Heavy-flavor contributions at NNLO in CTEQ PDF analysis

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Abstract. We discuss an NNLO realization of the general mass scheme S-ACOT-χ for treatment of heavy-flavour production in neutral current deep-inelastic scattering. Practical implementation of the NNLO calculation is illustrated on the example of semi-inclusive structure functions $F_{2c}(x, Q)$ and $F_{Le}(x, Q)$.

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Introduction. Correct computation of heavy-quark contributions to deep-inelastic scattering in the global PDF analysis is essential for predicting precision cross sections for $W$ and $Z$ boson production at the LHC [1].

Quark mass effects on DIS cross sections are comparable to next-to-next-to leading order (NNLO) contributions, therefore they must be included consistently in perturbative computations. The S-ACOT-χ scheme [2, 3, 4] is the default general-mass (GM) framework of CTEQ global PDF analyses; it is an improved formulation of the original ACOT scheme introduced in [5, 6].

S-ACOT-χ is an algorithmic procedure to account for heavy-quark masses in DIS structure functions that descends directly from the proof of QCD factorization for DIS with massive quarks [2]. Compared to the earlier ACOT and S-ACOT schemes, the S-ACOT-χ scheme adds a phenomenologically important requirement that all heavy-quark scattering contributions (including those with collinear approximation for heavy quarks) satisfy energy-momentum conservation near the quark production threshold.

In Ref. [7], we show that the constraints from energy-momentum conservation can be included directly in the QCD factorization theorem. Thus, the S-ACOT-χ scheme is proved to all orders on the same footing as the original ACOT scheme.

We also present, for the first time, S-ACOT-χ numerical predictions of NNLO accuracy for heavy-quark neutral-current DIS structure functions, $F_{2c}(x, Q)$ and $F_{Le}(x, Q^2)$.

S-ACOT-χ is attractive for phenomenological applications because of its relative simplicity compared to other schemes like BMSN [8] or TR [9]. It achieves a great simplification by replacing coefficient functions with incoming heavy-quark lines by their zero-mass (ZM) expressions, while requiring that the light-cone momentum fraction $\xi$
in the PDFs \( f_{a,p}(\xi, \mu) \) is always within the interval \( \chi < \xi < 1 \) that satisfies energy-momentum conservation \([4, 10]\). Here and in the following, a rescaled “Bjorken-\(x\)” variable \( \chi = x(1 + 4m_h^2/Q^2) \) is introduced. This arrangement allows to include all the physical scattering channels, while excluding kinematically prohibited \( \xi \) values.

The S-ACOT-\( \chi \) scheme assumes one value of the number of active quark flavors, \( N_f \), and one PDF set in each \( Q \) bin, in contrast to other possible GM schemes. Matching of massive 4-flavor predictions on massive 3-flavor predictions at low \( Q \), and on massless 4-flavor predictions at large \( Q \) is realized in S-ACOT-\( \chi \) through cancellations among certain classes of Feynman diagrams. These cancellations are improved by using the optimal rescaling variable \( \chi \), but also hold for other forms of the rescaling variable. Practical implementation is easy to handle, and all NNLO Wilson coefficient functions that are needed are available from literature.

**Summary of the computation.** If the components of inclusive \( F_{2,c}(x,Q^2) \equiv F \) are classified according to quark couplings to the photon \([11]\), \( F \) can be written as a sum of light and heavy-quark coupled contributions,

\[
F = \sum_{l=1}^{N_f} F_l + F_h, \tag{1}
\]

where

\[
F_l = e_l^2 \sum_a \left[ C_{l,a} \otimes f_{a/p} \right] (x, Q), \quad F_h = e_h^2 \sum_a \left[ C_{h,a} \otimes f_{a/p} \right] (x, Q). \tag{2}
\]

Here \( C_{l,h} \) are Wilson coefficient functions, and \( f_{a/p} \) are PDFs. Perturbative expansion up to \( \mathcal{O}(\alpha_s^2) \) leads to

\[
F_h^{(2)} = e_h^2 \left\{ c_{h,NS}^{(2)} \otimes (f_{h/p} + f_{\bar{h}/p}) + C_{h,l}^{(2)} \otimes \Sigma + C_{h,g}^{(2)} \otimes f_{g/p} \right\}, \tag{3}
\]

where lowercase \( c_{a,b}^{(2)} \) and uppercase \( C_{a,b}^{(2)} \) represent ZM coefficient functions and massive coefficient functions, constructed from results in Refs. \([12, 13, 14]\) and Refs. \([8, 15, 16, 17]\), respectively. \( \Sigma \) is the singlet PDF combination. A detailed derivation of these coefficient functions is presented in Ref. \([7]\). A similar expression for \( F_l \) is given by

\[
F_l^{(2)} = e_l^2 \left\{ C_{l,l}^{NS} \otimes (f_{l/p} + f_{\bar{l}/p}) + c_{l,g}^{PS} \otimes \Sigma + C_{l,g}^{(2)} \otimes f_{g/p} \right\}, \tag{4}
\]

where \( c_{l,g}^{(2)}, c_{l,g}^{PS} \) and \( C_{l,l}^{NS} \) are constructed from components available in Refs. \([12, 13, 14, 7]\).

**Numerical results.** In the following, we show representative NNLO predictions for \( F_{2,c} \) and \( F_{Lc} \), computed using Les Houches toy PDFs \([18, 19]\) that are evolved with 4 active flavors by HOPPET computer code \([20]\). In Fig.1, NNLO S-ACOT-\( \chi \) predictions for \( F_{2,c} \) (left panel) and \( F_{Lc} \) (right panel) are shown vs. \( Q \) by blue solid lines. ZM 4-flavor predictions at NNLO are shown by purple long-dashed lines, and 3-flavor (fixed-flavor-number, or FFN) predictions by red short-dashed lines. Fig.1 shows that S-ACOT-\( \chi \)
smoothly interpolates in between the FFN and ZM schemes, and that it reduces to the FFN scheme at $Q \approx m_c$ and to the ZM scheme when $Q \gg m_c$. Lower insets show ratios of the FFN and ZM predictions to the respective S-ACOT-$\chi$ predictions, to elucidate differences in the intermediate region.

Fig. 2 shows a remarkable reduction of the factorization scale dependence of $F_{2c}(x,Q)$.

Without extra tuning of the factorization scale, the S-ACOT-$\chi$ prediction is close to FFN and other NNLO schemes at $Q \approx m_c$. Here scattered symbols in the left panel correspond to predictions based on MSTW/TR’ NNLO coefficient functions (sea-green triangles) [21] and FONLL-C NNLO coefficient functions (blue circles) [11]. The solid black line is the S-ACOT-$\chi$ NNLO prediction corresponding to a reference factorization scale $\mu = \sqrt{Q^2 + m_c^2}$. The green band is the theoretical uncertainty in the S-ACOT-$\chi$ prediction due to the variation of the scale in the range $Q < \mu < \sqrt{Q^2 + 4m_c^2}$. The purple band represents scale variations in the FFN prediction at NNLO around the reference scale values indicated by the magenta short-dashed line. The light blue band around the blue-dashed line represents the S-ACOT-$\chi$ prediction at NLO and its scale uncertainty.

Conclusions. We have shown that the S-ACOT-$\chi$ scheme is fully compatible with the QCD factorization theorem, and that an NNLO computation of $F_{2c,Lc}$ in the S-ACOT-$\chi$ scheme is viable. S-ACOT-$\chi$ predictions at NNLO are stable and show significant reduction in the factorization scale dependence (see Fig.2), compared to NLO computations. This is the most challenging component of the CTEQ global analyses at NNLO. A full description of NNLO S-ACOT-$\chi$ computations is available in [7].
FIGURE 2. Factorization scale dependence for semi-inclusive $F_{2,Lc}(x,Q)$ at NNLO as a function of $x$ at $Q = 2$ GeV.

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