS) by Zijlstra and van Neerven in 1993 [2], using the so-called Larin scheme [3] with $\gamma_{5L} = \frac{i}{6} \epsilon_{\mu\nu\rho\sigma} \gamma_\mu \gamma_\nu \gamma_\rho$, where the resulting contractions of the $\epsilon$-tensor are evaluated in terms of the $D$-dimensional metric.

The complete matrix $\Delta P_{ij}^{(1)}$ was calculated in 1995 independently by Mertig and van Neerven [4] and by Vogelsang [5]. The former calculation was performed in the framework of the operator product expansion (OPE) and used the ‘reading-point’ scheme for $\gamma_5$ [6]. The latter calculation was carried out in the lightlike axial-gauge approach and employed primarily the ‘t Hooft/Veltman prescription for $\gamma_5$ of Refs. [7] which, in the present context, is equivalent to the Larin scheme.

The relation of the prescriptions of Refs. [3, 7] to the $\overline{\text{MS}}$ scheme was addressed to second order (NNLO) in 1998 in Ref. [8], where the transformation matrix is of the form

$$Z_{ik}(\alpha_s(\mu^2)) = \delta_{ij} \delta_{kg} (a_s z_{ns}^{(1)} + a_s^2 (z_{ns}^{(2)} + z_{ps}^{(2)})) + \ldots.$$  

Its non-singlet (ns) entries can be fixed by the relation between the corresponding coefficient functions for $g_1$ and the structure function $F_3$ which is known to order $\alpha_s^3$ [9]. The critical part is thus the pure-singlet (ps) part for which only that one calculation has been performed so far.

For reasons that will become obvious below, it is important for us to control the $x \to 1$ threshold limits of the splitting functions. Here it is reasonable to expect a helicity-flip suppression by a factor of $(1-x)^2$ or $1/N^2$ in Mellin space, cf. Ref. [10]. E.g., the differences $\delta_{ik}^{(0)} \equiv P_{ik}^{(0)} - \Delta P_{ik}^{(0)}$ of the (scheme-independent) leading-order (LO) unpolarized and polarized splitting functions read

$$\delta_{qg}^{(0)} = 0, \quad \delta_{ik}^{(0)} = \text{const} \cdot (1-x)^2 + \ldots \quad \text{for } ik = qg, gq, gg.$$
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Figure 1: The two-loop (NLO) splitting functions $\Delta P^{(1)}_{i \neq k}(x)$, compared to their unpolarized counterparts. The results are shown as published in Refs. [4, 5] (‘M’) and after an including an additional term $\varepsilon^{(1)}_{\text{gq}} = -\Delta \rho^{(0)}_{\text{gq}}$ in the transformation from the Larin scheme (‘A’), which removes all $(1-x)^0$ terms from $\delta^{(1)}_{\text{gq}}$. The corresponding NLO results are, in the standard version (denoted by ‘M’ below) of $\overline{\text{MS}}$ [4, 5],

$$\delta^{(1)}_{ik} = \Theta((1-x)^a) \quad \text{for} \quad ik = \text{qq, gg (with } a=1), \text{ qg (with } a=2) \quad (1.6)$$

$$\delta^{(1)}_{\text{gq}} = 8C_F(C_A-C_F)(2-x) \ln(1-x) + 4C_F\beta_0 - 6C_F^2 + (20/3C_F C_A + 2C_F^2 - 8/3C_F n_f)(1-x) + \Theta((1-x)^2). \quad (1.7)$$

The question arises whether these $(1-x)^0$ and $(1-x)^1$ terms are a physical feature or a scheme artifact. Flavour-singlet physical evolution kernels for structure functions in DIS, cf. Refs. [11, 12],

$$\frac{dF}{d\ln Q^2} = \frac{dC}{d\ln Q^2} f + C \rho f = (\beta a_s) \frac{dC}{da_s} + C \rho C^{-1} F = K F, \quad (1.8)$$

if available for corresponding quantities, can provide insight on this question.

2. $\alpha_S^3$ contributions via $g_1$ (at all $N$), and graviton-exchange DIS (for fixed $N$-values)

Following Refs. [13–17], our third-order calculation of polarized DIS proceeds via the optical theorem, which relates probe($q$)-parton($p$) total cross sections (with $Q^2 = -q^2 > 0$ and $p^2 = 0$) to forward amplitudes, and a dispersion relation in $x$, which provides the $N$-th Mellin moment

$$A^N = \int_0^1 dx x^{N-1} A(x) \quad (2.1)$$

from the coefficient of $(2p \cdot q)^N$. The unpolarized case was first computed at even $N \leq 10$ in the mid 1990s in Refs. [13, 14], using the Mincer program for three-loop self-energy integrals [18]. The corresponding all-$N$ and all-$x$ expressions were derived by us ten years ago [15–17].

A brief account of the extension of the latter calculations to the polarized structure function $g_1$ was presented at Loops & Legs 2008 [19], where we focused on the resulting expressions for $\Delta P^{(2)}_{\text{gq}}$ and $P^{(2)}_{\text{gq}}$, which can be extracted from the $\varepsilon^{-1}$ poles of the unfactorized structure functions.
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The resulting $C_{2n_f}^2$ contribution to the latter function, in the standard $M$ scheme, is given by

$$\frac{1}{8} \Delta P_{qg}^{(2)}(N) \big|_{C_{2n_f}^2} = 2 \Delta p_{qg} (-S_{-4} + 2 S_{-2}-2 + 4 S_{1,1} - 3 + 2 S_{1,1,1,1} - S_{1,1,2} - 5 S_{1,2,1}$$

$$+ 4 S_{1,3} + 2 S_{2,-2} - 6 S_{2,1,1} + 6 S_{2,2} + 7 S_{3,1} - 3 S_4 - 3 S_5 (2 D_0^2 + 4 D_1^2 - 9 D_0 + 12 D_1) + 4 S_{-3} (D_0^2 - 2 D_0 + 2 D_1) + 8 S_{1,-2} (2 D_1^2 - D_0 + D_1)$$

$$- 2 S_{2,1} (4 D_0^2 + 2 D_1^2 - 11 D_0 + 11 D_1) + S_{1,1,1} (5 D_0^2 - 2 D_1^2 - 21/2 D_0 + 12 D_1)$$

$$- 2 S_{1,2} (2 D_0^2 - 2 D_1^2 - 5 D_0 + 5 D_1) + 2 S_3 (3 D_0^2 + 6 D_1^2 - 11 D_0 + 11 D_1)$$

(2.2)

$$+ 2 S_{-2} (8 D_0^3 - 5 D_0^2 - 6 D_1^2 + 10 D_0 - 9 D_1) - S_{1,1} (10 D_0^3 + 6 D_1^2 - 35/2 D_0^2 - 5 D_1^2$$

$$+ 29 D_0 - 36 D_1) + 2 S_2 (4 D_0^3 + 6 D_1^2 - 10 D_0^2 - 4 D_1^2 + 17 D_0 - 22 D_1) - 6 D_2 (S_{-2} + 1)$$

$$+ S_1 (7 D_0^4 + 4 D_1^4 - 43/2 D_0^2 - 15 D_1^2 + 99/2 D_0^2 + 18 D_1^2 - 78 D_0 + 329/4 D_1) + 32 D_1^5$$

$$- 15/2 D_0^3 - 3 D_1^3 + 59/8 D_0^3 + 53/4 D_1^3 + 77/8 D_0^3 + 213/8 D_1^3 - 1357/32 D_0 + 777/16 D_1$$

in terms of $D_k = (N + k)^{-1}$ and $\Delta p_{qg} = 2 D_{1} - D_{0}$, with all harmonic sums [20] at argument $N$.

This result shows some interesting features. The weight-4 sums in the first two rows have the same coefficient in the unpolarized case of Ref. [16], where $\Delta p_{qg}$ is replaced by its counterpart $p_{qg}$. The lower-weight denominator structure is simpler in the present case, with only two terms with $D_2$ (third line from below) which do not lead to additional denominator primes at odd values of $N$. As in previous results in massless QCD, Eq. (2.2) does not include sums with index $-1$. The large-$N$ suppression of $\Delta_{qg}^{(2)}$ by two powers of $1/N$ holds separately for each harmonic sum. Finally the coefficients $D_{0,1}^2, D_{1,1}^4$ and $S_{1,1,1}$ are predictable in terms of $x \to 0$ and $x \to 1$ knowledge, i.e., by Ref. [21] and by extending Ref. [22], see also Ref. [23], and Ref. [12] to the present case.

The lower-row splitting functions $\Delta P_{qg}^{(2)}$ and $\Delta P_{qg}^{(2)}$ enter standard (electroweak gauge-boson exchange) DIS only at order $\alpha_s^2$. Hence an additional probe directly coupling to gluons is required. Following Ref. [11], the computation of $F_2$ has been complemented by DIS via a scalar $\phi$ with a $\phi G_{\mu\nu} G_{\mu\nu}$ coupling to gluons, i.e., the Higgs boson in the heavy-top limit, in Refs. [14, 16].

In the polarized case a non-(pseudo) scalar probe is required, in contrast to our statement in the penultimate paragraph of Ref. [19], which was based on an incorrectly simplified diagram database. One way to address this issue would be to extent the calculations to a supersymmetric case, as done in the context of NNLO antenna functions in Ref. [24]. Instead we consider graviton-exchange DIS, as described in Ref. [25], see also Ref. [26], which provides five relevant structure functions, $H_k, k = 1 - 4, 6$, that can be combined to provide unpolarized and polarized analogues of the system $(F_2, F_0)$, plus an analogue of the standard longitudinal structure function $F_L$.

A major drawback of this approach is that it leads to a very large number of higher tensor integrals, far beyond those tabulated during the calculation of $F_2$ and $F_0$ [15–17] and its later extension to $g_1$ [19]. We have therefore decided to (first) fall back to fixed-$N$ calculation using MINCER [18], for which we have improved our diagram management and, in particular, the high-$N$ efficiency of the MINCER program, see Ref. [27]. These improvements have allowed us to calculate polarized graviton-exchange DIS at the third order completely for the 12 odd moments $3 \leq N \leq 25$. The first moments are directly accessible neither in our calculation nor via operator matrix elements [25].

The calculations were performed on computers at DESY-Zeuthen (mainly for MINCER development), NIKHEF (hardest diagrams at highest values of $N$) and the ulgqcd cluster in Liverpool.
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(bulk production, using more than 200 cores), using the latest version of TFORM [28].

As an example, we here show the calculated moments of the $C_F^3$ part of $\Delta P_{gq}^{(2)}$ in the Larin scheme.

\[
\begin{align*}
N = 3: & \quad \frac{186505}{7776} \\
N = 5: & \quad \frac{9473569}{303750} \\
N = 7: & \quad -\frac{509428539731}{193616640000} \\
N = 9: & \quad -\frac{26684720969207}{56710659600000} \\
N = 11: & \quad -\frac{3349566589170829651}{608872292828640000} \\
N = 13: & \quad -\frac{7517747672901480225}{130490947198744678400000} \\
N = 15: & \quad -\frac{118907325528302937678830745102921869938637}{38642690852856502186336305851160000000000}
\end{align*}
\]

Returning to the large-$x$ limit, we note that the unpolarized structure functions $H_2$ and $H_3$) and $H_3$ (LO: gluons, from the outset) and their polarized counterparts $H_4, H_6$ form a set of quantities as mentioned at the end of Section 1. Comparing the NLO evolution kernel $K_{22}^{(1)}$ and $K_{64}^{(1)}$, which we have calculated at all $N_f/x$, we can conclude that the large-$x$ behaviour of $\Delta P_{gq}^{(1)}$ of Refs. [4, 5] discussed above is not physical.

Consequently one may expect the existence of a simple additional NNLO transformation that restores also the $1/N^2$ suppression of $\delta_{gq}^{(2)}(N) = P_{gq}^{(2)}(N) - \Delta P_{gq}^{(2)}(N)$. As shown in Fig. 2, where all non-$n_f$ and $n_f^1$ colour factors have been combined for brevity, this expectation appears to be justified. Hence the three-loop analogue of Eq. (1.7) can be predicted from lower-order information.

\[ z_{gq}^{(2)} = -\frac{1}{2} \Delta P_{gq}^{(1) L} \]

**Figure 2:** The moments of the three-loop (NNLO) splitting functions $\Delta P_{gq}^{(2)}$ in QCD determined using the MINCER program for graviton-exchange DIS. The results are shown separately for the $n_f^0$ and $n_f^1$ part in the Larin scheme (‘L’), the standard $\overline{\text{MS}}$ scheme according to Ref. [8] (‘M’) and with a NNLO additional term $z_{gq}^{(2)} = -\frac{1}{2} \Delta P_{gq}^{(1) L}$ in the transformation from the Larin scheme to $\overline{\text{MS}}$ (‘A’).
3. All-\( N \) expressions, using end-point knowledge and number-theory tools

We illustrate the determination of the all-\( N \) expressions for the critical \( n_f^0 \) parts of \( \Delta P_{\text{gg}}^{(2)}(N) \). Analogous to Eq. (2.2), the coefficients of the weight-4 sums are fixed by the unpolarized case. This leaves 2\( \times 32 \) coefficients of sums at weight three and below combined with powers of \( N \)\(^{-1} \) and \( (N+1)^{-1} \), plus up to 11 sums combined with \( (N-1)^{-1} \). Of these 75 unknowns, the 24 coefficients of \( D_0^1 \) and \( D_1^1 \) can be eliminated using the empirical \( 1/N^2 \) large-\( N \) suppression of \( S_{\text{gg}}^{(2)}(N) \) in the \( \Lambda \)-scheme, and a further 6 from small-\( x \) and large-\( x \) constraints as discussed below Eq. (2.2).

We have developed FORM tools which analyze the prime decomposition of the calculated moments and facilitate the derivation of relations between the remaining coefficients (which are all integer if suitably normalized) using the Chinese remainder theorem. These have proved sufficient, sometimes together with a brute-force scan of a few remaining variables, to solve simpler cases. It is however rather hard to get more than about ten relations for the difficult \( n_f^0 \) parts of \( \Delta P_{\text{gg}}^{(2)}(N) \).

Motivated by Ref. [29], we have turned to professional number-theory tools for these cases, in particular the program provided at www.numbertheory.org/php/axb.html which ‘Solves a system of linear Diophantine equations using the Hermite normal form of an integer matrix via the Havas-Majewski- Matthews LLL-based algorithm. . . . . We find . . . the solutions \( X \) in particular the program provided at www.numbertheory.org/php/axb.html which

\[ 1/8 \Delta P_{\text{gg}}^{(2)}(N)_{C_3^f} = 2 \Delta P_{\text{gg}}(−S_{−4} + 6S_{−2,+2} + 4S_{1−3} + 2S_{1,1,1,1} + S_{1,1,2} + 3S_{1,2,1} − 3S_{1,3} + 2S_{2,−2} + 2S_{2,1,1} − 2S_{2,2}) + 6c_3 \Delta P_{\text{gg}}(2S_1 − 3) − 4S_{−3}(2D_0^2 − D_0 + D_1) − 8S_{−2}(D_1^2 − 2D_0 + 2D_1) + S_{1,1,2}(2D_0^2 − 5D_1^2 − 6D_0 − 3/2D_1) − 2S_{1,2}(D_1^2 + 4D_0 − D_1) − S_{2,1}(4D_0^2 + 4D_1^2 − 4D_0 + 7D_1) + S_{3}(2D_0^2 + D_1^2 + 6D_0 − 3/2D_1) \]

(3.1)

\[-S_{−2}(8D_0^3 + 4D_0^2 + 18D_0^2 − 26D_0 + 24D_1) + 2S_2(D_1^3 + 2D_1^2 + 10D_0 − 4D_1) − S_{1,1}(6D_0^3 + 6D_1^2 + 4D_0^2 + 5D_1^2 + 2D_0 − 7/4D_1) − 6D_{−1}(S_{−2} + 1) − S_1(6D_0^4 + 7D_1^4 + 4D_0^3 + 23/2D_0^3 + 27/2D_0^2 + 39/4D_1^2 + 8D_0 + 23/4D_1) − 8D_0^5 − 12D_0^4 + 23D_0^3 − 28D_1^4 − 39/4D_0^3 − 427/8D_1^3 − 341/8D_0^5 − 1767/8D_1^5 + 2427/16D_0 − 4547/32D_1 \]

with \( \Delta P_{\text{gg}} = 2D_0 − D_1 \) and, again, \( D_k = (N+k)^{-1} \) and all harmonic sums taken at argument \( N \). The corresponding expressions for the \( C_F C_2^f \) and \( C_2^f C_A \) parts are somewhat lengthier; while the \( n_f \)-dependent terms are much simpler and do not require the \( N=25 \) moment. The determination of the all-\( N \) result for the NNLO gluon-gluon splitting function \( \Delta P_{\text{gg}}^{(2)}(N) \) proceeded in an analogous manner; finding the all-\( N \) form of its \( C_3^f \) part was the overall most difficult task.

While it is easy to recognize, by looking at the pattern of the coefficients, whether or not the correct all-\( N \) form is returned by the solution of a Diophantine system, it is necessary to validate
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the results. For this purpose the results are Mellin-inverted to $x$-space expressions $\Delta P^{(2)}_{gq}(x)$ and $\Delta P^{(2)}_{gg}(x)$ in terms of harmonic polylogarithms [31], from which arbitrary moments can be determined. The results can thus be compared to additional moments calculated using MINCER, such as

$$-\Delta P^{(2)}_{gq}(N=27) = \frac{4609770383587605432813291530849726335264810727}{98293450862721631896656577854990940800000000} C_F^3 + \cdots$$

with

Further high-$N$ checks have been performed for $\Delta P^{(2)}_{gq}(N=29)$ in the planar limit $C_A - 2C_F \to 0$ at $n_f=0$, which combines the three difficult all-$N$ expressions, and for the crucial $C_A^3$ parts of $\Delta P^{(2)}_{gg}(N)$ at $N=27$ and $N=29$. The functions $\Delta P^{(2)}_{gq}(x)$ and $\Delta P^{(2)}_{gg}(x)$ pass all these tests.

Finally these $x$-space expressions also facilitates the determination of the first moments,

$$\Delta P^{(2)}_{gq}(N=1) = \frac{1607}{12} C_F C_A^2 - \frac{461}{4} C_F^2 C_A + \frac{63}{2} C_F^3 + \left( \frac{41}{3} - 72 \xi_3 \right) C_F C_A n_f$$

$$- \left( \frac{107}{2} - 72 \xi_3 \right) C_F^2 n_f - \frac{13}{3} C_F n_f^2,$$

$$\Delta P^{(2)}_{gg}(N=1) = \frac{2857}{54} C_A^3 - \frac{1415}{54} C_A^2 n_f - \frac{205}{18} C_F C_A n_f + \frac{79}{54} C_A n_f^2 + \frac{11}{9} C_F n_f^2$$

$$= \beta_2^{\overline{MS}}.$$ (3.4)

The agreement, for all six colour factors, of $\Delta P^{(2)}_{gg}(N=1)$ with the NNLO contribution [32] to the $\beta$-function of QCD in the $\overline{MS}$ scheme provides another strong check of our results.

The new splitting functions $\Delta P^{(2)}_{gq}(x)$ and $\Delta P^{(2)}_{gg}(x)$ are shown in Fig. 3. As in the previous figures, the curves are scaled such that the results are approximately converted from the small parameter $\alpha_s = \alpha_s/(4\pi)$ in Eq. (1.3) to an expansion in $\alpha_s$. In Fig. 4 the impact of these results on the evolution is illustrated for a sufficiently realistic model input [33] at a rather large value of $\alpha_s$.

![Figure 3](image_url)

**Figure 3:** The NNLO splitting functions $\Delta P^{(2)}_{gq}(x)$ (left) and $\Delta P^{(2)}_{gg}(x)$ (right) compared to the corresponding unpolarized quantities. The results are shown in the $M$ and $A$ schemes for three light flavours $n_f$. 

Total execution time: 256 874 306.6 sec. Maximum disk space: 1 261 024 031 636 bytes.
4. Summary and outlook: more checks and calculations

We have finally, 10 years after publishing their unpolarized counterparts [15,16], derived all NNLO helicity-difference splitting functions \( \Delta F_{ij}^{(2)}(x) \). The last part, the lower row \( \Delta F_{gq}^{(2)} \) and \( \Delta F_{gg}^{(2)} \) of the flavour-singlet matrix, has been obtained by a combination of brute-force computations using M\textsc{incer} [18], insights into the structure of these functions, and number-theory tools [30].

The three-loop M\textsc{incer} computations of graviton-exchange DIS [25] have also been performed for the unpolarized case and, also to very high values of the Mellin moment \( N \), for the upper row for which we had calculated the all-\( N \) results before [19]. The resulting agreement with the corresponding splitting functions provides checks of our treatment of graviton-exchange DIS and of the M\textsc{incer} code as modified for much better large-\( N \) performance.

Our results agree with all previous partial results – if interpreted properly; in particular, the leading small-\( x \) terms of Ref. [21] apply to the NNLO physical kernels in the off-diagonal cases, not to the corresponding \( \overline{\text{MS}} \) splitting functions – and expectations for the high-energy and threshold limits, the first moments of \( \Delta F_{gq} \) and the leading large-\( n_f \) contributions [34].

As for the unpolarized case, the numerical effects of these NNLO contributions are small down to low values of \( x \) after the convolution with realistic quark and gluon initial distributions. The published version of the \( \overline{\text{MS}} \) scheme, defined by the transformation correcting for the use of, e.g., the Larin scheme for \( g_5 \) in dimensional regularization, is somewhat unphysical for \( x \to 1 \) already at NLO. However this does not appear to be a practically relevant problem, hence we see no reason to advocate a change of the scheme after almost 20 years of NLO data analyses.

Nevertheless, a re-calculation of the critical NNLO transformation quantity \( z_{ps}^{(2)} \) (and a check of \( z_{gq}^{(n)} = 0 \)) would be worthwhile. In fact, its extension to the third order would suffice to fix the \( \text{N}^3\text{LO} \) quark coefficient function for \( g_1 \), as we obtained the Larin-scheme result some years ago.
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