Mellin Representation for the Heavy Flavor Contributions to Deep Inelastic Structure Functions

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Abstract

We derive semi–analytic expressions for the analytic continuation of the Mellin transforms of the heavy flavor QCD coefficient functions for neutral current deep inelastic scattering in leading and next-to-leading order to complex values of the Mellin variable $N$. These representations are used in Mellin–space QCD evolution programs to provide fast evaluations of the heavy flavor contributions to the structure functions $F_2(x,Q^2)$, $F_L(x,Q^2)$ and $g_1(x,Q^2)$.

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1 Introduction

A major goal in investigating the scaling violations of the structure functions as measured in deeply inelastic scattering is to determine the QCD scale parameter $\Lambda_{\text{QCD}}$, or equivalently the strong coupling constant $\alpha_s(Q^2)$, at a typical reference scale $Q^2$. The QCD renormalization group equations for mass factorization at space–like momentum transfer are solved referring to either $x$–space \cite{1}\textsuperscript{2} or Mellin–space \cite{3,4} representations. \footnote{A series of these codes uses orthogonal polynomials to diagonalize the evolution equations \cite{2}.} The formulation of the evolution equations in Mellin space has the advantage that only \textbf{ordinary} differential equations, unlike integro-differential equations in $x$–space, have to be solved. Moreover, to maintain factorization–scheme invariance the evolution equations have to be consistently expanded in the strong coupling constant, which allows an analytic integration of the differential equations, i.e. a complete analytic solution. The only numerical element consists in the inverse Mellin transform of the solution to $x$–space via a contour integral around the singularities of the solution in the complex $N$–plane. The solution in fixed order perturbation theory has isolated poles on the real axis bounded by some positive number from above. Resummations of small–$x$ contributions can be easily implemented in this approach in a \textbf{consistent} way \cite{6}. In the QCD fit only the parameters of the non–perturbative input distributions and $\Lambda_{\text{QCD}}$ have to be varied and the evolution kernels consisting out of the anomalous dimensions and the Wilson coefficients to the respective order in the coupling constant need not to be recalculated but are kept fixed as (tabulated) $Q^2$–dependent arrays along the contour used for the numerical Mellin inversion. This makes QCD fits using Mellin–space programs particularly fast.

The analytic solution of the evolution equations in Mellin space allows to study factorization–scheme invariant evolution equations of different kind \cite{3,4}. These equations describe the evolution of \textbf{physical observables}. In the non–singlet case a flavor non–singlet combination of structure functions forms the input distribution, which can be measured at a starting scale $Q_0^2$. The usual flavor singlet evolution can be mapped into the evolution of two structure functions as e.g. $F_2(x, Q^2)$ and $F_L(x, Q^2)$, $F_2(x, Q^2)$ and $\partial F_2(x, Q^2)/\partial \ln(Q^2)$, or $g_1(x, Q^2)$ and $\partial g_1(x, Q^2)/\partial \ln(Q^2)$, \cite{4}. Here the non–perturbative input distributions are formed by the measured structure functions at a scale $Q_0^2$, and have therefore not to be determined in the QCD–analysis. The evolution kernels in $x$–space are complicated multiple Mellin convolutions of Wilson coefficients, splitting functions $P^{(k)}_{ij}(z)$ and of some Mellin–inverse splitting functions and Wilson coefficients in general, see \cite{8}. These physical evolution kernels can be easily calculated in analytic form in Mellin–$N$ space unlike in $x$–space, where, as is well known, already the Mellin–inverse of leading order splitting functions takes a complicated form \cite{9} and the convolutions to be performed were never done analytically. Due to the sizeable contribution of charm to the structure functions $F_2(x, Q^2)$ and $F_L(x, Q^2)$ in the kinematic regime of HERA ($x > 10^{-4}, Q^2 > 5 \text{ GeV}^2$) an exact treatment requires the account for heavy quark effects on $F_2(x, Q^2)$ and $F_L(x, Q^2)$ which is easiest described in analytic form in Mellin–$N$ space. The standard QCD analysis and fits using scheme–invariant evolution provide different methods to determine the strong coupling constant $\alpha_s(M_Z^2)$. In the upcoming high–precision analyses, which aim on measurement errors of $O(1\%)$, it is of particular importance to diminish all theoretical and conceptual uncertainties. For this purpose the use of both these methods will be essential.

So far no specific representation of the heavy flavor Wilson coefficients in Mellin–$N$ space, in the way used for those of the light flavors, were derived. It is the aim of the present paper to present these parameterizations in terms of a semi-analytic approach. The representation is
based on meromorphic functions in the Mellin variable \( N \). The \( \xi = Q^2/m^2 \) dependence is given by a series of numerical expansion coefficients until a desired accuracy is reached. Interpolations in the variable \( \xi \) are used along the inversion contour to keep the analysis as fast as possible. The present parameterizations enable to perform scheme–invariant evolutions including the effect of heavy flavor coefficient functions.

The paper is organized as follows. In section 2 we summarize the basic notations to describe the neutral–current heavy flavor contributions to deep–inelastic scattering up to next–to–leading order [10–14]. In section 3 we present the parameterization of the different contributions to the QCD Wilson coefficients for heavy flavor production for complex values of Mellin–\( N \) and apply these representations to calculate the heavy flavor structure functions using sample densities for the light partons, including the study of their accuracy. Section 4 contains the conclusions.

## 2 The Heavy Flavor Structure Functions

The Wilson–coefficients for heavy flavor production in deeply inelastic scattering depend on two different scales, which can be represented choosing different kinematic variables. Here we follow, for convenience, the notation of Ref. [14] and use the variables \( \xi \) and \( \eta \):

\[
\xi = \frac{Q^2}{m^2}, \quad \eta = \frac{s}{4m^2} - 1 \geq 0.
\]

\( s \) denotes the cms energy squared of the heavy quark system, \( Q^2 = -q^2 \) the four–momentum transfer squared, and \( m \) the heavy quark mass. The momentum fraction \( z \) carried by the struck parton in the nucleon is

\[
z = \frac{Q^2}{Q^2 + s} = \frac{\xi/4}{1 + \eta + \xi/4}, \quad z \in \left[ x, \frac{Q^2}{Q^2 + 4m^2} \right],
\]

and the cms velocity of the heavy quarks is

\[
v = \sqrt{1 - \frac{4m^2}{Q^2} \frac{z}{1 - z}} = \sqrt{\frac{\eta}{1 + \eta}}.
\]

The heavy flavor structure functions are given in leading (LO) and next-to-leading order (NLO) by

\[
F_k(x, Q^2, m^2) = F_k^{LO}(x, Q^2, m^2) + F_k^{NLO}(x, Q^2, m^2),
\]

\[
G_k(x, Q^2, m^2) = G_k^{LO}(x, Q^2, m^2),
\]

with \( k = 2, L \) for the unpolarized structure functions and \( k = 1 \) for the polarized structure functions. In the latter case the NLO corrections are not yet calculated. The heavy flavor contributions to the structure function \( g_2(x, Q^2) \) are obtained at leading twist from \( G_1(x, Q^2, m^2) \) via the Wandzura–Wilczek relation [15]. The leading order contributions are

\[
H_k^{LO}(x, Q^2, m^2) = \frac{Q^2}{\pi m^2} a_s(\mu^2) c_Q \int_x^{x_{\text{max}}} \frac{dz}{z} h_g \left( \frac{x}{z}, \mu^2 \right) c_g^{(0)}(\eta, \xi),
\]

with \( H = F, G, h = f, g, f_g(z, \mu^2) = G(z, \mu^2), g_g(z, \mu^2) = \Delta G(z, \mu^2) \) the unpolarized and polarized gluon distribution functions, resp., and an implicit \( z \) dependence of the Wilson–coefficients.
$c_{g,H_k}^{(0)}(\eta, \xi)$. $e_Q$ denotes the electric charge of the heavy quark, $\alpha_s = \alpha_s/(4\pi)$ the strong coupling constant, and $\mu^2$ the factorization scale. The LO Wilson coefficients are $[10–12]:$

$$
c_{g, F_L}^{(0)}(\eta, \xi) = \frac{\pi}{2} T_f \frac{\xi}{(1 + \eta + \xi/4)^3} \left\{ 2 \left[ (1 + \eta) \right]^{1/2} - L(\eta) \right\},$$  

$$
c_{g, F_T}^{(0)}(\eta, \xi) = \frac{\pi}{2} T_f \frac{1}{(1 + \eta + \xi/4)^3} \left\{ -2 \left[ (1 + \eta - \xi/4)^2 + 1 + \eta \left( \frac{\eta}{1 + \eta} \right)^{1/2} + \left[ 2(1 + \eta)^2 + \frac{\xi^2}{8} + 1 + 2\eta \right] L(\eta) \right\},$$  

$$
c_{g, F_L}(\eta, \xi) = c_{g, F_L}(\eta, \xi),$$  

$$
c_{g, F_T}(\eta, \xi) = c_{g, F_T}(\eta, \xi),$$  

$$
c_{g, g}(\eta, \xi) = \frac{4\pi}{\xi} T_f \frac{1}{1 + \eta + \xi/4} \left\{ \sqrt{\frac{\eta}{1 + \eta}} \left[ 3(1 + \eta) - \frac{\xi}{4} \right] - \left( 1 + \eta - \frac{\xi}{4} \right) L(\eta) \right\},$$

with $T_f = 1/2$ in $SU(N)$ and

$$L(\eta) = \ln \left[ \frac{(1 + \eta)^{1/2} + \eta^{1/2}}{(1 + \eta)^{1/2} - \eta^{1/2}} \right].$$

The NLO contributions $F_k^{NLO}(x, Q^2, m^2)$ are given by:

$$F_k^{NLO}(x, Q^2, m^2) = \frac{Q^2}{\pi m^2} \alpha_s^2(\mu^2) \int_x^{2\max} \frac{dz}{z^3} \left\{ e_Q f_g \left( \frac{x}{z}, \mu^2 \right) \left[ c_{k,g}^{(1)}(\xi, \eta) + \bar{c}_{k,g}^{(1)}(\xi, \eta) \ln \left( \frac{\mu^2}{m^2} \right) \right] \right.$$  

$$+ \sum_{i=q,\gamma}^3 \left\{ e_i^2 f_i \left( \frac{x}{z}, \mu^2 \right) \left[ c_{k,i}^{(1)}(\xi, \eta) + \bar{c}_{k,i}^{(1)}(\xi, \eta) \ln \left( \frac{\mu^2}{m^2} \right) \right] \right.$$  

$$+ e_i^2 f_i \left( \frac{x}{z}, \mu^2 \right) \left[ d_{k,i}^{(1)}(\xi, \eta) + \bar{d}_{k,i}^{(1)}(\xi, \eta) \right],$$

with $\bar{d}_{k,q}^{(1)}(\xi, \eta) = 0.4$. In [14] the functions $c_{k,j}^{(1)}, d_{k,j}^{(1)}$, and $\bar{c}_{k,j}^{(1)}, \bar{d}_{k,j}^{(1)}$ are parameterized in terms of analytic expressions for the threshold and asymptotic region and a tabulated numerical term interpolating between both.

### 3 Parameterization

The parameterization of the Mellin transform for the Wilson coefficients in section 2 shall be carried out for complex values of the Mellin variable $N$. Complete analytic results for the Mellin transforms of the heavy flavor coefficient functions are difficult to obtain even in lowest order in QCD. A very efficient method in representing higher order functions to high precision, cf. [16], consists in the MINIMAX–method, see also [17]. This polynomial representation uses Chebyshev–polynomials in the approximation. If compared to the Taylor–expansion of a function the coefficients are adapted in such a way that the convergence is significantly better comparing polynomials of the same degree. This method has been also successfully being used in representing analytic continuations [18] of Mellin transforms occurring in massless higher order calculations [19] before.

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4These functions emerge in case one would like to include photo-production as well.

5As shown in Ref. [11] for the unpolarized leading order coefficient functions analytic results for the Mellin transform can be calculated for integer $N$ are given in a form which does not allow analytic continuation.
The heavy quark structure function (4) are Mellin convolutions

\[
F(x) = (A \otimes C)(x) = \int_0^1 dx_1 \int_0^1 dx_2 A(x_1)C(x_2)\delta(x - x_1x_2) ,
\]

(13)

where the parton densities have support \(x_1 \in [0, 1]\) and the coefficient function \(x_2 \in [0, \xi/(\xi + 4)]\). (13) can be diagonalized by the Mellin transform

\[
M[F(x)](N) = \int_0^1 dx x^{N-1} F(x)
\]

(14)

\[
M[F(x)](N) = M[A(x_1)](N) \cdot M[C(x_2)](N) ,
\]

(15)

accounting for the support in \(C(x_2)\). The Wilson–coefficients \(C(z, \xi)\) are now parameterized as polynomials in \(z\) in the range \([0, \rho]\) with \(\rho = \xi/(\xi + 4)\) at fixed values of \(\xi\) using the MINIMAX–method to obtain optimal convergence. Sometimes it is useful to study the function

\[
C^{\text{MINIMAX}}(z, \xi)(\rho - z)^\kappa = \sum_{k=0}^{K} a_k(\rho)z^k
\]

(16)

instead of \(C(z, \xi)\) to improve the convergence.

The Mellin transform of \(C(z, \xi)\) is then obtained by a Riemann–Liouville fractional integral [20]

\[
M[C(z, \xi)](N) = \sum_{k=0}^{K} a_k(\rho)\rho^{N+k-\kappa}B(N+k, 1-\kappa) .
\]

(17)

Here, \(B(a, b)\) denotes the Euler Beta-function. As evident, (17) defines a meromorphic function in \(N\) with poles on the real axis bounded from above. For \(\kappa = 0\), \(B(N+k, 1) = 1/(N+k)\). In all representations below we refer to 15 expansion coefficients \(a_k(\rho)\), i.e. \(K = 14\). In a few cases a representation with \(\kappa \neq 0\) is chosen. We calculate the coefficients \(a_k(\rho)\) in 300 logarithmic steps in \(\xi \in [0.4, 10^4]\) and use numerical interpolation.

In Figures 1a–c we show the LO coefficient functions \(c_{gF_L}^{(0)}, c_{gF_2}^{(0)}\) and \(c_{g,g_1}^{(0)}\) and the absolute accuracy of their representation by the corresponding MINIMAX–polynomial (16). Figures 1d, e show examples for the MINIMAX–representation for NLO contributions to the heavy flavor Wilson coefficients. In Figures 1a–e below the accuracy of the representation \(\Delta C(\xi, \eta)\) is evaluated as

\[
\Delta C_i(\xi, \eta) = |C_i^{\text{MINIMAX}}(\xi, \eta) - C_i(\xi, \eta)| .
\]

(18)

Similar results as shown in Figures 1a–e are obtained for the other Wilson coefficients.

Table 1 gives a complete survey on the absolute accuracy of the representations of the Wilson coefficients in (6,12). In many of the cases very small maximal absolute errors, i.e. of \(O(10^{-5})\) and smaller, of the Wilson coefficients were obtained in the whole \(\xi\)–range. In some cases the errors may reach \(\sim 6 \cdot 10^{-2}\), however. Our main goal is to obtain sufficiently accurate representations for the heavy flavor structure functions.
Figure 1a: LO Wilson coefficient $c_{F,\eta}^{(0)}$ as a function of $z/\rho$ and $\xi = 1, 10, 10^2, 10^3, 10^4$ and the modulus of the error of the polynomial representation, $\Delta C$. 

Figure 1b: LO Wilson coefficient $c_{F,\eta}^{(0)}$. The MINIMAX-polynomial was determined choosing $\kappa = 0.5$ in (16). All other conditions are as in Figure 1a.
Figure 1c: LO Wilson coefficient \( c_{g_1,g}^{(0)} \). All other conditions are as in Figure 1a.

Figure 1d: Contribution to the NLO Wilson coefficient \( c_{F_2,g}^{(1)} \). The MINIMAX-polynomial was determined choosing \( \kappa = 0.4 \) in (16). All other conditions are as in Figure 1a.
Figure 1e: Contribution to the NLO Wilson coefficient $d_{L,q}^{(1)}$. All other conditions are as in Figure 1a.

| Wilson Coeff. | max. absolute errors of the MINIMAX-polynomials |
|---------------|-----------------------------------------------|
|               | $\kappa$ | $\xi = 1$ | $\xi = 10$ | $\xi = 10^2$ | $\xi = 10^3$ | $\xi = 10^4$ |
| $c_{F_{L,g}}^{(0)}$ | 0.0 | 2.1E-5 | 4.5E-5 | 2.5E-5 | 5.7E-6 | 2.9E-7 |
| $c_{F_{L,g}}^{(1)}$ | 0.5 | 1.4E-1 | 8.3E-3 | 3.0E-3 | 1.0E-3 | 3.8E-4 |
| $c_{g_{1,-g}}^{(0)}$ | 0.0 | 1.1E-3 | 6.7E-4 | 2.4E-4 | 8.3E-5 | 3.0E-5 |
| $c_{F_{L,q}}^{(1)}$ | 0.0 | 4.1E-5 | 5.0E-5 | 1.4E-5 | 8.9E-6 | 6.9E-7 |
| $d_{F_{L,q}}^{(1)}$ | 0.0 | 2.3E-5 | 5.0E-5 | 1.2E-6 | 1.8E-6 | 1.5E-7 |
| $c_{F_{L,q}}^{(1)}$ | 0.0 | 1.4E-5 | 2.2E-5 | 4.3E-6 | 3.3E-7 | 4.4E-7 |
| $d_{F_{L,q}}^{(1)}$ | 0.0 | 6.0E-7 | 2.1E-6 | 3.7E-7 | 3.7E-8 | 3.1E-8 |
| $d_{F_{L,q}}^{(1)}$ | 0.0 | 4.0E-6 | 2.6E-6 | 6.1E-7 | 1.5E-6 | 6.3E-7 |
| $c_{F_{2,g}}^{(1)}$ | 0.4 | 5.6E-2 | 2.6E-2 | 3.9E-3 | 1.0E-3 | 8.5E-4 |
| $d_{F_{2,g}}^{(1)}$ | 0.0 | 8.9E-4 | 5.3E-3 | 1.9E-3 | 6.6E-4 | 2.3E-4 |
| $c_{F_{2,q}}^{(1)}$ | 0.0 | 2.6E-3 | 1.2E-3 | 2.2E-4 | 2.2E-5 | 6.3E-6 |
| $d_{F_{2,q}}^{(1)}$ | 0.0 | 3.2E-4 | 1.3E-4 | 2.2E-5 | 1.8E-6 | 7.1E-7 |
| $d_{F_{2,q}}^{(1)}$ | 0.0 | 1.3E-4 | 5.1E-5 | 8.1E-6 | 1.0E-4 | 5.8E-4 |
| $d_{F_{2,q}}^{(1)}$ | 0.0 | 1.4E-14 | 8.5E-55 | -- | -- | -- |

Table 1: Maximal absolute errors of the MINIMAX–polynomials for the LO and NLO Wilson coefficients as a function of $\xi$. 
We illustrate the principal response of the Wilson coefficients for the heavy flavor structure functions by the following scale–independent ‘effective’ distribution $s$:

\[
\begin{align*}
    f_g(z) &= 1.8z^{-0.2}(1-z)^5 \\
    f_q(z) &= 0.6z^{-0.2}(1-z)^5 \\
    g_g(z) &= 20z^{1.4}(1-z)^6 \\
    \sum_{q,\bar{q}} c_q^2 f_q(z) &= 0.15z^{-0.2}(1-z)^5 .
\end{align*}
\]

for different structure functions for charm quark production choosing $m_c = 1.5\text{ GeV}$. The strong coupling constant is fixed to a value of $\alpha_s = 0.2$ for simplicity. All convolutions are performed in Mellin–$N$ space. Finally the structure functions in $x$–space are obtained by the contour integral

\[
F_i(x) = \frac{1}{\pi} \int_0^\infty dz \text{Im} \left[ e^{i\Phi} x^{-c(z)} F(c(z)) \right] , \quad c(z) = c_0 + ze^{i\Phi}, \quad \Phi \simeq (3/4)\pi .
\]

The absolute error of the MINIMAX–representation if compared to the numerical representation using the $x$–space parameterizations [14] and the sample distributions (19–22) in Figures 2a–e below are

\[
\Delta F_i(x, Q^2) = |F_i^{\text{MINIMAX}}(x, Q^2) - F_i(x, Q^2)| .
\]

As seen in the figures below the absolute errors $\Delta F_i(x, Q^2)$ are mostly smaller than $10^{-5}$ and reach $10^{-4}$ for $g_1(x, Q^2)$ in a range of $x < 10^{-2}$.

Figure 2a: $F_{L,c}^{LO}$ in dependence of $x$ and $Q^2$ and the absolute accuracy of the MINIMAX–representation $\Delta F_{L,c}^i$. 

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\[ F_{L,c}^{LO}(x,Q^2) \]
Figure 2b: $F_{2,c}^{LO}$ in dependence of $x$ and $Q^2$ and the absolute accuracy of the MINIMAX–representation $\Delta F_2^c$.

Figure 2c: $g_{1,c}^{LO}$ in dependence of $x$ and $Q^2$ and the absolute accuracy of the MINIMAX–representation $\Delta g_1^c$. 
Figure 2d: Contribution due to $c_{L,g}(\xi, \eta)$ to $F_{NLO}^{L,c}$ in dependence of $x$ and $Q^2$ and the absolute accuracy of the MINIMAX–representation $\Delta F_L^c$.

Figure 2e: Contribution due to $c_{2,q}(\xi, \eta)$ to $F_{NLO}^{2,c}$ in dependence of $x$ and $Q^2$ and the absolute accuracy of the MINIMAX–representation $\Delta F_2^c$. 
4 Conclusion

We derived semi-analytic representations for the MELLIN transforms of the Wilson coefficients for heavy flavor production in unpolarized and polarized deeply inelastic scattering to two-loop order for complex values of $N$. These representations are obtained using Riemann–Liouville fractional integrals and are meromorphic functions. The expansion coefficients were determined using the MINIMAX–method at fixed values of $\xi = Q^2/m^2$, which allows to obtain very precise approximations. This representation of the one– and two–loop massive Wilson coefficients is used in QCD evolution programs solving the renormalization group equations for mass factorization in MELLIN–space. These evolution programs are particularly fast due to the fact that all coefficient functions and anomalous dimensions are only once calculated during the initialization of the code. In the case of the heavy flavor coefficient functions the whole array in $\xi$ is stored for the inversion contour as a grid allowing for precise and fast numerical interpolations during the fit of the non–perturbative parton distribution functions. This representation of the Wilson coefficients can be directly used to implement the heavy–flavor effects into the physical evolution kernels for factorization scheme–invariant singlet evolution. The parameterization can be obtained from www-zeuthen.desy.de/theory/research/num.html

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