Three-Loop Contributions to the Gluonic Massive Operator Matrix Elements at General Values of N

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Recent results on the calculation of 3-loop massive operator matrix elements in case of one and two heavy quark masses are reported. They concern the $O(n_f T_F^2 C_F A)$ and $O(T_F^2 C_F A)$ gluonic corrections, two-mass quarkonic moments, and ladder- and Benz-topologies. We also discuss technical aspects of the calculations.

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1. Introduction

One of the most precise determinations of the strong coupling constant \( \alpha_s(M_Z) \) relies on the next-to-next-to-leading order (NNLO) QCD analysis of the world deep-inelastic data \([1, 2]\). Here currently the heavy flavor corrections to the structure function \( F_2(x,Q^2) \) and transversity are known for the first Mellin moments \( N = 2, \ldots, 10 \) \([3, 4]\). In the asymptotic region \( Q^2 \gg m^2 \) the heavy flavor Wilson coefficients can be represented in form of convolutions \([7]\) of massive operator matrix elements (OMEs) and the massless Wilson coefficients \([8]\). In case of the charm quark contribution the corresponding region is given by \( Q^2 / m_c^2 \gtrsim 10 \). To carry out complete NNLO QCD analyses in this region the heavy flavor Wilson coefficients have to be known for general values of \( N \). This also applies to precision measurements of the charm quark mass using the world deep-inelastic data \([9]\).

Since 2010 the systematic calculation of the asymptotic massive Wilson coefficients at general values of \( N \) have been carried out. Five massive Wilson coefficients contribute to \( F_2(x,Q^2) \) at NNLO \([3]\). Furthermore, there are other massive OMEs needed to compute the matching coefficients in the variable flavor number scheme in which the heavy quarks are assumed to decouple singly \([3, 10, 11]\). There are yet other contributions at NNLO from graphs containing both a massive charm and a bottom quark line, which extend the former representation in Ref. \([3]\) and are necessary because of the fact that charm quarks do not yet become massless at the mass scale of bottom quarks since \( m_c^2 / m_b^2 \approx 1/10 \) only. Results on first moments for these contributions are obtained in \([12–14]\). The extension of the renormalization of the massive OMEs is given in \([14]\). The logarithmic contributions at general values of \( N \) for the contributions to \( F_2(x,Q^2) \) are available \([15–17]\). Furthermore, the NNLO heavy flavor Wilson coefficients in the asymptotic region were calculated for the structure function \( F_L(x,Q^2) \) \([3, 20]\).

Two of the five massive Wilson coefficients contributing to \( F_2(x,Q^2) \) at NNLO are known completely \([21]\). They are of \( O(n_f T_F^2 C_{FA}) \). Likewise, these contributions to the further three Wilson coefficients and transversity were calculated for these color coefficients in \([21]\). Also the complete contribution \( O(T_F^2 C_{AF}) \) for the OMEs \( A_{Qq}^{PS}, A_{qq}^{NS}, A_{qq}^{TR} \) are available \([12]\).

In these proceedings we report on the calculation of the gluonic OMEs \( O(n_f T_F^2 C_{FA}) \) \([22]\) in Section 2 and on first results in \( O(T_F^2 C_{FA}) \) for this channel in Section 3. Furthermore, the scalar 3-loop integrals for all ladder type integrals were calculated \([23, 24]\). An extension of the method \([25]\) to calculate finite Feynman integrals to the case of massive quark lines with local operator insertions has been used to calculate ladder- and Benz-topologies \([23, 24]\), also leading to new types of finite nested sums extending the harmonic \([26]\), generalized harmonic \([27, 28]\), and cyclotomic sums \([29]\) and the associated polylogarithms, cf. Section 4. Section 5 contains the conclusions.

2. Gluonic OMEs \( O(n_f T_F^2 C_{FA}) \)

The calculation of all \( O(n_f T_F^2 C_{FA}) \) contributions to the massive OMEs has been completed with the computation of \( A_{qg,Q} \) and \( A_{gg,Q} \) at this order in \([22]\). In these and other computations described

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1. Present analyses use the NLO corrections in \( x \)-space \([5]\) or Mellin space implementations \([6]\).
2. The \( O(\alpha_s^2) \) and \( O(\alpha_s^2 \varepsilon) \) contributions, with \( \varepsilon = D - 4 \) the dimensional parameter, needed in the renormalization were given in \([7, 18, 19]\).
below we used the codes QGRAF [30], Form and tform [31], and color [32]. For the check of individual moments of the expressions derived we also used MATAD [33].

In the calculation of the $O(n_f T_F^2 C_F A)$-terms large amounts of nested sums emerge. An important step in the calculation consists in merging these individual sums to a smaller amount of sums containing very voluminous summands which are then solved with the codes used within the package Sigma [34], like EvaluateMultiSum and SumProduction [35], written in mathematica [36], cf. also [37]. Moreover, this compactification shall be performed for whole diagrams to avoid the intermediate emergence of a larger amount of generalized harmonic sums as was observed in [21]. Generalized harmonic sums do not contribute in this case.

The constant contributions to the unrenormalized massive OMEs $A_{gg,Q}$ and $A_{gq,Q}$, $d^{(3)}_{gq,Q}$, $j = q, g$, read:

$$d^{(3), n_f T_F^2}_{gq,Q} = C_F T_F^2 n_f \left\{ \frac{16 (N^2 + N + 2)}{9(N-1)N(N+1)} \left( \frac{1}{3} S_1^3 + S_2 S_1 + \frac{2}{3} S_3 + 14 \zeta_3 + 3 S_1 \zeta_2 \right) + \frac{16 (8N^3 + 13N^2 + 27N + 16)}{27(N-1)N(N+1)^2} (3 \zeta_2 + S_1^2 + S_2) - \frac{32 (35N^4 + 97N^3 + 178N^2 + 180N + 70)}{27(N-1)N(N+1)^3} S_1 + \frac{32 (1138N^5 + 4237N^4 + 8861N^3 + 11668N^2 + 8236N + 2276)}{243(N-1)N(N+1)^4} \right\}, \quad (2.1)$$

$$d^{(3), n_f T_F^2}_{gg,Q} = n_f T_F^2 \left\{ \frac{C_A}{(N-1)(N+2)} \left[ \frac{4 P_1}{27 N^2(2N+1)^2} S_1^3 + \frac{8 P_2}{729 N^3(N+1)^3} S_1^2 + \frac{160}{27} \frac{(N-1)(N+2) \zeta_2 S_1 - \frac{448}{27} \frac{(N-1)(N+2) \zeta_3 S_1 + \frac{P_3}{729 N^4(N+1)^4}}{\zeta_3 - \frac{4 P_3}{27 N^2(2N+1)^2} S_2} \right] + \frac{C_F}{(N-1)(N+2)} \left[ \frac{112 (N^2 + N + 2)^2}{27 N^2(2N+1)^2} S_1^3 - \frac{16 P_6}{27 N^3(N+1)^3} S_1^2 + \frac{16 P_7}{81 N^4(N+1)^4} S_1 + \frac{16 (N^2 + N + 2)^2}{3 N^2(N+1)^2} \zeta_2 S_1 + \frac{16 \zeta_5}{3 N^2(N+1)^2} S_2 S_1 \right] - \frac{16 P_6}{9 N^3(N+1)^3} S_2 + \frac{448 (N^2 + N + 2)^2}{9 N^2(N+1)^2} \zeta_3 + \frac{16 P_{10}}{9 N^3(N+1)^3} S_2 \right\}. \quad (2.2)$$

The corresponding $1/\varepsilon$ terms contain contributions of the 3-loop anomalous dimensions [38] which we have verified by an independent calculation. Moreover a prediction made in [39] has been confirmed.

The gluonic OMEs $A_{gg,Q}$ and $A_{gq,Q}$ are needed for correct flavor matching in case of the transition of a single heavy quark becoming light, cf. [3, 10]. Here the correct choice of the matching scale is of importance [40].
In extending the above calculation the computation of some topological classes of diagrams has been automated mapping the graph to expressions involving hypergeometric $p+1F_p$-functions. The $\varepsilon$-expansion leads to nested sums being calculated using the package $\Sigma$2 [41]. The automation will cover other classes soon, requiring more involved ways to match the initial functions.

3. Gluonic OMEs $O(T F_{F,A})$ and OMEs with massive fermion lines of two different masses

All basic scalar topologies contributing to the $O(T F_{F,A})$ of $A_{gg,Q}$ and $A_{gq,Q}$ have been calculated. An example is given in (3.1) for the graph containing two massive triangles with $m_1 = m_2$,

$$I_{D2}(N, \varepsilon) = (-1)^N \left\{ -\frac{1}{12N\varepsilon} + \frac{(27N^2 - 5N + 16)}{1440N(N + 1)(2N - 1)^4N} \left( \begin{array}{c} 2N \\ N \end{array} \right) \left[ \sum_{i_1=1}^{N} \frac{4^{i_1} S_1(i_1 - 1)}{i_1^2 \left( \begin{array}{c} 2i_1 \\ i_1 \end{array} \right)} - 7\zeta_3 \right] ight\}$$

$$- \left( \begin{array}{c} S_{2,1} - S_3 - 7\zeta_3 \\ 90N \end{array} \right) + \left( \begin{array}{c} S_1^2 - S_2 \\ 90(N - 1)N^2(N + 1) \end{array} \right)$$

$$+ \frac{(60N^3 - 19N^2 - 85N + 60)}{720(N - 1)N(N + 1)(2N - 1)} S_1 + \frac{(-162N^3 + 281N^2 - 187N + 30)}{720(N - 1)N^2(2N - 1)} \right\}.$$  \quad (3.1)

Here we chose a minimal representation of sums being pairwise transcendent, which is proven by $\Sigma$2 [41]. In these and similar diagrams sums of the kind

$$\sum_{i=1}^{N} \frac{4^i}{i^3 \left( \begin{array}{c} 2i \\ i \end{array} \right)} = \int_0^1 dx \frac{x^N - 1}{x - 1} H_{0w_3}^*(x) \quad (3.2)$$

$$\sum_{i=1}^{N} \frac{4^i}{i^2 \left( \begin{array}{c} 2i \\ i \end{array} \right)} S_1(i) = \int_0^1 dx \frac{x^N - 1}{x - 1} \left[ H_{0w_3}^*(x) - H_{0w_0}^*(x) - H_{w_1}^*(x) - 2\ln(2)H_{w_3}^*(x) \right] \quad (3.3)$$

emerge, which can be represented as Mellin transforms of iterated integrals, extending the usual harmonic polylogarithms (HPLs) [41], where $H_2^*(x) = 1, H_3^*(x) = \int_1^x dy f_{x} \int_1^y dy f_{y}$. The relative transcendence of the respective HPLs is proven using differential field methods [43]. In exceptional cases they may be obtained in terms of HPLs with root arguments. Eq. (3.1) obviously is recurrent in $N$. The asymptotic expansions of (3.2, 3.3) are given by

$$\sum_{i=1}^{N} \frac{4^i}{i^3 \left( \begin{array}{c} 2i \\ i \end{array} \right)} = 6\zeta_2 \ln(2) - \frac{7}{2} \zeta_3 - \sqrt{\pi} \left\{ \begin{array}{c} 2 \frac{1}{3N} - \frac{9}{20N^2} + \frac{199}{1344N^3} + O \left( \frac{1}{N^4} \right) \end{array} \right\} \quad (3.4)$$

$$\sum_{i=1}^{N} \frac{4^i}{i^2 \left( \begin{array}{c} 2i \\ i \end{array} \right)} S_1(i) = 6\zeta_2 \ln(2) + \frac{7}{2} \zeta_3 + \sqrt{\pi} \left\{ \begin{array}{c} 4 + \frac{7}{18N} = \frac{817}{2400N^2} + \frac{3835}{37632N^3} + O \left( \frac{1}{N^4} \right) \end{array} \right\}$$

$$- \frac{\ln(N)}{\sqrt{N}} \left\{ \begin{array}{c} 2 - \frac{5}{12N} + \frac{21}{320N^2} + \frac{223}{10752N^3} + O \left( \frac{1}{N^4} \right) \end{array} \right\} \quad (3.5)$$
with \( \gamma = Ne^{ik} \) and \( \gamma_k \) the Euler-Mascheroni number. The poles in the complex plane are situated at non-positive integers and half-integers and \((3.1)\) is thus a meromorphic function. The half-integer poles emerge algebraically and from structures like

\[
\left(2N\right)\frac{1}{4^N} = \frac{\Gamma(N + 1/2)}{\sqrt{\pi} (N + 1)}.
\]

With these properties it can be defined in the complex \( N \)-plane. By similar arguments the analytic continuation for the whole \( T_{CF}^2 \) contribution to \( A_{ggQ} \) is obtained.

First results on massive OMEs with two fermion lines for \( m_1 \neq m_2 \) have been reported in [12, 13] for the moments \( N = 2, 4, 6 \) for \( A_{Qg} \). The calculation has been performed by mapping the OMEs to tadpoles which were computed using \texttt{qexp} [45]. The renormalization of these matrix elements generalizes the case of \( n_f \) massless and one massive fermion [3] and is given in Ref. [14]. Since \( m_2^2/m_b^2 \sim 1/10 \), charm cannot be treated as massless at the scale \( m_b^2 \), which makes the use of the variable flavor scheme, see [3], built on this assumption, very problematic in case of these contributions. On the other hand, the fixed flavor number scheme which can be used in precision deep-inelastic world data analyses, cf. [1], can naturally accommodate these terms. The corresponding calculation in case of general values of \( N \) is underway [46].

4. Ladder and Benz Topologies

In the following we discuss higher topologies which contribute to the massive OMEs \( A_{ij} \) at 3–loop order. These are ladder-, Benz-, and crossed box topologies with the respective local operator insertions (of up to four lines). The basic ladder topologies have been calculated in Ref. [23] up to 3-leg operator insertions. Here we consider the case of only one massive fermion line. As has been described in [47] the Feynman diagrams can be represented as multiply nested sums. The ladder diagrams with six massive propagators have representations in terms of the Appell function \( F_1 \) [48]. Most of the integrals can be solved using \texttt{Sigma} [34], including the pole structure in \( \epsilon \). This is presently more involved in case of operator insertions with more than two legs at six massive lines.

For the non-divergent graphs the extension of the method [25] to local operators and massive lines allows the calculation. We consider the diagram shown in Fig. 1.

![Figure 1: 3-loop ladder diagram containing a 3-vertex local operator insertion.](image)

The local operator insertion can be resummed introducing a subsidiary parameter \( x \)

\[
\sum_{j=0}^{N} T_{4d}^{N-j} T_{4b}^j \to \sum_{N=0}^{\infty} \sum_{j=0}^{N} x^N T_{4d}^{N-j} T_{4b}^j = \sum_{N=0}^{\infty} \frac{(T_{4d}x)^N - (T_{4b}x)^N}{T_{4d} - T_{4b}} = \frac{1}{T_{4d} - T_{4b}} \left[ \frac{1}{1 - xT_{4d}} - \frac{1}{1 - xT_{4b}} \right] = \frac{x}{(1 - xT_{4d})(1 - xT_{4b})}.
\]

(4.1)
The integral may then be performed using the method [25] and is expressed in terms of hyperlogarithms $\mathbb{L}_a(x)$. They obey the relations

$$L_{b,a}(x) = \int_0^x \frac{dy}{y-b} L_{a}(y), \quad L_0(y) = 1; \quad L_{0,...,0}(x) = \frac{1}{n!} \ln^n(x), \quad a, b \in \mathbb{R}.$$  \hspace{1cm} (4.2)

As an intermediary result one obtains

$$I_4(x) = \left[ \frac{1+x}{x^3} L_{-1} - \frac{2x-1}{x^3} L_{1/2} - \frac{3(1-x)}{x^3} L_1 - \frac{1-2x+x^2}{(1-x)x^3} L_{0,-1} + \frac{1-2x^2}{x^3} L_{0,1/2} 
- \frac{3-4x-3x^2+3x^3}{(1-x)x^3} L_{0,1/2} - \frac{1-2x^2}{x^3} L_{1,1/2} + \frac{(1-x)(2+3x)}{x^3} L_{1,1} \right] \xi_3
+ \frac{(1+x)}{2x^3} \bigg[ 3L_{-1,0,0,1,1} - 2L_{-1,0,1,1,1} + 3L_{1,0,0,0,1} + \frac{1}{x} (6L_{0,0,1,1,1} - 4L_{0,1,0,1,1} - L_{0,1,1,1,1}) \bigg]
- \frac{3}{2x^2} L_{1,0,1,1,1} + \frac{2}{x^2} \left[ \frac{(1-x)}{x^3} L_{1,1,0,1,1} + \frac{L_{0,1,1,1,1}}{x} \right]
+ \frac{3}{2x^2} \left[ 3L_{0,-1,0,0,1,1} - 2L_{0,-1,0,1,1,1} \right]
- \frac{5}{1+x} L_{0,0,0,1,1,1} - \frac{5}{2(-1+x)} L_{0,0,1,0,1,1} + \frac{3(3+x)}{2(-1+x)} L_{0,0,1,1,1,1}
- \frac{(1+x)}{2x^3} \bigg[ 3L_{0,1/2,0,0,1} + L_{0,1/2,0,1,1} + 3L_{0,1/2,1,0,1} - L_{0,1/2,1,1,1} \bigg]
+ \frac{8}{2(-1+x)x^3} L_{0,1,0,0,1,1} + \frac{8-14x+5x^2+3x^3}{2(-1+x)x^3} L_{0,1,0,0,1,1}
+ \frac{8-15x+3x^2}{2(-1+x)x^3} L_{0,1,1,0,1,1} - \frac{3(-3+2x)}{2x^3} L_{0,1,1,1,1,1} + \frac{-6+3x+5x^2}{x^3} L_{1,0,0,0,1,1}
+ \frac{2(-1+x)}{x^3} L_{1,1,1,0,1,1} + \frac{4-2x+5x^2}{2x^3} L_{1,0,1,0,1,1} - \frac{-4+6x+3x^2}{2x^3} L_{1,0,1,1,1,1}
+ \frac{(1+x)}{2x^3} \bigg[ 3L_{1,1/2,0,0,1} - L_{1,1/2,0,1,1} \bigg] - \frac{3(-1+x)(4+3x)}{2x^3} L_{1,1,0,0,0,1}
- \frac{(1+x)}{2x^3} \left[ L_{1,1,2,0,1,1} + L_{1,1,1,1,1,1} \right] - \frac{(1-x)(5+3x)}{2x^3} L_{1,1,1,0,1,1}}}.$$  \hspace{1cm} (4.3)

Here iterated integrals over the alphabet \{0, 1, -1, 1/2\} contribute. Now the $\text{N}^\text{th}$ Taylor coefficient has to be obtained for $I_4(x)$, which is possible using the package HarmonicSums [28]:

$$\hat{I}_4(N) = \frac{P_1}{2(1+N)^5(2+N)^5(3+N)^5} + \frac{P_2}{(1+N)^2(2+N)^2(3+N)^2} \xi_3
+ \frac{(-1)^N (65 + 101N + 56N^2 + 13N^3 + N^4)}{2(1+N)^2(2+N)^2(3+N)^2} S_{-3} + \frac{(-24 - 5N + 2N^2)}{12(2+N)^2(3+N)^2} S_3
- \frac{1}{2(1+N)(2+N)(3+N)} S_2^2 + \frac{1}{(2+N)(3+N)} S_1^2 S_2
+ \frac{314 + 631N + 578N^2 + 288N^3 + 68N^4 + 5N^5}{4(1+N)^3(2+N)^2(3+N)^2} S_1 - \frac{3}{2} S_5.\quad (4.3)$$
Here $P_i$ denote polynomials, cf. [23]. The final expression contains individual terms which grow $\propto 2^N$ for $N \to \infty$. However, this singularity cancels in $\hat{I}_4(N)$. As an extension of the usual harmonic sums [26] also generalized sums [27, 28] contribute with weights $x_i \in \{1, 1/2, 2\}$.

Let us now turn to the graph shown in Fig. 2. It consists out of two contributions with respect to the operator insertion, cf. [3], which may be viewed as being obtained by contraction of the central lines of the ladder graph, resp. the graph of the crossed box, with central operator insertion.

![3-loop ladder diagram containing a 4-vertex local operator insertion.](image)

While the calculation of the former graph is rather straightforward, in the latter case root-letters appear in the integration formalism using the method of hyperlogarithms. Here it is possible, however, to move the corresponding root-expressions completely into the argument of the hyperlogarithms.
In the next step we would like to determine the $N$th Taylor coefficient of the expression obtained. A first possibility consists in calculating a large number of Mellin-moments for the expression in an efficient way, which needs the use of Form [31] beyond the representations in Maple [49]. In the present case about 1500 moments have been calculated. The method of guessing [50] allows to derive a corresponding difference equation, for which we needed $\sim 700$ moments in the present case. This equation can now be solved using Sigma [34] and the $N$th moment is obtained. In an earlier investigation we have determined all 3-loop anomalous dimensions and massless Wilson coefficients from their moments in this way, which required 5114 moments, [51]. Although not expected to fail with a significant probability, and having a large verification space with $\sim 1500$ moments available at $\sim 700$ needed, still the $N$th moment shall be derived having a proof certificate. A more involved calculation using HarmonicSums [28] and Sigma [34] provides this. Here, difference equations of up to order $o = 16$ and degree $d = 108$ have to be solved. The results are presented in [24].

The emergence of root-expressions in $x$ implies in the present result quite a series of new sums, which are of the nested binomial- and inverse-binomial type and also contain generalized harmonic sums. We have translated the result into $x$-space, where new iterated integrals with various root-type letters were obtained, extending those having appeared in [52]. Using the methods of Ref. [43] the relative transcendence of the different functions can be checked and we derived a corresponding basis for these functions, cf. [42]. In $N$-space the basis representation, including the new sums, is derived using Sigma, [34].

The method of hyperlogarithms also allows the calculation of non-singular Benz-graphs, which have representations in terms of harmonic sums and generalized harmonic sums, cf. [24, 53].

5. Conclusions

We reported on recent progress in calculating the asymptotic heavy flavor Wilson coefficients contributing to the deep-inelastic structure function $F_2(x, Q^2)$ at 3-loop order. As a first class all contributions of $O(n_f T_F^2 C_{A,F})$ have been completed and basis integrals for the class $O(T_F^2 C_{A,F})$ were obtained. Furthermore, the automatic calculation of related topology classes for other color factors started. We extended the former analysis to the case in which two heavy quarks of different mass contribute and obtained a series of Mellin moments. These contributions are no longer in accordance with the variable flavor number scheme, since charm does not decouple at the mass scale of the bottom quark. In case of two massive fermion lines with equal mass new sums and iterated integrals appear beyond the usual harmonic sums and polylogarithms, also leading to more singularities in the complex plane. We have also calculated the scalar graphs contributing to ladder-topologies for up to six massive fermion lines, including graphs with local 4-leg operators. Here the results are given in terms of special classes of generalized sums, which individually may even diverge exponentially for $N \to \infty$. This divergence is canceled between different terms contributing. In case of the graph shown in Fig. 2 a larger amount of nested binomial and inverse binomial sums weighted with harmonic sums and their generalization, also including cyclotomic sums, emerge, extending the known alphabets both for the sums and the associated iterated integrals. This all is invisible at the level of Mellin moments since the corresponding expressions are given in terms of rationals and single $\zeta$-values. It appears that in the presence of a single mass already at 3-loop
order rich new structures are contributing in the single differential case being characterized either by the Mellin variable $N$ or the momentum fraction $x$.

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