New Heavy Flavor Contributions to the DIS Structure Function $F_2(x,Q^2)$ at $O(\alpha_s^3)$

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We report on recent results obtained for the massive Wilson coefficients which contribute to the structure function $F_2(x,Q^2)$ at $O(\alpha_s^3)$ in the region $Q^2/m^2 \gtrsim 10$. In the calculation new species of harmonic sums and harmonic polylogarithms generated by cyclotomic polynomials arise in intermediary results which are briefly discussed.

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1. Introduction

The charm quark contributions to the nucleon structure functions are large in the small x region. To obtain a correct theoretical description of the structure function $F_2(x, Q^2)$, which is measured at an accuracy of 1% in this region, 3-loop (NNLO) corrections to the heavy flavor Wilson coefficients are needed. Present extractions of the strong coupling constant from deep inelastic data [1] and precision measurements of parton densities require this accuracy, with important consequences for precision measurements at Tevatron and LHC [2]. In previous calculations the Wilson coefficients were obtained to $O(\alpha_s^2)$ [3] [1]. If one considers the region $Q^2/m^2 \gtrsim 10$ the massive Wilson coefficients can be obtained through convolutions [5, 6] of massive operator matrix elements (OMEs) [7–13] and the massless Wilson coefficients [14]. Other massive OMEs play a role in higher order QED correction, [15]. Based on the 2-loop massive operator matrix elements, which are known for general values of N up to the linear term in the dimensional parameter ε [8, 10, 11] and the massless 3-loop Wilson coefficients [14] one may compute all logarithmic contributions at 3–loop order [16]. In the kinematic region of HERA, however, the logarithmic terms are not dominant over the yet unknown constant terms for general values of N, as demonstrated for the moments calculated in [6]. The $O(\alpha_s^3)$ corrections to the structure function $F_L(x, Q^2)$ in the asymptotic region were computed in [6, 17]. Heavy flavor corrections for charged current reactions in Mellin space were recently given in [18], correcting some errors in the literature.

The heavy flavor contributions to the structure function $F_2(x, Q^2)$ at $O(\alpha_s^3)$ in case of one massive quark are described by five massive Wilson coefficients $L_q^{\rm NS}, L_q^{\rm PS}, L_g^{\rm S}, H_q^{\rm PS}, H_q^{\rm S}$ [6] in the asymptotic region. Two of these Wilson coefficients, $L_q^{\rm PS}$ and $L_g^{\rm S}$ haven been computed completely for general values of N in [12], cf. also [16]. In [12] the contributions of the color factors $O(T_F^2 N_f C_{A,F})$ to the Wilson coefficients $L_q^{\rm NS}, H_q^{\rm PS}, H_q^{\rm S}$ were also calculated. The corresponding Feynman diagrams consist of graphs with a massless and a massive internal fermion line. After applying algebraic relations [19] these contributions to the massive Wilson coefficients can be represented in terms of the known $w = 4$ set of harmonic sums [20]. The calculations of the massive OMEs at general value of N were performed using tform [21] and C. Schneider's summation package Sigma [22], which has received continuous updates during the last years.

In this note we report on further progress of the 3-loop calculation of massive OMEs on contributions due to charm and bottom lines in single diagrams, massive gluonic OMEs, massive 3–loop ladder graphs, and cyclotomic harmonic sums and polylogarithms, which emerge in intermediate steps of present calculations.

2. Two massive quarks of unequal mass

Beginning at $O(\alpha_s^3)$, graphs with internal massive fermion lines carrying unequal finite masses contribute. Due to the mass ratio $x = m_c^2/m_b^2 \simeq 1/10$ for the case of charm and bottom quarks, one may expand the corresponding diagrams using this parameter. The results for the moments $N = 2$ and $N = 4$ of the gluonic operator matrix element A_{Qg} were given in [13] before, extending the code qexp [23] to higher moments applying projectors similar to those used in [6]. With rising

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[1]Precise numerical implementations in Mellin space were given in [4].

values of N the calculations become more and more time consuming even using `tform` [21]. Here we present the moment $N = 6$ which requested several months of run time :

$$
\begin{aligned}
a_{Qg}^{(3)} = T_F^2 C_A &\left\{ \frac{69882273800453}{367569090000} - \frac{395296}{19845}\zeta_3 + \frac{1316809}{39690}\zeta_2 + \frac{832369820129}{14586075000}x + \frac{1511074426112}{624023544375}x^2 \right.\\
&- \frac{84840004938801319}{690973782403905000}x^3 \\
&+ \ln\left(\frac{m_2^2}{\mu^2}\right)\left[\frac{11771644229}{194481000} + \frac{78496}{2205}\zeta_2 - \frac{1406143531}{69457500}x - \frac{105157957}{180093375}x^2 + \frac{2287164970759}{7669816654500}x^3\right] \\
&+ \ln^2\left(\frac{m_2^2}{\mu^2}\right)\left[\frac{2668087}{79380} + \frac{112669}{661500}x - \frac{49373}{51975}x^2 - \frac{31340489}{34054020}x^3\right] + \ln^3\left(\frac{m_2^2}{\mu^2}\right)\frac{324148}{19845} \\
&+ \ln^2\left(\frac{m_2^2}{\mu^2}\right)\ln\left(\frac{m_1^2}{\mu^2}\right)\frac{156992}{6615} \\
&+ \ln\left(\frac{m_2^2}{\mu^2}\right)\ln\left(\frac{m_1^2}{\mu^2}\right)\left[\frac{128234}{3969} - \frac{112669}{330750}x + \frac{98746}{51975}x^2 + \frac{31340489}{17027010}x^3\right] + \ln\left(\frac{m_2^2}{\mu^2}\right)\ln^2\left(\frac{m_1^2}{\mu^2}\right)\frac{68332}{6615} \\
&+ \ln\left(\frac{m_1^2}{\mu^2}\right)\left[\frac{83755534727}{583443000} + \frac{78496}{2205}\zeta_2 + \frac{1406143531}{69457500}x + \frac{105157957}{180093375}x^2 - \frac{2287164970759}{7669816654500}x^3\right] \\
&\left.+ \ln^2\left(\frac{m_1^2}{\mu^2}\right)\left[\frac{2668087}{79380} + \frac{112669}{661500}x - \frac{49373}{51975}x^2 - \frac{31340489}{34054020}x^3\right] + \ln^3\left(\frac{m_1^2}{\mu^2}\right)\frac{412808}{19845}\right\} \\
+ T_F^2 C_F &\left\{ -\frac{3161811182177}{71471767500} + \frac{447392}{19845}\zeta_3 + \frac{9568018}{4862025}\zeta_2 - \frac{64855635472}{2552563125}x + \frac{1048702178522}{97070329125}x^2 \right. \\
&+ \frac{1980566069882672}{2467763508585375}x^3 \\
&+ \ln\left(\frac{m_2^2}{\mu^2}\right)\left[\frac{1786067629}{204205050} - \frac{111848}{15435}\zeta_2 - \frac{128543024}{24310125}x - \frac{22957168}{3361743}x^2 - \frac{2511536080}{2191376187}x^3\right] \\
&+ \ln^2\left(\frac{m_2^2}{\mu^2}\right)\left[\frac{3232799}{4862025} + \frac{752432}{231525}x + \frac{177944}{40425}x^2 + \frac{127858928}{42567525}x^3\right] - \ln^3\left(\frac{m_2^2}{\mu^2}\right)\frac{111848}{19845} \\
&- \ln^2\left(\frac{m_2^2}{\mu^2}\right)\ln\left(\frac{m_1^2}{\mu^2}\right)\frac{223696}{46305} \\
&+ \ln\left(\frac{m_2^2}{\mu^2}\right)\ln\left(\frac{m_1^2}{\mu^2}\right)\left[\frac{22238456}{4862025} - \frac{1504864}{231525}x - \frac{355888}{40425}x^2 - \frac{255717856}{42567525}x^3\right] + \ln\left(\frac{m_2^2}{\mu^2}\right)\ln^2\left(\frac{m_1^2}{\mu^2}\right)\frac{223696}{46305} \\
&+ \ln\left(\frac{m_1^2}{\mu^2}\right)\left[-\frac{24797875607}{1021025250} - \frac{111848}{15435}\zeta_2 + \frac{128543024}{24310125}x + \frac{22957168}{3361743}x^2 + \frac{2511536080}{2191376187}x^3\right] \\
&\left.+ \ln^2\left(\frac{m_1^2}{\mu^2}\right)\left[\frac{3232799}{4862025} + \frac{752432}{231525}x + \frac{177944}{40425}x^2 + \frac{127858928}{42567525}x^3\right] - \ln^3\left(\frac{m_1^2}{\mu^2}\right)\frac{1230328}{138915}\right\} + O\left(x^4 \ln^3(x)\right).
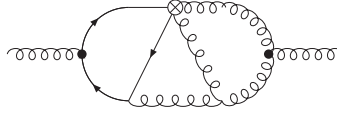\end{aligned}
$$

(2.1)

These contributions to the massive Wilson coefficients can be uniquely calculated in the fixed flavor number scheme with three massless quarks in the initial state. However they cannot be attributed either to the charm- or bottom distribution in a variable flavor scheme. [2] Despite all these contributions are universal, the so-called variable flavor scheme *ends at the 2-loop level.* In general we remark that the representation of the heavy flavor Wilson coefficients to $O(\alpha_s^3)$ are given in the

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[2]It was shown in [24] that the matching scale is rather process dependent and may differ significantly from the heavy quark mass m_Q, as comparisons to complete calculations show. This aspect, however, is often ignored.

fixed flavor number scheme. As has been shown e.g. in Refs. [25, 26] this choice is sufficient for the kinematic range at HERA.

3. Contributions due to 3-Loop Ladder Graphs

A next topology class consists of ladder graphs containing up to six massive lines and local operator insertions. The calculation of these graphs is underway [27]. Here we present, as an example, the result for the scalar Diagram shown in the following Figure :

$$\hat{I}_{10a} = \frac{1}{(N+3)(N+4)} \Bigg\{ \Bigg[-\frac{4\left(N^3+3N^2-N-5\right)}{(N+1)(N+2)(N+3)} S_1 + 2S_1^2 + \frac{4(-1)^N}{N+3} S_1 + 4S_{-2}$$

$$+2(2N+5)S_2 + \frac{4(-1)^N\left(2N^3+7N^2+4N-3\right)}{(N+1)^2(N+2)^2(N+3)} + \frac{4\left(6N^3+34N^2+63N+39\right)}{(N+1)^2(N+2)^2(N+3)} \Bigg] \frac{1}{\varepsilon^2}$$

$$+\Bigg[\frac{\left(-4N^4-25N^3-30N^2+49N+76\right)}{(N+1)(N+2)(N+3)(N+4)} S_1^2 - \frac{4\left(2N^4+14N^3+27N^2+5N-16\right)}{(N+1)(N+2)(N+3)(N+4)} S_{-2}$$

$$+\frac{\left(10N^4+73N^3+158N^2+73N-52\right)}{(N+1)(N+2)(N+3)(N+4)} S_2$$

$$+\frac{2(-1)^N\left(12N^5+127N^4+538N^3+1177N^2+1354N+648\right)}{(N+1)^2(N+2)^2(N+3)^2(N+4)} S_1$$

$$-\frac{2\left(8N^6+51N^5-72N^4-1330N^3-4062N^2-5151N-2436\right)}{(N+1)^2(N+2)^2(N+3)^2(N+4)} S_1$$

$$+S_1^3 + \frac{(-1)^N}{N+3}\left(S_1^2-S_2\right) + 4S_{-2}S_1 - 5S_2S_1 + 2(4N+15)S_{-3} + 2(N-1)S_3$$

$$-12S_{-2,1} + 8(N+4)S_{2,1}$$

$$+\frac{2(-1)^N\left(11N^6+60N^5-160N^4-1837N^3-5005N^2-5801N-2508\right)}{(N+1)^3(N+2)^3(N+3)^2(N+4)}$$

$$+\frac{2\left(70N^6+893N^5+4640N^4+12626N^3+19074N^2+15269N+5100\right)}{(N+1)^3(N+2)^3(N+3)^2(N+4)} \Bigg] \frac{1}{\varepsilon}$$

$$+\frac{7}{24}S_1^4 + \frac{\left(-10N^4-61N^3-68N^2+129N+188\right)}{6(N+1)(N+2)(N+3)(N+4)} S_1^3$$

$$+\frac{(-1)^N\left(12N^5+127N^4+538N^3+1177N^2+1354N+648\right)}{2(N+1)^2(N+2)^2(N+3)^2(N+4)} S_1^2$$

$$+\frac{P_{22}}{2(N+1)^2(N+2)^2(N+3)^2(N+4)^2} S_1^2 + \frac{3}{4}\zeta_2 S_1^2 - 4S_{-2}S_1^2 - \frac{13}{4}S_2S_1^2$$

$$
+\frac{(-1)^N P_{23}}{(N+1)^3(N+2)^3(N+3)^3(N+4)^2}S_1 + \frac{P_{24}}{(N+1)^3(N+2)^3(N+3)^3(N+4)^2}S_1
$$

$$
-\frac{3\left(N^3+3N^2-N-5\right)}{2(N+1)(N+2)(N+3)}\zeta_2 S_1 - 2S_{-3}S_1
$$

$$
-\frac{4\left(4N^4+41N^3+155N^2+254N+148\right)}{(N+1)(N+2)(N+3)(N+4)}S_{-2}S_1
$$

$$
+\frac{(-1)^N}{N+3}\left(-4S_{-2}S_1+\frac{9}{2}S_2 S_1+\frac{3}{2}\zeta_2 S_1+\frac{1}{6}S_1^3-2S_{-3}+\frac{10}{3}S_3+2S_{2,1}+12S_{-2,1}\right)
$$

$$
+\frac{\left(-14N^4-201N^3-936N^2-1715N-1044\right)}{2(N+1)(N+2)(N+3)(N+4)}S_2 S_1 - \frac{119}{3}S_3 S_1
$$

$$
-12S_{-2,1}S_1+22S_{2,1}S_1-2S_{-2}^2+\frac{1}{8}(32N+119)S_2^2
$$

$$
+\frac{(-1)^N P_{25}}{(N+1)^4(N+2)^4(N+3)^3(N+4)^2} + \frac{P_{26}}{(N+1)^4(N+2)^4(N+3)^3(N+4)^2}
$$

$$
+\frac{3(-1)^N\left(2N^3+7N^2+4N-3\right)}{2(N+1)^2(N+2)^2(N+3)}\zeta_2 + \frac{3\left(6N^3+34N^2+63N+39\right)}{2(N+1)^2(N+2)^2(N+3)}\zeta_2
$$

$$
+(8N+39)S_{-4}+\frac{2\left(8N^5+108N^4+558N^3+1365N^2+1553N+640\right)}{(N+1)(N+2)(N+3)(N+4)}S_{-3}
$$

$$
-\frac{4(-1)^N\left(2N^3+7N^2+4N-3\right)}{(N+1)^2(N+2)^2(N+3)}S_{-2}-\frac{4P_{27}}{(N+1)^2(N+2)^2(N+3)^2(N+4)^2}S_{-2}
$$

$$
+\frac{3}{2}\zeta_2 S_{-2}+\frac{(-1)^N\left(8N^5+79N^4+186N^3-279N^2-1426N-1224\right)}{2(N+1)^2(N+2)^2(N+3)^2(N+4)}S_2
$$

$$
+\frac{P_{28}}{2(N+1)^2(N+2)^2(N+3)^2(N+4)^2}S_2 + \frac{3}{4}(2N+5)\zeta_2 S_2 + 8S_{-2}S_2
$$

$$
+\frac{\left(-18N^5-229N^4-1498N^3-5558N^2-10017N-6460\right)}{3(N+1)(N+2)(N+3)(N+4)}S_3
$$

$$
+\frac{1}{4}(20N-29)S_4-14S_{-3,1}+\frac{4\left(4N^4+22N^3+11N^2-85N-96\right)}{(N+1)(N+2)(N+3)(N+4)}S_{-2,1}
$$

$$
-14S_{-2,2}+\frac{2\left(11N^4+107N^3+397N^2+640N+361\right)}{(N+1)(N+2)(N+3)}S_{2,1}+2(N+36)S_{3,1}
$$

$$
\left.+28S_{-2,1,1}+2(2N-7)S_{2,1,1}\right\}+O(\varepsilon)\,, \tag{3.1}
$$

$$
\begin{aligned}
P_{22} =\ & -6N^8-164N^7-1613N^6-7762N^5-19526N^4-22888N^3-2137N^2 \\
& +19968N+13264\,, \tag{3.2}
\end{aligned}
$$

$$
\begin{aligned}
P_{23} =\ & 119N^8+2250N^7+18755N^6+90365N^5+275464N^4+542281N^3+668958N^2 \\
& +469072N+142112\,, \tag{3.3}
\end{aligned}
$$

$$
\begin{aligned}
P_{24} =\ & 16N^{11}+448N^{10}+5568N^9+41171N^8+204092N^7+720291N^6+1858328N^5 \\
& +3504939N^4+4712624N^3+4272331N^2+2335952N+581072\,, \tag{3.4}
\end{aligned}
$$

$$
\begin{aligned}
P_{25} =\ & 78N^9+937N^8+2466N^7-17638N^6-155141N^5-538674N^4-1047495N^3 \\
& -1197445N^2-757472N-206256\,, \tag{3.5}
\end{aligned}
$$

$$P_{26} = 568N^9 + 11297N^8 + 98332N^7 + 492027N^6 + 1561688N^5 + 3266831N^4$$
$$+4516420N^3 + 3994885N^2 + 2061840N + 475824 \,, \tag{3.6}$$

$$P_{27} = 4N^8 + 96N^7 + 942N^6 + 4995N^5 + 15753N^4 + 30351N^3 + 34903N^2$$
$$+21844N + 5648 \,, \tag{3.7}$$

$$P_{28} = -32N^9 - 730N^8 - 7180N^7 - 40057N^6 - 139918N^5 - 317434N^4 - 466820N^3$$
$$-426421N^2 - 216416N - 45040 \,. \tag{3.8}$$

4. Contributions to Gluonic Matrix Elements

First results for general values of N have been obtained for the gluonic OMEs of $O(N_f T_F^2 C_{A,F})$. They are of importance to define the variable flavor scheme for the single heavy mass contributions, cf. [6, 11, 28]. As an example we show the renormalized result for $A_{gq,Q}^{(3)}(N)$, cf. [29]:

$$
\begin{aligned}
A_{gq,Q,C_F T_F^2 n_f}^{(3),\overline{\text{MS}}} = {}& C_F n_f T_F^2 \frac{1+(-1)^N}{2} \Bigg\{ \frac{88\left(N^2+N+2\right)}{27(N-1)N(N+1)} \log^3\left(\frac{m^2}{\mu^2}\right) \\
&+ \left(\frac{8\left(N^2+N+2\right)}{9(N-1)N(N+1)} S_1 - \frac{8\left(8N^3+13N^2+27N+16\right)}{27(N-1)N(N+1)^2} \right) \log^2\left(\frac{m^2}{\mu^2}\right) \\
&+ \Bigg[\frac{16\left(N^2+N+2\right)}{9(N-1)N(N+1)} \left(S_1^2 + S_2 - \frac{1}{2}\zeta_2 \right) - \frac{32\left(8N^3+13N^2+27N+16\right)}{27(N-1)N(N+1)^2} S_1 \\
&+ \frac{16\left(179N^4+489N^3+913N^2+925N+358\right)}{81(N-1)N(N+1)^3} \Bigg] \log\left(\frac{m^2}{\mu^2}\right) \\
&+ \Bigg[\frac{16(N^2+N+2)}{9(N-1)N(N+1)} \left(S_1^3 + 3S_2 S_1 + 2S_3 + 5S_1 \zeta_2 + \frac{11}{2}\zeta_3 \right) \\
&- \frac{16(8N^3+13N^2+27N+16)}{9(N-1)N(N+1)^2} \left(S_1^2 + S_2 + \frac{5}{3}\zeta_2 \right) \\
&+ \frac{32(160N^4+408N^3+827N^2+845N+320)}{81(N-1)N(N+1)^3} S_1 \\
&- \frac{32(1189N^5+4276N^4+9248N^3+12289N^2+8668N+2378)}{243(N-1)N(N+1)^4} \Bigg] \Bigg\}. \tag{4.1}
\end{aligned}
$$

5. Cyclotomic Harmonic Sums and Harmonic Polylogarithms

In various calculations of the massive OMEs harmonic sums emerged, which are associated to cyclotomic harmonic polylogarithms. It appeared therefore as useful to generalize the usual harmonic polylogarithms [30] based on the alphabet $\{1/x, 1/(1-x), 1/(1+x)\}$ to that of the alphabet

$$\mathfrak{A} = \left\{ \frac{1}{x} \right\} \cup \left\{ \frac{x^l}{\Phi_k(x)} \,\middle|\, k \in \mathbb{N}_+, 0 \le l < \varphi(k) \right\}, \tag{5.1}$$

with Φ_k the kth cyclotomic polynomial and φ Euler's totient function, cf. [31]. The cyclotomic harmonic polynomials are obtained as iterated integrals of the letters in $\mathfrak{A}$. The corresponding harmonic sums[3] iterate the letters of the type

$$\frac{(-1)^k}{(nk+m)^l}, \quad n \geq 1, m \leq n, l \geq 1 \,, \tag{5.2}$$

which can also be related to usual harmonic sums at numerator weights being nth roots of unity. The properties of these harmonic polylogarithms, harmonic sums and associated generalizations of the multiple zeta values [33], as well as the relations of these quantities, are given in [31]. They are implemented in the package `HarmonicSums` [34].

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