First results for three-loop deep-inelastic structure functions in QCD

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As a first step towards the complete calculation of deep-inelastic scattering at third order of massless perturbative QCD, we have computed the fermionic ($n_f$) contributions to the flavour non-singlet structure functions in unpolarized electromagnetic scattering. We briefly discuss the approach chosen for this calculation, the problems we encountered and the status of the project. We show the results for the corresponding anomalous dimension in both Mellin- and Bjorken-$x$. Together with the $n_f$ part of $A_3$, our calculation facilitates the complete determination of the threshold-resummation coefficients $B_2$ and $D^{DIS}_2$. The latter quantity vanishes in the $\overline{\text{MS}}$ scheme.

1. Introduction

The computation of the three-loop contributions to the anomalous dimensions is needed to complete the next-to-next-to-leading order (NNLO) calculations for deep-inelastic scattering (DIS). These in their turn are required for the NNLO determination of the parton distribution functions (PDFs) that describe the quark and gluon contents of the proton. The accuracy of the experiments has become such that this order of perturbation theory is needed to match it. In turn, the PDF’s at NNLO accuracy are required for precise QCD predictions for the future experiments at the LHC.

The method we use for obtaining the three-loop structure functions is based on the calculation of all Mellin moments as a function of the Mellin moment number $N$. Once either all even or all odd moments are known, we can obtain the results in Bjorken-$x$ space by means of an inverse Mellin transformation. This method has been employed for structure functions since the early days of QCD. Only the coefficient functions are the two-loop level were first obtained by a different approach. However, the $N$-space method was later used to confirm those results.

Until the calculation of the two-loop anomalous dimensions, this method could still be applied in a rather direct way. The two-loop computation of $\sigma_L/\sigma_T$ required more finesse, and recursion relations, also called difference equations, entered the scene. The various mixings of the flavour contributions were solved in the calculation of a number of fixed moments at the three-loop level. This method turned out to be so powerful that not only the anomalous dimensions could be obtained, but also the three-loop coefficient functions as the beginning of the NNLO calculation. Hence it seemed best to continue along this path and obtain all moments. This avoids the difficult problem of operator mixings and gets us the whole three-loop order in one go.

2. Eight Problems

In this section we discuss eight of the main problems that were encountered. Basically these are problems that occur in any high-order calculation. Their solution however depends of the particular calculation.

Problem 1
For the current calculation the mathematics of the answer had to be understood better. Hence
first the properties of harmonic sums [10, 16, 17, 18] and harmonic polylogarithms [19, 20, 21] had to be studied. In addition procedures were obtained to go from one to the other by means of an inverse Mellin transform [21, 22]. All this was programmed in FORM [22]. The answer of our calculations will comprise harmonic sums of up to weight 6 for the Mellin moments. In Bjorken-$x$ space we will obtain harmonic polylogarithms with weights up to 5.

Problem 2
Next we need a scheme in which all integrals are reduced to a set of master integrals. To find these reduction algorithms in a way that they can handle any integral of the necessary topologies is much work. We have to deal with $O(70)$ (sub) topologies. For some the algorithms are trivial, but for the most difficult cases it may take a few months to derive a good algorithm. In general the equations are based on integration by parts [23, 24, 25, 26], scaling equations, form-factor analysis [27] and some equations that fall in a special category because they involve a careful study of the parton-momentum limit $P \cdot P \rightarrow 0$.

Problem 3
The master integrals can usually be determined by difference equations. For the determination of the $n_f$ part of the non-singlet structure functions we needed only first-order and second-order difference equations. For the complete calculation we have encountered equations up to fourth order. These equations are solved with a special FORM program in which we substitute a sufficiently general combination of harmonic sums and then solve for the (some times thousands of) coefficients. The boundary values are provided by the Mincer program [28] that was also used for obtaining the fixed moments.

Problem 4
The reduction equations have to be derived in a way that avoids spurious poles. Some equations may introduce powers of $1/\epsilon$ that are superfluous. The general rule is that one has to introduce at most one power of $1/\epsilon$ for each line that is eliminated. If there are more poles, the integrals by which they are multiplied will be needed to a corresponding number of extra powers of $\epsilon$. This is not always feasible. One usually avoids such extra poles by tedious combinations of equations. This is the most difficult part of the reduction scheme.

Problem 5
Next the equations have to be programmed in a way that produces results. Brute force application leads eventually to programs that run unacceptably long or produce intermediate results that exceed the size of the available disks. The solution here is a very careful tabulation of integrals of lower complexity. For this one has to define a hierarchy of complexity. Currently we have already more than 20000 tabulated integrals.

Problem 6
Because the integrals are functions of a parameter and involve harmonic sums of weight 6 (of which there are 486 different ones) each tabulated integral typically takes about 20 Kbytes. This means that the tables are rather large, $O(500\text{ Mbytes})$. It is not convenient to have to compile such an amount of code for each of the about 10000 diagrams to be computed, even though the FORM compiler is very fast (about 2 Mbytes per second on a 1.7 GHz Pentium processor). The solution to this problem lies in the use of the new tablebase facilities of FORM [29].

Problem 7
All topologies and subtopologies have to be programmed, debugged and run. Here the old Mincer program [28] for the fixed moments forms an indispensable tool. At any moment we can replace the Mellin moment $N$ by a fixed integer value and continue with the Mincer program. This way we can locate errors rather efficiently. Without this method the chances of obtaining the correct answer soon would be virtually zero.

Problem 8
Manage FORM [22]. Rare bugs occur. Also for a problem of this complexity sometimes new features can bring relief. The above-mentioned feature of the tablebases is an example.
3. Status

On the level of integrals we distinguish basic building blocks (BBB’s) and composite building blocks (CBB’s). The BBB’s are integrals in which the parton momentum \( P \) flows only through a single line in the diagram. These have been programmed completely and the vast majority of necessary integrals have been tabulated. Occasionally we still have to add some integrals to the tables. We have reduction schemes for all CBB’s. They are switched on and debugged one by one at the moment. As there exists a rather strict hierarchy in the complexity of diagrams the most complicated will be done last, but that does not necessarily imply that the most complicated are the most difficult. The easier topologies have all been debugged and most of their diagrams have been run. At the moment the more complicated topologies are being treated and run.

4. Some results

We have completed the diagrams which contribute to the \( n_f \) part of the non-singlet structure functions. The results for the anomalous dimension and some parameters of the soft-gluon resummation are presented below. We hope to finish the complete non-singlet part early in the 2003. Later that year the singlet results should follow. All diagrams we have run check with the Mincer results for several fixed moments. Our results include both the anomalous dimensions and the coefficient functions. For the latter the reader is referred to ref. [5].

The fermionic three-loop contribution to the even-\( N \) non-singlet MS anomalous dimension, with the expansion parameter normalized as \( \alpha_s/(4\pi) \), is given by

\[
\gamma_n^{(2)}(N) = 16 C_A C_F n_f \left( \frac{3}{2} \zeta_3 - \frac{5}{4} + \frac{10}{9} S_{-3} - \frac{10}{9} S_3 + \frac{4}{3} S_{1,-2} - \frac{2}{3} S_{-4} + 2 S_{1,1} - \frac{25}{9} S_2 + \frac{257}{27} S_1 - \frac{2}{3} S_{-3,1} - N_+ \left[ S_{2,1} - \frac{2}{3} S_{3,1} - \frac{2}{3} S_4 \right] \right) + (1 - N_+) \left[ \frac{23}{18} S_3 - S_2 \right] \times (N_- + N_+) \times \left[ S_{1,1} + \frac{1237}{1216} S_1 + \frac{11}{18} S_3 - \frac{317}{108} S_2 \right] + \frac{16}{9} S_{1,-2} - \frac{2}{3} S_{1,-2,1} - \frac{1}{3} S_{1,-3} - \frac{1}{2} S_{1,3} - \frac{1}{2} S_{2,1} - \frac{1}{3} S_{2,-2} + S_1 \zeta_3 + \frac{1}{2} S_{3,1} \right) \\
+ 16 C_F n_f^2 \left( \frac{17}{144} - \frac{13}{27} S_1 + \frac{2}{9} S_2 \right) + (N_- + N_+) \left[ \frac{2}{9} S_1 - \frac{11}{54} S_2 + \frac{1}{18} S_3 \right] \\
+ 16 C_F^2 n_f^2 \left( \frac{23}{16} - \frac{3}{2} S_3 + \frac{4}{3} S_{-3,1} - \frac{59}{36} S_2 \right) + \frac{4}{3} S_{-4} - \frac{20}{9} S_{-3} + \frac{20}{9} S_1 - \frac{8}{3} S_{1,-2} - \frac{8}{3} S_{1,1} - \frac{4}{3} S_{1,2} + N_+ \left[ \frac{25}{9} S_3 - \frac{4}{3} S_{3,1} - \frac{1}{3} S_4 \right] \\
+ (1 - N_+) \left[ \frac{67}{36} S_2 - \frac{4}{3} S_{2,1} + \frac{4}{3} S_3 \right] + (N_- + N_+) \left[ \frac{325}{144} S_1 - \frac{2}{3} S_{1,-3} + \frac{32}{9} S_{1,-2} - \frac{4}{3} S_{1,-2,1} + \frac{4}{3} S_{1,1} + \frac{16}{9} S_{1,2} - \frac{4}{3} S_{1,3} + \frac{11}{18} S_2 - \frac{2}{3} S_{2,-2} + \frac{10}{9} S_{2,1} + \frac{1}{2} S_4 - \frac{2}{3} S_{2,2} - \frac{8}{9} S_3 \right] \right).
\]

Here we have suppressed the argument \( N \) of the harmonic sums and used the notation

\[
N_{\pm} f(N) = f(N \pm 1) \\
N_{\pm i} f(N) = f(N \pm i).
\]

The corresponding splitting function, as usual defined with a relative sign, reads

\[
P_{n_s}^{(2)}(x) = 16 C_A C_F n_f \left( p_{qq}(x) \left[ \frac{5}{9} \zeta_2 - \frac{209}{216} - \frac{3}{2} \zeta_3 + \frac{167}{108} \ln(x) + \frac{1}{3} \ln(x) \zeta_2 \right] - \frac{1}{4} \ln^2(x) \ln(1-x) - \frac{7}{12} \ln^2(x) - \frac{1}{18} \ln^3(x) \right) - \frac{1}{2} \ln(x) \text{Li}_2(x) + \frac{1}{3} \text{Li}_3(x) \\
+ p_{qq}(-x) \left[ \frac{1}{2} \zeta_3 - \frac{5}{9} \zeta_2 - \frac{2}{3} \ln(1+x) \zeta_2 \right]
\]
\[
\begin{align*}
+ \frac{1}{6} \ln(x) \zeta_2 & - \frac{10}{9} \ln(x) \ln(1+x) + \frac{5}{18} \ln^2(x) \\
- \frac{1}{6} \ln^2(x) \ln(1+x) & + \frac{1}{18} \ln^3(x) - \frac{10}{9} \text{Li}_2(-x) \\
- \frac{1}{3} \text{Li}_3(-x) & - \frac{1}{3} \text{Li}_3(x) + \frac{2}{3} H_{-1,0,1}(x) \\
+ (1 + x) \left[ \frac{1}{6} \zeta_2 + \frac{1}{2} \ln(x) - \frac{1}{2} \text{Li}_2(x) \\
- \frac{2}{3} \text{Li}_2(-x) & - \frac{2}{3} \ln(x) \ln(1+x) + \frac{1}{24} \ln^2(x) \\
+ (1 - x) \left[ \frac{1}{3} \zeta_2 - \frac{257}{54} + \ln(1+x) - \frac{17}{9} \ln(x) \\
- \frac{1}{24} \ln^2(x) & + \delta(1-x) \left[ \frac{5}{4} - \frac{167}{54} \zeta_2 + \frac{1}{20} \zeta_2^2 \\
+ \frac{25}{18} C_F & \right] + 16 C_F n_f^2 \left( p_{qq}(x) \frac{5}{54} \ln(x) \\
- \frac{1}{54} & + \frac{1}{36} \ln^2(x) \right) + (1 - x) \left[ \frac{13}{54} + \frac{1}{9} \ln(x) \\
- \delta(1-x) \left[ \frac{17}{144} - \frac{5}{27} \zeta_2 + \frac{1}{9} \zeta_3 \right] \\
+ 16 C_F^2 n_f & \right] \left( p_{qq}(x) \frac{5}{54} \zeta_2 - \frac{55}{48} \right) \\
+ \frac{5}{24} \ln(x) & + \frac{1}{3} \ln(x) \zeta_2 - \frac{10}{9} \ln(x) \ln(1-x) \\
+ \frac{1}{4} \ln^2(x) & + \frac{2}{3} \ln^2(x) \ln(1-x) \\
+ \frac{1}{3} \ln(x) \text{Li}_2(x) & - \frac{2}{3} \text{Li}_3(x) - \frac{1}{18} \ln^3(x) \\
+ p_{qq}(-x) \left[ \frac{10}{9} \zeta_2 - \zeta_3 + \frac{4}{3} \ln(1+x) \zeta_2 \\
- \frac{1}{3} \ln(x) \zeta_2 & - \frac{5}{9} \ln^2(x) + \frac{20}{9} \ln(x) \ln(1+x) \\
- \frac{1}{9} \ln^3(x) & + \frac{1}{3} \ln^2(x) \ln(1+x) + \frac{20}{9} \text{Li}_2(-x) \\
+ \frac{2}{3} \text{Li}_3(-x) & + \frac{2}{3} \text{Li}_3(x) - \frac{4}{3} H_{-1,0,1}(x) \\
+ (1 + x) \left[ \frac{7}{36} \ln^2(x) - \frac{67}{72} \ln(x) \\
+ \frac{4}{3} \ln(x) & \ln(1+x) + \frac{1}{12} \ln^3(x) + \frac{2}{3} \text{Li}_2(x) \\
+ \frac{4}{3} \text{Li}_2(-x) & + (1 - x) \left[ \frac{1}{9} \ln(x) - \frac{10}{9} \right]
\right]
\end{align*}
\]

where we have used

\[
p_{qq}(x) = 2 (1 - x)^{-1} - 1 - x
\]

and all divergences for \( x \to 1 \) are understood in the sense of + - distributions. The \( n_f^2 \) part of eqs. (1) and eqs. (3) has been derived before by Gracey [3] and we agree with his result.

Our results also facilitate the determination of coefficients governing the soft-gluon (threshold) resummation [22, 33, 34] at next-to-next-to-leading logarithmic accuracy [35].

The coefficient \( A_3 \) arising from initial-state collinear emissions is the coefficient of \( 1/\ln(1-x)_+ \) in \( P_{22}^{(2)}(x) \). Its fermionic part reads

\[
A_3 \bigg|_{n_f} = C_A C_F n_f \left[ -\frac{836}{27} + \frac{160}{9} \zeta_2 - \frac{112}{3} \zeta_3 \right] \\
+ C_F n_f \left[ -\frac{110}{3} + 32 \zeta_3 \right] \\
+ C_F n_f^2 \left[ -\frac{16}{27} \right].
\]

Simultaneously to our work Carola Berger [36] has used a method based on eikonal expansions to obtain this coefficient. The calculations have been performed independently and put on the internet before comparison. The result agrees.

From the coefficient of \( \ln(1-x)/\ln(1-x)_+ \) in the \( n_f \) part of the three-loop coefficient function we can furthermore determine the (complete) resummation coefficients \( B_2 \) and \( D_2^{DIS} \) which are due to final-state collinear and large-angle soft gluons, respectively. Previously only the sum of these two parameters had been determined [33] from the two-loop coefficient function of ref. [3]. Our result involves a different linear combination (with a prefactor \( \beta_0 \)), and hence we can extract both individually, yielding

\[
B_2 = C_F \left[ -\frac{3}{2} - 24 \zeta_2 + 12 \zeta_3 \right] \\
+ C_F C_A \left[ -\frac{3155}{54} + 40 \zeta_3 + \frac{44}{3} \zeta_2 \right]
\]
\[ D^\text{DIS}_2 = 0. \tag{5} \]

The last result is intriguing and calls for further studies.

REFERENCES