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The complete three-loop unpolarized and polarized massive operator matrix elements and asymptotic Wilson coefficients

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We report on the three-loop unpolarized and polarized massive operator matrix elements, with single- and two-mass corrections, and the associated deep-inelastic massive Wilson coefficients in the region $Q^2 \gg m_Q^2$, the calculation of which has been completed recently. We also provide fast and precise numerical representations of the massless Wilson coefficients, splitting functions to tree-loop order, and target-mass corrections in x -space well suited for QCD-fitting codes.

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1. Introduction

The precision measurement of the strong coupling constant $a_s(M_Z^2) = \alpha_s(M_Z^2)/(4\pi)$ [1–4] and the mass of the charm quark m_c [5] using deep-inelastic scattering data needs to be performed under well-defined experimental conditions. Only for the twist-2 contributions, sufficiently precise calculations were performed. The higher twist corrections have therefore to be removed by kinematic cuts [6–9]. At an intended precision of $O(1\%)$ and better, this requires to refer to data $Q^2 \gtrsim 20 \text{ GeV}^2$ and $W^2 = Q^2(1-x)/x \gtrsim 15 \text{ GeV}^2$ for the virtuality and the hadronic mass squared in the deep-inelastic scattering process. This is also the region for which it has been shown in Ref. [10] that the asymptotic heavy-flavor corrections for the structure function $F_2(x, Q^2)$ at $O(a_s^2)$ agree at the level of $O(1\%)$ with the full phase-space calculation in Refs. [11–13].

In the asymptotic region, analytic results can be calculated at $O(a_s^3)$ in the single- and two-mass cases. Here, simple alphabet structures ruling the massless case, such as harmonic sums [14, 15], are not sufficient anymore. The solution spaces are spanned by generalized harmonic sums [16, 17], cyclotomic harmonic sums [18], nested binomial harmonic sums [19], iterated integrals over letters implied by quadratic forms [20], and ${}_2F_1$ - or complete elliptic letters (which are modular forms) [21].

Even more involved structures appear in the two-mass case. Of course, one can derive the corresponding iterated-noniterative integrals [22]. In the end one needs, however, fast and precise numerical implementations.¹ For this purpose, the analytic method described in Ref. [29] is very well suited. It is based on overlapping deep local analytic expansions of logarithmically modulated Taylor expansions, allowing to reach any precision.

Analytic results in the full phase space were computed to $O(a_s^2)$ for the non-singlet and pure-singlet contributions both in the unpolarized and polarized cases in Refs. [10, 30–33]. This is also possible for the gluonic cases, at the expense of alphabets containing higher transcendental letters. The non-singlet contributions at $O(a_s^2)$ already contain root-valued letters [19] and the iterated integrals in the pure-singlet case contain incomplete elliptic integrals [32, 33]. In Ref. [34] a complete Mellin-space implementation of the $O(a_s^2)$ results [11–13] has been derived for $N \in \mathbb{C}$ at high precision for the use in Mellin-space QCD analysis programs. The corresponding phase-space integrals at $O(a_s^3)$ will contain even more of these structures, and imply various thresholds and pseudo-thresholds to be dealt with in their numerical quantification. Furthermore, in part of the contributions one faces a three-scale problem due to the presence of both the charm and bottom quark masses.

In the following we will give a survey on the quantitative three-loop results of the heavy-flavor corrections to deep-inelastic scattering for larger virtualities both in the unpolarized and polarized case to three-loop order. We describe the computation methods used in Section 2. A survey on the single-mass corrections is given in Section 3, and the two-mass corrections are described in Section 4. In Section 5, we discuss the implications for the structure function $F_2(x, Q^2)$. In Refs. [35, 36] we also presented fast and precise numerical implementations for all unpolarized and polarized single-mass operator matrix elements (OMEs) and asymptotic massive Wilson coefficients

¹Even for the numerical quantification of harmonic polylogarithms [23] over a simple alphabet [24] of only three (non-singular) letters, efficient numerical implementations have to be found [25–27], consisting of the Bernoulli-method or Hölder convolution [28], despite having a formal representation as iterative integrals.

as public codes. In Section 6, we supplement these for the massless three-loop Wilson coefficients and splitting functions in the same form, for convenient use for x -space QCD-analysis codes. Moreover, we add a numerical implementation for the target-mass corrections. Section 7 contains the conclusions.

2. The Computation Methods

The massive three-loop operator matrix elements A_{ij} are propagator integrals containing local operator insertions [37, 38]. Their renormalization includes mass-, coupling constant-, and operator-renormalization, as well as the subtraction of the collinear singularities of massless sub-graphs, see Ref. [38] in the single-mass case and Refs. [39, 40] in the two-mass case. The factorization relations valid for virtualities $Q^2 \gg m_Q^2$, with m_Q the heavy-quark mass, cf. Refs. [35, 41], imply the representation of the heavy-flavor Wilson coefficients in terms of polynomials of respective pieces of the massive OMEs and the massless Wilson coefficients [42–44] in Mellin space in this kinematic region.

The calculation of the contributing Feynman diagrams from their generation to the reduction to the master integrals has been described in Ref. [45]. We use the packages QGRAF, Form, Color and Reduze 2 [46–51]. In the polarized case we compute the OME in the Larin scheme [52].

For the calculation of the different diagram classes, different calculation methods were used. The simpler topologies can be computed directly using the method of (generalized) hypergeometric functions [53–56], paired with direct summation methods [57, 58]. Here algorithms of difference ring theory were used [59–70].

In the more involved cases, the spanning functions both in Mellin- and x -space were not known a priori, but had to be derived algorithmically. Here the method of arbitrary high Mellin moments [71] is essential, since it allows to find the input required to obtain the corresponding recursions from a finite number of moments. These are determined using guessing methods [72–75]. Next, it has to be analyzed by using the package Sigma [76, 77] whether the recursion is first-order-factorizing or not. In the former case, one finds sum-product representations of the solution. This has to be the case for the *whole* physical set of Mellin-moments, cf. Ref. [78]. In the case of the OMEs $A_{gg,Q}^{(3)}$ and $\Delta A_{gg,Q}^{(3)}$ [79] this turned out not to be the case down to the lowest moment for a single diagram, for which x -space technologies had to be used to obtain the correct physical expression. The evanescent sum-product solution valid for all higher moments thus turns out to be a special case of a global higher transcendental solution. Techniques implemented in the package HarmonicSums.m [14, 15, 17–19, 23, 24, 80–91] allow to derive the associated x -space representations and offers various methods to simplify the results.

In the case of the single- and two-mass OMEs $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$ these representations are not sufficient. Although one may obtain recurrences for these quantities in N -space, they are not first-order-factorizable. Also the differential equations in x -space do not factorize to first order. The corresponding iterated integrals contain higher transcendental letters. They can be calculated using the method described in Ref. [29]. The local operators defined for discrete integer values of N are resummed into a generating function which depends on the continuous real variable $t \in [0, \infty[$, cf. Refs. [55, 92]. Furthermore, before treating the regular part, one has to subtract the distribution-valued contributions.

The master integrals are computed in this variable by solving linear systems of coupled differential equations, see also Refs. [45, 93–96]. The initial values are provided by the Mellin moments, which are the expansion coefficients at $t = 0$ or $x \rightarrow \infty$. One solves the differential equations in t and performs then the analytic continuation from the region $t \in [0, 1]$ to $t \in [1, \infty[$. For $t < 1$ the amplitude does not contain an imaginary part. Still one has to perform a series of matchings of local expansions until one reaches the point $t = 1$. The variables t and x are related via $x = 1/t$. In the region $x \in [0, 1]$ the solutions are expanded into different overlapping logarithmic modulated Taylor series. This representation also provides the numerical results.

In the two-mass cases the gluonic OMEs can be represented by iterated integrals over root-valued letters, see Refs. [97, 98]. Also many new special constants beyond the multiple zeta values [80] are contributing. In the pure-singlet case, only the x -space representations obey first-order-factorizing differential equations [99, 100], which have to be solved for sub-intervals in $x \in [0, 1]$. Finally, the two-mass corrections for $A_{Q_g}^{(3)}$ and $\Delta A_{Q_g}^{(3)}$ [39] are calculated in a similar way as the ones in the single-mass case. The best convergence is obtained by expanding in the mass ratio around $m_c = m_b$ and by additional use of convergence acceleration due to Aitken extrapolation [101].

There is a variety of other calculation methods which have been developed and used in this project. A survey on these computer-algebraic and mathematical techniques are given in Refs. [102, 103].

3. The single-mass corrections

The extrinsic inclusive heavy-quark corrections to deep-inelastic scattering in the unpolarized and polarized case were obtained in Refs. [104–107] and [108]. At two-loop order, numerical results for the complete kinematics in the unpolarized case were obtained in Refs. [11–13], and in the polarized case in Ref. [109]. Mellin-space implementations were given in Ref. [34]. Analytic two-loop calculations were performed in the unpolarized and polarized non-singlet cases in Refs. [10, 30, 31] and in the pure-singlet cases in Refs. [32, 33].

Analytic two-loop calculations of the heavy-flavor Wilson coefficients in the region $Q^2 \gg m_Q^2$ were independently performed in Refs. [10, 54] in the unpolarized case and Refs. [30, 110] in the polarized case. Further massive OMEs contributing to the variable flavor number scheme were calculated to two-loop orders in Refs. [41, 111].

The logarithmic three-loop corrections are based on the complete two-loop results for the massive OMEs and the three-loop massless Wilson coefficients [42–44]. These contributions were given in Refs. [112, 113] in the unpolarized case and in Ref. [114] in the polarized case.

Also the asymptotic three-loop corrections to the structure function $F_L(x, Q^2)$ depend only on the two-loop massive OMEs and were calculated in Ref. [115]. It turns out that these corrections, already at NLO, describe the full phase-space results only for $Q^2/m_Q^2 > 800 \text{ GeV}^2$, i.e. in a kinematic region, where there are currently no data.

The asymptotic massive three-loop Wilson coefficients for the unpolarized structure function $F_2(x, Q^2)$ and polarized structure function $g_1(x, Q^2)$ were calculated in Refs. [36, 45, 113, 116–118]. and Refs. [36, 45, 114, 116, 118–120]. Where necessary, we used the Larin scheme. Here, also the parton distributions have to be evolved in this scheme, see Ref. [121] for a parameterization.

Also the heavy-flavor corrections to deep-inelastic charged current structure functions were calculated. Here, also flavor excitation processes, e.g. for $s \rightarrow c$, contribute. For the one-loop order cross sections see Refs. [122, 123]. At two-loop order, there are results in the asymptotic region [124, 125]. Furthermore, there are three-loop heavy-flavor corrections to the non-singlet structure functions $x F_3(x, Q^2)$ [126] and the differences $F_L^{W^+ - W^-}(x, Q^2)$ and $F_2^{W^+ - W^-}(x, Q^2)$ [127].

The massive OMEs also determine the flavor matching in the variable flavor number scheme (VFNS). The two-loop single-mass matching relations were given in Ref. [41] with corrections given in Ref. [111] in the unpolarized case. The further two-loop massive OMEs in the polarized case were calculated in Ref. [110]. At three-loop order the VFNS was studied in Ref. [35].² The additional OMEs A_{gq} and A_{gg} were calculated in Refs. [79, 129] in the unpolarized case and Refs. [79, 130] in the polarized case.

Finally, also the massive three-loop corrections have been calculated to the massive OME for transversity in Refs. [116, 131].

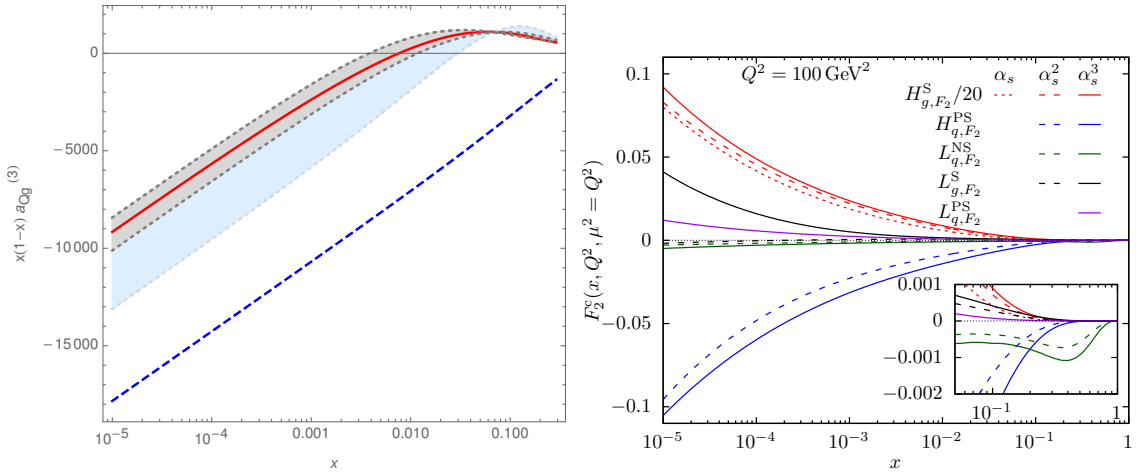


Figure 1: Left panel: the constant part of the massive OME $A_{Qg}^{(3)}$, $a_{Qg}^{(3)}(x)$, as a function of x , rescaled by the factor $x(1-x)$ in the region of smaller values of x . Full line (red): $a_{Qg}^{(3)}(x)$; dashed line (blue): leading small- x term $\propto \ln(x)/x$ [132]; light blue region: estimates of [112]; gray region: estimates of [133]; from Ref. [118]. Right panel: the charm contributions to the structure function $F_2(x, Q^2)$ by the Wilson coefficients $H_g^S, H_q^{PS}, L_q^{NS}, L_g^S$ and L_g^{PS} at $Q^2 = 100 \text{ GeV}^2$ at different orders in the strong coupling constant up to $O(\alpha_s), O(\alpha_s^2)$ and $O(\alpha_s^3)$; from Ref. [36]. For the notations of the massive Wilson coefficients see Ref. [38].

In Figure 1, we illustrate the constant part of the unpolarized unrenormalized three-loop single-mass OME A_{Qg} , $a_{Qg}^{(3)}(x)$, Ref. [45, 118]. Previous approximate estimates with error bands are now replaced by the exact result. We also show the result for the leading small- x term $\propto \ln(x)/x$, which does not describe the result. As also in various other cases [134–136] even in the small- x region a series of sub-leading terms are of the same size as the leading term or even larger and cause this difference. In an earlier analysis, there was a theory error of $\delta_T m_c = 70 \text{ MeV}$, much larger than the experimental error [5]. This error can now be significantly reduced.

²For the use in evolution codes see e.g. Ref. [128].

We also illustrate the different contributions to the heavy-flavor corrections, e.g. for the charm contributions in Figure 1. The positive gluonic terms are largest, followed by the negative pure-singlet terms in the small- x region. There are three other contributions which are smaller but are relevant at resolutions of $O(1\%)$. In the large- x region the non-singlet contribution dominates and is negative. That means that there the massless contributions to $F_2(x, Q^2)$ are diminished by the heavy-flavor contributions. The structure function is still positive.

4. The two-mass corrections

Two-mass heavy-flavor corrections arise first at two-loop order as factorizable vacuum polarization contributions in one-loop graphs for the OMEs A_{Qg} and $A_{gg,Q}$, cf. Ref. [137], in the unpolarized case and Ref. [110] in the polarized case. Genuine two-mass corrections arise from three-loop order and contribute to the OMEs $A_{qq,Q}^{\text{NS}}$, $A_{qq,Q}^{\text{NS,trans}}$ and $A_{gq,Q}$, calculated in Ref. [40]. The unpolarized and polarized two-mass OMEs A_{Qq}^{PS} were calculated in Refs. [98, 99], the ones for $A_{gg,Q}$ in Refs. [97, 98], for $\Delta A_{gq,Q}$ in Ref. [130]. Finally, the two-mass corrections to A_{Qg} in the unpolarized and polarized case were computed in Ref. [39].

Because the charm and bottom mass are very similar, one may consider to decouple both contributions together in a two-mass VFNS, cf. [40, 137]. The two-mass corrections to the structure functions emerge as $O(T_F^2 C_{F,A})$ contributions. We computed the relative two-mass part in all T_F^2 contributions. On average it amounts to $O(50\%)$ for all processes. We illustrate this for the two-mass contributions to $A_{gq}^{(3)}$ in Figure 2.

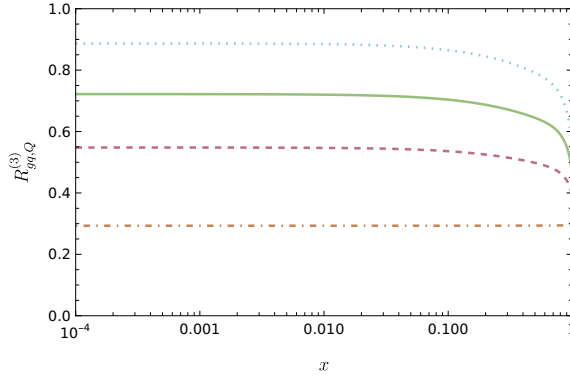


Figure 2: The ratio of the three-loop two-mass contributions to $A_{gq,Q}$ to the complete gq $O(T_F^2)$ corrections. Dotted line: $Q^2 = 30 \text{ GeV}^2$; Full line: $Q^2 = 50 \text{ GeV}^2$; Dashed line: $Q^2 = 100 \text{ GeV}^2$; Dashed-dotted: $Q^2 = 1000 \text{ GeV}^2$.

5. The structure functions

The present results on the asymptotic heavy-flavor Wilson coefficients allow the NNLO QCD-analysis of the deep-inelastic structure function data on $F_2(x, Q^2)$ at large enough virtualities for the first time. Corresponding results were also obtained for the polarized structure function $g_1(x, Q^2)$.

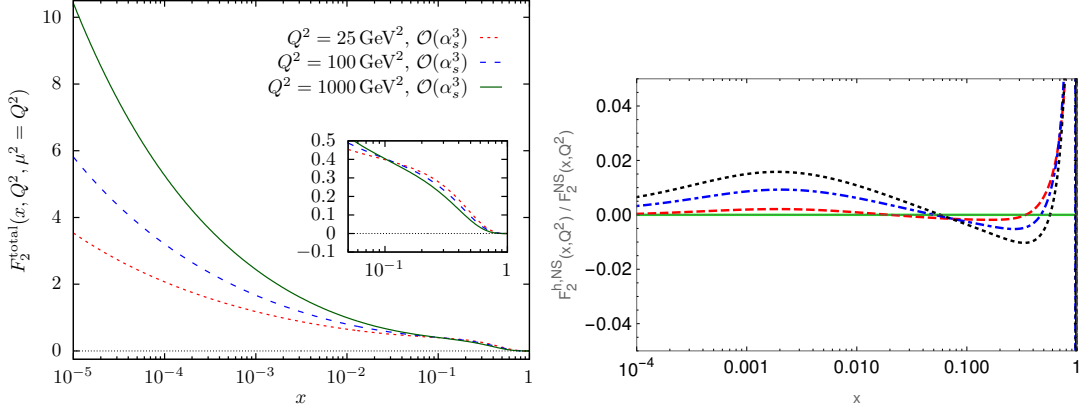


Figure 3: Left panel: The structure function $F_2(x, Q^2)$ at NNLO containing the massless and the asymptotic single-mass contributions due to charm and bottom quarks as a function of x and Q^2 , using the parton distribution functions of Ref. [133]; from Ref. [36]. Right panel: The relative contribution of the heavy-flavor contributions due to c and b quarks to the structure function F_2^{NS} ; dashed lines: 100 GeV²; dashed-dotted lines: 1000 GeV²; dotted lines: 10000 GeV². massless: N³LO contributions and single- and two-mass contributions: $\mathcal{O}(\alpha_s^3)$; from Ref. [139].

Previous analyses were still lacking parts of the heavy-flavor corrections. Since the heavy-flavor corrections have different scaling violations than the massless ones, these corrections are essential. In Figure 3, we show the prediction of the scale evolution of $F_2(x, Q^2)$ in a wide range of x and Q^2 , referring to the parton distribution functions of Ref. [133].

As well-known, the measured values of $\alpha_s(M_Z)$ from deep-inelastic scattering data of different analyses do not yet agree. In the future there will be dedicated measurements at the EIC [138], using both proton and deuteron data. From those, by performing deuteron wave-function corrections, one can extract a flavor non-singlet structure function. For this quantity one may study scheme-invariant scale evolution, by measuring the input at a scale Q_0^2 and parameterizing it to sufficient precision. The scale evolution is then driven by the QCD-scale Λ_{QCD} only, still being correlated to the measured input. These data are not affected by the gluon distribution and various sea-quark distributions. Here, the heavy-flavor corrections are rather small and predictions have been made at N³LO in Ref. [139] already, see Figure 3.³ We regard this as the cleanest way to extract $\alpha_s(M_Z^2)$ from deep-inelastic scattering data, through which the present debates can be settled.⁴ It is needless to say, that also here the region of higher twist corrections has to be cut out in the analysis.

6. Numerical Implementations of Massless Wilson Coefficients, Splitting Functions and Target-Mass Corrections

We provide the Fortran libraries WILS3, SPLIT_U, and SPLIT_P for the massless Wilson coefficients of deep-inelastic scattering and the unpolarized and polarized splitting functions to three-loop

³The study of electron-deuteron scattering has also been considered [140] and later proposed for HERA [141] but was not realized.

⁴A measurement of this kind had been proposed for an upgrade of the BCDMS experiment in 1989 by C. Guyot et al. in Ref. [142] amounting to 35 million CHF. This proposal was not realized. The proposed experiment could have answered the still open question on the value of $\alpha_s(M_Z^2)$ from deep-inelastic data.

order as fast and precise numerical implementations, in a similar form as for the implementation of the massive asymptotic Wilson coefficients and massive operator matrix elements as given in Refs. [35, 36]. For the polarized splitting functions we provide both the splitting functions in the M-scheme [143] and the Larin scheme [52]. We also include the code TARGM for the target-mass corrections for the structure functions F_2, F_L, xF_3, g_1 and g_2 , see Ref. [144]⁵ and Refs. [146, 147]. They are well suited to be used in x -space evolution codes for the QCD analysis of deep-inelastic scattering data.⁶

The Wilson coefficients are represented as polynomials in the parameters

$$\{\text{IO}, a_s, x, N_F, \ln(Q^2/\mu^2), \text{flav}\},$$

see Ref. [36]. The x -dependence is described by elementary functions and polynomial interpolations. The order in the coupling constant is selected by the parameter $\text{IO} = 1, 2, 3$. We include the Wilson coefficients for the structure functions $F_2(x, Q^2), F_L(x, Q^2), xF_3(x, Q^2)$ [42–44] and $g_1(x, Q^2)$ [44]. For the splitting functions, we refer to Refs. [117, 151–156] in the unpolarized case and Refs. [157–160] in the polarized case. The representations are based on analytic expansions in the small and large- x regions and a numerical representation of the remainder part, see Ref. [36] for details. Unlike the case in Mellin- N space, one has to split the parts $\propto \delta(1-x)$ DEL...f, the +-distribution contributions PLU...f, and the regular parts into different functions in x -space, because of the different Mellin-convolutions in x -space, cf. Eqs. (12–14) of Ref. [36]. The regular parts are given by a superposition of the small- x SX...f, large- x LX...f, and a remainder contribution GR...f, based on cubic spline-interpolation [161] of fine grids for the individual polynomial contributions. The $\delta(1-x)$ - and +-function terms, as well as the small and large- x expansions are coded as analytic expressions, for which we used code-optimization [162]. In the case of the polarized splitting functions, the above argument list is extended by the parameter $\text{LARIN} = 0$ (M-scheme), $= 1$ (Larin scheme). The parameterization of the splitting functions is given with a factor of 1/2 relative to the ones in Refs. [153, 158]. For the target-mass corrections, we also include the numerical integration routines DAIND of Ref. [163].

The license conditions for any use of these codes require the citation of this paper and the references on which their implementation have been based. They are given in separate files along with the other parts of the codes.

7. Conclusions

Given the current precision of the World deep-inelastic data and facing high luminosity data taken at the EIC in the near future, the theoretical description of the scale evolution of the deep-inelastic structure function has to be more precise than the $O(1\%)$ -level. Here one missing asset has been the three-loop heavy-flavor corrections, now being available in the region of large Q^2 . Future dedicated

⁵Here we correct the known typographical errors in the expressions for the structure functions F_1 and xF_3 , see also Ref. [145].


⁶As target-mass corrections are structure-function related, one may consider to correct the data for these effects prior to QCD-fits, as has been done Ref. [148]. Because of the emerging double-integrals, this will save time in the QCD-fitting codes. Likewise, one also performs QED radiative corrections [149, 150] on the data before analyzing the scaling violations.

precision measurements of $\alpha_s(M_Z^2)$ will be performed under these conditions to unambiguously determine this fundamental coupling constant.

Along with this calculation project, various new computer-algebraic and mathematical algorithms, tools and techniques were developed, which are of wider use in other perturbative higher order calculations in QED, QCD, and the Standard Model.

The results of the project allow the analysis of both unpolarized and polarized precision data and will help to improve the accuracy of the extraction of m_c and m_b using upcoming high luminosity data. With this new level of precision also more precise parton distributions will be obtained and a deeper insight into the nucleon spin problem is possible. The presently available theoretical framework will improve re-analyses of the current deep-inelastic data and play a central role in analyzing upcoming data at the EIC and for proposed projects like the LHeC [164, 165].

We also provide fast and precise numerical implementations of the unpolarized and polarized three-loop massless Wilson coefficients and splitting functions in terms of public codes.

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