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Heavy flavour corrections to polarised and unpolarised deep-inelastic scattering at 3-loop order*

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We report on progress in the calculation of 3-loop corrections to the deep-inelastic structure functions from massive quarks in the asymptotic region of large momentum transfer Q^2 . Recently completed results allow us to obtain the $O(\alpha_s^3)$ contributions to several heavy flavour Wilson coefficients which enter both polarised and unpolarised structure functions for lepton-nucleon scattering. In particular, we obtain the non-singlet contributions to the unpolarised structure functions $F_2(x, Q^2)$ and $xF_3(x, Q^2)$ and the polarised structure function $g_1(x, Q^2)$. From these results we also obtain the heavy flavour contributions to the Gross-Llewellyn-Smith and the Bjorken sum rules.

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1. Introduction

Deep-inelastic scattering provides a valuable way to both test the theory of quantum chromodynamics (QCD) and to extract theory parameters from experiments. Among these are in particular the strong coupling constant α_s [1], the parton distribution functions (PDFs) [2–4] and the masses of the charm and bottom quarks [5, 6]. To harness the full potential of the experimental data, it is necessary to have predictions at hand for which the theoretical uncertainties keep up with the experimental accuracy. Currently, the corrections from massive quarks are still missing for a complete next-to-next-to-leading order (NNLO) analysis of the deep-inelastic scattering World data. They can be calculated analytically at NNLO in the kinematic limit $Q^2 \gg m^2$ [7], where Q^2 is the virtuality of the electro-weak gauge boson and m is the mass of the heavy quark. In this paper, we report on progress in the calculation of these heavy flavour corrections.

In Section 2 we describe the framework for the heavy flavour corrections to deep-inelastic scattering in the limit $Q^2 \gg m^2$. In this limit, the massive operator matrix elements of the light-cone operators are the key quantities which have not been completely computed yet. Thus, we sketch the steps involved in their calculation. Section 3 contains several applications of the results which have been obtained so far. In particular, we illustrate the impact of the heavy flavour Wilson coefficients on the structure function $F_2(x, Q^2)$, $g_1(x, Q^2)$ and $xF_3(x, Q^2)$, as well as their consequences for the polarised Bjorken sum rule and the Gross-Llewellyn-Smith sum rule. Finally, we comment on our results for the massive operator matrix element of the non-singlet operator for transversity in Section 4 and conclude in Section 5

2. Framework of calculation

The structure functions of deep-inelastic scattering can in general be written as convolutions of PDFs and Wilson coefficients (cf., e.g., [8]). The Wilson coefficients carry the process-dependent information about the particular scattering process at hand and can be calculated in perturbation theory. They receive contributions from massless quarks and gluons as well as from massive quarks. In the following, we will refer to the contributions of a single massive quark species (i.e. charm or bottom quarks) as the heavy flavour contributions. Starting at 3-loop order, there are also contributions from diagrams with two different massive quarks. Their calculation poses quite different challenges and is discussed elsewhere [9]. The heavy flavour contributions to the structure function $F_2(x, Q^2)$, for example, can be written as [7, 10, 11]

$$\begin{aligned}
 F_2^h(x, N_F + 1, Q^2, m^2) = & \\
 & x \left\{ \sum_{k=1}^{N_F} e_k^2 \left[L_{q,2}^{\text{NS}} \left(x, N_F + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) \otimes \left[f_k(x, \mu^2, N_F) + \bar{f}_k(x, \mu^2, N_F) \right] \right. \right. \\
 & + \frac{1}{N_F} L_{q,2}^{\text{PS}} \left(x, N_F + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) \otimes \Sigma(x, \mu^2, N_F) \\
 & \left. \left. + \frac{1}{N_F} L_{g,2}^{\text{S}} \left(x, N_F + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) \otimes G(x, \mu^2, N_F) \right] \right\}
 \end{aligned}$$

$$\begin{aligned}
& + e_Q^2 \left[H_{q,2}^{\text{PS}} \left(x, N_F + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) \otimes \Sigma(x, \mu^2, N_F) \right. \\
& \left. + H_{g,2}^{\text{S}} \left(x, N_F + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) \otimes G(x, \mu^2, N_F) \right] \Bigg\}. \tag{2.1}
\end{aligned}$$

Here, f_k , \bar{f}_k and G refer to the PDFs for quarks and anti-quarks of flavour k and the gluon PDF, respectively. The singlet PDF combination is defined as $\Sigma = \sum_{k=1}^{N_F} (f_k + \bar{f}_k)$ and μ^2 is the factorisation scale. The number of light quark flavours is denoted by N_F and e_k and e_Q represent the charges of the light and heavy quarks. The heavy flavour Wilson coefficients are denoted by $L_{i,a}$ and $H_{i,a}$, where the L and H distinguish the cases where the electro-weak gauge boson couples to a light or a heavy quark, respectively, and the subscripts i and a label the initial state parton (q, g) and the structure function under consideration. The symbol \otimes represents the Mellin convolution, which turns into a simple product of moments if we apply to it a Mellin transformation

$$M[f](N) = \int_0^1 dx x^{N-1} f(x). \tag{2.2}$$

This introduces the Mellin variable N , to which we will refer in several places in the following.

The massless Wilson coefficients have been calculated up to 3-loop order [12], while the massive ones are available only semi-numerically up to 2-loop order [13].¹ However, it was observed in [7] that the heavy-flavour Wilson coefficients factorise into the massless Wilson coefficients and massive operator matrix elements (OME) in the kinematic limit where $Q^2 \gg m^2$. In this limit, the heavy flavour Wilson coefficients $\mathcal{C}_{i,a}^{\text{asympt}}$ can be written schematically as [7]

$$\mathcal{C}_{i,a}^{\text{asympt}} \left(x, N_F + 1, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2} \right) = \sum_j C_{j,a} \left(x, N_F + 1, \frac{Q^2}{\mu^2} \right) \otimes A_{ij,Q} \left(x, N_F + 1, \frac{m^2}{\mu^2} \right) + \mathcal{O} \left(\frac{m^2}{Q^2} \right). \tag{2.3}$$

The massless Wilson coefficients $C_{i,a}$ are evaluated for $N_F + 1$ massless flavours and the massive OMEs $A_{ij,Q}$ are calculated with N_F massless and one massive quark. More details on the formalism can be found in [7, 15, 10, 11]. Below, we will frequently refer to the expansion coefficients of the OMEs in powers of $a_s = \frac{\alpha_s}{4\pi}$, where the coefficient of a_s^k is denoted by $A_{ij,Q}^{(k)}$.

The massive OMEs are known analytically up to 2-loop order [7, 16, 15, 17] including linear terms in the dimensional regulator $\varepsilon = D - 4$, where D is the dimensionality of space-time in dimensional regularisation [18]. The extension of these results to 3-loop order is the topic of our project and here we report on progress in this regard.

The massive OMEs can be extracted from calculating two-point functions with external on-shell partons and operators, which introduce additional Feynman rules beyond those of QCD. Our calculation follows a diagrammatic approach, where all relevant diagrams are generated using QGRAF [19]. After inserting the Feynman rules, we simplify the colour and Dirac algebra using FORM [20] and `color.h` [21]. In this way, we express the diagrams in terms of roughly 10^5 scalar loop integrals. In order to compute those, we first reduce them to a smaller number of master integrals using integration-by-parts relations [22, 23]. For this task we use the program `Reduze 2` [24].² A major task is then to actually calculate the master integrals. Over the years a number of

¹For a precise implementation in Mellin space see [14].

²`Reduze 2` uses the packages `GiNaC` [25] and `Fermat` [26].

techniques have proven to be very useful for this task:

- *Higher hypergeometric functions* [27]: After deriving a Feynman parameter representation for the loop integrals, they can sometimes be brought in a form which can be integrated in terms of generalised hypergeometric (${}_pF_q$) or Appell functions that have convergent series representations. If this is the case, we can expand them in ϵ and the resulting sum representations can be simplified using the summation algorithms [28, 29] implemented in `Sigma` [28, 30, 31], `EvaluateMultiSums` and `SumProduction` [32] with support from `HarmonicSums` [33–38] for dealing with the nested sums that arise.
- *Mellin-Barnes integrals* [39, 40]: Even if a direct evaluation of the Feynman parameter integrals in terms of hypergeometric functions is not possible, it may still be feasible to derive a sum representation that can be simplified using `Sigma` and related packages: We split up suitably formed sums of Feynman parameters at the cost of complex contour integrals [40, 41]. Afterwards, the Feynman parameter integrals can usually be done in terms of Beta and Gamma functions, while the contour integrals give rise to infinite sums via the residue theorem.
- *Almkvist-Zeilberger algorithm* [42, 34]: If it is possible to confine the Mellin variable N in the integrand of the Feynman parameter integrals to only one or a small number of places, it can be advantageous to employ the multi-variable Almkvist-Zeilberger algorithm, implemented in the package `MultiIntegrate` [34]. It allows to derive recurrence relations for the integrals which can subsequently be solved using the algorithms implemented in `Sigma`.
- *Differential equations and difference equations* [43, 44]: Based on the integration-by-parts relations it is possible to derive coupled systems of differential equations for the master integrals. We translate these into coupled systems of difference equations and uncouple them using Zürcher’s algorithm [45], which is implemented in `OreSys` [46]. Once suitable initial conditions are available (e.g. from direct calculations using other methods), the difference equations can be solved using the package `SolveCoupledSystem` [47].

More details on the application of these techniques to the calculation of massive OMEs can be found in [44, 48–53]. The results obtained so far for the OMEs can be expressed in terms of nested sums. In particular harmonic sums [54], generalised harmonic sums [55, 36], cyclotomic sums [35] and binomially weighted sums [56, 37] appear both in the intermediate steps and in the results. These structures are related to corresponding iterated integrals [57, 55, 36, 35, 37] via an inverse Mellin transformation. Finally, the results for the master integrals can be inserted into the diagrams, yielding the unrenormalised expressions for the operator matrix elements.

The renormalisation procedure for the massive OMEs at $\mathcal{O}(a_s^3)$ was worked out in [10]. Since we calculate matrix elements of the local light-cone operators, it comes at no surprise that their renormalisation involves the anomalous dimensions of the operators. Using known results for the beta function, mass anomalous dimensions and lower order OMEs, we can use the pole terms of our 3-loop results to calculate the N_F -dependent part of the anomalous dimensions.

3. Results for structure functions

Over the course of the recent years, a number of analytic results for the operator matrix elements have been completed. In particular, the OMEs $A_{qg,Q}^{(3)}$ [48], $A_{gq,Q}^{(3)}$ [51], $A_{qq,Q}^{\text{PS},(3)}$ [48], $A_{Qq}^{\text{PS},(3)}$ [58], $A_{qq,Q}^{\text{NS},(3)}$ [59] have been calculated. Moreover, the gluonic OME $A_{gg,Q}^{(3)}$ is known for even values of the Mellin variable N [60]. These results allow for a numerical illustration of their impact on the heavy flavour Wilson coefficients of different structure functions. For the structure function $F_2(x, Q^2)$ there are five different Wilson coefficients (see Eq. (2.1)), each of which requires the knowledge of the 3-loop term of one OME. Since $A_{Qg}^{(3)}$ is not yet fully known, the Wilson coefficient $H_{g,2}$ cannot be given yet at 3-loop order at this point. Nevertheless, we can illustrate the impact of the remaining Wilson coefficients, supplemented by the contribution of $H_{g,2}$ up to 2-loop order for comparison. Figure 1 shows the heavy flavour contributions to $F_2(x, Q^2)$ for a fixed value of

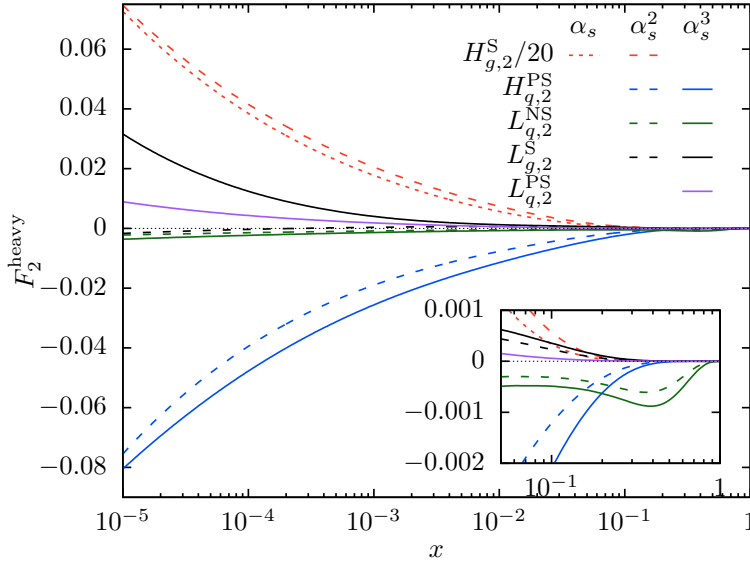


Figure 1: Illustration of the contributions to the structure function $F_2(x, Q^2)$ from the individual Wilson coefficients. The plot shows the values for $Q^2 = 100 \text{ GeV}^2$ and the scale choice $\mu^2 = Q^2$ with PDFs from [2]. The charm quark mass is $m_c = 1.59 \text{ GeV}^2$ in the on-shell scheme [5]. The inset enlarges the region of $0.05 \leq x \leq 1$.

$Q^2 = 100 \text{ GeV}^2$. The biggest contribution comes from $H_{g,2}$. Contributions to this Wilson coefficient start at $\mathcal{O}(a_s)$ and are the only contribution at that order. Due to this and the fact that it involves the gluon PDF, it is quite large in the small- x region and we have scaled down the curve by a factor 20. The second largest contribution in the small- x region is the pure-singlet Wilson coefficient $H_{q,2}^{\text{PS}}$. It starts at $\mathcal{O}(a_s^2)$ and is negative, except for very large values of x (not visible in the plot). The large- x region is dominated by the non-singlet Wilson coefficient, which also starts at $\mathcal{O}(a_s^2)$ and is negative throughout the whole x -range. Here, the even moments of the non-singlet OME $A_{qq,Q}^{\text{NS},(3)}$ enter. Somewhat smaller contributions arise from the gluon- and quark-initiated singlet Wilson coefficients $L_{g,2}^{\text{S}}$ and $L_{q,2}^{\text{PS}}$, which start at $\mathcal{O}(a_s^2)$ and $\mathcal{O}(a_s^3)$, respectively.

The non-singlet OME $A_{qq,Q}^{\text{NS},(3)}$ was calculated also for odd moments in [59]. This allows for applications to other structure functions besides $F_2(x, Q^2)$: In particular the non-singlet contribution

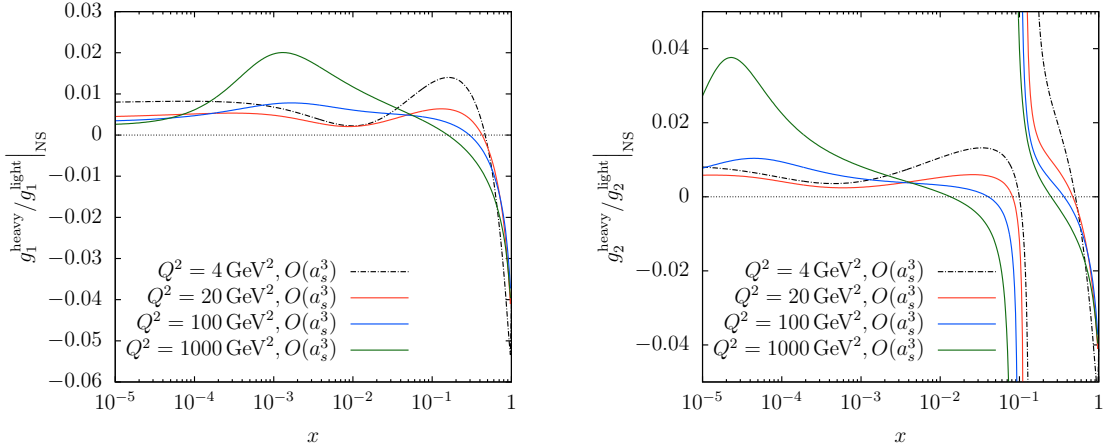


Figure 2: Ratio of the heavy over the light flavour contributions to the polarised structure functions $g_1(x, Q^2)$ (left panel) and $g_2(x, Q^2)$ (right panel) for different values of Q^2 . Here, the PDFs from [61] were used; plots from [62].

to the polarised structure function $g_1(x, Q^2)$ was explored in [62]. Figure 2 illustrates the impact of the charm quarks on this structure function. Compared to the contributions from massless quarks and gluons, the charm quark constitutes around +1% to 2% to -5% of the non-singlet structure function. This is below the current experimental accuracy but may be of interest at future high-luminosity colliders [63].

At the level of twist 2, the structure function $g_2(x, Q^2)$ is also related to $g_1(x, Q^2)$ by the Wandzura-Wilczek relation [64],

$$g_2(x, Q^2) = -g_1(x, Q^2) + \int_x^1 \frac{dy}{y} g_1(y, Q^2). \quad (3.1)$$

This allows us to show also the impact of the charm quarks there. As can be seen in the right panel of Figure 2, the heavy quark contributions are about 1% to 4% the size of the massless contribution. The pole in the plot is due to a change of sign of g_2^{light} .

Another application of the non-singlet OME is the polarised Bjorken sum rule [65]. It is defined as the difference of the first moments of $g_1(x, Q^2)$ in electron-proton and electron-neutron scattering,

$$\int_0^1 dx [g_1^{ep}(x, Q^2) - g_1^{en}(x, Q^2)] = \frac{1}{6} \left| \frac{g_A}{g_V} \right| C_{\text{pBj}}(a_s), \quad (3.2)$$

where g_A and g_V denote the axial-vector and vector decay constants. The perturbative coefficient C_{pBj} arises from first moment of the Wilson coefficients. For the massless contributions it has been calculated up to $\mathcal{O}(a_s^4)$ [66–68]. Our result for the non-singlet heavy flavour Wilson coefficient leads us to the conclusion that in the limit $Q^2 \gg m^2$ the polarised Bjorken sum rule for N_F massless quarks and one massive quark is given completely by the massless contributions for $N_F + 1$ quarks: The massive non-singlet OME, which could modify the sum rule compared to the completely massless case, has a vanishing first moment due to fermion number conservation. However, away

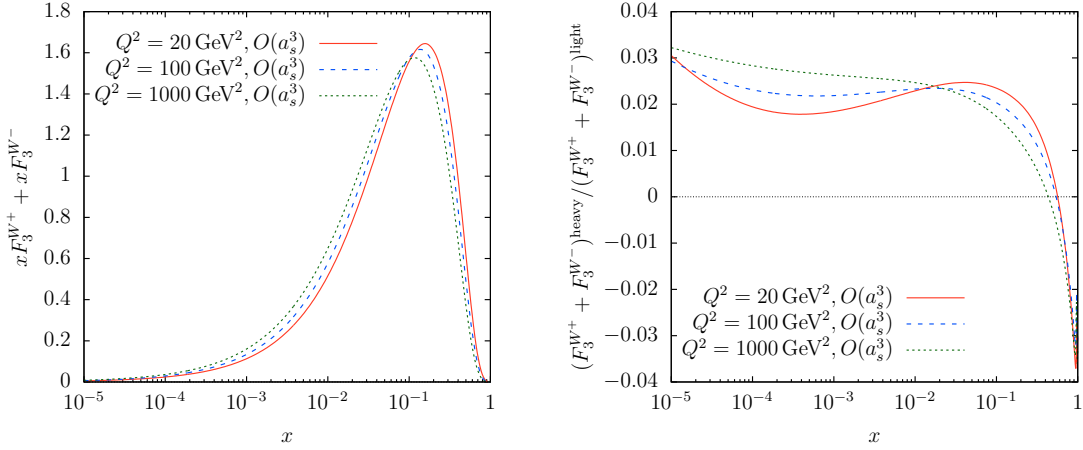


Figure 3: *Left panel:* Illustration of the structure function combination $x F_3^{W^+ - W^-}(x, Q^2)$ including the contributions from a massive charm quark with a mass of $m_c = 1.59 \text{ GeV}^2$ in the on-shell scheme [5]. *Right panel:* Ratio of the heavy quark contributions over the massless part of the same structure function; plots from [70].

from the limit $Q^2 \gg m^2$, the behaviour described above no longer holds and genuine heavy flavour contributions to the polarised Bjorken sum rule arise, cf. [69].

Moreover, the same non-singlet OME enters also the charged-current structure function combination

$$x F_3^{W^+ - W^-}(x, Q^2) = x F_3^{W^+}(x, Q^2) + x F_3^{W^-}(x, Q^2). \quad (3.3)$$

For an explanation of the notation we refer to [71, 70]. This structure function receives contributions from two non-singlet Wilson coefficients: On the one hand, there is $L_{q,3}^{\text{NS}}$, which describes reactions in which the W boson couples to a light quark and mediates a flavour transition between light quark species. This is analogous to the case of photon exchange, except for the flavour change. On the other hand, there is $H_{q,3}^{\text{NS}}$, which describes flavour excitation reactions (e.g. $s \rightarrow c$). Here, the W boson couples to a heavy quark. This part has no analogy in the photon-mediated case. The impact of both Wilson coefficients on $x F_3^{W^+ - W^-}(x, Q^2)$ is illustrated in Figure 3. The size of the heavy quark contribution is again of the order of about 3%. Also in the charged current sector, there is a sum rule arising from the first moment of the structure functions: The Gross-Llewellyn-Smith sum rule [72] is given by

$$\int_0^1 dx \left[F_3^{\bar{v}p}(x, Q^2) + F_3^{vp}(x, Q^2) \right] = 6 C_{\text{GLS}}(a_s). \quad (3.4)$$

The massless QCD corrections to C_{GLS} are again known to $\mathcal{O}(a_s^4)$ [66, 73, 74] and the situation in the heavy quark sector is similar to the polarised case: Due to the vanishing first moment of $A_{qq,Q}^{\text{NS}}$, the influence of the heavy quark in the asymptotic region $Q^2 \gg m^2$ reduces to incrementing the number of massless flavours ($N_F \rightarrow N_F + 1$). For the power corrections in m^2/Q^2 up to 2-loop order, we refer to [69].

4. Operator matrix element for transversity

The non-singlet results discussed so far involve the flavour non-singlet vector or axial-vector operators. A very similar calculation can be performed for the non-singlet tensor operator

$$O_{q,r}^{\text{TR,NS},\mu\mu_1\dots\mu_N}(z) = i^{N-1} S \left[\bar{\psi}(z) \sigma^{\mu\mu_1} D^{\mu_2} \dots D^{\mu_N} \frac{\lambda_r}{2} \psi(z) \right] - \text{trace terms}, \quad (4.1)$$

where D^μ is the covariant derivative, ψ is the quark field operator, λ_r denotes the Gell-Mann matrices of $\text{SU}(3)_{\text{flavour}}$, $\sigma^{\mu\nu} = \frac{i}{2}(\gamma^\mu \gamma^\nu - \gamma^\nu \gamma^\mu)$ and $S[\dots]$ denotes the symmetrisation of the Lorentz indices.

The operator in Eq. (4.1) is related to the transversity distribution $\Delta_T f_k$ which appears in the transversity structure function $h_1(x, Q^2)$ [75]. It can be measured in semi-inclusive deep-inelastic scattering [76] and polarised Drell-Yan processes [77]. The massive OME of this operator is denoted by $A_{qq,Q}^{\text{NS,TR,(3)}}$ and involves the same diagrams as the vector non-singlet operator $A_{qq,Q}^{\text{NS,(3)}}$. Of course, different Feynman rules and a different projector have to be used, but the required master integrals turn out to be the same. Our calculation allows to extract the N_F -dependent parts of the anomalous dimensions of the transversity operator up to 3-loop order. The result for the anomalous dimensions and the complete OME $A_{qq,Q}^{\text{NS,TR,(3)}}$ are given in [59]. In principle the heavy flavour Wilson coefficients could be constructed in a similar fashion as for the other structure functions, but at this point the light flavour Wilson coefficients have not been calculated to a sufficient order yet.

5. Conclusions

Up to now, seven out of eight 3-loop massive operator matrix elements have been calculated analytically for general values of the Mellin variable N . Here, we discussed both the framework of calculation as well as a selected number of applications. The analytic calculation of the required 3-loop master integrals with additional local operator insertions led to the development and improvement of computer-algebraic and mathematical methods and tools. The packages `Sigma`, `HarmonicSums`, `EvaluateMultiSums`, `SumProduction` and `SolveCoupledSystem` both enabled the calculation and have benefited greatly from the challenges posed by the tasks arising from the project.

The largest contribution to the heavy flavour corrections to the structure function $F_2(x, Q^2)$ is expected to come from the Wilson coefficient $H_{g,2}^S$, which is not yet known due to the missing OME $A_{Qg}^{(3)}$. Nonetheless, a first impression of the impact of the heavy flavour corrections can be seen from our illustrations in Section 3. We also discussed the influence of the massive OME $A_{qq,Q}^{\text{NS,(3)}}$ on the non-singlet polarised and charged-current structure functions $g_1(x, Q^2)$ and $xF_3(x, Q^2)$, which is of the order of a few percent in both cases. Due to the vanishing first moment of the non-singlet OME, the polarised Bjorken and Gross-Llewellyn-Smith sum rules are only modified by shifting N_F to $N_F + 1$ if compared to the purely massless case with N_F quark flavours in the region $Q^2 \gg m^2$. Finally, we also calculated the massive OME for the non-singlet transversity operator, which enabled us to obtain the N_F -dependent parts of the 3-loop anomalous dimension of this operator.

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