Variable-flavor number scheme for next-to-next-to-leading order

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At NNLO it is particularly important to have a Variable-flavor Number Scheme (VFNS) to deal with heavy quarks because there are major problems with both the zero-mass variable-flavor number scheme and the fixed-flavor number scheme. I illustrate these problems and present a general formulation of a Variable-flavor Number Scheme (VFNS) for heavy quarks that is explicitly implemented up to NNLO in the strong coupling constant α_S, and may be used in NNLO global fits for parton distributions. The procedure combines elements of the ACOT(χ) scheme and the Thorne-Roberts scheme. Despite the fact that at NNLO the parton distributions are discontinuous as one changes the number of active quark flavors, all physical quantities are continuous at flavor transitions and the comparison with data is successful.

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I. INTRODUCTION

While up, down and strange quarks may be treated as being effectively massless partons, the heavy quarks, charm ~1.5 GeV, bottom ~4.3 GeV, top ~175 GeV, must have their mass, m_H taken into account in any QCD calculations. In particular it is essential to treat charm and bottom correctly in global fits for parton distributions. There are two distinct regimes that can be considered. Near threshold, $Q^2 \sim m_H^2$, massive quarks are not treated as parton constituents of the proton but are created in the final state. Any processes may be described using the Fixed-flavor Number Scheme (FFNS). For example, structure functions are given by

$$F(x, Q^2) = C_k^{FF}(Q^2/m_H^2, Q^2/\mu^2) \otimes f_k^{n_f}(\mu^2), \qquad (1)$$

up to higher twist ($\mathcal{O}(\Lambda^2/Q^2)$) corrections, where n_f is the number of light partons and all the mass dependence is in the hard coefficient functions which have been calculated up to NLO (i.e. $\mathcal{O}(\alpha_S^2)$) [1]. This is reliable for scales not much greater than m_H^2, but increasing orders in α_S contain increasing logarithms in Q^2/m_H^2, and order-by-order perturbation theory is not guaranteed to be accurate. Also, the FFNS coefficient functions are not known yet at NNLO, rendering an NNLO FFNS impossible to define.

At high scales, i.e. Q^2, $\mu^2 \gg m_H^2$, the heavy quarks are expected to behave like massless partons. The heavy quark is treated like the other partons and $\ln(\mu^2/m_H^2)$ terms are then automatically summed via evolution. The simplest approach is the Zero Mass Variable-flavor Number Scheme (ZMVFNS) [2]. This ignores all $\mathcal{O}(m_H^2/Q^2)$ corrections for each of the n_H heavy quarks, and the structure functions are given by

$$F(x, Q^2) = C_j^{ZMVF}(Q^2/\mu^2) \otimes f_j^{n_f+n_H}(\mu^2), \qquad (2)$$

where the hard coefficient functions are mass independent. Although this is called a "scheme" it is important to note that unlike usual scheme definitions, which are alternative ways to order the perturbative series, the ZMVFNS is incorrect by terms of $\mathcal{O}(m_H^2/Q^2)$, and is really only an approximation in the region $m_H^2 \sim Q^2$. The approximation in this region may indeed be very important in practice, as I will demonstrate later. A correct variable-flavor number scheme should not have these inaccuracies, but should correct the coefficient functions for the mass effects.

As we go from an n_f-flavor to an $n_f + 1$-flavor scheme, the partons in the different number regions are related to each other perturbatively,

$$f_j^{n_f+1}(\mu^2) = A_{jk}(\mu^2/m_H^2) \otimes f_k^{n_f}(\mu^2), \qquad (3)$$

where the perturbative matrix elements $A_{jk}(\mu^2/m_H^2)$ contain the $\ln(\mu^2/m_H^2)$ terms which relate $f_k^{n_f}(\mu^2)$ and $f_k^{n_f+1}(\mu^2)$ and lead to the correct evolution for both. There is then a similar relationship as we go from an $n_f + 1$-flavor to an $n_f + 2$-flavor scheme, but I will consider the transitions one at a time in this paper. At the bottom quark transition point n_f is effectively equal to 4, i.e. the charm quark is already evolving like a massless partons below this point.

At LO, i.e. zeroth order in α_S, the relationship is trivial,

$$q(g)_k^{n_f+1}(\mu^2) \equiv q(g)_k^{n_f}(\mu^2). \qquad (4)$$

At NLO, i.e. first order in α_S, the nontrivial contributions are

$$\begin{aligned}(h + \bar{h})(\mu^2) &= \frac{\alpha_S}{4\pi} P_{qg}^0 \otimes g^{n_f}(Q^2) \ln(\mu^2/m_H^2),\\ g^{n_f+1}(\mu^2) &= \left(1 - \frac{\alpha_S}{6\pi} \ln(\mu^2/m_H^2)\right) g^{n_f}(\mu^2),\end{aligned} \qquad (5)$$

where $h(x, \mu^2)$ is the heavy quark parton distribution. Hence, the heavy flavor evolves from zero at $\mu^2 = m_H^2$ according to standard massless quark evolution and the gluon loses corresponding momentum. It is natural to choose $\mu^2 = m_H^2$ as the transition point from the n_f-flavor to the $n_f + 1$-flavor scheme, since at this order the partons are then continuous and the heavy quark starts

evolving from a zero value. At NNLO, i.e. second order in α_S, there is much more complication

$$f^{n_f+1}_{i,NNLO}(\mu^2) = \left(\frac{\alpha_S}{4\pi}\right)^2 \sum_{ij} (A^{2,0}_{ij} + A^{2,1}_{ij} \ln(\mu^2/m_H^2) + A^{2,2}_{ij} \ln^2(\mu^2/m_H^2)) \otimes f^{n_f}_j(\mu^2), \quad (6)$$

where the $A^{2,0}_{ij}$ [3] are generally nonzero. There is no longer any possibility of a smooth transition at $\mu^2 = m_H^2$. Since each of the $A^{k,0}_{ij}$ is a different function there is no smooth turn on of the flavor distribution at any alternative value of μ^2, hence, for technical simplicity, it seems sensible to keep the transition point at $\mu^2 = m_H^2$, though any other point can be chosen if desired. Making this choice it turns out that $A^{2,0}_{Hg}$, the matrix element giving the gluon contribution to the heavy quark distribution, is negative at small x, even though the structure function is always positive, and the heavy quark starts evolving from a negative value in the $\overline{\rm MS}$ scheme. This highlights the fact that parton distributions are not physical quantities. However, it also illustrates a major problem with the zero-mass variable-flavor number scheme.

In order to make a concrete illustration of the effect we must choose a factorization and renormalization scale. For light partons both of these are conventionally chosen to be $\mu^2 = Q^2$. It is most natural to place the heavy flavor on the same footing, and choose the same scale, e.g. it is difficult to think of momentum conservation at a given scale if the factorization scale is different for different partons. Hence, for the remainder of this article I will set $\mu^2 = Q^2$. Having made a choice, we see that in the ZMVFNS the coefficient functions already lead to a discontinuity in the structure functions at NLO, i.e.

$$F_2^H(x, Q^2) = 0 \qquad Q^2 < m_H^2,$$
$$= \frac{\alpha_S}{4\pi} C_{2,g} \otimes g^{n_f+1}(Q^2) \qquad Q^2 > m_H^2. \quad (7)$$

However, this is a very small effect at NLO. It is larger at NNLO, since the coefficient function makes a larger contribution, even though it is nominally of higher order, and it is negative at smallish x ($x \sim 0.001$), as is the starting value of the partons. Hence, $F_2^H(x, Q^2)$ is also negative for $Q^2 = m_H^2$. This shows that the ZMVFNS is not really feasible at NNLO. It leads to huge discontinuities in the charm structure function $F_2^c(x, Q^2)$, and even significant discontinuities in the total structure function $F_2(x, Q^2)$. These are shown in Fig. 1, where a small discontinuity in $F_2(x, Q^2)$ at $Q^2 = m_b^2$ is also seen. This is a measure of the mistake made in omitting the $\mathcal{O}(m_H^2/Q^2)$ corrections in this approximate scheme. One really needs a general Variable-flavor Number Scheme (VFNS) joining the two well-defined limits of $Q^2 \leq m_H^2$ and $Q^2 \gg m_H^2$ in a theoretically correct manner. We will outline such a scheme, which has been implemented explicitly up to NNLO, in the remainder of this article.[1]

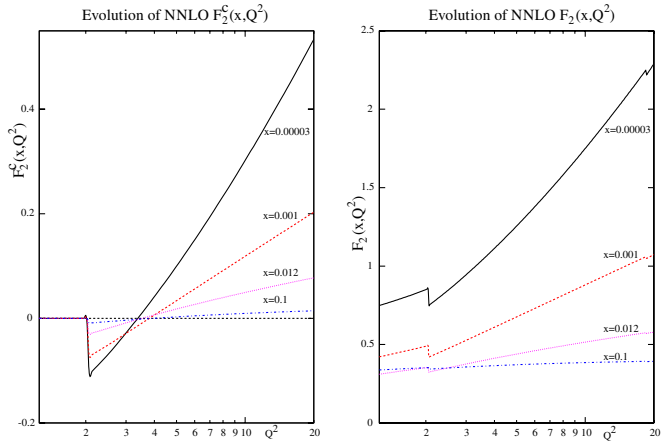


FIG. 1 (color online). The discontinuity in $F_2^c(x, Q^2)$ (left) and $F_2(x, Q^2)$ (right) using the zero-mass variable-flavor number scheme at NNLO.

II. THE VARIABLE-FLLAVOR NUMBER SCHEME

A correct VFNS can be defined by demanding equivalence of the n_f (FFNS) and $n_f + 1$-flavor descriptions at all orders, i.e.

$$F(x, Q^2) = C_k^{FF}(Q^2/m_H^2, Q^2/\mu^2) \otimes f_k^{n_f}(\mu^2)$$
$$= C_j^{VF}(Q^2/m_H^2, Q^2/\mu^2) \otimes f_j^{n_f+1}(\mu^2)$$
$$\equiv C_j^{VF}(Q^2/m_H^2, Q^2/\mu^2) \otimes A_{jk}(\mu^2/m_H^2) \otimes f_k^{n_f}(\mu^2). \quad (8)$$

Hence, the VFNS coefficient functions have to satisfy

$$C_k^{FF}(Q^2/m_H^2, Q^2/\mu^2) = C_j^{VF}(Q^2/m_H^2, Q^2/\mu^2) \otimes A_{jk}(\mu^2/m_H^2), \quad (9)$$

at all orders. It is important to remember that the left-hand side of this expression is expanded in the n_f-flavor coupling α_{S,n_f}, while the right-hand side is most naturally expanded in the $n_f + 1$-flavor coupling α_{S,n_f+1}. The two are related by

$$\alpha_{S,n_f+1}(\mu^2) = \alpha_{S,n_f} + \frac{1}{6\pi} \ln(\mu^2/m_H^2) \alpha^2_{S,n_f} + \mathcal{O}(\alpha^3_{S,n_f}). \quad (10)$$

The coupling is therefore continuous up to $\mathcal{O}(\alpha_S^2)$, but at $\mathcal{O}(\alpha_S^3)$ there is a small discontinuity. This discontinuity does not influence the VFNS up to NNLO.

[1]The scheme has previously been outlined in a very brief form in [4].

At $\mathcal{O}(\alpha_S)$ Eq. (9) becomes, for example, for the structure function $F_2(x, Q^2)$

$$C_{2,g}^{FF,1}(Q^2/m_H^2) = C_{2,HH}^{VF,0}(Q^2/m_H^2) \otimes P_{qg}^0 \ln(\mu^2/m_H^2) + C_{2,g}^{VF,1}(Q^2/m_H^2, Q^2/\mu^2), \quad (11)$$

The VFNS coefficient functions automatically tend to the massless limits as $Q^2/m_H^2 \to \infty$ [5] and, if we use the zeroth order cross-section for photon-heavy quark scattering,

$$C_{2,HH}^{VF,0}(Q^2/m_H^2, z) = (1 + 4m_H^2/Q^2)\delta(z - 1/(1 + m_H^2/Q^2)), \quad (12)$$

this is the original ACOT scheme [6].

However, $C_{2,HH}^{VF,i}(Q^2/m_H^2)$ (we set $\mu^2 = Q^2$ explicitly for simplicity) is only uniquely defined in the massless limit $Q^2/m_H^2 \to \infty$. One can swap $\mathcal{O}(m_H^2/Q^2)$ terms between $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ and $C_{2,g}^{VF,1}(Q^2/m_H^2)$ while still satisfying Eq. (11), i.e. $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ is not uniquely defined. This is true for all $C_{2,HH}^{VF,n}(Q^2/m_H^2)$. The original ACOT prescription removed the ambiguity by defining $C_{2,HH}^{VF,i}(Q^2/m_H^2)$ as the calculated coefficient function for an incoming massive quark. However, this violates the physical production threshold $W^2 > 4m_H^2$ since it only needs one quark in the final state rather than a quark-antiquark pair. Hence, there is not a smooth transition at $Q^2 = m_H^2$ as $n_f \to n_f + 1$. The Thorne-Roberts Variable-flavor Number Scheme (TR-VFNS) first recognized this ambiguity in the definition of $C_{2,HH}^{VF,0}(Q^2/m_H^2)$ [7] and removed it by imposition of the physically motivated constraint of $(dF_2/d\ln Q^2)$ being continuous at the transition point $Q^2 = m_H^2$ (in the gluon sector). Hence, it guaranteed smoothness at $Q^2 = m_H^2$, but the approach to $Q^2/m_H^2 \to \infty$ is a little odd—the VFNS result overshooting the zero-mass result before approaching it asymptotically from above. This effect diminishes at higher orders but more of a problem is the complicated form of the scheme—$C_{2,HH}^{VF,0}(Q^2/m_H^2) \propto (P_{qg}^0)^{-1}$, which is not a simple function. This makes the scheme very involved at higher orders and it is also not well suited to charged currents [8].

There have been various other alternatives since this. Most recently Tung, Kretzer and Schmidt have devised the ACOT(χ) prescription [9] which may be interpreted as

$$C_{2,HH}^{VF,0}(Q^2/m_H^2, z) = \delta(z - Q^2/(Q^2 + 4m_H^2)),$$
$$F_2^{H,0}(x, Q^2) = (h + \bar{h})(x/x_{\max}, Q^2), \quad (13)$$
$$x_{\max} = Q^2/(Q^2 + 4m_H^2).$$

Hence, the zeroth-order coefficient function tends to the standard $C_{2,HH}^{ZM,0}(z) = \delta(1 - z)$ for $Q^2/m_H^2 \to \infty$ but respects the threshold requirement $W^2 = Q^2(1 - x)/x \geq 4m_H^2$ for quark-antiquark production. Moreover, it is very simple. For the VFNS to remain simple (and physically motivated) at all orders n in α_S it is necessary to choose

$$C_{2,HH}^{VF,n}(Q^2/m_H^2, z) = C_{2,HH}^{ZM,n}(z/x_{\max}). \quad (14)$$

It is also important to choose

$$C_{L,HH}^{VF,n}(Q^2/m_H^2, z) \propto C_{L,HH}^{ZM,n}(z/x_{\max}), \quad (15)$$

and to impose the condition that $C_{L,HH}^{VF,0}(Q^2/m_H^2, z) \equiv 0$ (as is done in [7]), despite the fact that one obtains

$$C_{L,HH}^{0}(Q^2/m_H^2, z) = 4z\frac{m_H^2}{Q^2}\delta(z - 1/(1 + m_H^2/Q^2)) \quad (16)$$

for single quark-photon scattering. Because the heavy-flavor contribution to $F_L(x, Q^2)$ is highly suppressed at low values of Q^2, compared to that for $F_2(x, Q^2)$, we choose

$$C_{L,HH}^{VF,n}(Q^2/m_H^2, z) = \frac{5}{4}\left(\frac{1}{1 + 4m_H^2/Q^2} - \frac{1}{5}\right)C_{L,HH}^{ZM,n}(z/x_{\max}). \quad (17)$$

The prefactor is zero at $Q^2 = m_H^2$ and tends to unity as $Q^2/m_H^2 \to \infty$, but is suppressed by the physical threshold of $4m_H^2$ for intermediate values of Q^2. This factor guarantees that the heavy-flavor parton contribution to $F_L^H(x, Q^2)$ is heavily moderated for Q^2 just above m_H^2. Failure to do this results in a kink in $F_L^H(x, Q^2)$ just above $Q^2 = m_H^2$. The fact that this is a function of Q^2/m_H^2 only avoids any additional complications when obtaining higher-order coefficient functions by convolutions with matrix elements which the definition in Eq. (9) requires.

Adopting this convention for the heavy-flavor coefficient functions at NNLO we have, for example,

$$C_{2,Hg}^{VF,2}(Q^2/m_H^2, z) = C_{2,Hg}^{FF,2}(Q^2/m_H^2, z) - C_{2,HH}^{ZM,1}(z/x_{\max}) \otimes A_{Hg}^1(Q^2/m_H^2) - C_{2,HH}^{ZM,0}(z/x_{\max}) \otimes A_{Hg}^2(Q^2/m_H^2) - \frac{1}{6\pi}\ln(Q^2/m_H^2)C_{2,HH}^{ZM,0}(z/x_{\max}) \otimes A_{Hg}^1(Q^2/m_H^2). \quad (18)$$

The last term comes from the change in the coupling constant as we go across the transition point, i.e. from Eq. (10). This would be absent if we used (somewhat unnaturally) the n_f-flavor renormalization scheme above $Q^2 = m_H^2$, as is sometimes done, but this means the definition of $A_{Hg}^2(Q^2/m_H^2, z)$ is different in the two renormalization schemes (compare that in [3] with that in [10]). There is also in principle a contribution of the form

$$-\frac{1}{6\pi}\ln(Q^2/m_H^2)C_{2,Hg}^{VF,1}(Q^2/m_H^2, z) - C_{2,Hg}^{VF,1}(Q^2/m_H^2, z) \otimes A_{gg}^1(Q^2/m_H^2) \quad (19)$$

on the right-hand side, but

$$A^1_{gg}(Q^2/m_H^2, z) = -\frac{1}{6\pi}\ln(Q^2/m_H^2)\delta(1-z), \qquad (20)$$

as seen in Eq. (5), so these terms cancel. Both would be absent if we used the n_f-flavor renormalization scheme above $Q^2 = m_H^2$.

From the definition in Eq. (18) we see that since $A^2_{Hg}(1, z) \neq 0$, the coefficient function $C^2_{2,Hg}(Q^2/m_H^2, z)$ is discontinuous as we go across $Q^2 = m_H^2$. This compensates exactly for the $\mathcal{O}(\alpha_S^2)$ discontinuity arising from that in the heavy-flavor parton distribution, i.e. for the term $C^{VF,0}_{2,HH} \otimes (h + \bar{h})$, and $F_2^H(x, Q^2)$ is continuous.[2] In practice this requires the knowledge of $C^{FF,2}_{2,Hg}(Q^2/m_H^2, z)$. An expression for this exists as semianalytic code [11] where the dominant contributions for $W^2 \to \infty$ and $W^2 \to 4m_H^2$ (from above) are analytic and the rest numerical. I have produced much faster analytic expressions which are exact for $Q^2/m_H^2 \to \infty$ and in some cases for $W^2 \to 4m_H^2$, and the (m_H^2/Q^2) remainders are provided by fitting the values to analytic functions with a number of free parameters. These final expressions are slightly approximate, but the error in $F_2^H(x, Q^2)$ is only $\sim 1\%$ even in the most extreme cases.

There is one more problem in defining the VFNS. The ordering for $F_2^H(x, Q^2)$ is different for the n_f and $n_f + 1$ regions. This can be illustrated by the following table which shows the order-by-order expressions both below and above the transition point.

	n_f − flavor	$n_f + 1$ − flavor
LO	$\frac{\alpha_S}{4\pi} C^{FF,1}_{2,Hg} \otimes g^{n_f}$	$C^{VF,0}_{2,HH} \otimes (h + \bar{h})$
NLO	$(\frac{\alpha_S}{4\pi})^2 (C^{FF,2}_{2,Hg} \otimes g^{n_f} + C^{FF,2}_{2,Hq} \otimes \Sigma^{n_f})$	$\frac{\alpha_S}{4\pi}(C^{VF,1}_{2,HH} \otimes (h + \bar{h}) + C^{VF,1}_{2,Hg} \otimes g^{n_f+1})$
$NNLO$	$(\frac{\alpha_S}{4\pi})^3 \sum_i C^{FF,3}_{2,Hi} \otimes f_i^{n_f}$	$(\frac{\alpha_S}{4\pi})^2 \sum_j C^{VF,2}_{2,Hj} \otimes f_j^{n_f+1}$.

The issue is that the series expansion begins at zeroth order above the transition point, where there is a heavy-flavor distribution, but at $\mathcal{O}(\alpha_S)$ below the transition point. Hence, what is meant by LO, NLO etc. is different by one power of α_S as one changes the number of active quark flavors. Therefore, making the transition directly from a given fixed order to the same relative order when going from n_f to $n_f + 1$ flavors leads to a different order in α_S and discontinuities which may be rather significant—for example, LO is nonzero as one approaches the transition point from below, but zero when approaching it from above. One must make some decision on how to deal with this problem.

Up to now ACOT have used the same order of α_S above and below the transition point, e.g. at NLO

$$\frac{\alpha_S}{4\pi} C^{FF,1}_{2,Hg} \otimes g^{n_f} \to C^{VF,0}_{2,HH} \otimes (h + \bar{h}) + \frac{\alpha_S}{4\pi}(C^{VF,1}_{2,HH} \otimes (h + \bar{h}) + C^{FF,1}_{2,Hg} \otimes g^{n_f+1}). \qquad (21)$$

The structure function is then automatically continuous. However, there is effectively LO evolution below the transition point—$C^{FF,1}_{2,Hg}$ contains only information on P^0_{qg}, not on P^1_{qg}—and NLO evolution above it. Hence the slope $dF_2^H(x, Q^2)/d\ln Q^2$ is discontinuous.

The Thorne-Roberts scheme used the same relative order above and below the transition point, but added a uniquely determined Q^2-independent term above the transition point to maintain continuity of the structure function. For example, at LO

$$\frac{\alpha_S(Q^2)}{4\pi} C^{FF,1}_{2,Hg}(Q^2/m_H^2) \otimes g^{n_f}(Q^2) \to \frac{\alpha_S(M^2)}{4\pi} C^{FF,1}_{2,Hg}(1) \otimes g^{n_f}(M^2) + C^{VF,0}_{2,HH}(Q^2/m_H^2) \otimes (h + \bar{h})(Q^2), \qquad (22)$$

i.e. this prescription freezes the higher order α_S term when going upwards through $Q^2 = m_H^2$. This difference in choice is extremely important at low Q^2 (if using $\mu^2 = Q^2$), as is illustrated in Fig. 2 which compares the two choices at NLO. The $\mathcal{O}(\alpha_S^2)$ part is dominant at low x for $Q^2 \leq m_c^2$ because the $\mathcal{O}(\alpha_S^2)$ coefficient functions diverge at small x whereas the $\mathcal{O}(\alpha_S)$ coefficient function is finite in this limit. Indeed, the "frozen" part is very significant for $m_c^2 \leq Q^2 \leq 12\ \mathrm{GeV}^2$. Its inclusion clearly improves the match to the data [12,13]. It is also clear that switching from the standard n_f-flavor NLO to the standard $n_f + 1$-flavor NLO would lead to a large discontinuity in

[2] In principle there are $\mathcal{O}(\alpha_S^3)$ discontinuities due to terms such as $C^{VF,1}_{2,HH} \otimes (h + \bar{h})$ and $C^{VF,1}_{2,Hg} \otimes g^{n_f+1}$, i.e. $\mathcal{O}(\alpha_S)$ coefficient functions convoluted with $\mathcal{O}(\alpha_S^2)$ discontinuities in partons. These would be cancelled at NNNLO by discontinuities in $\mathcal{O}(\alpha_S^3)$ coefficient functions, but are actually tiny in practice.

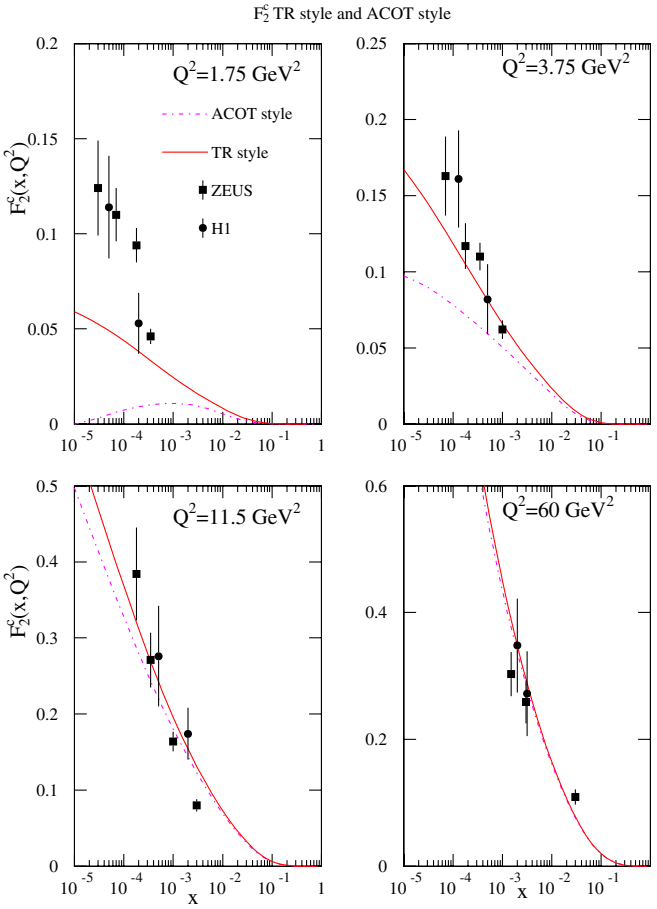


FIG. 2 (color online). Comparison between the ACOT choice of ordering and the Thorne-Roberts choice at NLO.

$F_2^H(x, Q^2)$. Hence we choose to continue using the Thorne-Roberts approach for the matching at the transition point. However, this is a place where there is a definite freedom of choice, and there are various possibilities available.

With the type of choice made for the definition of the heavy-flavor coefficient functions $C_{L,HH}^{VF,n}(Q^2/m_H^2, z)$ in Eq. (17) there is no problem with ordering across the transition point for the longitudinal structure function. This is because both the FFNS and VFNS coefficient functions begin at $\mathcal{O}(\alpha_S)$ for both the gluon and heavy quarks. It is possible to choose a nonvanishing value for $C_{L,HH}^{VF,0}(Q^2/m_H^2, z)$, and indeed some VFNS definitions do so, but this is contrary to the spirit of this approach, and will lead to extra complications.

In order to define fully the VFNS at NNLO, this choice for ordering above and below the transition point means that we need the $\mathcal{O}(\alpha_S^3)$ heavy-flavor coefficient functions for $Q^2 \leq m_H^2$ and that the contribution from these should be frozen for $Q^2 > m_H^2$. However, these coefficient functions are not yet known. Nevertheless, we do know the leading threshold logarithms [14], i.e. the leading contribution for W^2 not much above $4m_H^2$. This is given by

$$C_{2,Hg}^{FF,3,\text{thresh}}(Q^2/m_H^2, z) \sim \frac{1}{z(1+\eta)} \frac{Q^2}{Q^2+4m_H^2} \rho(\eta, Q^2/m_H^2),$$
$$\eta = \frac{Q^2(1-z)}{z4m_H^2} - 1, \tag{23}$$

i.e. $\eta \to 0$ at threshold and $\eta \to \infty$ as $W^2 \to \infty$. $\rho(\eta, Q^2/m_H^2)$ is a function which models the contribution from the dominant threshold logarithms. This contribution occurs only in the gluon sector.

We can also derive the leading $\ln(1/x)$ term from k_T-dependent impact factors derived by Catani, Ciafaloni and Hautmann [15]. With a little work these can be shown to give

$$C_{2,Hg}^{FF,3,\text{low}x}(Q^2/m_H^2, z) = 96 \frac{\ln(1/z)}{z} \kappa_2(Q^2/m_H^2), \tag{24}$$

where $\kappa_2(Q^2/m_H^2)$ may be calculated and $\kappa_2(1) \approx 4$. We also know that in this small-x limit $C_{2,Hq}^{FF,3,\text{low}x}(Q^2/m_H^2, z) = 4/9 C_{2,Hg}^{FF,3,\text{low}x}(Q^2/m_H^2, z)$. By analogy with the known NNLO coefficient functions and splitting functions it is reasonable to propose that this be modified to

$$C_{2,Hg}^{FF,3,\text{low}x}(Q^2/m_H^2, z) = \frac{96}{z} \beta(\ln(1/z) - 4) \times (1 - z/x_{\max})^{20} \kappa_2(Q^2/m_H^2). \tag{25}$$

$\beta = (1 - 4m_H^2 z/(Q^2(1-z)))^{1/2}$ is the velocity of a heavy quark in the center-of-mass frame and its introduction ensures that this contribution $\to 0$ smoothly at threshold. The leading $\ln(1/z)$ is accompanied by ~ -4, i.e. a $1/z$ term of similar size to that in other known coefficient functions and splitting functions is introduced. Finally, the effect of the this entire small z term is damped as $z \to 1$ by the large power of $(1 - z/x_{\max})$. The power of 20 is chosen in order to make the contribution in Eq. (25) very suppressed until $x < 0.1$, which is in line with the values of x above which the small-x divergent terms tend to be suppressed in the complete NNLO splitting functions [16]. The total approximate NNLO coefficient function is obtained by adding the contributions in Eqs. (23) and (25). The amount of information is similar to (though a little weaker than) that used previously to derive approximate NNLO splitting functions [17], which turned out to be a very good approximation once the exact expressions became known.

These expressions could also be used to provide an approximate NNLO FFNS definition. However, in this case they would have to be used over a far wider range of Q^2, rather than the small range here. In particular the

frozen NNLO contribution becomes a proportionally very small contribution to the total $F_2^H(x, Q^2)$ at high Q^2, whereas there is no reason to believe the $\mathcal{O}(\alpha_S^3)$ contribution in the FFNS is small since it contains terms of order $\ln^3(Q^2/m_H^2)$. The NNLO FFNS would therefore be more genuinely approximate. For $F_L^H(x, Q^2)$ we can approximate the $\mathcal{O}(\alpha_S^3)$ coefficient functions at $Q^2 \leq m_H^2$ using the same approach. In this case there is no large threshold contribution and the small-x contribution is estimated to be

$$C_{L,Hg}^{FF,3,\mathrm{low}x}(Q^2/m_H^2, z) = \frac{96}{z}\beta^3(\ln(1/z) - 4)(1 - z/x_{\max})^{20} \times \kappa_L(Q^2/m_H^2), \quad (26)$$

where $\kappa_L(1) \approx 0.16$ and the β^3 reflects the fact that the longitudinal heavy-flavor coefficients are much more suppressed near threshold. For the VFNS for $F_L^H(x, Q^2)$ one can then extrapolate smoothly to the exact massless $\mathcal{O}(\alpha_S^3)$ coefficient functions used in the VFNS at high Q^2. Explicitly, for $Q^2 > m_H^2$

$$F_L^H(x, Q^2) = \frac{5}{4}\left(1 - \frac{1}{1 + 4m_H^2/Q^2}\right)\left(\left(\frac{\alpha_S}{4\pi}\right)^3 \sum_i C_{L,Hi}^{FF,3} \otimes f_i^{n_f} - C_{L,Hg}^{FF,1} \otimes A_{gg,H}^2 \otimes g^{n_f}\right)_{Q^2=m_H^2} + \frac{5}{4}\left(\frac{1}{1 + 4m_H^2/Q^2} - \frac{1}{5}\right)\left(\frac{\alpha_S(Q^2)}{4\pi}\right)^3 \times \sum_i C_{L,Hi}^{ZM,3} \otimes f_i^{n_f+1}(Q^2), \quad (27)$$

where the term $\propto C_{L,Hg}^{FF,1} \otimes A_{gg,H}^2 \otimes g^{n_f}$ maintains continuity of the structure function across the transition point despite the discontinuity in the gluon distribution. Again the degree of modelling and approximation is far less than in a NNLO FFNS.

Using these approximate $\mathcal{O}(\alpha_S^3)$ coefficient functions one can produce full NNLO predictions for structure functions with discontinuous partons and coefficient functions but continuous $F^H(x, Q^2)$. The results are not very sensitive to the choices made in this approximation, as long as they are within a sensible range. Note also that the definition of the VFNS, relying only on Eqs. (9), (14), and (17) and the ordering across the transition point, may be straightforwardly generalised to any choice of factorization and renormalization scales. For the simplest choice of $\mu^2 = Q^2$ the NNLO corrections are seen in Fig. 3. They clearly improve the match to the lowest Q^2 data, where NLO is always too low. This large increase at low x is because the NNLO coefficient functions are more divergent than the NLO coefficient functions. The comparison with the recent bottom quark production data [18] from H1 is also shown

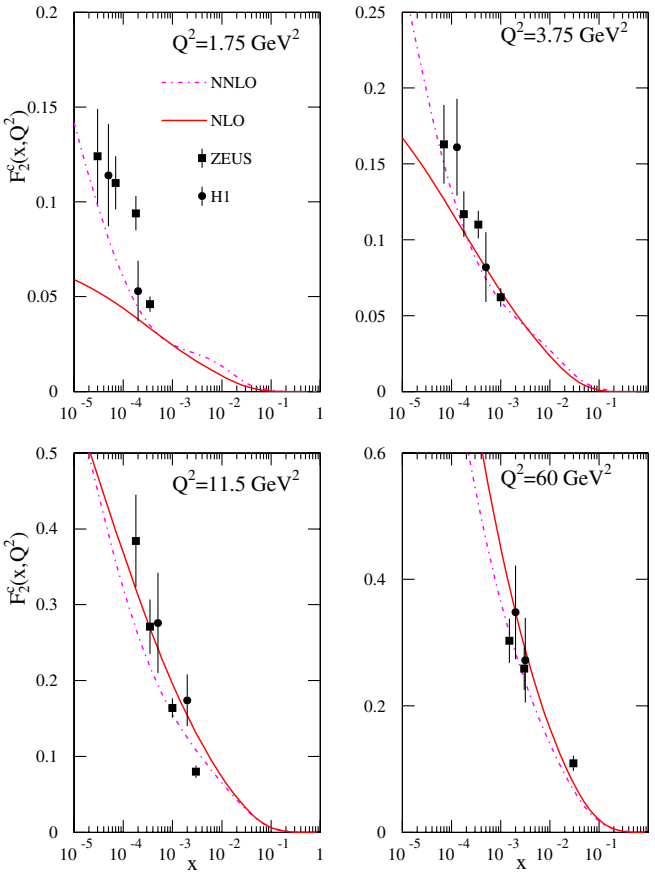


FIG. 3 (color online). Comparison of the NLO and NNLO predictions for $F_2^c(x, Q^2)$ compared with data.

in Fig. 4.[3] The agreement is good, but one can clearly see that the slope $(dF_2^b(x, Q^2)/d\ln Q^2)$ is smaller at NNLO than at NLO, and the same is true for charm. This is because one is interpolating from a higher value at low Q^2, due to the NNLO coefficient function contribution, to lower values at high Q^2, where the quark content is dominant and has a relative reduction compared to NLO because the evolution has started from a negative value rather than zero. Hence, this tendency for a reduction in the slope of the heavy-flavor structure function at NNLO is a generic feature of NNLO. The detailed phenomenology of the global fit with the NNLO VFNS prescription will appear in the account our next global parton analysis [20].

[3]This is an updated version of Fig. 8 in [18]. This previous figure used the MRST04 NNLO partons which applied a rather approximate NNLO treatment of heavy flavors. The updated figure is constructed using NNLO partons from a fit which applies the NNLO VFNS. This leads to a generally slightly increased prediction for $F_2^b(x, Q^2)$. The gluons from this new fit are exhibited in Fig. 3 of [19], and are more negative than our previous, approximate NNLO partons at low Q^2 and very small x.

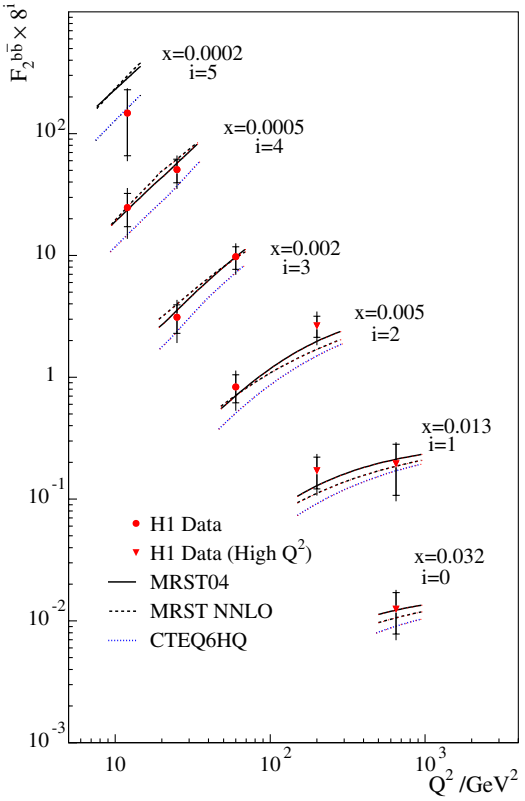
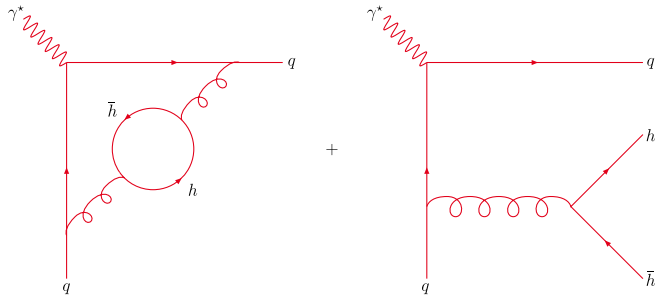


FIG. 4 (color online). Comparison of the NLO and NNLO predictions for $F_b^c(x, Q^2)$ compared with H1 data.

III. LIGHT-FLAVOR SECTOR

At NNLO it is no longer possible to think of heavy-flavor effects as only associated with heavy-flavor production, as has already been discussed in [21]. At this order we also get contributions due to heavy flavors away from the photon vertex. Examples of such contributions are shown below.



In the light-flavor sector the VFNS is defined as before. There are matrix elements changing the light flavors as we go from n_f flavors to $n_f + 1$ flavors and contributions to light-flavor coefficient functions in the FFNS from the type of diagrams above. The exact expressions for these, as well as the asymptotic limits, can be found in [10]. Defining the consistent VFNS according to Eq. (9) then leads to a discontinuity in the coefficient functions across the transition point, which again cancels that in the light quark distributions, leaving the total structure function continuous. In this sector there are peculiar complications due to the occurrence of $(\ln^m(1-z)/(1-z))_+$ terms at the threshold. For example, from the type of diagrams on the right-hand side we get contributions to the structure function of the form

$$\alpha_S^2 \ln^2(Q^2/m_H^2)\left(\frac{\ln^m(1-z)}{1-z}\right) \otimes q(x, Q^2) = \alpha_S^2 \ln^3(Q^2/m_H^2) q(x, Q^2) + \alpha_S^2 \ln^2(Q^2/m_H^2) \times \left(\frac{\ln^m(1-z)}{1-z}\right)_+ \otimes q(x, Q^2) + \mathcal{O}(\ln^2(Q^2/m_H^2)). \tag{28}$$

The maximum value of z in the convolution is $1/(1 + 4m_H^2/Q^2)$ so the divergence at $z = 1$ is not reached. However, the convolution on the left-hand side does produce an additional power of $\ln(Q^2/m_H^2)$. The $\ln^3(Q^2/m_H^2)$ contributions then cancel exactly with contributions from terms of the form $\alpha_s^2 \ln^3(Q^2/m_H^2)\delta(1-z)$ in the coefficient functions from the type of diagrams on the left-hand side, leaving the remainder, including the "+"-distributions. This is an added complication compared to the case where the heavy quark appears at the photon vertex, requiring particular care in a numerical implementation of the VFNS. However, it is only really a technical problem rather than producing any fundamentally new features. In the light-flavor sector there is no problem with ordering. The light-flavor contribution to $F_2(x, Q^2)$ begins at zeroth order in the FFNS and VFNS.

Furthermore, if one is being totally correct, the left-hand type diagram and the soft parts of the right-hand type diagram should contribute to the light-flavor structure function, and the hard part of the right-hand type diagram contributes to $F_2^H(x, Q^2)$ [21]. This can be implemented (it depends on a separation parameter, determining "hard" and "soft"), but each contribution is in practice tiny. At the moment we include all such contributions in the light flavors. This leads to a very small underestimate of the heavy-flavor structure functions.

IV. CHARGED-CURRENT STRUCTURE FUNCTIONS

The VFNS works, in principle, in much the same way for charged currents. The zeroth-order coefficient function for single (anti)charm production from a (anti)strange quark is now

$$C_{2,sc}^{VF,0}(Q^2/m_c^2, z) = \delta(z - Q^2/(Q^2 + m_c^2)), \tag{29}$$

i.e. the threshold is now for a single heavy quark production. The same is obviously true for (anti)charm production from a (anti)down quark. This is far simpler than the prescription in [8]. At higher orders the generalization is

again trivial. Using the ACOT(χ) reasoning one simply uses the light coefficient function with argument z replaced by $z/(1 + m_c^2/Q^2)$. However, there is a major problem in defining the full VFNS, even at NLO. The FFNS coefficient functions are calculated at $\mathcal{O}(\alpha_S)$ [22] but are not yet calculated exactly at $\mathcal{O}(\alpha_S^2)$ for the charged-current case.[4] The generalization from the neutral current case is not simple because the divergences in the final state are different, i.e. one more particle is massless and regularized by dimensional regularization, and one fewer is regularized by the mass.

Hence, in defining the VFNS for the charged-current case it is necessary to make an approximation. In practice we have used the $\mathcal{O}(\alpha_S^2)$ neutral current cross-sections but altered the threshold dependence in all expressions so that all dependence on $Q^2/(Q^2 + 4m_H^2)$ is replaced by dependence on $Q^2/(Q^2 + m_H^2)$. This guarantees that all terms respect the true kinematic threshold. The approximation occurs mainly at low Q^2 where the $\mathcal{O}(\alpha_S^2)$ FFNS coefficient functions are most important in the VFNS. This is not peculiar to this definition of a VFNS, but will be present in any current approach.[5] There is an uncertainty at low Q^2 at $\mathcal{O}(\alpha_S^2)$ that can only be removed by an explicit calculation. At higher Q^2 the VFNS tends to the zero-mass limit for all coefficient functions, so all expressions become exact. Hence the HERA charged-current data are very insensitive indeed to the approximation. The charged-current data at low Q^2 only exist down to $x \sim 0.01$, much higher than for the neutral current HERA data, and at low Q^2 and high-x heavy-flavor production is very small. Hence any errors in the approximation are not very important phenomenologically.

[4]They have been determined in the $Q^2 \gg m_H^2$ limit in [23].

[5]This is except for the ZMVFNS, which will simply be completely wrong by terms of $\mathcal{O}(m_c^2/Q^2)$ and will have incorrect kinematic thresholds, whereas the approximation here is guaranteed to have the correct general form.

V. CONCLUSIONS

There are discontinuities in both the parton distributions and the coefficient functions at NNLO. This makes a variable-flavor number scheme more necessary than ever. The ZMVFNS is badly discontinuous at the transition point $Q^2 = m_H^2$, and the FFNS is only approximate at NNLO. A generalization of the ACOT(χ) prescription leads to a physically sensible and simple VFNS, in principle defined to all orders. One must still be careful about matching when going across the transition point of $Q^2 = m_H^2$. If this matching is done properly it guarantees the continuity of the physical structure functions and maximizes the smoothness of the function. We choose the Thorne-Roberts method of matching above and below the transition, i.e. choose the correct order for the region of n_f flavors and add an additional, uniquely defined constant for the region of $n_f + 1$ flavors to guarantee continuity. This choice is significant and leads to a much better match to the low Q^2 data. We have devised an explicit, full NNLO VFNS for $F_2(x, Q^2)$ and $F_L(x, Q^2)$, with a small amount of necessary modelling of NNLO fixed-flavor coefficient functions. The NNLO variable-flavor number scheme seems to improve the fit to lowest x and Q^2 data greatly and is not very sensitive to this modelling. It is essential to use such an NNLO VFNS in NNLO global analysis of data, and indeed the construction of the NNLO VFNS makes such a precise analysis possible [20].

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