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Nuclear Physics B (Proc. Suppl.) 222–224 (2012) 35–40
NUCLEAR PHYSICS B PROCEEDINGS SUPPLEMENTS
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DIS heavy-flavor contributions at two loops in a general mass scheme

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Abstract

We discuss an NNLO realization of the general mass scheme S-ACOT-χ for treatment of heavy-flavor production in neutral current deep-inelastic scattering. The connection of this scheme to the QCD factorization theorem with massive quarks is elucidated. As a new feature, kinematical constraints on collinear production of heavy quarks that are crucial near the heavy-quark threshold are included in the amended QCD factorization theorem. Practical implementation of the NNLO calculation is illustrated on the example of semi-inclusive structure functions $F_{2c}(x, Q)$ and $F_{Lc}(x, Q)$.

1. Introduction

Among several factors comparable to the next-to-next-to-leading order (NNLO) corrections in a global analysis of parton distribution functions (PDFs), dependence of QCD cross sections on masses of heavy quarks, m_c and m_b, can be significant. Precision predictions for W and Z boson production at the LHC are sensitive to the choice of the theoretical framework for describing production of massive quarks in deep inelastic scattering at HERA [1]. Accurate predictions for heavy-quark DIS contributions, accounting for full mass dependence at all DIS momentum scales Q, are therefore essential. The general-mass (GM) factorization scheme [2] systematically implements the mass dependence at each order of the QCD coupling strength, in the whole range of energies accessed by the global PDF analysis. In this contribution, we elucidate theoretical aspects of the heavy-quark treatment at NNLO accuracy in neutral-current DIS in the S-ACOT-χ scheme [2, 3, 4, 5], the default GM scheme of CTEQ PDF fits. Technical details of the study are documented in Ref. [6].

While DIS calculations in the GM scheme at NLO are well understood, their extension to the NNLO accuracy was more subtle and followed a number of theoretical approaches [7, 8, 9, 10, 11, 12, 13]. Given a variety of opinions expressed in these references, our main goal was to identify and document the key, most indispensable, steps that a GM calculation for DIS at NNLO must follow. The other goal was to clarify requirements on the structure of the NNLO terms in the GM scheme that are imposed by the QCD factorization theorem for DIS with massive quarks proved by Collins [2]. Both of these goals are naturally pursued in the context of the S-ACOT-χ scheme, which has a relatively simple structure and is organized along the logical lines suggested by the Collins' proof of QCD factorization. Based on this study, we obtained a stable implementation of NNLO heavy-quark DIS contributions that is now employed in CTEQ NNLO fits.

The S-ACOT-χ scheme is an advanced formulation of the Aivazis-Collins-Olness-Tung (ACOT) scheme that was originally introduced in [3]. Recent general-purpose CTEQ NLO fits, such as CTEQ6.6 [14] or CT10 [15], are based on this scheme. Compared to the original ACOT scheme, the S-ACOT-χ scheme allows simpler computations by using zero-mass (ZM) matrix elements for many Feynman diagrams [2, 4]. In addition, the slow rescaling (χ) prescription is introduced in contributions with incoming heavy quarks [5], with

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doi:10.1016/j.nuclphysbps.2012.03.005

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the goal to better approximate kinematical dependence in the energy region close to the threshold for massive quark production. Suppression of heavy-quark cross sections in the threshold region results from energy-momentum conservation in production of massive pairs, and its effect numerically dominates over other mass-dependent contributions [16]. Slow rescaling is equivalent to requiring that the approximate Wilson coefficient functions with incoming heavy quarks comply with energy-momentum conservation. Although slow rescaling was initially proposed as a means to improve the kinematical behavior of *leading-order* cross sections [17], in our latest paper, we explicitly demonstrate that the χ rescaling is compatible with the QCD factorization theorem for heavy-quark DIS *to all orders of* α_s, including NNLO.

We use a nomenclature convention according to which "NNLO" refers to the two-loop $O(\alpha_s^2)$ accuracy in Wilson coefficient functions at all Q scales and in all considered mass schemes, including the fixed-flavor-number, or FFN, scheme [18]. In each category of processes included in the global fit (DIS, vector boson production, jet production,...), we identify a hard subprocess described by a Feynman cut diagram with the smallest number of loops, *e.g.*, $\gamma^* q \to q$ with no QCD radiation in NC DIS. The order of another radiative contribution in the same class is equal to the number of the extra QCD loops that it contains. Since each QCD loop suppresses the event rate by one power of α_S, such counting provides a uniform measure of the relative magnitude of the radiative contributions in each class, and of the relative strength of the resulting constraints that they place on the PDFs.

The S-ACOT-χ NNLO cross sections are constructed from massive and massless coefficient functions that are readily available from literature, using a few explicit formulas that are close in their structure to the NNLO DIS cross sections in the zero-mass (ZM) scheme [19, 20, 21]. Wilson coefficient functions with incoming heavy quarks h are evaluated using ZM matrix elements, but with the light-cone variable x replaced by $\chi = x\left(1 + 4m_h^2/Q^2\right)$ according to the slow rescaling convention. Slow rescaling suppresses production of $h\bar{h}$ pairs when the energy $\widehat{W}^2 = Q^2\,(1/\widehat{x} - 1)$ of photon-parton scattering is barely above the production threshold. In charm production, this produces smooth matching of the 4-flavor GM prediction on the 3-flavor FFN prediction as $\widehat{W}$ approaches the threshold. The basic requirement of energy-momentum conservation is thus entirely sufficient for the matching of the 4-flavor prediction on the 3-flavor prediction. It does not require introducing extra constraints on Q scale derivatives of the structure functions or a damping factor that are used to enable matching in the context of other schemes [11, 13].

In the same paper, we present, for the first time, the NNLO S-ACOT-χ numerical predictions for heavy-quark neutral-current DIS structure functions, $F_{2c}(x, Q)$ and $F_{Lc}(x, Q^2)$. Near the threshold, the two-loop S-ACOT-χ predictions for heavy-quark DIS contributions are numerically close to predictions of the same order in the fixed-flavor number (FFN) and alternative variable flavor number (VFN) schemes, notably in the FONLL-C scheme that is close to the NNLO S-ACOT-χ scheme by its design [13]. At larger Q values, the S-ACOT-χ cross sections interpolate between the FFN and ZM $\overline{MS}$ predictions. The S-ACOT-χ results turn out to be perturbatively stable both at low and high Q values.

In each Q bin, the S-ACOT-χ scheme operates with one value of the number of active quark flavors, N_f, and one PDF set. This facile arrangement is easier to implement than, for example, the BMSN scheme [7], which requires to compute cross sections for N_f and $N_f + 1$ values simultaneously in each Q region. 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-χ through cancellations among certain classes of Feynman diagrams. These cancellations are improved at low Q by using the optimal rescaling variable χ, but also occur without the slow rescaling. The universality of the resulting PDFs is immediately confirmed by examining the QCD factorization theorem for the S-ACOT-χ scheme.

2. Summary of the computation

If the components of inclusive $F_{2,L}(x, Q^2) \equiv F$ are classified according to quark couplings to the photon [13], F can be written as a sum of light and heavy-quark coupled contributions,

$$F = \sum_{l=1}^{N_l} F_l + F_h,$$

where

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

Here $C_{a,b}$ are Wilson coefficient functions, and $f_{a/p}$ are the PDFs. h represents a heavy (anti)quark (*e.g.*, $h = c$ or $\bar{c}$), and l stands for gluons (g) and light quarks, such

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as $\overset{(-)}{u}$, $\overset{(-)}{d}$, and $\overset{(-)}{s}$. Perturbative expansion up to $O(\alpha_s^2)$ leads to the following NNLO contributions:

$$F_h^{(2)} = e_h^2 \Big\{ c_{h,h}^{NS,(2)} \otimes (f_{h/p} + f_{\bar{h}/p}) + C_{h,l}^{(2)} \otimes \Sigma + C_{h,g}^{(2)} \otimes f_{g/p} \Big\},$$

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. [20, 21, 22] and Refs. [7, 23, 24, 25], respectively. Σ is the singlet PDF combination. A detailed derivation of these coefficient functions is presented in Ref. [6]. A similar expression for F_l is given by

$$F_l^{(2)} = e_l^2 \Big\{ C_{l,l}^{NS,(2)} \otimes (f_{l/p} + f_{\bar{l}/p}) + c^{PS,(2)} \otimes \Sigma + c_{l,g}^{(2)} \otimes f_{g/p} \Big\},$$

where $c_{l,g}^{(2)}$, $c^{PS,(2)}$ and $C_{l,l}^{NS,(2)}$ are constructed from components available in Refs. [20, 21, 22]. Among these components, one must include subtractions that correspond to two-loop approximations for heavy-quark PDFs. The subtractions coincide with matching coefficient functions $A_{Hg}^{(2)}$ and $A_{Hg}^{(2)}$ computed in Ref. [7]. They cancel the contributions with initial-state heavy quarks at $Q \to m_h$, as well the contributions describing collinear production of $h\bar{h}$ pairs in hard cross sections with initial-state light partons at $Q \gg m_h$. The net result of these cancellations is the matching of the S-ACOT-χ predictions on the FFN and ZM $\overline{MS}$ predictions at low and high Q, respectively.

2.1. The role of the rescaling convention

To see why the χ convention is needed, consider the heavy-quark contribution to $F(x, Q)$,

$$F_h(x,Q) = e_h^2 \sum_{a=1}^{N_f} \int_\chi^1 \frac{d\xi}{\xi} C_{h,a}\left(\xi p, m_h, \frac{Q}{\mu}\right) f_{a/p}(\xi,\mu),$$

and focus on the case when the initial-state parton is *light*: $a = g, \overset{(-)}{u}, \overset{(-)}{d}, \overset{(-)}{s}$. The center-of-mass energy $\widehat{W}$ of the photon scattering on a light parton (in so called "flavor-creation subprocesses") is obtained as

$$\widehat{W}^2 \equiv (p_a + q)^2 = Q^2\,(\xi/x - 1)\,.$$

It must be larger than the mass of the $h\bar{h}$ pair for the $h\bar{h}$ production subprocess to occur:

$$4m_h^2 \le \widehat{W}^2 \le W^2 = Q^2(1/x - 1).$$

According to this condition, the scattering probability is non-zero only if the momentum fraction ξ is in the range

$$\chi \le \xi \le 1,$$

where $\chi = x\,(1 + 4m_h^2/Q^2) \ge x$. The energy-momentum conservation imposes a lower limit χ on the light-cone momentum fraction ξ in the convolution integral.

In Wilson coefficient functions with initial-state *heavy* quarks ("flavor-excitation" functions, such as $C_{h,h}$) and corresponding subtraction terms, the energy-momentum conservation is not automatic. If it is strongly violated, large spurious contributions from the unphysical kinematical region $x \le \xi < \chi$ cancel to each order of α_s, but survive in higher-order terms. This leads to deteriorating convergence of GM perturbative predictions near the threshold. The violation is prevented by imposing a supplemental requirement on the flavor-excitation contributions that the exact integration limits are always to be preserved.

This goal is achieved by slow rescaling of the light-cone momentum variable ξ in the convolutions of $C_{a,h}$.

Since the flavor-excitation terms always involve an approximation for heavy-quark collinear production, the flavor-excitation coefficient function $C_{a,h}$ is also *approximate* and can be defined in a number of ways. In this regard, the flavor excitation contributions, such as $\gamma^* c \to c$, are different from the "flavor creation" contributions, such as $\gamma^* g \to c\bar{c}$, which are defined unambiguously by the QCD Feynman rules.

The slow rescaling [5] uses this flexibility to discard all mass dependence in flavor-excitation Wilson coefficient functions [$C_{h,h}$, etc.], with the exception of the mass-dependent constraints on the convolution limits. If we denote the mass-dependent and massless quantities by uppercase and lowercase letters, the S-ACOT-χ convention for the flavor-excitation contributions is summarized as

$$C_{a,h}\left(\frac{x}{\xi}, \frac{Q}{\mu}, \frac{m_h}{Q}\right) = c_{a,h}\left(\frac{\chi}{\xi}, \frac{Q}{\mu}, m_h = 0\right) \times \theta(\chi \le \xi \le 1). \quad (1)$$

Given the importance of energy-momentum conservation in scattering processes, it is essential that the factorized QCD predictions obey it. Slow rescaling provides the effective means to enforce it. We emphasize again that the slow rescaling is introduced only in the approximate flavor-excitation coefficient functions (with initial-state heavy quarks) that cancel near the threshold. It does not affect the flavor-creation terms that determine physical $c\bar{c}$ production processes near the threshold, in which the energy-momentum conservation is exact.

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It can be further shown [6] that the slow rescaling is compatible with the QCD factorization theorem for DIS with massive quarks [2] to an arbitrary order of α_s. The following desirable properties are realized:

1. The proof of QCD factorization for the ACOT and S-ACOT schemes given in [2] also applies to the S-ACOT-χ scheme. This proof validates the S-ACOT-χ scheme to all order of α_s, including the definition for the flavor-excitation functions in Eq. (1) that the S-ACOT-χ scheme implies.
2. The integration over ξ proceeds over the physical range $\chi \le \xi \le 1$ in all channels. It includes all physically possible scattering channels, but excludes kinematically prohibited ξ values.
3. The S-ACOT-χ coefficient functions $C_{a,h}$ in the flavor-excitation channels are given by ZM expressions evaluated at $\widehat{x} = \chi/\xi$. Kinematical prefactors in front of the coefficient functions that are independent of ξ are not modified.
4. The Feynman subgraphs corresponding to the PDFs are given by *universal* operator matrix elements that are the same in all ACOT-like schemes.
5. When Q is much larger than m_h, the S-ACOT-χ scheme reduces to the zero-mass $\overline{\text{MS}}$ scheme, without additional finite renormalizations.
6. When Q is of order m_h, the S-ACOT-χ scheme with the slow rescaling approaches the FFN scheme faster than the (S-)ACOT scheme without rescaling. The matching on the FFN scheme is a consequence solely of the energy conservation included in the factorization theorem, and it does need additional matching conditions such as relationships between the Q derivatives at the threshold or a damping factor.

3. Numerical results

In order to illustrate phenomenological applications of the NNLO S-ACOT-χ calculation, we show representative NNLO predictions for F_{2c} and F_{Lc}, computed using Les Houches toy PDFs [26, 27] that are evolved with 4 active flavors by HOPPET computer code [28].

Mass-dependent NNLO coefficient functions are computed using a program available from [24]. This program tabulates two-loop massive coefficient functions in a form that allows fast evaluation of convolution integrals in the Q range covered by the experimental data. Other input parameters are $\alpha_s(Q_0) = 0.36$ and the pole mass $m_c = \sqrt{2}$ GeV. Our program can alternatively read $\overline{\text{MS}}$ masses as the input. In this case, the $\overline{\text{MS}}$ masses are later converted into pole masses that are required as an input in the code by Riemersma et al [24].

Similar comparisons have been repeated for bottom-quark functions F_{2b} and F_{Lb}, as well as for the full inclusive functions $F = \sum_{l=1}^{N_l} F_l + \sum_{h=N_l+1}^{N_f^{fs}} F_h$ and alternative values of Bjorken x. The results of other tests show similar patterns and can be viewed at [29].

In Fig.1, NNLO S-ACOT-χ predictions for F_{2c} (upper figure) and F_{Lc} (lower figure) are shown vs. Q by blue solid lines (in color online). 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. Lower insets show ratios of the FFN and ZM predictions to the respective S-ACOT-χ predictions, to elucidate differences in the intermediate region. The upper figure shows that the S-ACOT-χ theory prediction for $F_{2c}(x, Q)$ (blue solid line) is numerically close to the FFN prediction (red short-dashed line) at $Q \approx m_c$ and to the ZM prediction (magenta long-dashed line) at $Q > 10$ GeV. In the lower figure, the S-ACOT-χ prediction for the longitudinal function $F_{Lc}(x, Q)$ coincides with the corresponding FFN prediction at $Q \approx m_c$ and approaches the ZM prediction at $Q > 30$ GeV. $F_{Lc}(x, Q)$ is sensitive to mass-dependent corrections to scattering off longitudinally polarized photons. Its matching on the ZM prediction happens at higher Q values than in F_{2c}. The S-ACOT-χ prediction interpolates between the FFN and ZM predictions at intermediate Q values, precisely as expected.

Fig. 2 (in color online) shows a remarkable reduction of the factorization scale dependence of $F_{2,Lc}$. Without extra tuning of the factorization scale, the S-ACOT-χ prediction is close to FFN and other NNLO schemes at $Q \approx m_c$. Here scattered symbols in the upper panel correspond to predictions based on MSTW/TR' NNLO coefficient functions (sea-green triangles) [30] and FONLL-C NNLO coefficient functions (blue circles) [13]. The solid black line is the S-ACOT-χ NNLO prediction corresponding to a reference factorization scale $\mu = \sqrt{Q^2 + m_c^2}$. The green band around this line is the theoretical uncertainty in the S-ACOT-χ 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-χ prediction at NLO and its scale uncertainty.

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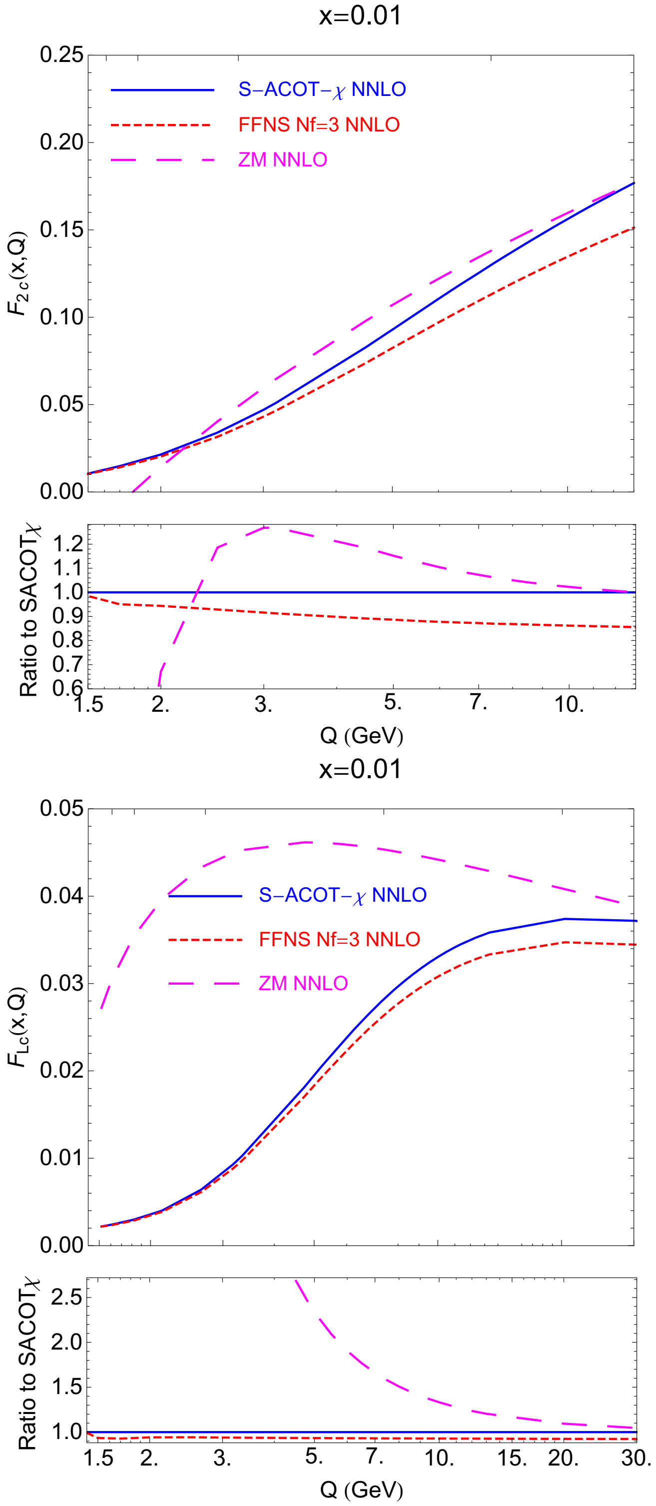

Figure 1: (color online). Upper insets: semi-inclusive $F_{2c}(x,Q)$ and $F_{Lc}(x,Q)$ at NNLO as a function of Q at $x = 10^{-2}$. Lower insets: ratios of ZM and FFN predictions to the respective S-ACOT-χ predictions.

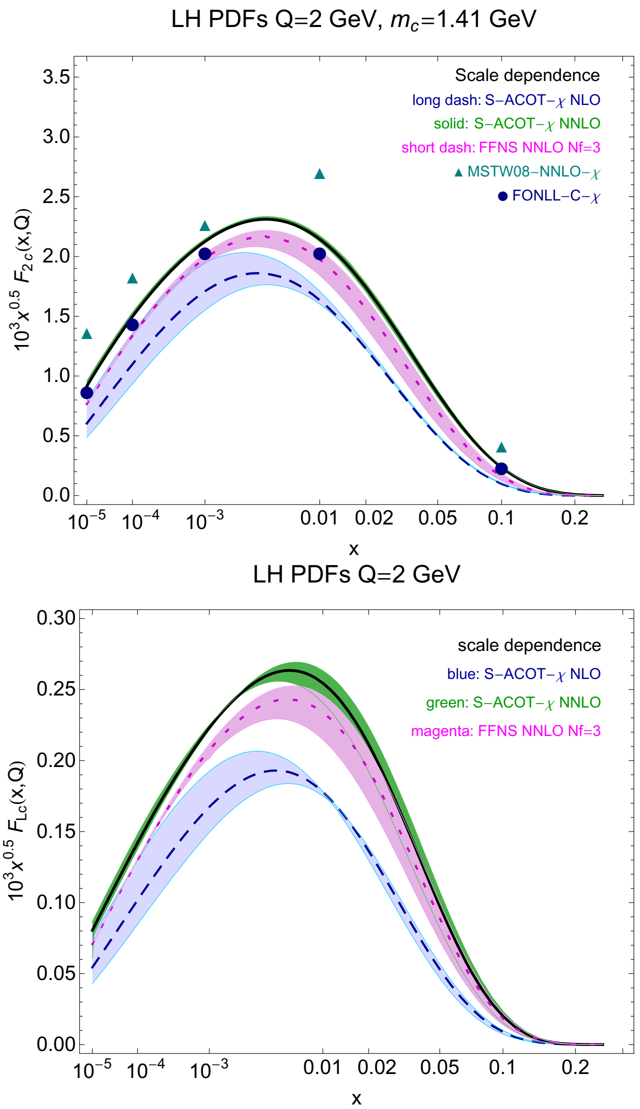

Figure 2: (color online). Factorization scale dependence for semi-inclusive $F_{2,Lc}(x,Q)$ at NNLO as a function of x at $Q = 2$ GeV.

4. Conclusions

We have shown that the S-ACOT-χ scheme is fully compatible with the QCD factorization theorem, and that an NNLO computation of $F_{2,Lc}$ in the S-ACOT-χ scheme is viable. An NNLO calculation for neutral-current DIS with massive quarks was documented in a form that is structurally similar to the NNLO computation in the zero-mass scheme [19, 20, 21]. Constraints from energy-momentum conservation are important phenomenologically and can be satisfied in all channels as a part of the QCD factorization theorem. These constraints are included in the amended version of Collins' factorization theorem by rescaling the partonic momentum fraction in flavor-excitation Wilson

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coefficients. The S-ACOT-χ scheme thus realizes correct kinematical dependence solely by the means of the QCD factorization theorem and momentum conservation.

S-ACOT-χ 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 analysis at NNLO. A full description of NNLO S-ACOT-χ computations is available in [6].

Acknowledgments

P. N. is grateful to the organizers of the workshop and Max-Planck-Society for the kind invitation to present these results, financial support, and stimulating and supportive atmosphere created at the beautiful workshop's venue. This work was supported in part by the U.S. DOE Early Career Research Award DE-SC0003870 and by Lightener-Sams Foundation.

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