Heavy quark production in variable flavor number schemes

A Dissertation Presented

by

Anton Alexeevich Chuvakin

to

The Graduate School

in Partial Fulfillment of the Requirements

for the Degree of

Doctor of Philosophy

in

Physics

State University of New York
at
Stony Brook

May 2001

State University of New York
at Stony Brook

The Graduate School

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Abstract of the Dissertation

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The dissertation deals with the calculation of heavy flavor parton densities and deep inelastic structure functions. The three flavor parton densities are evolved from a small value of the scale μ^2 up to the heavy quark threshold where the heavy quark densities are generated using the leading, next-to-leading or next-to-next-to leading order matching conditions. These densities are then used to compute the heavy quark structure functions $F_{2,H}(x,Q^2)$ and $F_{L,H}(x,Q^2)$ for charm and bottom quarks in both fixed order perturbation theory and in variable flavor number schemes (VFNS).

The question of choosing the best VFNS scheme is discussed. A comparison with the recent experimental data from the ZEUS and H1 experiments at DESY, Hamburg is provided.

To my parents, Alexei Chuvakin and Lyubov Koshchey for helping me to become who I am now.

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Acknowledgements

I would like to sincerely thank my advisor professor John Smith who guided my research work.

Chapter 1

Introduction

1.1 Introduction

The concept of quarks was introduced into physics by Gell-Mann and Zweig in 1964 [1] before the first evidence for proton and neutron internal structure was discovered in experiments at the Stanford Linear Accelerator Center (SLAC) [2] late in the 1960s.

Quarks were used to classify the huge number of "elementary" particles that were discovered in the 1950s using high-energy particle accelerators and detectors. As the energy of the accelerators increased so did the masses of particles found, up to several times the proton mass. Most particles that were discovered belonged to groups of "hadrons" (strongly interacting particles). The attempts to classify hadrons into some sort of "Mendeleev periodic table" failed, so theorists started to look for a more fundamental picture. This led to the $SU(3)$ (flavor) quark model where u,d and s (up, down and strange) quarks together with their anti-particles were used to build up the multiplets of hadrons. Quarks are fermions that is they have spin 1/2. The Ω-baryon consisting of 3 s quarks with total spin 3/2 was actually predicted several years before it was discovered. A wave function for three identical quarks with spin 1/2 in the same state violates the Pauli exclusion principle for fermions. The unusual composition of the particle was solved by the addition of a new "color" quantum number.

After many experiments it became clear that quarks cannot be observed directly. Since hadrons carry no color quantum number they are defined to be "white" (either by combining quarks of all primary colors - red, green, blue in baryons or by combining color and anti-color quarks in mesons). The precise reasons why quarks are not observed outside of hadrons were proposed much later.

The SLAC experiments (deep inelastic scattering of electrons on protons) revealed that protons contain point-like objects of spin 1/2. "Deep" in the previous sentence refers to the large virtuality of Q^2 (the four-momentum squared of the virtual photon exchanged between the incoming electron and target proton) which allowed the probe to penetrate deep within the hadron. Later the partons were identified with the quarks (and gluons) of an $SU(3)$ (color) gauge theory introduced by Gell-Mann, Fritzsch and Leutwyler [3]. The u and d quarks have constituent masses of about 150 MeV and the s about 300 MeV. However, it should be noted that since quarks are not observed outside of hadrons their masses are only approximate (roughly one half the mass of the meson containing them).

The quark table was later enlarged by the addition of the c quark (charm, discovered in the J/Ψ particle containing $c\bar{c}$, 1974 [4]), the b quark (bottom, discovered in Υ meson containing $b\bar{b}$, 1977 [5]) and the t quark (top, discovered at Fermilab in 1994, [6]). These "heavy" quarks were actually predicted by the parton model prior to their experimental discovery to make the number of quarks equal to the number of leptons.

Another important result of deep inelastic scattering (DIS) experiments was that the measured cross-section was found to be essentially flat in Q^2, but dependent upon the ratio $x = Q^2/2M\nu$ where ν is the energy loss between the incoming and outgoing electron and M denotes the mass of the proton. The x variable ranges between 0 and 1. This observation was called scaling (also known as Bjorken scaling). This property was observed for $0.15 < x < 0.25$ and $2 < Q^2 < 40\,\mathrm{GeV}^2$ which was all the kinematic range of the experiments in the 1960s.

In 1969 Feynman [7] proposed his parton model to explain the scaling phenomenon. Partons were considered to be massless objects inside the proton that interacted with the photons and the total DIS cross-section was just the incoherent sum of these individual cross-sections. In the large proton momentum p limit, x is the fraction of the proton longitudinal momentum carried by each elastically scattered parton and the size of the cross-section is proportional to the sum of probabilities of finding partons of corresponding type (up, down, etc) with momentum xp within the proton [8]. This collision is assumed to be completely unaffected by the presence of neighboring partons. These constituents were assumed to have very small transverse momenta. Scaling was later observed in all hard (large momentum transfer) scattering experiments. The cross sections in the parton model are typically ([9]):

$$\sigma_H(p,q) = \int \sigma_i(xp,q)\phi_{i/H}(x)\,dx \tag{1.1.1}$$

where p is hadron momentum, x is the fraction of x that the parton i carries, $\sigma_i(xp, q)$ is a parton level Born cross section and $\phi_{i/H}(x)$ is a parton distribution function (PDF)which gives the probability to find a parton i in a hadron H carrying the fraction x of the momentum p.

Color was incorporated later when the parton model was extended into quantum chromodynamics (QCD) which is an unbroken non-abelian (thus allowing self-interaction of gluons) $SU(3)$ (color) gauge theory with a running coupling α_S. There are three possible colors for quarks of six flavors and eight color combinations for gluons.

In the years that followed significant progress was achieved in describing the collision processes of partons especially with regard to the production of jets of particles measured in hadronic reactions. This was possible due to two important properties of QCD, namely asymptotic freedom and confinement. Asymptotic freedom refers to the weakness of the interaction between quarks at small distances (confirmed by measurements of scattering cross-sections at large momentum transfer). This feature is explained by the behavior of the QCD running coupling which is large at small momentum scales and small at large momentum scales. Confinement refers to the increase of the interaction strength between quarks at longer distances (leading to the non-existence of free quarks). So the force between quarks is relatively weak at small distances and grows as the distance increases. At some point it becomes energetically more efficient to form a new bound state (a meson) rather than keep straining the color bond between the quarks. This is exactly the opposite to what happens in QED where forces decrease with distance. The physical explanation applied in QED is that a screening effect takes place and the interaction between, say, a pair of electrons becomes weaker as the distance increases. The similar explanation of the growing coupling in QCD is based on the "paramagnetism" analogy due to gluonic spin. The running coupling also depends upon the number of quark flavors. That means that we have to distinguish between a 3-flavor α_s valid for small scales below the mass of the charm quark and a 4-flavor α_s, valid for larger scales.

Quark masses in QCD also depend upon the energy scale. Their running follows from the renormalization group equation in a manner similar to the running of the coupling α_S.

The renormalization procedure removes ultraviolet (high energy) divergences from a quantum field theory such as QCD. That procedure introduces a renormalization scale, typically denoted by μ. The physical meaning of this scale can be viewed as the separation of the divergent energy range from the rest of the calculation. The statement that a result for a physics quantity R is independent of this arbitrary parameter μ leads to the renormalization group

equation

$$\mu^2 dR(Q^2/\mu^2, \alpha_s)/d\mu^2 = (\mu^2 \partial/\partial\mu^2 + \beta\partial/\partial\alpha_S)R = 0 \qquad (1.1.2)$$

where $\beta = \mu^2 d\alpha_S/d\mu^2$, because the running coupling is a function of μ^2. This is a partial differential equation which can be solved by standard methods.

Factorization is the property of QCD which allows the separation of the long-distance (soft) processes, such as interaction of quarks within the hadron from short-distance (hard) processes such as the electromagnetic or weak interaction between the incoming high energy electrons and the quarks inside the hadron. The factorization theorem was proven by Collins, Soper and Sterman ([10]). It was based on QCD which elevates the parton model to a field theory. The parton model corresponds to only incorporating tree level graphs in the calculation (no loops). The charm quark density can be described in terms of two structure functions $F_{2,c}(x, Q^2)$ and $F_{L,c}(x, Q^2)$, which can then be written as convolutions (the convolution operation $\otimes$ is defined as $f \otimes g = \int f(x/y)g(y)dy/y$ with $x \leq y \leq 1$) of coefficient functions with parton density functions (PDFs). The most important applications of factorization are ([9]):

- coefficient functions are infrared-safe (no collinear or soft divergences), calculable in perturbative QCD and independent of long distance effects such as the internal structure of the particular hadron. They can be thought of as generalizations of partonic scattering cross-sections.

- every theoretically defined PDF is infrared-divergent (goes to infinity in the soft and collinear region) and thus not calculable in perturbative QCD. They are extracted from the experimental data. PDFs contain all the information about quarks and gluons within the particular hadron and are process-independent i.e. PDFs are the same for both DIS and Drell-Yan processes.

The divergences that are moved from the partonic scattering cross-sections into the PDFs can be of two different types: infrared (soft) and collinear. The former occurs when gluon is emitted with very low energy, while the latter is due to gluon emission parallel to the quarks with zero transverse momentum k_T [11].

Initially, due to the relatively large strength of strong interaction and thus the large size of the running coupling α_S the applicability of perturbation theory to hadron processes was questioned. No small-parameter expansion was thought possible. However in QCD there are reactions where α_S is small

enough for the perturbation theory approach to work. This is still a subject of considerable interest for theorists.

Perturbative QCD (pQCD) gives good predictions for three types of processes:

- e^+e^- annihilation, $e^+e^- \to X$
- deep inelastic scattering (DIS), $e^-p \to e^-X$
- Drell - Yan production, $pp \to e^+e^-X$

The process of e^+e^- annihilation involves no quarks in the initial state and can be used to measure fragmentation functions of quarks into hadrons. The DIS process is ideal for QCD studies since it only has one hadron in the initial state. Parton densities can be measured in DIS and Drell-Yan processes.

Parton distribution functions (PDFs) only have a clear physical meaning in the Born approximation. They are interpreted as probabilities to find a particular parton (quark or gluon) inside the hadron carrying the fraction x of its momentum at the scale μ^2.

We summarize some of their properties:

- the PDFs are not physical. They depend upon the renormalization scheme (for example, the modified minimum subtraction $\overline{\rm MS}$ scheme) and on the scale. One should convolute them with coefficient functions (that are pQCD calculable) to get experimentally measurable quantities.
- the PDFs are not pQCD-calculable - they contain 'soft' (low momentum transfer) physics
- the PDFs can be expressed as matrix elements of number operators between quark (and gluon) states in particular gauges
- the PDFs are universal (process-independent)
- the PDFs are subject to sum rules such as

$$\int_0^1 dx \left(\phi_{u/p}(x) - \bar{\phi}_{u/p}(x)\right) = 2 \qquad (1.1.3)$$
$$\int_0^1 dx \left(\phi_{d/p}(x) - \bar{\phi}_{d/p}(x)\right) = 1$$

  and others which usually have higher order corrections in α_S.

In order to perform rigorous calculations in pQCD the operator product expansion formalism ([12]) is used for DIS. The formalism describes the parton cross-sections in terms of matrix elements of composite operators taken between parton states [11]. While we can write PDFs in terms of matrix elements we cannot calculate such objects. They have to be obtained from experimental data. For example, DIS cross-sections depend on matrix elements of the product of two electromagnetic currents between proton states. The extraction of PDFs from the wide range of experimental data is sometimes called "global analysis".

In the 1970s the first deviations from the naive parton model predictions were discovered experimentally. In contradiction to the expectations of the parton model when Q^2 increased to a large value a small Q^2 dependence appeared in the experimental data. The search for the possible explanation began. It turns out that the parton transverse momentum is in fact not small. For example a quark can emit a gluon and therefore acquire a large transverse momentum so terms in $\ln(Q^2/\mu^2)$ become visible at order α_S. That shows that partons inside the proton are not behaving exactly like free particles. Also it was noted that charged partons i.e. the quarks only account for about 50% of the proton's momentum. This demonstrated the existence of gluons (to carry the rest of the momentum) which had previously been postulated to provide the interaction between quarks. Using the renormalization group equation the parton distributions are calculable at a given Q^2 from knowing them at another (smaller or larger) ${Q^2}_0$ value as long as α_S is sufficiently small to be in perturbative QCD region for both ${Q^2}_0$ and Q^2. The evolution is described by the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) evolution equations [13]. These equations can be directly derived from factorization (as in [11]) or from the renormalization group equation for the deep inelastic scattering functions $F_a(x, \mu^2)$ [9]. Each evolution equation has the following properties:

- it describes *scale breaking* by logarithms in μ^2 which means that the parton transverse momentum is not small as assumed in the parton model
- the sum in the equation is over all 'active' flavors- ones that exist on the current μ^2 scale

The evolution kernels or splitting functions (since they describe the splitting of partons into other partons) $P_{ij}(x/y, \alpha_s(\mu^2))$ are subject to symmetry relations such as

$$P_{q_i\, q_j} = P_{\bar{q}_i\, \bar{q}_j} \qquad (1.1.4)$$
$$P_{q_i\, \bar{q}_j} = P_{\bar{q}_i\, q_j}$$

$$P_{q_i\,g} = P_{\bar{q}_i\,g} = P_{q\,g}$$
$$P_{g\,q_i} = P_{g\,\bar{q}_i} = P_{g\,q} \tag{1.1.5}$$

that depend upon the order in perturbative QCD[11]. The physical interpretation for the splitting functions ${P^0}_{ab}(x)$ (only in leading order in α_S) is that they are probability functions to find a parton a in a parton b with a fraction x of the longitudinal momentum of a parent parton and transverse momentum much less than μ^2 [13].

There are separate evolution equations for the flavor singlet (that mix with the gluon) and flavor non-singlet parton densities that are described in more detail in Chapter 2.

A number of methods to solve the evolution equations have been proposed, including direct x-space methods, Mellin-transform methods and orthogonal polynomial methods. More details are given in Chapter 2.

So far we have only discussed inclusive processes. The measurements of heavy quarks (namely c, b and t) require the detection of a final heavy quark meson so it is called a single particle inclusive reaction. There are three main approaches to the computation of heavy quark production in DIS:

- the three flavor number scheme - only three initial state PDFs are evolved so the charm (and anticharm) are in the final state. Structure functions for charm are calculated via the photon-gluon fusion process both on the Born level and in higher orders of pQCD. For example, in LO:

$$F_{2,c}(x, Q^2, {m_c}^2) = (\alpha_S/2\pi){C^{(1)}}_g(Q^2/{m_c}^2) \otimes g(\mu^2) \tag{1.1.6}$$

  where $C_g^{(1)}(Q^2/{m_c}^2)$ is a coefficient function which is calculable in pQCD. It is anticipated that this description fails at large Q^2 due to the presence of large logarithms so that $\alpha_S \ln(Q^2)$ is no longer small and we cannot apply perturbation theory. However the exact impact of those logarithms on physically measured quantities is not entirely clear due to the convolution used in the calculation. This production mechanism is sometimes is referred to as "extrinsic" charm production, in contrast with "intrinsic" charm quarks existing in the hadron wave function.

- variable flavor number schemes (in particular the zero-mass VFNS)- all quarks are taken to be massless, but massless charm only contributes above a threshold scale so that its density $c(x, \mu^2) = \phi_{c/h}(x, \mu^2)$ is zero for $\mu^2 < {m_c}^2$. The (massless) charm PDF is generated for $\mu^2 > {m_c}^2$ via the evolution equation with appropriate boundary conditions. In this

case charm structure functions are calculated using the charm parton density. For example, in LO:

$$F_{2,c}(x,Q^2) = C_H^{(1)} \otimes c(x,\mu^2) + C_g^{(1)} \otimes g(x,\mu^2) \qquad (1.1.7)$$

where $\otimes$ denotes the convolution operation defined as above. Note that the dependence on m_c vanishes from $F_{2,c}$ since charm is treated just like a light quark density i.e. has zero mass. This is usually called "intrinsic" charm production and the dominant mechanism is often called flavor excitation. This scheme is inadequate in the threshold region $m_c^2 < Q^2 < 4m_c^2$ where the three flavor scheme is superior.

- non-zero-mass VFNS - where the number of light flavors changes by one unit while going from the threshold region for that parton flavor to the asymptotic region and the heavy quark masses are retained in the coefficient functions to improve the behavior near threshold.

This thesis deals with the construction of VFNS schemes and the comparison of their predictions with experimental data for various regions of x and Q^2. As was mentioned above there are three approaches to this problem.

The next to leading order (NLO) coefficient functions for the three flavor number scheme were constructed by Laenen et al [14]. The first three flavor densities were produced by Glück, Reya and Vogt (in [15] and [16]) which allowed the reliable computation of heavy flavor cross-sections for wide ranges of Q^2 and x in NLO perturbation theory. In this approach, initial PDFs are chosen at some low scale (sometimes as low as $0.26\,\mathrm{GeV}^2$) and then evolved upwards. Then they are convoluted with appropriate LO or NLO coefficient functions to produce the charm structure functions $F_{2,c}(x,Q^2)$ and $F_{L,c}(x,Q^2)$. This approach requires careful selection of initial conditions and evolution parameters such as the heavy quark mass m_c and scale parameter Λ. The number of flavors is kept fixed at all higher scales although the running coupling does change around the b heavy flavor threshold. Calculations in this scheme are conceptually simple however the inclusion of the higher order corrections requires a lot of technical effort [17]. It is important to note that NLO corrections are of the same order of magnitude as LO terms. This scheme also exhibits a significant μ scale dependence that does not always decrease with order [18]. Also it is sometimes impossible to match the experimental data over a wide region of x and Q^2 for any value of μ [19]. This three flavor scheme is considered to be the best scheme achievable in the low Q^2 region where Q^2 is approximately equal to ${m_c}^2$ (for charm production case) so there we can

ignore logarithmic terms in $\ln(Q^2/{m_c}^2)$. Since most experimental data for charm production is for much higher Q^2 some other method might be needed.

If we treat the charm quark in the same manner as all other (light) densities i.e. we assume that a massless charm density exists above its production threshold and does not exist below the threshold we get the zero-mass VFNS. This scheme is very easy to implement since the treatment of charm is the same as other densities. In this case the number of flavors (called "number of active flavors") grows as the momentum transfer increases above the threshold. The (supposedly) large logarithms in $Q^2/{m_c}^2$ are resummed in this case into the evolution of the charm density. This scheme is unphysical in the region of small Q (order of m_c) where the structure functions $F_{2,c}$ usually become negative.

The history of VFNS started with the paper of Aivazis, Collins, Olness and Tung (ACOT) [20]. Their scheme implemented the leading order matching condition between the regions of applicability of three and four flavor schemes. The idea was to provide a scheme that coincides with the fixed flavor number scheme for low Q^2, approximates the behavior of zero-mass VFNS at high Q^2 and has reasonable behavior in the intermediate region. ACOT only developed their scheme for matching in the leading order (i.e. ${\alpha_S}^1$). Their four flavor scheme was also leading order in α_S. There have been attempts to improve this by adding NLO vertex corrections such as in [18] and [21].

The method used by the CTEQ group ([22]) in their global analysis of experimental data involves using the ACOT prescription [20] to fit structure functions $F_{2,c}(x,Q^2)$ and $F_{L,c}(x,Q^2)$. This "global analysis" in perturbative QCD allows them to produce consistent sets of parton densities and heavy and light quark structure functions. The analysis includes processing the ever-increasing amount of experimental data from a wide range of hard-scattering processes and producing improved PDF sets which also serve to test pQCD [22]. The CTEQ group has produced both fixed three and four flavor density sets as well as VFNS (using ACOT prescription) PDFs from fits to data from the H1 and ZEUS experiments at HERA and from other experiments. The emphasis is made on the precise extraction of the gluon density from the data since heavy quark production in leading order (LO) is determined only by the gluon density.

A scheme proposed by Thorne and Roberts [23] uses the matching of structure functions similar to the ACOT prescription, but adds a condition that their derivatives in Q^2 also match at the heavy flavor thresholds. The matching used in their global analysis is performed also in leading order in α_S [24].

The above discussion demonstrates that there is no unique choice for a

precise scale where a massive three flavor scheme is replaced by a massless four flavor scheme nor a unique method to connect them. The switching of scales should not have any influence on the physically measurable results at higher Q^2 due to its arbitrary nature (in spite of the typical choice of ${m_c}^2$, the role of the switching point is also studied in [25]).

The higher-order VFNS schemes presented in this dissertation aim to increase the accuracy of pQCD predictions. The available schemes differ in the choice of heavy quark masses, choice of α_S, method and order of the threshold treatment. Also the leading order schemes should be better at reproducing certain experimental results. Unfortunately, at the time of this writing the accuracy of the experimental data is still insufficient to make a definite choice of the best VFNS scheme. We can however argue that our schemes provide the best theoretical foundation for a pQCD description of heavy quark production in DIS since they are higher order in α_S.

Note that the NLO and NNLO threshold matching condition as well as pieces of NNLO splitting functions are now available. Approximations to NNLO splitting functions are developed ([26],[27]). Global analysis using LO, NLO and NNLO densities was done by MRST ([28]). Although the full NNLO splitting functions are not known yet this paper draws some conclusions about the role of NNLO parton densities in heavy quark production.

The research presented in this thesis deals with the study of two VFNS for heavy flavor (charm and bottom) electroproduction (via photons and not W or Z bosons) and their application to computing total and differential cross-sections in x and Q^2 in higher orders (up to NNLO) of perturbation theory.

The first scheme further referred to as the BMSN scheme (Buza-Matiounine-Smith-Neerven) [29], requires the asymptotic three flavor NLO coefficient functions which manifest correct limiting behavior for high and low Q^2. They are extracted from an analysis of the three flavor structure functions for low Q^2 and four flavor massless coefficient functions for high Q^2. In this way the scheme gives an interpolation from low to high Q^2. The scheme is based on an all-orders proof of heavy quark factorization presented in [29] and more details are given [30] and [31].

The second scheme, which is called the CSN scheme (Chuvakin-Smith-Neerven) [32] utilizes massive coefficient functions to yield a better treatment of the low Q^2 region. For higher Q^2 the m^2/Q^2 terms introduced vanish as $Q^2 \to \infty$ so we match the zero mass four flavor scheme. The iterative procedure to include massive coefficient functions was suggested in [33]. Further details on the above schemes are presented in Chapters 4 and 5.

In Chapter 2 we present a new multifunctional evolution code that allows fast and accurate evolution of all parton densities in leading order, next-to-

leading order and next-to-next-to-leading order (LO, NLO and NNLO) in α_s using the direct x-space method of solving the spin-averaged evolution equations for parton densities. The important features of the code include the analytic computation of the LO, NLO and NNLO weights, the NNLO heavy flavor threshold matching conditions and NNLO evolution. This work is already available [34] and will be submitted for publication.

In Chapter 3 we apply the above mentioned code to create our own density set in NNLO. The chapter deals with charm and bottom flavor matching conditions for parton densities. Using a modified minimum renormalization scheme ($\overline{\rm MS}$) based on dimensional regularization and starting from a three-flavor density set, where the scale $\mu < m_c$, we use our two-loop matching conditions and our evolution code described in Chapter 2 to generate a new set of four-flavor parton densities where $m_c \leq \mu < m_b$ and five-flavor densities where $\mu \geq m_b$. We also study the effect of the NNLO matching conditions on the evolution equations which is important for scales just above the transition regions. This includes the small x and small Q^2 domain recently studied by the H1 and ZEUS experiments at HERA. We found that at small x the effects of the matching conditions never die away even for large μ^2. This work is published in [35].

Chapter 4 deals with calculation of charm structure functions using the BMSN and CSN variable flavor number schemes in deep inelastic electron-proton scattering. In these schemes the coefficient functions are derived from mass factorization of the heavy quark coefficient functions presented in a fixed three flavor number scheme. Since the coefficient functions in the variable flavor number schemes have to be finite in the limit $m \to 0$ we have defined a prescription for those processes where the virtual photon is attached to a light quark. Furthermore one has to construct a parton density set with four active flavors (u,d,s,c) out of a set which only contains three light flavors (u,d,s). This is done using the code from Chapter 2. In order α_s^2 the two sets are discontinuous at $\mu = m_c$ which follows from mass factorization of the heavy quark coefficient functions. The charm component of the structure function $F_{2,c}$ is insensitive to the different variable flavor number schemes. In particular the BMSN and CSN schemes both agree in the threshold region with a three flavor scheme description in fixed order perturbation theory. However one version does not lead to a correct description of the threshold behavior of the longitudinal structure function $F_{L,c}$. This happens when one requires a non-vanishing zeroth order longitudinal coefficient function. This work is published in [32].

Chapter 5 extends the treatment in Chapter 4 to the bottom structure functions $F_{2,b}(x, Q^2, {m_c}^2)$ and $F_{L,b}(x, Q^2, {m_c}^2)$. We again use the BMSN and

CSN schemes to describe bottom quark production. For structure function generation we use our new five flavor parton density set created by our evolution code. This set satisfies the requirements from Chapter 4. Both the BMSN and CSN schemes give almost identical predictions for the bottom structure functions. Also they both agree well with the corresponding results based on NLO four-flavor perturbation theory over a wide range in x and Q^2. This work is published in [36].

The x and Q^2 differential cross sections for charm particle production are provided in Chapter 6. Data for $D^{*\pm}(2010)$ meson electroproduction in the range $10 < Q^2 < 1350$ GeV^2 has recently been presented by the H1 and ZEUS collaborations at HERA. We use these results together with previously published data for $Q^2 > 1$ GeV^2 to test whether one can distinguish between different theoretical schemes for charm quark electroproduction based on the differential cross-sections measurements. We find that it is not possible at present to make such a differentiation up to the largest measured Q^2. Then we point out the regions where differences between the various schemes arise. Future experiments with higher luminosity should be able to make more precise measurements. This work is published in [37].

We conclude by noting that VFNS provide viable descriptions for deep inelastic heavy quark production but more experimental data is needed to make conclusions about the best scheme and the role of the NNLO corrections in the predictions.

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Chapter 2

Evolution program for parton densities with perturbative heavy flavor boundary conditions

2.1 Introduction

Deep-inelastic lepton-hadron scattering experiments probe the internal structure of hadrons. The lepton-hadron inclusive cross sections may be written in terms of structure functions, which depend on the virtuality of the probe Q^2. Three structure functions F_1, F_2 and F_L are necessary to describe neutral current (photon and Z-boson exchange) and charged current (W-boson exchange) reactions. In perturbative quantum chromodynamics (pQCD) the probe interacts with partonic constituents of the hadron. There are probability densities $f(x,\mu^2)$ to find partons carrying a fraction x ($0 < x \leq 1$) of the longitudinal momentum of the hadron at a mass factorization scale μ. Therefore the F_i, $i = 1, 2, L$ also depend on x and μ.

The operator product expansion (OPE) allows the structure functions to be written as convolutions of the parton (quark and gluon) probability densities with partonic hard scattering cross sections (or coefficient functions). The latter can be calculated in pQCD. Even though the former cannot be calculated in pQCD, their μ dependence is determined by a set of integro-differential equations, the (Dokshitzer-Gribov-Lipatov)-Altarelli-Parisi evolution equations [1], which follow from renormalization group analysis. Discussions of the pQCD description of deep inelastic scattering reactions are available in [2] and [3]. The probability densities and splitting functions are defined in the modified-minimal-subtraction ($\overline{\rm MS}$) scheme.

For simplicity we will call the above equations the evolution equations. They describe processes where a massless parton (quark or gluon) carrying a fraction of the longitudinal momentum of the incoming hadron radiates a massless parton and becomes a (different) massless parton with a different momentum fraction. The probability for this process to happen is determined by splitting functions which are computed order-by-order in pQCD. The leading-order (LO) and next-to-leading order (NLO) splitting functions have been known for some time [4], [5], [6], [7], [8], [9] and the results are summarized in a convenient form in [3]. Recently some moments of the next-to-next-to-leading order (NNLO) splitting functions have been calculated in [10], see also [11] and [12] . If the x-dependence of the quark and gluon densities in a hadron are parametrized at one value of μ, (say at μ_0,) then the solutions of the evolution equations with the above LO, NLO or NNLO splitting functions yield the x dependence of the massless parton densities at a different μ. There is a second scale in the pQCD theory, the renormalization scale, which appears in argument of the the running coupling α_s. It is usually set to be the same as the mass factorization scale μ so $\alpha_s = \alpha_s(\mu^2)$.

The flavor dependence of the quark and anti-quark densities is governed

by the flavor group, which is SU(2) for the up and down quarks, SU(3) for the up, down and strange quarks etc. Therefore is is convenient to form flavor non-singlet and flavor (pure) singlet combinations of densities. The former have their own evolution equations. The latter mix with the gluons and the combined evolution is described by matrices which obey coupled integro-differential equations.

A number of methods to solve the evolution equations for the parton densities have been proposed, including direct x-space methods, [13], [14], [15], [16], [17], [18], orthogonal polynomial methods [19], [20], and Mellin-transform methods [21], [22]. A compilation of parton density sets is available in [23].

The best method, which should be both accurate and fast, depends on region chosen in x and μ^2. Currently the requirements are that the code be able to evolve densities from a minimum μ^2 near 0.26 GeV^2 up to a maximum μ^2 near 10^6 GeV^2 required for QCD studies for the future Large Hadron Collider at CERN. The range in x is from a minimum value near 10^{-5} up to a maximum near unity. We use the direct x-space method, with the following additional features.

One of our aims is a better treatment of parton density evolution for "light" u, d and s quarks near the heavy flavor thresholds chosen to be at the charm and the bottom quark masses (m_c and m_b respectively). The parton density description must be modified to incorporate new c and b "heavy" quark densities as the evolution scale increases. The implementation of the NLO and NNLO matching conditions across heavy flavor thresholds in the variable flavor number schemes (VFNS) [24], [25], [26], [27] involve large cancellations between various terms in the expressions for the structure functions. Poor numerical accuracy in the solution for the evolution of the parton densities at small scales would spoil these cancellations and ruin the VFNS predictions. We achieve the required accuracy by avoiding one numerical integration in our program so we analytically calculate the weights for the exact LO, the exact NLO and the approximate NNLO splitting functions. The approximate NNLO splitting functions are taken from [28],[29], while the relevant operator matrix elements (OMEs), which provide the matching conditions on the parton densities across heavy flavor thresholds, are taken from [30].

Since we start the scale evolution from a set of densities (input boundary conditions) at a low scale $\mu = \mu_0 \ll m_c$, the running coupling $\alpha_s(\mu^2)$ is large. We therefore use the exact solution of the NLO equation for α_s and match the values on both sides of the heavy flavor thresholds to three decimal places. We mention here that the NNLO matching conditions on α_s across heavy flavor thresholds are available in [31] and [32]. Our program evolves both light and heavy parton densities in LO, NLO and NNLO from a minimum x equal to

10^{-7} to a maximum x equal to unity, a mimimum $\mu^2 = 0.26$ (GeV)^2 in LO and $\mu^2 = 0.40$ (GeV)^2 in NLO and NNLO and and a maximum $\mu^2 = 10^6$ (GeV)^2. Results have been published in [25], [26], [27] and [33]. Here we give a detailed write up of the program.

2.2 The evolution equations

2.2.1 Definitions of densities

We evolve combinations of up (u), down (d), strange (s), charm (c) and bottom (b) quark densities which transform appropriately under the flavor group. Hence we define flavor-non-singlet valence quark densities by

$$f_{k-\bar{k}}(n_f, x, \mu^2) \equiv f_k(n_f, x, \mu^2) - f_{\bar{k}}(n_f, x, \mu^2)\,,\ k = u, d\,. \tag{2.2.1}$$

The flavor-singlet quark densities

$$f_q^{\rm S}(n_f, x, \mu^2) = \sum_{k=1}^{n_f} f_{k+\bar{k}}(n_f, x, \mu^2) \tag{2.2.2}$$

are defined in terms of the expression

$$f_{k+\bar{k}}(n_f, x, \mu^2) \equiv f_k(n_f, x, \mu^2) + f_{\bar{k}}(n_f, x, \mu^2)\,,\ k = u, d, s, c, b\,, \tag{2.2.3}$$

when $n_f = 5$. Then the flavor-non-singlet sea quark densities are

$$f_q^{\rm NS}(n_f, x, \mu^2) = f_{k+\bar{k}}(n_f, x, \mu^2) - \frac{1}{n_f} f_q^{\rm S}(n_f, x, \mu^2)\,. \tag{2.2.4}$$

These equations will be discussed further in the next section.

2.2.2 The evolution equations

A typical evolution equation is that for a flavor-non-singlet parton density $f^{NS}(x, \mu^2)$

$$\frac{\partial}{\partial \ln \mu^2}\ f^{NS}(y, \mu^2)\ = \frac{\alpha_s(\mu^2)}{2\pi}\ \int_y^1 \frac{dx}{x}\ P_{NS}(\frac{y}{x}, \mu^2)\ f^{NS}(x, \mu^2) \quad , \tag{2.2.5}$$

where $P^{NS}(y/x, \mu^2)$ is a non-singlet splitting function, and $\alpha_s(\mu^2)$ is the running coupling.

The splitting functions in the evolution equations can be expanded in a perturbation series in α_s into LO, NLO and NNLO terms as follows

$$P(z, \mu^2) = P^{(0)}(z, \mu^2) + (\frac{\alpha_s(\mu^2)}{2\pi}) P^{(1)}(z, \mu^2) + (\frac{\alpha_s(\mu^2)}{2\pi})^2 P^{(2)}(z, \mu^2). \tag{2.2.6}$$

The non-singlet combinations of the $q_r(\bar{q}_r)$ to $q_s(\bar{q}_s)$ splitting functions, where the subscripts r, s denote the flavors of the (anti)quarks q and $\bar{q}$ respectively

and satisfy $r, s = 1, \cdots, n_f$, can be further decomposed into flavor diagonal parts proportional to δ_{rs} and flavor independent parts. In LO there is only one non-singlet splitting function P_{qq} but in NLO it is convenient to form two combinations from P_{qq} and $P_{q\bar{q}}$ as follows

$$\begin{aligned} P_+ &= P_{qq} + P_{q\bar{q}}\,, \\ P_- &= P_{qq} - P_{q\bar{q}}\,. \end{aligned} \tag{2.2.7}$$

These splitting functions are used to evolve two independent types of non-singlet densities, which will be called plus and minus respectively. They are given by

$$\begin{aligned} f_i^+ &= f_q^{\rm NS}(n_f, x, \mu^2)\,, \\ f_j^- &= f_{k-\bar{k}}(n_f, x, \mu^2)\,. \end{aligned} \tag{2.2.8}$$

Since the general formulae in Eqs. (3.1)-(3.4) are rather involved the easiest way to explain the indices is by explicitly giving the combinations we use. For $j = 1, 2$ we have

$$f_1^- = u - \bar{u}\,,\; f_2^- = d - \bar{d}\,, \tag{2.2.9}$$

which are used for all flavor density sets. Then for three-flavor densities $i = 1, 2, 3$ and we define

$$\begin{aligned} f_1^+ &= u + \bar{u} - \Sigma(3)/3\,, \qquad f_2^+ = d + \bar{d} - \Sigma(3)/3\,, \\ f_3^+ &= s + \bar{s} - \Sigma(3)/3\,, \end{aligned} \tag{2.2.10}$$

where $\Sigma(3) = f_q^S(3) = u + \bar{u} + d + \bar{d} + s + \bar{s}$. These densities should be used for scales $\mu < m_c$. For four-flavor densities $i = 1, 2, 3, 4$ and we define

$$\begin{aligned} f_1^+ &= u + \bar{u} - \Sigma(4)/4\,, \qquad f_2^+ = d + \bar{d} - \Sigma(4)/4\,, \\ f_3^+ &= s + \bar{s} - \Sigma(4)/4\,, \qquad f_4^+ = c + \bar{c} - \Sigma(4)/4\,, \end{aligned} \tag{2.2.11}$$

where $\Sigma(4) = f_q^S(4) = c + \bar{c} + \Sigma(3)$. These should be used for scales in the region $m_c \le \mu < m_b$. For five-flavor densites $i = 1, 2, 3, 4, 5$ and we define

$$\begin{aligned} f_1^+ &= u + \bar{u} - \Sigma(5)/5\,, \qquad f_2^+ = d + \bar{d} - \Sigma(5)/5\,, \\ f_3^+ &= s + \bar{s} - \Sigma(5)/5\,, \qquad f_4^+ = c + \bar{c} - \Sigma(5)/5\,, \\ f_5^+ &= b + \bar{b} - \Sigma(5)/5\,, \end{aligned} \tag{2.2.12}$$

where $\Sigma(5) = f_q^S(5) = b + \bar{b} + \Sigma(4)$. These should be used for scales $\mu \ge m_b$.

If we define $t = \ln(\mu^2/(1\,\mathrm{GeV}^2)$ then we need to solve the four evolution equations

$$\frac{\partial f_i^+(y,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi}\int_y^1 \frac{dx}{x} P_+(\frac{y}{x},t) f_i^+(x,t)\,, \tag{2.2.13}$$

$$\frac{\partial f_j^-(y,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi}\int_y^1 \frac{dx}{x} P_-(\frac{y}{x},t) f_j^-(x,t)\,, \tag{2.2.14}$$

$$\frac{\partial f_g(y,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi}\int_y^1 \frac{dx}{x}\left[P_{gq}(\frac{y}{x},t) f_q^S(x,t) + P_{gg}(\frac{y}{x},t) f_g^S(x,t)\right] \tag{2.2.15}$$

$$\frac{\partial f_q^S(y,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi}\int_y^1 \frac{dx}{x}\left[P_{qq}(\frac{y}{x},t) f_q^S(x,t) + P_{qg}(\frac{y}{x},t) f_g^S(x,t)\right] \tag{2.2.16}$$

where for $\mu < m_c$ we set $i = 1,2,3$, $j = 1,2$, $f_q^S = \Sigma(3)$ and the gluon is a three-flavor gluon. When $m_c \le \mu < m_b$, we use $i = 1,2,3,4$, $j = 1,2$, $f_q^S = \Sigma(4)$ and the gluon is a four-flavor gluon. Finally when $\mu \ge m_b$, we set $i = 1,2,3,4,5$, $j = 1,2$, $f_q^S = \Sigma(5)$ and the gluon is a five-flavor gluon. Note that since NNLO splitting functions are approximate we provide the high and low estimate for each splitting functions labeled A and B. For all calculations we use their average so that the error is minimized.

The densities satisfy the momentum conservation sum rule which we write in terms of the $u, d, ..b$ (anti)-quark and gluon densities as

$$\begin{aligned}\int_0^1 dx\, x\Big[&u(x,\mu^2) + \bar{u}(x,\mu^2) + d(x,\mu^2) + \bar{d}(x,\mu^2)\\ &+ s(x,\mu^2) + \bar{s}(x,\mu^2) + [c(x,\mu^2) + \bar{c}(x,\mu^2)]\theta(\mu^2 - m_c^2)\\ &+ [b(x,\mu^2) + \bar{b}(x,\mu^2)]\theta(\mu^2 - m_b^2) + g(x,\mu^2)\Big] = 1\,.\end{aligned} \tag{2.2.17}$$

Also the quark constituents carry all the charge, isospin, strangeness, charm and bottom quantum numbers of the nucleon so they also satisfy the other standard sum rules for the conservation of these quantities, see [2], [3].

2.3 Direct x-space method of solution and initial conditions

2.3.1 The method

Our choice of the direct x-space method is motivated by the necessity to step densities across heavy flavor thresholds using LO, NLO and NNLO boundary conditions. The procedure of doing this with Mellin moments would involve taking moments of the densities and then inverting moments several times. The direct x-space method is much more intuitive and straightforward. The main features of this method are linear interpolation over a grid in x and second-order interpolation over a grid in t. Let us describe it in more detail to point out where we differ from the method in [14].

First we consider the x-variable in the evolution and write the right-hand-side of the evolution equation Eq.(4.3.5) for the non-singlet density as

$$I(x_0) = \int \frac{dx}{x} \frac{x_0}{x} P\left(\frac{x_0}{x}\right) q\left(x\right) , \tag{2.3.1}$$

where $x_0 \leq x \leq 1$,

$$q(x) = xf(x) , \tag{2.3.2}$$

and

$$x_0 < x_1 < ... < x_n < x_{n+1} \equiv 1 , \tag{2.3.3}$$

with $q(x_{n+1}) = q(1) \equiv 0$. Between grid points x_i and x_{i+1}, x is chosen so that

$$q(x) = (1 - \bar{x})q(x_i) + \bar{x}q(x_{i+1}) , \tag{2.3.4}$$

with $\bar{x} = (x - x_i)/(x_{i+1} - x_i)$. Using this relation we convert the integral into a sum

$$I(x_0) = \sum_{i=0}^{n+1} w(x_i, x_0) q(x_i) , \tag{2.3.5}$$

where the weights are (in all orders LO, NLO and NNLO)

$$\begin{aligned} w(x_0, x_0) &= S_1(s_1, s_0) \\ w(x_i, x_0) &= S_1(s_{i+1}, s_i) - S_2(s_i, s_{i-1}) , \end{aligned} \tag{2.3.6}$$

where $s_i = x_0/x_i$ and

$$\begin{aligned} S_1(u, v) &= \frac{v}{v-u} \int_u^v (z-u) P(z) \frac{dz}{z} , \\ S_2(u, v) &= \frac{u}{v-u} \int_u^v (z-v) P(z) \frac{dz}{z} . \end{aligned} \tag{2.3.7}$$

In the above formula $P(z)$ denotes the splitting function of the corresponding order in α_s and type (non-singlet, singlet, etc.) We use the LO and NLO splitting functions in [19] and the approximations to the NNLO splitting functions from [28] and [29]. For completeness the latter are given in Appendix A. We have calculated the integrals in Eq.(2.3.7) analytically and the results are in the computer program. This yields the formula in Eq.(2.3.5) describing the grid for the x variable. Note that the weights $w^{(0)}$, $w^{(1)}$ and $w^{(2)}$ are those for the exact LO, the exact NLO and the approximate NNLO splitting functions respectively. Thus, for the singlet case, we have

$$\begin{aligned}\frac{d(x_0\Sigma(x_0))}{dt} &= \frac{\alpha_s}{2\pi}\sum_{i=0}^{n+1}\Big[[w_{qq}^{(0)}(x_i,x_0)+\frac{\alpha_s}{2\pi}w_{qq}^{(1)}(x_i,x_0)+(\frac{\alpha_s}{2\pi})^2 w_{qq}^{(2)}(x_i,x_0)] \\ &\quad\times\ x_i\Sigma(x_i) \\ &\quad+[w_{qg}^{(0)}(x_i,x_0)+\frac{\alpha_s}{2\pi}w_{qg}^{(1)}(x_i,x_0)+(\frac{\alpha_s}{2\pi})^2 w_{qg}^{(2)}(x_i,x_0)] \\ &\quad\times\ x_i g(x_i)\Big]\,, \end{aligned} \tag{2.3.8}$$

where Σ is either $\Sigma(3)$, $\Sigma(4)$ or $\Sigma(5)$ depending on the scale.

Now consider the variation in the variable t. For each x_i we pick a grid in t labelled by distinct points t_j. Then, for example, the non-singlet equation becomes

$$\begin{aligned}q^{'}(x_i,t_j) = \frac{\alpha_s(t_j)}{2\pi}\sum_{k=1}^{n}[w_{\pm}^{(0)}(x_k,x_i)+\frac{\alpha_s(t_j)}{2\pi}w_{\pm}^{(1)}(x_k,x_i) \\ +(\frac{\alpha_s(t_j)}{2\pi})^2 w_{\pm}^{(2)}(x_k,x_i)]q(x_k,t_j)\,,\end{aligned} \tag{2.3.9}$$

where $q^{'}(x_i,t_j)$ denotes the derivative with respect to t evaluated at $t=t_j$. In compact notation this equation can be rewritten as

$$q_j^{'} = wq_j + S\,, \tag{2.3.10}$$

with S being the sum of the terms on the right hand side of Eq.(2.3.9) excluding the j-th term.

For t between the grid points t_{j-1} and t_j we interpolate the parton density using quadratic interpolation as follows:

$$q(x_i,t) = at^2+bt+c\,. \tag{2.3.11}$$

Thus we relate the value of q at the point t_j to that of q at the point t_{j-1} by

$$q(x_i,t_j) = q(x_i,t_{j-1})+\frac{1}{2}[q^{'}(x_i,t_j)+q^{'}(x_i,t_{j-1})]\Delta t_j\,, \tag{2.3.12}$$

where $\Delta t_j = t_j - t_{j-1}$. This equation can also be written more compactly as

$$q_j = q_{j-1} + \frac{1}{2}(q'_{j-1} + q'_j)\Delta t_j \,. \tag{2.3.13}$$

The resulting system of two linear equations in Eq.(2.3.10) and Eq. (2.3.13) for q_j and q'_j has the solution

$$q_j = \frac{2q_{j-1} + (q'_{j-1} + S)\Delta t_j}{2 - w\Delta t_j} \,. \tag{2.3.14}$$

Then we find q'_j from Eq.(2.3.10). Applying the same procedure to the gluon and singlet combinations involves four equations because we have to compute both the densities and their derivatives.

The evolution proceeds from the initial $\mu_0^2 = \mu_{\rm LO}^2$ (or $\mu_0^2 = \mu_{\rm NLO}^2$) to the first heavy flavor threshold at the scale $\mu^2 = m_c^2$. Next the charm density is introduced in NNLO (α_s^2-order terms) and all the four-flavor densities are evolved from the new boundary conditions in Section 4.2. This evolution continues up to the transition point $\mu^2 = m_b^2$, where the same procedure is applied to generate the bottom quark density. From that matching point all five-flavor densities are evolved up to all higher μ^2 scales starting from the boundary conditions in Appendix B.

Since the weights for the calculation are computed analytically from the LO, NLO [19] and NNLO ([28],[29]) $\overline{\rm MS}$ splitting functions we remove possible instabilities in the numerical integrations. Hence the program is very efficient and fast. The results from the evolution code have been thoroughly checked against the tables in the HERA report [16] and they agree to all five decimal places.

2.3.2 The initial conditions

The GRV98 [22] three-flavor LO and NLO parton density sets contain input formulae at low scales $\mu < m_c$ which are ideal as initial values for our parametrizations. Therefore we start our LO evolution using the following input at $\mu_0^2 = \mu_{\rm LO}^2 = 0.26$ GeV^2

$$\begin{aligned}
xf_{u-\bar{u}}(3,x,\mu_0^2) &= xu_v(x,\mu_{\rm LO}^2) \\
&= 1.239\; x^{0.48}\,(1-x)^{2.72}\,(1-1.8\sqrt{x}+9.5x) \\
xf_{d-\bar{d}}(3,x,\mu_0^2) &= xd_v(x,\mu_{\rm LO}^2) \\
&= 0.614\;(1-x)^{0.9}\;xu_v(x,\mu_{\rm LO}^2)
\end{aligned}$$

$$
\begin{aligned}
x(f_{\bar{d}}(3,x,\mu_0^2) - f_{\bar{u}}(3,x,\mu_0^2)) &= x\Delta(x,\mu^2_{\rm LO}) \\
&= 0.23\ x^{0.48}\,(1-x)^{11.3}\,(1-12.0\sqrt{x}+50.9x) \\
x(f_{\bar{d}}(3,x,\mu_0^2) + f_{\bar{u}}(3,x,\mu_0^2)) &= x(\bar{u}+\bar{d})(x,\mu^2_{\rm LO}) \\
&= 1.52\ x^{0.15}\,(1-x)^{9.1}\,(1-3.6\sqrt{x}+7.8x) \\
x f_g(3,x,\mu_0^2) &= xg(x,\mu^2_{\rm LO}) \\
&= 17.47\ x^{1.6}\,(1-x)^{3.8} \\
x f_s(3,x,\mu_0^2) = x f_{\bar{s}}(3,x,\mu_0^2) &= xs(x,\mu^2_{\rm LO}) \\
&= x\bar{s}(x,\mu^2_{\rm LO}) = 0\,. \qquad (2.3.15)
\end{aligned}
$$

Here $\Delta \equiv \bar{d} - \bar{u}$ is used to construct the non-singlet combination.

We start the corresponding NLO evolution using the following GRV98 input at $\mu_0^2 = \mu^2_{\rm NLO} = 0.40$ GeV^2

$$
\begin{aligned}
x f_{u-\bar{u}}(3,x,\mu_0^2) &= x u_v(x,\mu^2_{\rm NLO}) \\
&= 0.632\ x^{0.43}\,(1-x)^{3.09}\,(1+18.2x) \\
x f_{d-\bar{d}}(3,x,\mu_0^2) &= x d_v(x,\mu^2_{\rm NLO}) \\
&= 0.624\ (1-x)^{1.0}\ x u_v(x,\mu^2_{\rm NLO}) \\
x(f_{\bar{d}}(3,x,\mu_0^2) - f_{\bar{u}}(3,x,\mu_0^2)) &= x\Delta(x,\mu^2_{\rm NLO}) \\
&= 0.20\ x^{0.43}\,(1-x)^{12.4}\,(1-13.3\sqrt{x}+60.0x) \\
x(f_{\bar{d}}(3,x,\mu_0^2) + f_{\bar{u}}(3,x,\mu_0^2)) &= x(\bar{u}+\bar{d})(x,\mu^2_{\rm NLO}) \\
&= 1.24\ x^{0.20}\,(1-x)^{8.5}\,(1-2.3\sqrt{x}+5.7x) \\
x f_g(3,x,\mu_0^2) &= xg(x,\mu^2_{\rm NLO}) \\
&= 20.80\ x^{1.6}\,(1-x)^{4.1} \\
x f_s(3,x,\mu_0^2) = x f_{\bar{s}}(3,x,\mu_0^2) &= xs(x,\mu^2_{\rm NLO}) \\
&= x\bar{s}(x,\mu^2_{\rm NLO}) = 0. \qquad (2.3.16)
\end{aligned}
$$

We start the corresponding NNLO evolution using the same NLO input and starting scale as above.

2.3.3 The calculation of the running coupling

The heavy quark masses $m_c = 1.4$ GeV^2, $m_b = 4.5$ GeV^2 are used throughout the calculation. We also use the exact solution (as opposed to a perturbative solution in inverse powers of $\ln(\mu^2/\Lambda^2)$) of the differential equation

$$
\frac{d\,\alpha_s(\mu^2)}{d\,\ln(\mu^2)} = -\frac{\beta_0}{4\pi}\,\alpha_s^2(\mu^2) \;-\; \frac{\beta_1}{16\pi^2}\,\alpha_s^3(\mu^2)\,, \qquad (2.3.17)
$$

for the running coupling $\alpha_s(\mu^2)$. Here $\beta_0 = 11 - 2n_f/3$ and $\beta_1 = 102 - 38n_f/3$. Another way of writing this equation is

$$\ln \frac{\mu^2}{(\tilde{\Lambda}^{(n_f)}_{\rm EXACT})^2} = \frac{4\pi}{\beta_0 \alpha_s(\mu^2)} - \frac{\beta_1}{\beta_0^2} \ln \left[\frac{4\pi}{\beta_0 \alpha_s(\mu^2)} + \frac{\beta_1}{\beta_0^2} \right] . \tag{2.3.18}$$

The values for $\tilde{\Lambda}^{(n_f)}_{\rm EXACT}$ are carefully chosen to obtain accurate matching of α_s at the scales m_c^2 and m_b^2. We used the values $\tilde{\Lambda}^{(3,4,5,6)}_{\rm EXACT} = 299.4,\ 246,\ 167.7,\ 67.8$ MeV$/c^2$ respectively in the exact formula (which yields $\alpha_s^{\rm EXACT}(m_Z^2) = 0.114$, $\alpha_s^{\rm EXACT}(m_b^2) = 0.205$, $\alpha_s^{\rm EXACT}(m_c^2) = 0.319$, $\alpha_s^{\rm EXACT}(\mu^2_{\rm NLO}) = 0.578$) and $\Lambda^{(3,4,5,6)}_{\rm LO} = 204,\ 175,\ 132, 66.5$ MeV$/c^2$ respectively (which yields $\alpha_s^{\rm LO}(m_Z^2) = 0.125$, $\alpha_s^{\rm LO}(m_b^2) = 0.232$, $\alpha_s^{\rm LO}(m_c^2) = 0.362$, $\alpha_s^{\rm LO}(\mu^2_{\rm LO}) = 0.763$) for the LO formula (where $\beta_1 = 0$). There is a NNLO discontinuity of aproximately two parts in one thousand in the running coupling across heavy flavor thresholds [31], [32]. We have ignored this effect to focus on the numerically more significant matching of the flavor densities.

2.3.4 The evolution process

Three flavor evolution proceeds from the initial μ_0^2 to the scale $\mu^2 = m_c^2 = 1.96$ (GeV^2)^2. At this point the charm density is then defined by

$$\begin{aligned} f_{c+\bar{c}}(n_f+1, m_c^2) &= a_s^2(n_f, m_c^2) \Big[\tilde{A}^{\rm PS}_{Qq}(1) \otimes f_q^{\rm S}(n_f, m_c^2) \\ &\quad + \tilde{A}^{\rm S}_{Qg}(1) \otimes f_g^{\rm S}(n_f, m_c^2) \Big] , \end{aligned} \tag{2.3.19}$$

with $n_f = 3$ and $a_s = \alpha_s/4\pi$. We have suppressed the x dependence to make the notation more compact. The $\otimes$ symbol denotes the convolution integral $f \otimes g = \int f(x/y) g(y) dy/y$, where $x \le y \le 1$. The OME's $\tilde{A}^{\rm PS}_{Qq}(\mu^2/m_c^2)$, $\tilde{A}^{\rm S}_{Qg}(\mu^2/m_c^2)$ are given in [30] and are also listed in Appendix B. The reason for choosing the matching scale μ at the mass of the charm quark m_c is that all the $\ln(\mu^2/m_c^2)$ terms in the OME's vanish at this point leaving only the nonlogarithmic pieces in the order α_s^2 OME's to contribute to the right-hand-side of Eq.(4.19). Hence the LO and NLO charm densities vanish at the scale $\mu = m_c$. The NNLO charm density starts off with a finite x-dependent shape in order α_s^2. Note that we then order the terms on the right-hand-side of Eq. (2.3.19) so that it contains a product of NLO OME's and LO parton densities. The result is then of order α_s^2 and should be multiplied by order α_s^0 coefficient functions when forming the deep inelastic structure functions.

The four-flavor gluon density is also generated at the matching point in the same way. At $\mu = m_c$ we define

$$\begin{aligned} f_g^{\rm S}(n_f+1,m_c^2) &= f_g^{\rm S}(n_f,m_c^2) \\ &\quad +a_s^2(n_f,m_c^2)\Big[A_{gq,Q}^{\rm S}(1)\otimes f_q^{\rm S}(n_f,m_c^2)\,, \\ &\quad +A_{gg,Q}^{\rm S}(1)\otimes f_g^{\rm S}(n_f,m_c^2)\Big]\,. \end{aligned} \tag{2.3.20}$$

The OME's $A_{gq,Q}^{\rm S}(\mu^2/m_c^2)$, $A_{gg,Q}^{\rm S}(\mu^2/m_c^2)$ are given in [30] and are also listed in the Appendix B. The four-flavor light quark (u,d,s) densities are generated using

$$\begin{aligned} f_{k+\bar{k}}(n_f+1,m_c^2) &= f_{k+\bar{k}}(n_f,m_c^2) \\ &\quad +a_s^2(n_f,m_c^2)A_{qq,Q}^{\rm NS}(1)\otimes f_{k+\bar{k}}(n_f,m_c^2)\,. \end{aligned} \tag{2.3.21}$$

The OME $A_{qq,Q}^{\rm NS}(\mu^2/m_c^2)$ is given in [30] (as well as in Appendix B) and the *total* four-flavor singlet quark density folows from the sum of Eqs. (2.3.19) and (2.3.21). In Eqs. (2.3.20) and (2.3.21) we set $n_f = 3$. The remarks after Eq. (2.3.19) are relevant here too.

Next the resulting four-flavor densities are evolved using the four-flavor weights in either LO, NLO and NNLO up to the scale $\mu^2 = m_b^2 = 20.25$ $(\mathrm{GeV}^2)^2$. The bottom quark density is then generated at this point using

$$\begin{aligned} f_{b+\bar{b}}(n_f+1,m_b^2) &= a_s^2(n_f,m_b^2)\Big[\tilde{A}_{Qq}^{\rm PS}(1)\otimes f_q^{\rm S}(n_f,m_b^2) \\ &\quad +\tilde{A}_{Qg}^{(\rm S)}(1)\otimes f_g^{\rm S}(n_f,m_b^2)\Big]\,, \end{aligned} \tag{2.3.22}$$

and the gluon and light quark densities (which now include charm) are generated using Eqs.(2.3.19)-(2.3.21) with $n_f = 4$ and replacing m_c^2 by m_b^2. Therefore only the nonlogarithmic terms in the order a_s^2 OME's contribute to the matching conditions on the bottom quark density. Then all the densities are evolved up to higher μ^2 as a five-flavor set with either LO, NLO and NNLO splitting functions. This is valid until $\mu = m_t \approx 175$ GeV^2 above which one should switch to a six-flavor set. We do not implement this step because the top quark density would be extremely small.

The procedure outlined above generates a full set of parton densities (gluon, singlet, non-singlet light and heavy quark densities,) for any x and μ^2 from the three-flavor LO, NLO and NNLO inputs in Eqs.(2.3.15) and (2.3.16). Note that we have used μ^2 for the factorization and renormalization scales in the above discussion. In the computer program we use the notation that Q^2 denotes these scales, since this is done in all the previous computer codes for the parton densities.

2.4 Input parameter description and usage

To prepare the program for use unpack the distribution package **adens-24.tar.gz** by typing tar -xzf adens-24.tar.gz. The resulting directory will contain the following files

```
head.h
main.h
main.c
l-a-w.c
nl-a-w.c
alpha.c
init.c
polylo.c
intpol.c
evolver.c
thresh.c
a-coefs.c
loader.c
quadrat.c
daind.c
integrands.c
grids.c
weights.c
nnl-a-w.c
wgplg.c
evolution_parameters.input
makefile
my_howto.tex
sample.out
```

To build the executable on a machine with a gcc compiler type *make* . The executable named **adens.x** will be produced. To run the code just run the file **adens.x**. Some debugging information may appear on the standard output.

Here is the parameter file (**evolution_parameters.input**) explanation with default values shown:

0.204e0	LambdaLO-3	LO Λ for N_f =3
0.175e0	LambdaLO-4	LO Λ for N_f =4
0.132e0	LambdaLO-5	LO Λ for N_f =5
0.306e0	LambdaNLO3	NLO Λ for N_f =3
0.257e0	LambdaNLO4	NLO Λ for N_f =4
0.1734e0	LambdaNLO5	NLO Λ for N_f =5
0.2994e0	LambdaENLO3	Exact Λ for N_f =3
0.246e0	LambdaENLO4	Exact Λ for N_f =3
0.1677e0	LambdaENLO5	Exact Λ for N_f =3
0.40e0	Qinitial2	Initial Q^2 to start evolution
1.96e0	QcharmMass	Mass of first heavy quark c
20.25e0	QbottomMass	Mass of second heavy quark b
1.96e0	QcharmThreshold	Charm threshold
1.96e0	AlphaCharmThreshold	C threshold used for α_s
20.25e0	QbottomThreshold	Bottom threshold
20.25e0	AlphaQbottomThreshold	B threshold used for α_s
1000.0e0	Qfinal2	Final Q^2
130	tGridSize	Q^2 grid size
200	xGridSize	x grid size
130	xGridSplit	x split between log and linear
1.0e-5	xInitial	x initial
0.2e0	xSplit	x at the split btw log and linear
1.00e0	xFinal	x final (always 1)
0	DebugLevel	Error message detail (0-5)
1	GraphVsX	Plotting data files are versus x (1) or Q^2 (0)
1	Order	LO/NLO/NNLO for 0,1,2
0	DoFortran	Produce (1) or no (0) data files for CSN/BMSN Fortran programs (1-yes, 0-no)
1	AlphaDoSeparateThreshold	Use separate thresholds for α_s (1-yes, 0-no)

1	AlphaUseExact	Use exact GRV98-style α_s (1-yes, 0-no)
0	ThreeFlavorMode	Calculate GRV98-style densities with no heavy flavors (1-yes, 0-no)
0	GraphAll	Plot all data points (1-yes, 0-no)
0	NNLOmultiOrderCHARM	Use our proper order NNLO heavy flavors (1-yes, 0-no)
1	DoBottomThreshold	Generate bottom (1-yes, 0-no)
0	LoadWeightsMadeBefore	Use ready weights if available (1-yes, 0-no)
1	DoNotDumpWeights	Dump weight for future use as the option above (1-yes, 0-no)
0	NLO4NNLO	Use NLO weights for NNLO calculation (1-yes, 0-no)

The first set of Lambdas are used for LO calculations. The second set are used for NLO and NNLO calculations if the exact α_s is not requested (AlphaUseExact=0). The next set (LambdaENLO3, LambdaENLO4, LambdaENLO5) are used for the exact solution of the differential equation for α_s as proposed in the GRV98 paper [22]. The code that calculates the exact α_s might use its own set of flavor thresholds (which means that the number of flavors used for α_s can be reset independently from the regular heavy flavor threshold as done in [22]).

Next we give the Q^2 limits and the heavy masses: the initial and final Q^2, the charm and bottom masses (used in threshold calculations), the heavy flavor thresholds and the separate α_s thresholds. Next follow the grid sizes in x and Q^2 together with x initial and final (always 1) and the switch point between logarithmic and linear grids in the x dimension. The x grid always starts as logarithmic and then becomes linear at higher x, usually at a value of the order of 0.1 (xGridSplit parameter).

The last group of parameters contains various control values that set the modes of the computation:
DebugLevel , controls the amount of generated error, warning and information messages,
GraphVsX , controls the printing of the output data for plotting (first column is either x or Q^2, then subsequent columns will contain density values for various Q^2 or x),
Order, sets calculation order (use 0,1,2 for LO,NLO,NNLO),
DoFortran, sets whether to dump interpolated densities on a special grid for

future use in Fortran code for the calculation of structure functions ; CSN and BMSN refer to VFNS schemes which are explained in [25],
AlphaDoSeparateThreshold, sets whether we use a separate threshold for α_s (used, for instance for GRV98 set where n_f for densities is always 3 and n_f for α_s goes from 3 to 5,
AlphaUseExact, sets whether to use exact (differential equation solution) α_s for NLO and NNLO calculation,
ThreeFlavorMode, sets whether to run GRV98 mode (no heavy flavors, $n_f = 3$ for all Q^2),
GraphAll, controls the amount of graphing and printing output (either all data points or the special grid defined in the file **main.h**, that contains some favorite values (for more see Section 7)),
NNLOmultiOrderCHARM, activates NNLO threshold calculation using proper order combinations (this mode requires one to first run the LO and NLO calculations),
DoBottomThreshold, enables the bottom density,
LoadWeightsMadeBefore, turns on and off the loading of weights computed in the prior runs,
DoNotDumpWeights, sets whether to save computed weights to disk for future use,
NLO4NNLO, sets whether NLO weights are used for the NNLO calculation (thus having only the boundary condition in NNLO).

Some common parameter settings and typical grid sizes for popular evolutions are shown in Section 7.

2.5 Description of the program

2.5.1 Program module summary

main.c	The main program, input and output
l-a-w.c	Calculation of LO weights
nl-a-w.c	Calculation of NLO weights
alpha.c	Calculation of α_s
init.c	Definition of initial functions
polylo.c	Calculation of polylogarithms
intpol.c	Interpolation routine
evolver.c	Evolution process subroutine
thresh.c	Threshold handling subroutine
a-coefs.c	OMEs for thresholds
loader.c	Datafile reading subroutine
quadrat.c	Gaussian integration subroutine
daind.c	Another integration subroutine
integrands.c	Heavy flavor integrand calculation routine
grids.c	Grid generation routine and memory management routines
weights.c	Weight table handling routine
nnl-a-w.c	Calculation of NNLO weights
wgplg.c	Calculation of high order polylogarithms

2.5.2 main.c

subroutines:
none.

The main program module contains input handling from the parameter file, parameter verification, calls to grid generating routines (**MakeXGrid, MakeTGrid**), resets for all density arrays (array q) and their derivatives (array qp). It also includes calls to the generation of weights (**analowgts, ananlowgts**), the calls to evolution and threshold routines (**evolver, threshold**) that do the actual work. Also it contains some pre-output density processing and the results provided in various formats for both viewing and plotting.

2.5.3 l-a-w.c

subroutines:

int analowgts(int nf,int loadWgts),
int computeLOwgts(int nf),
double sqq(double x,double y),
double sgg(double x,double y).

Analytically computes or reads from the file the LO weights for the evolution equations.

2.5.4 nl-a-w.c

subroutines:
int ananlowgts(int nf,int loadWgts),
int computeNLOwgts(int nf),
double s1ff(double x,double y, int nf),
double s2ff(double x,double y, int nf),
double s1fg(double x,double y, int nf),
double s2fg(double x,double y, int nf),
double s1gf(double x,double y, int nf),
double s2gf(double x,double y, int nf),
double s1gg(double x,double y, int nf),
double s2gg(double x,double y, int nf),
double s1ff_plus(double x, int nf),
double s1gg_plus(double x, int nf),
double s1p(double x,double y, int nf),
double s2p(double x,double y, int nf),
double s1m(double x,double y, int nf),
double s2m(double x,double y, int nf),
double s1p_plus(double x, int nf),
double s1m_plus(double x, int nf),
double s1gf_lim(double sp,double nf),
double s1fg_lim(double sp,double nf),
double s2ff_lim(double sp,double nf),
double s2fg_lim(double sp,double nf),
double s2gf_lim(double sp,double nf),
double s2gg_lim(double sp,double nf),
double s2p_lim(double sp,double nf),
double s2m_lim(double sp,double nf).

Analytically computes or reads from the file the NLO weights for the evolution equation. These routines are grouped into 3 kinds: the s1,2xx

routines calculate the regular weights, the s1,2xx_lim routines calculate the regular weights called at 1 and s1,2xx_plus do the weights that contain the plus-distributions.

2.5.5 alpha.c

subroutines:
double alpha(double tt, int nf), double alphae (double tt,int nf).

Calculates LO, NLO and exact running coupling α_s using corresponding parameters from the input file.

2.5.6 init.c

subroutines:
double initq_uv(double xx),
double initq_dv(double xx),
double init_gl(double xx),
double initq_ss(double xx),
double initq_del(double xx),
double initq_udbar(double xx).

Sets initial values for all parton densities using the GRV98 input for LO and NLO densities from [22].

2.5.7 polylo.c

subroutines:
double Li2(double x),
double Li3(double x),
double S12(double x).

Calculates these three polylogarithms using a fast routine with Bernouilli numbers. .

2.5.8 intpol.c

subroutines:
double int_q(int j,double xx,int it),
double interpolate(double xx,double *xt, double *yt,int points).

Interpolation routines used to calculate densities between grid points and for integration at the threshold.

2.5.9 evolver.c

subroutines:
evolver(int it1,int it2,int ic,int ib).

The main routine that performs the evolution between thresholds for all densities. It updates the main density array q and the density derivatives array qp.

2.5.10 thresh.c

subroutines:
int threshold(int what,int itt),
int fdens4(double xx,int ittc,double *u,double *d,double *s),
double light_charm(double xx,int ittc),
double fcharm(double xx,int ittc),
double fbottom(double xx,int ittc),
double fsigma(double xx,int ittc),
double fgluon(double xx,int ittc),
double fcharm(double xx,int ittc),
double fbottom(double xx,int ittc).

Threshold handling routines to implement LO, NLO and NNLO matching conditions for light and heavy densities at the charm and bottom thresholds. The density routines are calls to convolution integrals that generate new densities for $n_f + 1$ flavors.

2.5.11 a-coefs.c

subroutines:
double a1qg(double z,double fs2,double hm2),

double a2qq(double z,double fs2,double hm2),
double a2qg(double z,double fs2,double hm2),
double a2qqns(double z,double fs2,double hm2),
double softq(double z,double fs2,double hm2),
double corq(double z,double fs2,double hm2),
double a2gg(double z,double fs2,double hm2),
double softg(double z,double fs2,double hm2),
double corg1(double fs2,double hm2),
double corg2(double z,double fs2,double hm2),
double a2gq(double z,double fs2,double hm2).

The OME routines used for NNLO threshold matching. These contain the formulae in Appendix B.

2.5.12 loader.c

subroutines:
int loadOrd(int what).

Functions to handle threshold datafile loading, saving and verification. This file allows one the ability to use previously computed density values at the threshold in a new computation.

2.5.13 quadrat.c

subroutines:
double qadrat(double *x, double a, double b, double (*fx)(double), double e[]),
double lint(double *x, double (*fx)(double), double e[], double x0, double xn, double f0, double f2, double f3, double f5, double f6, double f7, double f9, double f14, double hmin, double hmax, double re, double ae).

Backup integration routine used as a check for the actual one used in the threshold integration.

2.5.14 daind.c

subroutines:
double daind(double *x,double a,double b, double (*fun)(double),double eps,int

key,int max).

Main Gaussian integration routine, see [34].

2.5.15 integrands.c

subroutines:
inline double fcharm_integrand(double x1),
inline double fgluon_integrand(double x1),
inline double fsigma_integrand(double x1),
inline double us_integrand(double x1),
inline double ds_integrand(double x1),
inline double ss_integrand(double x1),
inline double fbottom_integrand(double x1),
inline double light_charm_integrand(double x1).

Functions containing integrands for the threshold integration. They use the density values and the coefficient functions from a-coefs.c to produce the integrands that are then fed into the Gaussian integration program.

2.5.16 grids.c

subroutines:
int MakeXGrid(void),
int MakeTGrid(void),
int merge(double *a,double *b,int na, int nb,char w),
int check_grid(double *a,int n,char w),
int MakeFortranGrid(int test_mode),
double **allocate_real_matrix(int ur, int uc),
void free_real_matrix(double **m,int ur).

Subroutines for making (and also merging and verifying) the initial grids in x and Q^2 and the final grids for Fortran-code compatible output. The grid merging is used to combine the evenly spaced grid generated automatically from the initial and final values with the premade grid containing several x and Q^2 values for plotting and outputting the data. Two routines are added for deallocating memory.

2.5.17 weights.c

subroutines:
int readWeights(int nf,int order),
int dumpWeights(int nf,int order).

Routines dealing with loading and saving computed NLO and NNLO weight tables to do a fast calculation on the same grids. LO weights are not saved as it is very fast to compute them every time.

2.5.18 nnl-a-w.c

subroutines:
int anannlowgts(int nf,int loadWgts),
int computeNNLOwgts(int nf),
double nn_s1ff(double x,double y, int nf),
double nn_s2ff(double x,double y, int nf),
double nn_s1fg(double x,double y, int nf),
double nn_s2fg(double x,double y, int nf),
double nn_s1gf(double x,double y, int nf),
double nn_s2gf(double x,double y, int nf),
double nn_s1gg(double x,double y, int nf),
double nn_s2gg(double x,double y, int nf),
double nn_s1ff_plus(double x, int nf),
double nn_s1gg_plus(double x, int nf),
double nn_s1p(double x,double y, int nf),
double nn_s2p(double x,double y, int nf),
double nn_s1m(double x,double y, int nf),
double nn_s2m(double x,double y, int nf),
double nn_s1p_plus(double x, int nf),
double nn_s1m_plus(double x, int nf),
double nn_s1gf_lim(double sp,double nf),
double nn_s1fg_lim(double sp,double nf),
double nn_s2ff_lim(double sp,double nf),
double nn_s2fg_lim(double sp,double nf),
double nn_s2gf_lim(double sp,double nf),
double nn_s2gg_lim(double sp,double nf),
double nn_s2p_lim(double sp,double nf),
double nn_s2m_lim(double sp,double nf).

Analytically computes or reads from files the approximate NNLO weights for the evolution equations. Here the routines are grouped into three kinds: the nn_s1,2xx routines calculate the regular weights, the nn_s1,2xx_lim routines calculate the regular weights called at 1 and nn_s1,2xx_plus do the weights that contain the plus-distributions.

2.5.19 wgplg.c

subroutines:
double wgplg(int n,int p,double x).

The routines which calculate polylogarithms using the method from CERN-LIB [35]. They are only used for the higher order polylogarithms because the routines for Li2, Li3 and S12 in polylo.c are faster.

2.6 Results

The code can be used in several modes of operation.

For all of them there is some optimum grid size in x and Q^2. Internally, the grid with the sizes entered in the parameter file is merged with another grid (that is used for plotting the output data at the end), thus increasing the resulting grid size. This internal grid size contains all "popular" values, like $x = 0.1$, 0.01, 0.001 etc., and is 38 in Q^2 and 64 in x. The corresponding values are located in file **main.h** (arrays xpr[] and q2pr[]). This grid is then merged with the automatically generated equidistant grid and the equal values are weeded out. Shown in the table are the resulting grid sizes as shown in the output file. The table uses the calculation for all flavors as opposed to the GRV98-like (only three-flavor) densities. In general, the evolution time grows quadratically in n_x and linearly in n_{Q^2}. The numbers we give below are for an alpha PC with a 21164 processor unit running at 500 MHz, 1 Gbyte of memory and rated at an Specfp = 20.4.

order	n_x	n_{Q^2}	accuracy,digits	time,sec
LO	162	96	5	15
NLO	162	96	3	113
NNLO	162	96	3	385
LO	262	136	6	31
NLO	262	136	5	275
NNLO	262	136	5	1021
LO	362	136	6	44
NLO	362	136	6	529
NNLO	362	136	5	1537

1. Set parameters to the following values to produce LO and NLO GRV98-style fixed three-flavor densities for the whole range of Q^2 (only parameters essential for this calculation are provided, the rest can be set to whatever one wishes since they control the form of the output and similar features, not the physically meaningful ones):

LO	
0.26	Qinitial2
0	Order
1	ThreeFlavorMode
NLO	
0.40	Qinitial2
1	Order
1	AlphaUseExact
1	ThreeFlavorMode

2. To generate regular VFNS densities with all heavy flavors (both charm and bottom) one sets:

LO	
0.26	Qinitial2
0	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
0	NNLOmultiOrderCHARM
1	DoBottomThreshold
NLO	
0.40	Qinitial2
1	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	AlphaUseExact
0	NNLOmultiOrderCHARM
1	DoBottomThreshold

3. To generate VFNS densities involving proper order mixing at heavy thresholds with all heavy flavors (both charm and bottom) but without using NNLO weights (as done in our previous papers [25], [26], [27], [33]) one sets:

LO	
0.26	Qinitial2
0	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	DoBottomThreshold
NLO	
0.40	Qinitial2
1	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	AlphaUseExact
1	DoBottomThreshold
NNLO	
0.40	Qinitial2
2	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	AlphaUseExact
1	NNLOmultiOrderCHARM
1	DoBottomThreshold
1	NLO4NNLO

In this mode it is necessary to generate LO and NLO sets by running the program before running the NNLO set on the same grid! Those will be dumped in special data files
(**agrv99lo.BO.threshold**, **agrv99lo.CH.threshold**,
agrv99nlo.BO.threshold, and **agrv99nlo.CH.threshold**)
that will later be read for the NNLO calculation whenever
NNLOmultiOrderCHARM=1.

4. To generate VFNS densities involving proper order mixing at heavy thresholds with all heavy flavors (both charm and bottom) and using LO, NLO and NNLO (approximate) weights one sets:

LO	
0.26	Qinitial2
0	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	DoBottomThreshold
NLO	
0.40	Qinitial2
1	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	AlphaUseExact
1	DoBottomThreshold
NNLO	
0.40	Qinitial2
2	Order
0	ThreeFlavorMode
1	AlphaDoSeparateThreshold
1	AlphaUseExact
1	NNLOmultiOrderCHARM
1	DoBottomThreshold
0	NLO4NNLO

In this mode it is also necessary to generate LO and NLO sets by running the program before running the NNLO set on the same grid! Those will be dumped in special data files
(**agrv99lo.BO.threshold**, **agrv99lo.CH.threshold**,
agrv99nlo.BO.threshold, and **agrv99nlo.CH.threshold**)
that will later be read for NNLO calculation whenever
NNLOmultiOrderCHARM=1.

Program output is arranged in several forms. First, the default output in normal readable form goes into **resLO.dat, resNLO.dat or resNNLO.dat** or for GRV98-mode into **resLO3.dat, resNLO3.dat or resNNLO3.dat** depending upon the set calculation order. This file contains the input parameters, calculation time and the columns of data versus Q^2 and x for all densities (uv,dv,us,ds,ss,ch and bt, described in previous chapters). Here is the sample:

```
========================== Q2=    1.960 ======================
```

```
Alpha(Q2=    1.96 GeV2)=0.318513 for nf=4
------------------------- x=0.000010  ----------------------
SI(x= 0.0000100)=3.4695646e+00  GL(x= 0.0000100)=1.3074834e+01
UV(x= 0.0000100)=6.1120367e-03  DV(x= 0.0000100)=3.7959190e-03
US(x= 0.0000100)=5.9818110e-01  DS(x= 0.0000100)=5.9988948e-01
SS(x= 0.0000100)=5.3175774e-01
CH(x= 0.0000100)=0.0000000e+00  BT(x= 0.0000100)=0.0000000e+00
------------------------- x=0.000020  ----------------------
SI(x= 0.0000200)=3.1153438e+00  GL(x= 0.0000200)=1.1469641e+01
UV(x= 0.0000200)=8.2564168e-03  DV(x= 0.0000200)=5.1210226e-03
US(x= 0.0000200)=5.4149612e-01  DS(x= 0.0000200)=5.4372565e-01
SS(x= 0.0000200)=4.6576141e-01
CH(x= 0.0000200)=0.0000000e+00  BT(x= 0.0000200)=0.0000000e+00
```

The above sample was produced with GraphAll=0 thus printing only values on a small grid with minimum $Q^2 = 1.96$ GeV^2 and not all values from minimum $Q^2 = 0.40$ GeV^2. For convenience, SI denotes singlet, GL gluon, UV and DV are valence densities $u - \bar{u}$, $d - \bar{u}$, US, DS, SS are of the $q + \bar{q} - \Sigma(n_f)/n_f$ kind and CH and BT are $(c + \bar{c})/2$ and $(b + \bar{b})/2$.

For graphing purposes, the output also goes into several datafiles with names formed as **g_densityORDER.dat** where ORDER is LO, NLO or NNLO respectively e.g. **g_glLO.dat** or **g_uvNNLO.dat**. Those contains columns of the particular density with the first column being x or Q^2, depending upon GraphVsX parameter (1-x, 0-Q^2). Then the other parameter is varied across columns. Here is the piece of **g_cpNLO.dat** file. The first column contains the x value, the second is the charm density for $Q^2 = 1.96$ GeV^2 (where it is zero) and then the charm density for $Q^2 = 2, 3, ..$ GeV^2:

```
0.0000100000 0.0000000000e+00   1.0468420825e-02   1.3022045486e-01
0.0000200000 0.0000000000e+00   8.8559755303e-03   1.0970003578e-01
0.0000300000 0.0000000000e+00   8.0049032415e-03   9.8909559249e-02
0.0000400000 0.0000000000e+00   7.4395488912e-03   9.1758900075e-02
0.0000500000 0.0000000000e+00   7.0219632243e-03   8.6487022224e-02
0.0000600000 0.0000000000e+00   6.6940248888e-03   8.2352079221e-02
0.0000700000 0.0000000000e+00   6.4257535493e-03   7.8973989377e-02
0.0000800000 0.0000000000e+00   6.1998499386e-03   7.6132631291e-02
0.0000900000 0.0000000000e+00   6.0054517691e-03   7.3690103826e-02
```

The above sample was produced with GraphVsX=1 thus printing x, not Q^2 values in the first column. The GraphAll=0 was also set, thus only nice values of x are used (0.00001, 0.00002, 0.00003, etc).

Also, if the necessary option (DoFortran=1) is set the output also goes into the file suitable for reading by a GRV98-like Fortran program that interpolates the data points and makes parton density functions. This program is used in structure function calculations (the code is written in Fortran). The datafile format has eight columns with all densities on the fixed grid (hard-coded into the both evolution code and the interpolation program) in x and Q^2.

The sample follows:

```
Information line: first
+6.112E-03 +3.796E-03 +5.982E-01 +5.999E-01 +5.318E-01 +1.307E+01
+6.128E-03 +3.806E-03 +6.084E-01 +6.101E-01 +5.419E-01 +1.333E+01
+6.303E-03 +3.912E-03 +7.251E-01 +7.268E-01 +6.581E-01 +1.634E+01
+6.440E-03 +3.996E-03 +8.260E-01 +8.278E-01 +7.586E-01 +1.901E+01
+6.553E-03 +4.064E-03 +9.151E-01 +9.169E-01 +8.473E-01 +2.140E+01
+6.649E-03 +4.122E-03 +9.949E-01 +9.967E-01 +9.269E-01 +2.357E+01
+6.731E-03 +4.172E-03 +1.067E+00 +1.069E+00 +9.990E-01 +2.556E+01
+6.804E-03 +4.216E-03 +1.134E+00 +1.135E+00 +1.065E+00 +2.740E+01
+6.869E-03 +4.255E-03 +1.195E+00 +1.197E+00 +1.126E+00 +2.910E+01
+6.927E-03 +4.291E-03 +1.252E+00 +1.253E+00 +1.183E+00 +3.070E+01
```

Sample pictures of bottom densities are provided in [26] and also below in Figs. 2.1 - 2.4.

2.7 Error code descriptions

Program error code description:

message	filename	refer to
Threshold LO datafile is missing	loader.c	NNLO calculation with proper orders requires the datafile from a previous run in LO
Threshold NLO datafile is missing	loader.c	NNLO calculation with proper orders requires the datafile from a previous run in NLO
Wrong Multicharm factor	main.c	NNLOmultiOrderCHARM should be 1 or 0
Wrong order factor	several modules	should be 0,1,2 for LO, NLO, NNLO
File evolution_parameters.input does not exist	main.c	find the file and put into working directory
Wrong INI Q2:increase it!	main.c	order and initial Q^2 are incompatible
Wrong INI Q2:decrease it!	main.c	order and initial Q^2 are incompatible
Evolver: dont know how to proceed	main.c	wrong doBottom factor
Wrong Alpha switch factor!	main.c	check AlphaDoSeparateThreshold value
Wrong order factor while graphing	main.c	check Order to be 0,1,2
Wrong graphing factor	main.c	check GraphAll value to be 0,1
Wrong loadWgts factor	l-a-w.c, nl-a-w.c	check loadWgts to be 0,1

2.8 Conclusions

We have presented a multifunctional code for the direct x-space method of solving the spin-averaged evolution equations for parton densities. The distinctive features of this code include analytic computation of the LO, NLO and NNLO weights, NNLO heavy flavor threshold matching and NNLO evolution.

The code is very fast and accurate. For example for grid sizes not exceeding 200 in Q^2 and 150 in x the NLO calculation with full weighs computed for three values of n_f and up to five decimal accuracy has a runtime well below 200 seconds. Also it is the only code that does the proper NNLO evolution with NNLO heavy flavor matching conditions.

The program is also easy to use and complete documentation is available. The code is well-tested both on specific test functions (e.g. see [16]) and on actual densities (e.g. see [25]) in all (LO, NLO and NNLO) orders.

2.9 Acknowledgments

The work was partially supported by the National Science Foundation grant PHY-9722101. We thank Michael Botje for valuable comments on his method of solving the evolution equations and providing us with his evolution code. We also thank Andreas Vogt for help with testing the code in NNLO and for providing comparison data. Thanks are also due to Brian Harris for testing the code and comments on the manuscript.

2.10 Appendix A

Here we give the NNLO parametrizations of the splitting functions from [29]. Note that $L_0 = \ln z$ and $L_1 = \ln(1-z)$.

First the parametrizations for the non-singlet splitting functions $P_{\rm NS}^{(2)\pm}$ are:

$$\begin{aligned}
P_{{\rm NS},A}^{(2)-}(z) &= 1185.229\,(1-z)_+^{-1} + 1365.458\,\delta(1-z) - 157.387\,L_1^2 - 2741.42\,z^2 \\
&\quad - 490.43\,(1-z) + 67.00\,L_0^2 + 10.005\,L_0^3 + 1.432\,L_0^4 \\
&\quad + N_f\,\{-184.765\,(1-z)_+^{-1} - 184.289\,\delta(1-z) + 17.989\,L_1^2 + 355.636\,z^2 \\
&\quad - 73.407\,(1-z)L_1 + 11.491\,L_0^2 + 1.928\,L_0^3\} \;+\; P_{{\rm NS},2}^{(2)}(z), \\
P_{{\rm NS},B}^{(2)-}(z) &= 1174.348\,(1-z)_+^{-1} + 1286.799\,\delta(1-z) + 115.099\,L_1^2 + 1581.05\,L_1 \\
&\quad + 267.33\,(1-z) - 127.65\,L_0^2 - 25.22\,L_0^3 + 1.432\,L_0^4 \\
&\quad + N_f\,\{-183.718\,(1-z)_+^{-1} - 177.762\,\delta(1-z) + 11.999\,L_1^2 + 397.546\,z^2 \\
&\quad + 41.949\,(1-z) - 1.477\,L_0^2 - 0.538\,L_0^3\} \;+\; P_{{\rm NS},2}^{(2)}(z), \qquad (2.10.1)
\end{aligned}$$

and

$$\begin{aligned}
P_{{\rm NS},A}^{(2)+}(z) &= 1183.762\,(1-z)_+^{-1} + 1347.032\,\delta(1-z) + 1047.590\,L_1 - 843.884\,z^2 \\
&\quad - 98.65\,(1-z) - 33.71\,L_0^2 + 1.580\,(L_0^4 + 4L_0^3) \\
&\quad + N_f\,\{-183.148\,(1-z)_+^{-1} - 174.402\,\delta(1-z) + 9.649\,L_1^2 + 406.171\,z^2 \\
&\quad + 32.218\,(1-z) + 5.976\,L_0^2 + 1.60\,L_0^3\} \;+\; P_{{\rm NS},2}^{(2)}(z), \\
P_{{\rm NS},B}^{(2)+}(z) &= 1182.774\,(1-z)_+^{-1} + 1351.088\,\delta(1-z) - 147.692\,L_1^2 - 2602.738\,z^2 \\
&\quad - 170.11 + 148.47\,L_0 + 1.580\,(L_0^4 - 4\,L_0^3) \\
&\quad + N_f\,\{-183.931\,(1-z)_+^{-1} - 178.208\,\delta(1-z) - 89.941\,L_1 + 218.482\,z^2 \\
&\quad + 9.623 + 0.910\,L_0^2 - 1.60\,L_0^3\} \;+\; P_{{\rm NS},2}^{(2)}(z)\;. \qquad (2.10.2)
\end{aligned}$$

The parametrizations for $P_{\rm NS}^{(2),S}(z)$ and $P_{\rm PS}^{(2)}(z)$ are

$$\begin{aligned}
P_{{\rm NS},A}^{(2)S}(z) &= N_f\,\{(1-z)(-1441.57\,z^2 + 12603.59\,z - 15450.01) + 7876.93\,zL_0^2 \\
&\quad - 4260.29\,L_0 - 229.27\,L_0^2 + 4.4075\,L_0^3\} \\
P_{{\rm NS},B}^{(2)S}(z) &= N_f\,\{(1-z)(-704.67\,z^3 + 3310.32\,z^2 + 2144.81\,z - 244.68) \\
&\quad + 4490.81\,z^2L_0 + 42.875\,L_0 - 11.0165\,L_0^3\}, \qquad (2.10.3)
\end{aligned}$$

and

$$
\begin{aligned}
P^{(2)}_{\mathrm{PS},A}(z) &= N_f\,\{(1-z)(-229.497\,L_1 - 722.99\,z^2 + 2678.77 - 560.20\,z^{-1}) \\
&\quad + 2008.61\,L_0 + 998.15\,L_0^2 - 3584/27\,z^{-1}L_0\} \;+\; P^{(2)}_{\mathrm{PS},2}(z), \\
P^{(2)}_{\mathrm{PS},B}(z) &= N_f\,\{(1-z)(73.845\,L_1^2 + 305.988\,L_1 + 2063.19\,z - 387.95\,z^{-1}) \\
&\quad + 1999.35\,zL_0 - 732.68\,L_0 - 3584/27\,z^{-1}L_0\} \\
&\quad +\; P^{(2)}_{\mathrm{PS},2}(z), \qquad (2.10.4)
\end{aligned}
$$

with

$$
\begin{aligned}
P^{(2)}_{\mathrm{PS},2}(z) &= N_f^2\,\{(1-z)(-7.282\,L_1 - 38.779\,z^2 + 32.022\,z - 6.252 + 1.767\,z^{-1}) \\
&\quad + 7.453\,L_0^2\}\ . \qquad (2.10.5)
\end{aligned}
$$

Next we show the parametrizations of the off-diagonal singlet splitting functions:

$$
\begin{aligned}
P^{(2)}_{qg,A}(z) &= N_f\,\{-31.830\,L_1^3 + 1252.267\,L_1 + 1999.89\,z + 1722.47 + 1223.43\,L_0^2 \\
&\quad - 1334.61\,z^{-1} - 896/3\,z^{-1}L_0\} \;+\; P^{(2)}_{qg,2}(z), \\
P^{(2)}_{qg,B}(z) &= N_f\,\{19.428\,L_1^4 + 159.833\,L_1^3 + 309.384\,L_1^2 + 2631.00\,(1-z) \\
&\quad - 67.25\,L_0^2 - 776.793\,z^{-1} - 896/3\,z^{-1}L_0\} \;+\; P^{(2)}_{qg,2}(z), \qquad (2.10.6)
\end{aligned}
$$

with

$$
\begin{aligned}
P^{(2)}_{qg,2}(z) &= N_f^2\,\{-0.9085\,L_1^2 - 35.803\,L_1 - 128.023 + 200.929\,(1-z) \\
&\quad + 40.542\,L_0 + 3.284\,z^{-1}\}\ , \qquad (2.10.7)
\end{aligned}
$$

and

$$
\begin{aligned}
P^{(2)}_{gq,A}(z) &= 13.1212\,L_1^4 + 126.665\,L_1^3 + 308.536\,L_1^2 + 361.21 - 2113.45\,L_0 \\
&\quad - 17.965\,z^{-1}L_0 \;+\; N_f\,\{2.4427\,L_1^4 + 27.763\,L_1^3 + 80.548\,L_1^2 \\
&\quad - 227.135 - 151.04\,L_0^2 + 65.91\,z^{-1}L_0\} \;+\; P^{(2)}_{gq,2}(z), \\
P^{(2)}_{gq,B}(z) &= -4.5108\,L_1^4 - 66.618\,L_1^3 - 231.535\,L_1^2 - 1224.22\,(1-z) + 240.08\,L_0^2 \\
&\quad + 379.60\,z^{-1}(L_0+4) \;+\; N_f\{-1.4028\,L_1^4 - 11.638\,L_1^3 + 164.963\,L_1 \\
&\quad - 1066.78\,(1-z) - 182.08\,L_0^2 + 138.54\,z^{-1}(L_0+2)\} \\
&\quad +\; P^{(2)}_{gq,2}(z), \qquad (2.10.8)
\end{aligned}
$$

with

$$P^{(2)}_{gq,2}(z) = N_f^2 \{1.9361\ L_1^2 + 11.178\ L_1 + 11.632 - 15.145\ (1-z) + 3.354\ L_0 - 2.133\ z^{-1}\}\ . \quad (2.10.9)$$

Last we show the parametrizations of the diagonal singlet splitting functions

$$\begin{aligned} P^{(2)}_{gg,A}(z) &= 2626.38\ (1-z)_+^{-1} + 4424.168\ \delta(1-z) - 732.715\ L_1^2 - 20640.069\ z \\ &\quad - 15428.58\ (1-z^2) - 15213.60\ L_0^2 + 16700.88\ z^{-1} + 2675.85\ z^{-1} L_0 \\ &\quad + N_f \{-415.71\ (1-z)_+^{-1} - 548.569\ \delta(1-z) - 425.708\ L_1 + 914.548\ z^2 \\ &\quad - 1122.86 - 444.21\ L_0^2 + 376.98\ z^{-1} + 157.18\ z^{-1} L_0\} \\ &\quad + \ P^{(2)}_{gg,2}(z), \\ P^{(2)}_{gg,B}(z) &= 2678.22\ (1-z)_+^{-1} + 4590.570\ \delta(1-z) + 3748.934\ L_1 + 60879.62\ z \\ &\quad - 35974.45\ (1+z^2) + 2002.96\ L_0^2 + 9762.09\ z^{-1} + 2675.85\ z^{-1} L_0 \\ &\quad + N_f \{-412.00\ (1-z)_+^{-1} - 534.951\ \delta(1-z) + 62.630\ L_1^2 + 801.90 \\ &\quad + 1891.40\ L_0 + 813.78\ L_0^2 + 1.360\ z^{-1} + 157.18\ z^{-1} L_0\} \\ &\quad + \ P^{(2)}_{gg,2}(z), \end{aligned} \quad (2.10.10)$$

with

$$P^{(2)}_{gg,2}(z) = N_f^2 \{-16/9\ (1-z)_+^{-1} + 6.4882\ \delta(1-z) + 37.6417\ z^2 - 72.926\ z + 32.349 - 0.991\ L_0^2 + 2.818\ z^{-1}\}\ . \quad (2.10.11)$$

2.11 Appendix B

Shown below are the renormalized OME's used for threshold matching calculations in NLO and NNLO (they correspond to the unrenormalized expressions given in Appendix C of [36] and in Appendix A of [30]). All OME'S have been renormalized in the $\overline{\rm MS}$-scheme.

In particular the renormalized coupling α_s is presented in the above scheme for $n_f + 1$ light flavors. Here the heavy quark $H = (c, b)$ is treated on the same footing as the light flavors and it is not decoupled from the running coupling in the VFNS approach. The $(\alpha_s/4\pi)^2$ coefficient in the heavy-quark OME $\tilde{A}_{Hq}^{\rm PS}$ is given by

$$\begin{aligned}
\tilde{A}_{Hq}^{\rm PS,(2)}\left(\frac{m^2}{\mu^2}\right) = C_F T_f \Bigg\{ & \Bigg[-8(1+z)\ln z - \frac{16}{3z} - 4 \\
& + 4z + \frac{16}{3} z^2 \Bigg] \ln^2 \frac{m^2}{\mu^2} + \Bigg[8(1+z)\ln^2 z - \left(8 + 40z + \frac{64}{3} z^2 \right) \ln z \\
& - \frac{160}{9z} + 16 - 48z + \frac{448}{9} z^2 \Bigg] \ln \frac{m^2}{\mu^2} \\
& + (1+z) \Bigg[32 {\rm S}_{1,2}(1-z) + 16 \ln z {\rm Li}_2(1-z) - 16 \zeta(2) \ln z \\
& - \frac{4}{3} \ln^3 z \Bigg] + \left(\frac{32}{3z} + 8 - 8z - \frac{32}{3} z^2 \right) {\rm Li}_2(1-z) \\
& + \left(-\frac{32}{3z} - 8 + 8z + \frac{32}{3} z^2 \right) \zeta(2) + \left(2 + 10z + \frac{16}{3} z^2 \right) \ln^2 z \\
& - \left(\frac{56}{3} + \frac{88}{3} z + \frac{448}{9} z^2 \right) \ln z - \frac{448}{27z} - \frac{4}{3} - \frac{124}{3} z + \frac{1600}{27} z^2 \Bigg\} \qquad (2.11.1)
\end{aligned}$$

The $\alpha_s/4\pi$ and the $(\alpha_s/4\pi)^2$ coefficients of the heavy quark OME's $\tilde{A}_{Hg}^{\rm S}$ are

$$\tilde{A}_{Hg}^{\rm S,(1)}\left(\frac{m^2}{\mu^2}\right) = T_f \left[-4(z^2 + (1-z)^2) \ln \frac{m^2}{\mu^2} \right], \qquad (2.11.2)$$

and

$$\tilde{A}_{Hg}^{\rm S,(2)}\left(\frac{m^2}{\mu^2}\right) = \Bigg\{ C_F T_f [(8 - 16z + 16z^2) \ln(1-z)$$

$$
\begin{aligned}
&-(4-8z+16z^2)\ln z-(2-8z)]\\
&+C_AT_f\Bigg[-(8-16z+16z^2)\ln(1-z)-(8+32z)\ln z\\
&-\frac{16}{3z}-4-32z+\frac{124}{3}z^2\Bigg]+T_f^2\Bigg[-\frac{16}{3}(z^2+(1-z)^2)\Bigg]\Bigg\}\ln^2\frac{m^2}{\mu^2}\\
&+\Bigg\{C_FT_f\Bigg[(8-16z+16z^2)[2\ln z\ln(1-z)-\ln^2(1-z)+2\zeta(2)]\\
&-(4-8z+16z^2)\ln^2 z-32z(1-z)\ln(1-z)\\
&-(12-16z+32z^2)\ln z-56+116z-80z^2\Bigg]\\
&+C_AT_f\Bigg[(16+32z+32z^2)[\mathrm{Li}_2(-z)+\ln z\ln(1+z)]\\
&+(8-16z+16z^2)\ln^2(1-z)+(8+16z)\ln^2 z\\
&+32z\zeta(2)+32z(1-z)\ln(1-z)-\left(8+64z+\frac{352}{3}z^2\right)\ln z\\
&-\frac{160}{9z}+16-200z+\frac{1744}{9}z^2\Bigg]\Bigg\}\ln\frac{m^2}{\mu^2}\\
&+C_FT_f\Big\{(1-2z+2z^2)[8\zeta(3)+\frac{4}{3}\ln^3(1-z)\\
&-8\ln(1-z)\mathrm{Li}_2(1-z)+8\zeta(2)\ln z-4\ln z\ln^2(1-z)\\
&+\frac{2}{3}\ln^3 z-8\ln z\mathrm{Li}_2(1-z)+8\mathrm{Li}_3(1-z)-24\mathrm{S}_{1,2}(1-z)]\\
&+z^2\Bigg[-16\zeta(2)\ln z+\frac{4}{3}\ln^3 z+16\ln z\mathrm{Li}_2(1-z)+32\mathrm{S}_{1,2}(1-z)\Bigg]\\
&-(4+96z-64z^2)\mathrm{Li}_2(1-z)-(4-48z+40z^2)\zeta(2)\\
&-(8+48z-24z^2)\ln z\ln(1-z)+(4+8z-12z^2)\ln^2(1-z)\\
&-(1+12z-20z^2)\ln^2 z-(52z-48z^2)\ln(1-z)\\
&-(16+18z+48z^2)\ln z+26-82z+80z^2\Big\}\\
&+C_AT_f\Big\{(1-2z+2z^2)[-\frac{4}{3}\ln^3(1-z)\\
&+8\ln(1-z)\mathrm{Li}_2(1-z)-8\mathrm{Li}_3(1-z)]+(1+2z+2z^2)\\
&\times[-8\zeta(2)\ln(1+z)-16\ln(1+z)\mathrm{Li}_2(-z)-8\ln z\ln^2(1+z)\\
&+4\ln^2 z\ln(1+z)+8\ln z\mathrm{Li}_2(-z)-8\mathrm{Li}_3(-z)-16\mathrm{S}_{1,2}(-z)]
\end{aligned}
$$

$$+(16+64z)[2\mathrm{S}_{1,2}(1-z)+\ln z\mathrm{Li}_2(1-z)]-\left(\frac{4}{3}+\frac{8}{3}z\right)\ln^3 z$$
$$+(8-32z+16z^2)\zeta(3)-(16+64z)\zeta(2)\ln z+(16+16z^2)$$
$$\times[\mathrm{Li}_2(-z)+\ln z\ln(1+z)]+\left(\frac{32}{3z}+12+64z-\frac{272}{3}z^2\right)\mathrm{Li}_2(1-z)$$
$$-\left(12+48z-\frac{260}{3}z^2+\frac{32}{3z}\right)\zeta(2)-4z^2\ln z\ln(1-z)$$
$$-(2+8z-10z^2)\ln^2(1-z)+\left(2+8z+\frac{46}{3}z^2\right)\ln^2 z$$
$$+(4+16z-16z^2)\ln(1-z)-\left(\frac{56}{3}+\frac{172}{3}z+\frac{1600}{9}z^2\right)\ln z$$
$$-\frac{448}{27z}-\frac{4}{3}-\frac{628}{3}z+\frac{6352}{27}z^2\Bigg\}, \qquad (2.11.3)$$

respectively. Now we present the renormalized expressions for the heavy-quark loop contributions to the light-parton OME's denoted by $A_{kl,H}$. The coefficients of the $(\alpha_s/4\pi)^2$ terms in $A_{qq,H}$ and $A_{gq,H}$ are

$$A_{qq,H}^{\mathrm{NS},(2)}\left(\frac{m^2}{\mu^2}\right)=C_F T_f\Bigg\{\left[\frac{8}{3}\left(\frac{1}{1-z}\right)_+-\frac{4}{3}-\frac{4}{3}z+2\delta(1-z)\right]\ln^2\frac{m^2}{\mu^2}$$
$$+\left[\frac{80}{9}\left(\frac{1}{1-z}\right)_+ +\frac{8}{3}\frac{1+z^2}{1-z}\ln z+\frac{8}{9}-\frac{88}{9}z\right.$$
$$\left.+\delta(1-z)\left(\frac{16}{3}\zeta(2)+\frac{2}{3}\right)\right]\ln\frac{m^2}{\mu^2}$$
$$+\frac{1+z^2}{1-z}\left(\frac{2}{3}\ln^2 z+\frac{20}{9}\ln z\right)$$
$$+\frac{8}{3}(1-z)\ln z+\frac{224}{27}\left(\frac{1}{1-z}\right)_+ +\frac{44}{27}-\frac{268}{27}z$$
$$+\delta(1-z)\left(-\frac{8}{3}\zeta(3)+\frac{40}{9}\zeta(2)+\frac{73}{18}\right)\Bigg\}, \qquad (2.11.4)$$

and

$$A_{gq,H}^{\mathrm{S},(2)}\left(\frac{m^2}{\mu^2}\right)=C_F T_f\Bigg\{\left[\frac{16}{3z}-\frac{16}{3}+\frac{8}{3}z\right]\ln^2\frac{m^2}{\mu^2}$$
$$+\left[\frac{160}{9z}-\frac{160}{9}+\frac{128}{9}z+(\frac{32}{3z}-\frac{32}{3}+\frac{16}{3}z)\ln(1-z)\right]\ln\frac{m^2}{\mu^2}$$

$$+\frac{4}{3}\left(\frac{2}{z}-2+z\right)\ln^2(1-z)+\frac{8}{9}\left(\frac{10}{z}-10+8z\right)\ln(1-z)$$
$$+\frac{1}{27}\left(\frac{448}{z}-448+344z\right)\Bigg\}. \qquad (2.11.5)$$

respectively. The coefficients of the $\alpha_s/4\pi$ and $(\alpha_s/4\pi)^2$ terms in $A_{gg,H}$ are

$$A^{\mathrm{S},(1)}_{gg,H}\left(\frac{m^2}{\mu^2}\right)=T_f\left[\frac{4}{3}\delta(1-z)\ln\frac{m^2}{\mu^2}\right], \qquad (2.11.6)$$

and

$$\begin{aligned}A^{\mathrm{S},(2)}_{gg,H}\left(\frac{m^2}{\mu^2}\right)=&\Bigg\{C_FT_f\left[8(1+z)\ln z+\frac{16}{3z}+4-4z-\frac{16}{3}z^2\right]\\
&+C_AT_f\left[\frac{8}{3}\left(\frac{1}{1-z}\right)_+ +\frac{8}{3z}-\frac{16}{3}+\frac{8}{3}z-\frac{8}{3}z^2\right]\\
&+T_f^2\left[\frac{16}{9}\delta(1-z)\right]\Bigg\}\ln^2\frac{m^2}{\mu^2}\\
&+\Bigg\{C_FT_f\left[8(1+z)\ln^2 z+(24+40z)\ln z-\frac{16}{3z}+64-32z\right.\\
&\left.-\frac{80}{3}z^2+4\delta(1-z)\right]+C_AT_f\left[\frac{16}{3}(1+z)\ln z+\frac{80}{9}\left(\frac{1}{1-z}\right)_+\right.\\
&\left.+\frac{184}{9z}-\frac{232}{9}+\frac{152}{9}z-\frac{184}{9}z^2+\frac{16}{3}\delta(1-z)\right]\Bigg\}\ln\frac{m^2}{\mu^2}\\
&+C_FT_f\Bigg\{\frac{4}{3}(1+z)\ln^3 z+(6+10z)\ln^2 z+(32+48z)\ln z\\
&-\frac{8}{z}+80-48z-24z^2-15\delta(1-z)\Bigg\}\\
&+C_AT_f\Bigg\{\frac{4}{3}(1+z)\ln^2 z+\frac{1}{9}(52+88z)\ln z-\frac{4}{3}z\ln(1-z)\\
&+\frac{1}{27}\left[224\left(\frac{1}{1-z}\right)_+ +\frac{556}{z}-628+548z-700z^2\right]\\
&+\frac{10}{9}\delta(1-z)\Bigg\},\end{aligned} \qquad (2.11.7)$$

respectively.

The definitions for the polylogarithms $\mathrm{Li}_n(z)$ and the Nielsen functions $\mathrm{S}_{n,p}(z)$, which appear in the above expressions, can be found in [37].

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Chapter 3

$\overline{\text{MS}}$ Parton densities with NNLO heavy flavor matching conditions

3.1 Introduction

Quantum chromodynamic predictions for experimental cross sections and distributions in perturbation theory rely heavily on accurate knowledge of parton densities. Several groups [1], [2], [3] have extracted these densities from global fits to data with the latest theoretical information on $\overline{\rm MS}$ coefficient functions. At present the evolution of these densities via the Altarelli-Parisi (AP) equations [4] uses the information on leading order (LO) and next-to-leading order (NLO) [5] splitting functions. Unfortunately the next-to-next-to-leading order (NNLO) splitting functions are not known but some interesting pieces of information are available [6], [7], [8]. The complete splitting functions should be known soon.

The description of heavy quarks within this analysis recently received a lot of attention due to the data on deep inelastic production of D^* mesons from HERA [9], [10]. The global fitting groups have adopted different approaches. The CTEQ5 analysis describes charm and bottom densities via the so-called ACOT prescription [11], which is a one-loop matching condition between three-flavor and four-flavor densities at the scale $\mu = m_c$ and a corresponding one-loop matching between the four-flavor and five-flavor densities at the scale $\mu = m_b$. This is not done in the MRST density sets. Instead they impose matching conditions that the logarithmic derivative of the deep inelastic structure functions with regard to the scale μ should be continuous, see [12] for details. This yields different charm and bottom densities. The GRV group [13] adopt the approach that one does not need any densities other than a three-flavor $\overline{\rm MS}$ set because the convolution of these densities with the NLO heavy quark coefficient functions provided in [14] yields an excellent fit to the presently available data on $F_{2,c}(x, Q^2, m_c^2)$, which is stable under scale variations. By never taking the limit that $m_c \to 0$ the theoretical prediction has no collinear singularity problem. Note that the physical threshold for a heavy quark antiquark pair is at $Q^2(1-x)/x = 4m^2$. However the physical threshold is distinct from the matching scale where one switches between parton density sets.

The parton densities with n_f and $n_f + 1$ flavors are related by a set of operator matrix elements (OME's). The order α_s^2 OME's were recently derived in [15]. They contain terms with $\ln^i(\mu^2/m^2)$ $i = 1, 2$ as well as non-logarithmic terms. They have the property that the $n_f + 1$ flavor densities vanish in LO and in NLO when the scale $\mu = m$. In NNLO there are finite x-dependent discontinuities at this scale, which we refer to as NNLO matching conditions. In this respect the matching conditions on the parton densities are similar to those for the two-loop running coupling constant derived in

[19], [20]. These NNLO matching conditions can be important numerically. Note that the running coupling constant is not small at the scale $\mu = m_c$. The charm density constructed from the two-loop matching conditions has been used in a recent study of variable flavor number schemes for the charm component of the deep inelastic structure functions [16]. Here we would like to present a complete set of parton densities for light (u,d,s,g) and heavy (c,b) partons which satisfy the NNLO boundary conditions and are evolved with NLO splitting functions. When the three-loop anomalous dimensions become available they can be included in this analysis. At present our study primarily focuses on the effects of the discontinuous matching conditions and the differences between the resulting three, four and five-flavor parton densities as the scale μ increases through the regions $m_c \leq \mu < m_b$ and $\mu \geq m_b$ respectively.

In Sec. II we present some technical details about our choice of input parton densities and the two-loop matching conditions. All densities are derived in the $\overline{\rm MS}$ scheme. Then in Sec.III we give plots of the parton densities. Finally comparisons are made between the presently available NLO sets and our (NNLO) set. A discussion of the solutions of the evolution equations is given in the Appendix. We intend to make our computer package for these densities available in due course.

3.2 The parton densities

We present a consistent set of $\overline{\rm MS}$ parton densities containing three, four and five flavors for scales satisfying $\mu < m_c$, $m_c \leq \mu < m_b$ and $\mu \geq m_b$ respectively. The evolution of the densities is done with our own computer code written in C++ and some details are given in the Appendix. The code uses the direct x-space method to solve the evolution equation [4] similar to that in [17] and allows us to evolve both light and heavy parton densities in LO, NLO and NNLO (the latter using the NLO weights). The weights for the calculation are computed analytically from the LO and NLO [5] $\overline{\rm MS}$ splitting functions thus removing possible instabilities in the numerical integrations. Hence the program is very efficient and fast. The results from the evolution code have been thoroughly checked against the tables in the HERA report [18]. We use weights in LO and NLO for $n_f = 3, 4, 5$ for evolving the gluon $f_g^{\rm S}(n_f, x, \mu^2)$, the singlet quark densities $f_q^{\rm S}(n_f, x, \mu^2)$, the non-singlet valence quark densities $f_{k-\bar{k}}(n_f, x, \mu^2)$ and the non-singlet sea quark densities $f_q^{\rm NS}(n_f, x, \mu^2)$. As the scale increases across the charm and bottom matching points the sets are redefined to include densities for the c and b heavy quarks. The program allows us to use LO, NLO or NNLO matching conditions for the generation of the heavy flavor densities.

The number densities are defined as

$$\begin{aligned} f_{k-\bar{k}}(n_f, x, \mu^2) &\equiv f_k(n_f, x, \mu^2) - f_{\bar{k}}(n_f, x, \mu^2)\,,\ k = u, d \\ f_{k+\bar{k}}(n_f, x, \mu^2) &\equiv f_k(n_f, x, \mu^2) + f_{\bar{k}}(n_f, x, \mu^2)\,,\ k = u, d, s, c, b \end{aligned} \tag{3.2.1}$$

$$f_q^{\rm S}(n_f, x, \mu^2) = \sum_{k=1}^{n_f} f_{k+\bar{k}}(n_f, x, \mu^2) \tag{3.2.2}$$

$$f_q^{\rm NS}(n_f, x, \mu^2) = f_{k+\bar{k}}(n_f, x, \mu^2) - \frac{1}{n_f} f_q^{\rm S}(n_f, x, \mu^2)\,. \tag{3.2.3}$$

We start our LO evolution using the following input from [2] at $\mu_0^2 = \mu_{\rm LO}^2 = 0.26\ ({\rm GeV/c}^2)^2$

$$\begin{aligned} x f_{u-\bar{u}}(3, x, \mu_0^2) &= x u_v(x, \mu_{\rm LO}^2) \\ &= 1.239\ x^{0.48} (1-x)^{2.72} (1 - 1.8\sqrt{x} + 9.5x) \\ x f_{d-\bar{d}}(3, x, \mu_0^2) &= x d_v(x, \mu_{\rm LO}^2) \\ &= 0.614\ (1-x)^{0.9}\ x u_v(x, \mu_{\rm LO}^2) \end{aligned}$$

$$
\begin{aligned}
x(f_{\bar{d}}(3,x,\mu_0^2) - f_{\bar{u}}(3,x,\mu_0^2)) &= x\Delta(x,\mu^2_{\rm LO}) \\
&= 0.23\ x^{0.48}\,(1-x)^{11.3}\,(1-12.0\sqrt{x}+50.9x) \\
x(f_{\bar{d}}(3,x,\mu_0^2) + f_{\bar{u}}(3,x,\mu_0^2)) &= x(\bar{u}+\bar{d})(x,\mu^2_{\rm LO}) \\
&= 1.52\ x^{0.15}\,(1-x)^{9.1}\,(1-3.6\sqrt{x}+7.8x) \\
x f_g(3,x,\mu_0^2) &= xg(x,\mu^2_{\rm LO}) \\
&= 17.47\ x^{1.6}\,(1-x)^{3.8} \\
x f_s(3,x,\mu_0^2) = x f_{\bar{s}}(3,x,\mu_0^2) &= xs(x,\mu^2_{\rm LO}) \\
&= x\bar{s}(x,\mu^2_{\rm LO}) = 0\,. \qquad (3.2.4)
\end{aligned}
$$

Here $\Delta \equiv \bar{d} - \bar{u}$ is used to construct the non-singlet combination. We start the corresponding NLO evolution using the following input from [2] at $\mu_0^2 = \mu^2_{\rm NLO} = 0.40\ ({\rm GeV/c^2})^2$

$$
\begin{aligned}
x f_{u-\bar{u}}(3,x,\mu_0^2) &= xu_v(x,\mu^2_{\rm NLO}) \\
&= 0.632\ x^{0.43}\,(1-x)^{3.09}\,(1+18.2x) \\
x f_{d-\bar{d}}(3,x,\mu_0^2) &= xd_v(x,\mu^2_{\rm NLO}) \\
&= 0.624\ (1-x)^{1.0}\ xu_v(x,\mu^2_{\rm NLO}) \\
x(f_{\bar{d}}(3,x,\mu_0^2) - f_{\bar{u}}(3,x,\mu_0^2)) &= x\Delta(x,\mu^2_{\rm NLO}) \\
&= 0.20\ x^{0.43}\,(1-x)^{12.4}\,(1-13.3\sqrt{x}+60.0x) \\
x(f_{\bar{d}}(3,x,\mu_0^2) + f_{\bar{u}}(3,x,\mu_0^2)) &= x(\bar{u}+\bar{d})(x,\mu^2_{\rm NLO}) \\
&= 1.24\ x^{0.20}\,(1-x)^{8.5}\,(1-2.3\sqrt{x}+5.7x) \\
x f_g(3,x,\mu_0^2) &= xg(x,\mu^2_{\rm NLO}) \\
&= 20.80\ x^{1.6}\,(1-x)^{4.1} \\
x f_s(3,x,\mu_0^2) = x f_{\bar{s}}(3,x,\mu_0^2) &= xs(x,\mu^2_{\rm NLO}) \\
&= x\bar{s}(x,\mu^2_{\rm NLO}) = 0. \qquad (3.2.5)
\end{aligned}
$$

From the above densities we form the combinations that we evolve and step across thresholds. The NNLO densities for $\mu^2_{\rm NLO} < \mu^2 < m_{\rm c}^2$ are replaced with NLO densities. The heavy quark masses $m_c = 1.4\ {\rm GeV/c^2}$, $m_b = 4.5\ {\rm GeV/c^2}$ are used throughout the calculation together with the exact expression for the running coupling constant $\alpha_s(\mu^2)$, represented as the solution of the following differential equation

$$
\frac{d\,\alpha_s(\mu^2)}{d\,\ln(\mu^2)} = -\frac{\beta_0}{4\pi}\,\alpha_s^2(\mu^2) \;-\; \frac{\beta_1}{16\pi^2}\,\alpha_s^3(\mu^2) \qquad (3.2.6)
$$

or in the implicit form

$$
\ln\frac{\mu^2}{(\tilde{\Lambda}^{(n_f)}_{\rm EXACT})^2} = \frac{4\pi}{\beta_0\alpha_s(\mu^2)} \;-\; \frac{\beta_1}{\beta_0^2}\,\ln\left[\frac{4\pi}{\beta_0\alpha_s(\mu^2)} \;+\; \frac{\beta_1}{\beta_0^2}\right], \qquad (3.2.7)
$$

where $\beta_0 = 11 - 2n_f/3$ and $\beta_1 = 102 - 38n_f/3$. The values for $\tilde{\Lambda}^{(n_f)}_{\rm EXACT}$ are carefully chosen to obtain accurate matching at the scales m_c^2 and m_b^2 respectively. We used the values $\tilde{\Lambda}^{(3,4,5,6)}_{\rm EXACT} = 299.4,\ 246,\ 167.7,\ 67.8$ MeV/c^2 respectively in the exact formula (which yields $\alpha_s^{\rm EXACT}(m_Z^2) = 0.114$, $\alpha_s^{\rm EXACT}(m_b^2) = 0.205$, $\alpha_s^{\rm EXACT}(m_c^2) = 0.319$, $\alpha_s^{\rm EXACT}(\mu^2_{\rm NLO}) = 0.578$) and $\Lambda^{(3,4,5,6)}_{\rm LO} = 204,\ 175,\ 132, 66.5$ MeV/c^2 respectively (which yields $\alpha_s^{\rm LO}(m_Z^2) = 0.125$, $\alpha_s^{\rm LO}(m_b^2) = 0.232$, $\alpha_s^{\rm LO}(m_c^2) = 0.362$, $\alpha_s^{\rm LO}(\mu^2_{\rm LO}) = 0.763$) for the LO formula. Note that we have not used the two-loop matching of the running coupling constant $\alpha_s(\mu^2)$ at the same scales from [19],[20] to focus on the matching conditions on the flavor densities. Numerically the discontinuity in the running coupling constant across the charm threshold is aproximately two parts in one thousand, which is far too small to affect our results.

Three flavor evolution proceeds from the initial μ_0^2 to the scale $\mu^2 = m_c^2 = 1.96$ (GeV/c^2)^2. At this point the charm density is then defined by

$$\begin{aligned} f_{c+\bar{c}}(n_f+1, m_c^2) &= a_s^2(n_f, m_c^2)\Big[\tilde{A}^{\rm PS}_{Qq}(1) \otimes f_q^{\rm S}(n_f, m_c^2) \\ &\quad + \tilde{A}^{\rm S}_{Qg}(1) \otimes f_g^{\rm S}(n_f, m_c^2)\Big], \end{aligned} \tag{3.2.8}$$

with $n_f = 3$ and $a_s = \alpha_s/4\pi$. We have suppressed the x dependence to make the notation more compact. The $\otimes$ symbol denotes the convolution integral $f \otimes g = \int f(x/y)g(y)dy/y$, where $x \le y \le 1$ The OME's $\tilde{A}^{\rm PS}_{Qq}(\mu^2/m_c^2)$, $\tilde{A}^{\rm S}_{Qg}(\mu^2/m_c^2)$ are given in [15]. The reason for choosing the matching scale μ at the mass of the charm quark m_c is that all the $\ln(\mu^2/m_c^2)$ terms in the OME's vanish at this point leaving only the nonlogarithmic pieces in the order α_s^2 OME's to contribute to the right-hand-side of Eq.(2.8). Hence the LO and NLO charm densities vanish at the scale $\mu = m_c$. The NNLO charm density starts off with a finite x-dependent shape in order a_s^2. Note that we then order the terms on the right-hand-side of Eq.(2.8) so that the result contains a product of NLO OME's and LO parton densities. The result is then of order a_s^2 and should be multiplied by order a_s^0 coefficient functions when forming the deep inelastic structure functions.

The four-flavor gluon density is also generated at the matching point in the same way. At $\mu = m_c$ we define

$$\begin{aligned} f_g^{\rm S}(n_f+1, m_c^2) &= f_g^{\rm S}(n_f, m_c^2) \\ &\quad + a_s^2(n_f, m_c^2)\Big[A^{\rm S}_{gq,Q}(1) \otimes f_q^{\rm S}(n_f, m_c^2), \\ &\quad + A^{\rm S}_{gg,Q}(1) \otimes f_g^{\rm S}(n_f, m_c^2)\Big]. \end{aligned} \tag{3.2.9}$$

The OME's $A^{\rm S}_{gq,Q}(\mu^2/m_c^2)$, $A^{\rm S}_{gg,Q}(\mu^2/m_c^2)$ are given in [15]. The four-flavor light quark (u,d,s) densities are generated using

$$\begin{aligned} f_{k+\bar{k}}(n_f+1,m_c^2) &= f_{k+\bar{k}}(n_f,m_c^2) \\ &\quad + a_s^2(n_f,m_c^2) A^{\rm NS}_{qq,Q}(1) \otimes f_{k+\bar{k}}(n_f,m_c^2). \end{aligned} \tag{3.2.10}$$

The OME $A^{\rm NS}_{qq,Q}(\mu^2/m_c^2)$ is given in [15] and the *total* four-flavor singlet quark density in Eq.(2.2) follows from the sum of Eqs.(2.8) and (2.10). The nonsinglet density then follows from Eq.(2.1). In Eqs.(2.9) and (2.10) $n_f = 3$. The remarks after Eq.(2.8) are relevant here too.

Next the resulting four-flavor densities are evolved using the four-flavor weights in either LO or NLO up to the scale $\mu^2 = 20.25$ $(\mathrm{GeV/c^2})^2$. The bottom quark density is then generated at this point using

$$\begin{aligned} f_{b+\bar{b}}(n_f+1,m_b^2) &= a_s^2(n_f,m_b^2)\Big[\tilde{A}^{\rm PS}_{Qq}(1) \otimes f_q^{\rm S}(n_f,m_b^2) \\ &\quad + \tilde{A}^{(\rm S)}_{Qg}(1) \otimes f_g^{\rm S}(n_f,m_b^2)\Big], \end{aligned} \tag{3.2.11}$$

and the gluon and light quark densities (which now include charm) are generated using Eqs.(5.2.8)-(5.2.10) with $n_f = 4$ and replacing m_c^2 by m_b^2. Therefore only the nonlogarithmic terms in the order a_s^2 OME's contribute to the matching conditions on the bottom quark density. Then all the densities are evolved up to higher μ^2 as a five-flavor set with either LO or NLO splitting functions. This is valid until $\mu = m_t \approx 175$ $\mathrm{GeV/c^2}$ above which one should switch to a six-flavor set. We do not implement this step because the top quark density would be extremely small.

The procedure outlined above generates a full set of parton densities (gluon, singlet, non-singlet light and heavy quark densities,) for any x and μ^2 from the three-flavor LO and NLO inputs in Eqs.(5.2.4) and (5.2.5). Note that one could also use the formulae above in fixed order perturbation theory. In this case the four-flavour densities are defined by extending the integrals on the right-hand sides of Eqs.(2.8)-(2.11) to

$$\begin{aligned} f_{c+\bar{c}}(n_f+1,\mu^2) &= a_s(n_f,\mu^2)\tilde{A}^{\rm S}_{Qg}\Big(\frac{\mu^2}{m_c^2}\Big) \otimes f_g^{\rm S}(n_f,\mu^2) \\ &\quad + a_s^2(n_f,\mu^2)\Big[\tilde{A}^{\rm PS}_{Qq}\Big(\frac{\mu^2}{m_c^2}\Big) \otimes f_q^{\rm S}(n_f,\mu^2) \\ &\quad + \tilde{A}^{\rm S}_{Qg}\Big(\frac{\mu^2}{m_c^2}\Big) \otimes f_g^{\rm S}(n_f,\mu^2)\Big], \end{aligned} \tag{3.2.12}$$

$$
\begin{aligned}
f_g^{\rm S}(n_f+1,\mu^2) &= f_g^{\rm S}(n_f,\mu^2) \\
&+a_s(n_f,\mu^2)A_{gg,Q}^{\rm S}(\frac{\mu^2}{m_c^2})\otimes f_g^{\rm S}(n_f,\mu^2) \\
&+a_s^2(n_f,\mu^2)\Big[A_{gq,Q}^{\rm S}(\frac{\mu^2}{m_c^2})\otimes f_q^{\rm S}(n_f,\mu^2)\,, \\
&+A_{gg,Q}^{\rm S}(\frac{\mu^2}{m_c^2})\otimes f_g^{\rm S}(n_f,\mu^2)\Big]\,, \qquad (3.2.13)
\end{aligned}
$$

and

$$
\begin{aligned}
f_{k+\bar{k}}(n_f+1,\mu^2) &= f_{k+\bar{k}}(n_f,\mu^2) \\
&+a_s^2(n_f,\mu^2)A_{qq,Q}^{\rm NS}\Big(\frac{\mu^2}{m_c^2}\Big)\otimes f_{k+\bar{k}}(n_f,\mu^2)\,, \\
& \qquad (3.2.14)
\end{aligned}
$$

for $n_f = 3$ and $m_c^2 \leq \mu^2 < m_b^2$. Then the five-flavor densities are defined by

$$
\begin{aligned}
f_{b+\bar{b}}(n_f+1,\mu^2) &= a_s(n_f,\mu^2)\tilde{A}_{Qg}^{\rm S}\Big(\frac{\mu^2}{m_b^2}\Big)\otimes f_g^{\rm S}(n_f,\mu^2) \\
&+a_s^2(n_f,\mu^2)\Big[\tilde{A}_{Qq}^{\rm PS}\Big(\frac{\mu^2}{m_b^2}\Big)\otimes f_q^{\rm S}(n_f,\mu^2) \\
&+\tilde{A}_{Qg}^{\rm S)}\Big(\frac{\mu^2}{m_b^2}\Big)\otimes f_g^{\rm S}(n_f,\mu^2)\Big]\,, \qquad (3.2.15)
\end{aligned}
$$

for $n_f = 4$ and $\mu^2 \geq m_b^2$. Also one should replace $n_f = 4$ and m_c^2 by m_b^2 in Eqs.(2.12)-(2.14). In this case no four-flavor or five-flavour evolution is made so the logarithmic terms in μ^2/m_c^2 and/or μ^2/m_b^2 are not summed. We will show the differences between this fixed order perturbation theory (FOPT) treatment and the evolved treatment in the next Section.

3.3 Results

Here we present results from the evolution of the parton densities. The inputs are the three-flavor densities at μ_0 in Eqs.(2.4),(2.5) which are evolved up to the scale $\mu = m_c = 1.4$ GeV/c^2. During this evolution the number of light flavors $n_f = 3$ in both the $\overline{\rm MS}$ splitting functions and the running coupling constant.

We start by giving the four-flavor densities, where $n_f = 4$, in the region between $m_c \leq \mu < m_b$ which follow by evolution from the matching conditions in Eqs. (2.8)-(2.10). We present results at the scales $\mu^2 = 1.96$, 2, 3, 4, 5, 10 and 20 in units of (GeV/c^2)^2. First we show the charm density $xc^{\rm NNLO}(4, x, \mu^2)$ in two ranges (a) $10^{-5} < x < 1$ and (b) $10^{-2} < x < 1$ in Figs. 3.1(a) and 3.1(b) respectively. We notice that this density starts off negative at small x but it is positive at large x so that the momentum sum rule is satisfied. To show the effect of resumming the logarithmic terms via the evolution equation from the charm threshold as compared with just computing the integrals in Eq. (2.12) at all scales μ we show in Fig. 3.1(c) the ratios $R_c^{\rm NNLO}(x, \mu^2) = xc_{\rm EVOLVED}(4, x, \mu^2)/xc_{\rm FOPT}(4, x, \mu^2)$. Here FOPT stands for fixed order perturbation theory. The effects of the evolution are especially significant at small x and large x. Notice that the discontinuity at $x \approx 0.01$ is caused by the change in sign of the NNLO charm quark density. For a comparison we have also shown the NLO results from the MRST98 set 1 [3] and CTEQ5HQ [1] parton density sets in Figs. 3.1(d) and (e). These groups use different input densities so a direct comparison does not have any true significance. Nevertheless our density is larger than the MRST98 set 1 result and smaller than the CTEQ5HQ result at small x and large μ^2.

In Fig. 3.2(a) we show the four-flavor gluon density $xg^{\rm NNLO}(4, x, \mu^2)$ in the same range $10^{-5} < x < 1$ for the same scales as in Fig. 3.1. We also show in Fig. 3.2(b) the ratios $R_g^{\rm NNLO}(x, \mu^2) = xg_{\rm EVOLVED}(4, x, \mu^2)/xg_{\rm FOPT}(4, x, \mu^2)$ for the same scales, where we use Eq.(2.13) for the FOPT density. The effect of the suppression of the charm density at small x translates into an increase of the gluon density at small x. For comparison we show the three-flavor NLO gluon density in Fig. 3.2(c). We have also shown the NLO results from the MRST98 set 1 and CTEQ5HQ parton density sets in Figs. 3.2(d) and (e). These densities do not increase as rapidly at large μ^2 because they use different inputs.

In Fig. 3.3(a) we show the singlet quark density $x\Sigma^{\rm NNLO}(4, x, \mu^2)$ in the range $10^{-5} < x < 1$ for the same scales as above. Then is Fig. 3.3(b) we show the ratios $R_\Sigma^{\rm NNLO}(x, \mu^2) = x\Sigma_{\rm EVOLVED}(4, x, \mu^2)\ /x\Sigma_{\rm FOPT}(4, x, \mu^2)$, where we use Eq.(2.14) for the FOPT density. This ratio shows increases or decreases

depending on the x and μ^2 values. It is appreciably smaller at large μ^2, which reflects the differences between the three-flavor and four-flavor gluon densities. For comparison we show the three-flavor NLO density in Fig. 3.3(c).

Next in Fig. 3.4(a) we show the nonsinglet density $x\sigma^{\rm NNLO}(4,x,\mu^2)$, where $\sigma=(u+\bar{u})/2$, in the range $10^{-5}<x<1$ for the same scales. In Fig. 3.4(b) we show the ratios $R_\sigma^{\rm NNLO}(x,\mu^2)=x\sigma_{\rm EVOLVED}(4,x,\mu^2)/x\sigma_{\rm FOPT}(4,x,\mu^2)$ for the same scales, where we use Eq.(2.14) for the FOPT density. The ratio is significantly below unity at large x. In Fig. 3.4(c) we show the three-flavor NLO result. The difference is small.

We complete our presentation of four-flavor densities by showing in Fig. 3.5(a) the strange quark density $xs^{\rm NNLO}(4,x,\mu^2)$ in the range $10^{-5}<x<1$. In Fig. 3.5(b) we show the ratios $R_g^{\rm NNLO}(x,\mu^2)=xs^{\rm EVOLVED}(4,x,\mu^2)/xs^{\rm FOPT}(4,x,\mu^2)$ for the same scales. In Fig. 3.5(c) we show the three-flavor NLO density, where again the difference is small. We have checked that these densities satisfy the momentum sum rule for four flavors.

Now we move up in scale to consider $\mu>m_b=4.5$ GeV/c^2 which is the five-flavor region. The parton densities in this region are now generated from the previous four-flavor set by using the conditions in the Eqs.(2.8) -(2.10) with $n_f=4$ at $\mu^2=m_b^2$ and replacing m_c^2 by m_b^2. Here we show plots for the scales μ^2 =20.25, 25, 30, 40, and 100 in units of (GeV/c^2)^2.

The first density to consider is the bottom quark density. We show in Fig. 3.6(a) $xb^{\rm NNLO}(5,x,\mu^2)$ in the range $10^{-5}<x<1$ for the scales mentioned above. Notice that it is negative for small x and small μ^2, The region $10^{-2}<x<1$ is shown in Fig. 3.6(b) to demonstrate that the density is positive for large x. In this respect it is like the charm density in the region just above the four-flavor matching point. In Fig. 3.6(c) we show the ratios $R_g^{\rm NNLO}(x,\mu^2)=xb^{\rm EVOLVED}(5,x,\mu^2)/xb^{\rm FOPT}(5,x,\mu^2)$, where Eq.(2.15) is used for the FOPT density. Here it is clear that the effect of the evolution is appreciable at small x. For a comparison we have also shown the NLO results from the MRST98 set 1 and CTEQ5HQ parton density sets in Figs. 3.1(d) and (e). Note that these groups use different input densities so a direct comparison does not have any true significance. Nevertheless both bottom densities are larger than ours at small x and large μ^2.

The five-flavor charm density $xc^{\rm NNLO}(5,x,\mu^2)$ is shown in Fig. 3.7(a) in the range $10^{-5}<x<1$ for the same scales. In this case the ratios of the evolved densities to the FOPT densities is very close to unity for all x and μ^2 values so we do not show a plot. For a comparison we have also shown the NLO results from the MRST98 set 1 and CTEQ5HQ parton density sets in Figs. 3.1(b) and (c). The former has a smaller density at large μ^2 and the latter a larger density.

Next we show in Fig. 3.8(a) the gluon density $xg^{\rm NNLO}(5,x,\mu^2)$ in the range $10^{-5} < x < 1$ for the same scales. In this case the ratios of the evolved densities to the FOPT densities is very close to unity for all x and μ^2 values so we do not show a plot. In Fig. 3.8(b) we show the corresponding three-flavor NLO density. The latter is larger at small x and large μ^2.

In Fig. 3.9(a) we show the nonsinglet quark density $x\Sigma^{\rm NNLO}(5,x,\mu^2)$, where $\sigma = (u+\bar{u})/2$, in the range $10^{-5} < x < 1$ for the same scales. Also in this case the ratios of the evolved densities to the FOPT densities is very close to unity for all x and μ^2 values so we do not show any plot. In Fig. 3.9(b) we show the corresponding three-flavor NLO density.

In Fig. 3.10(a) we show the nonsinglet quark density $x\sigma^{\rm NNLO}(5,x,\mu^2)$ in the range $10^{-5} < x < 1$ for the same scales. Also in this case the ratios of the evolved densities to the FOPT densities is very close to unity for all x and μ^2 values so we do not show any plot. In Fig. 3.10(b) we show the corresponding three-flavor NLO density.

In Fig. 3.11(a) we show the strange quark density $xs^{\rm NNLO}(5,x,\mu^2)$ in the range $10^{-5} < x < 1$ for the same scales. Also in this case the ratios of the evolved densities to the FOPT densities is very close to unity for all x and μ^2 values so we do not show any plot. In Fig. 3.11(b) we show the corresponding three-flavor NLO density. We have checked that the five-flavour densities satisfy the momentum sum rule.

The above plots demonstrate that the NNLO matching conditions do influence the parton densities appreciably in regions just above $\mu = m_c$ and $\mu = m_b$. This has consequences for the analysis of HERA experiments because a lot of the data is at small x and small values of the scale Q^2. In fact all of the data for $x < 10^{-4}$ has $Q^2 < 100$ $(\mathrm{GeV/c^2})^2$. Even for the scale μ much larger than m_b the boundary conditions are still important. For $\mu \geq 10$ $\mathrm{GeV/c^2}$ for example the rapid rise of the five-flavour gluon density means that it dominates over all the other parton densities at small x. There is roughly a ten percent difference between the three-flavor and five-flavor densities at small x and large μ^2, which can be important for precision phenomenology.

ACKNOWLEDGMENTS

This research was partially supported by the National Science Foundation grant PHY-9722101. We thank M. Botje, E. Laenen and W.L. van Neerven for very useful discussions.

3.4 Appendix A

All the splitting functions in the Altarelli-Parisi (AP) equations can be expanded as a perturbation series in α_s into LO and NLO terms as follows

$$P = P^{(0)} + \frac{\alpha_s}{2\pi} P^{(1)}. \tag{3.1.1}$$

The non-singlet combinations of the $q_r(\bar{q}_r)$ to $q_s(\bar{q}_s)$ splitting functions, where the subscripts r, s denote the flavors of the (anti)quarks and satisfies $r, s = 1, \cdots, n_f$, can be further decomposed into a flavor diagonal part proportional to δ_{rs} and a flavor independent part. In LO there is only one non-singlet splitting function P_{qq} but in NLO it is convenient to form two combinations from P_{qq} and $P_{q\bar{q}}$ as follows

$$\begin{aligned} P_+ &= P_{qq} + P_{q\bar{q}} \\ P_- &= P_{qq} - P_{q\bar{q}}. \end{aligned} \tag{3.1.2}$$

These splitting functions are used to evolve two independent types of non-singlet densities, which will be called plus and minus respectively. They are given by

$$\begin{aligned} f_i^+ &= f_q^{\rm NS}(n_f, x, \mu^2) \\ f_j^- &= f_{k-\bar{k}}(n_f, x, \mu^2). \end{aligned} \tag{3.1.3}$$

The easiest way to explain the indices in these equations is by explicitly giving the combinations we use. For $j = 1, 2$

$$f_1^- = u - \bar{u}\,,\; f_2^- = d - \bar{d}\,, \tag{3.1.4}$$

which are used for all flavour density sets. Then for three-flavor densities $i = 1, 2, 3$ and we define

$$\begin{aligned} f_1^+ &= u + \bar{u} - \Sigma(3)/3\,, \qquad f_2^+ = d + \bar{d} - \Sigma(3)/3\,, \\ f_3^+ &= s + \bar{s} - \Sigma(3)/3\,, \end{aligned} \tag{3.1.5}$$

where $\Sigma(3) = f_q^S(3) = u + \bar{u} + d + \bar{d} + s + \bar{s}$. These densities should be used for $\mu < m_c$. For four-flavor densities $i = 1, 2, 3, 4$ and we define

$$\begin{aligned} f_1^+ &= u + \bar{u} - \Sigma(4)/4\,, \qquad f_2^+ = d + \bar{d} - \Sigma(4)/4\,, \\ f_3^+ &= s + \bar{s} - \Sigma(4)/4\,, \qquad f_4^+ = c + \bar{c} - \Sigma(4)/4\,, \end{aligned} \tag{3.1.6}$$

where $\Sigma(4) = f_q^S(4) = c + \bar{c} + \Sigma(3)$. These should be used for $m_c \leq \mu < m_b$. For five-flavor densites $i = 1, 2, 3, 4, 5$ and we define

$$\begin{aligned} f_1^+ &= u + \bar{u} - \Sigma(5)/5\,, \qquad & f_2^+ &= d + \bar{d} - \Sigma(5)/5\,, \\ f_3^+ &= s + \bar{s} - \Sigma(5)/5\,, \qquad & f_4^+ &= c + \bar{c} - \Sigma(5)/5\,, \\ f_5^+ &= b + \bar{b} - \Sigma(5)/5\,, \end{aligned} \tag{3.1.7}$$

where $\Sigma(5) = f_S^q(5) = b + \bar{b} + \Sigma(4)$. These should be used for $\mu \geq m_b$.

If we define $t = \ln(\mu^2/(1(\mathrm{GeV/c}^2)^2)$ then the AP equations that we need to solve are

$$\frac{\partial f_i^+(x,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi} \int_x^1 \frac{dz}{z} P_+(\frac{x}{z}) f_i^+(z,t)\,, \tag{3.1.8}$$

$$\frac{\partial f_j^-(x,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi} \int_x^1 \frac{dz}{z} P_-(\frac{x}{z}) f_j^-(z,t)\,, \tag{3.1.9}$$

$$\frac{\partial f_g(x,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi} \int_x^1 \frac{dz}{z} \left[P_{gq}(\frac{x}{z}) f_q^S(z,t) + P_{gg}(\frac{x}{z}) f_g^S(z,t) \right], \tag{3.1.10}$$

$$\frac{\partial f_q^S(x,t)}{\partial t} = \frac{\alpha_s(t)}{2\pi} \int_x^1 \frac{dz}{z} \left[P_{qq}(\frac{x}{z}) f_q^S(z,t) + P_{qg}(\frac{x}{z}) f_g^S(z,t) \right], \tag{3.1.11}$$

where for $\mu < m_c$ we set $i = 1, 2, 3$, $j = 1, 2$, $f_q^S = \Sigma(3)$ and the gluon is a three-flavor gluon. When $m_c \leq \mu < m_b$, we use $i = 1, 2, 3, 4$, $j = 1, 2$, $f_q^S = \Sigma(4)$ and the gluon is a four-flavor gluon. Finally when $\mu \geq m_b$, we set $i = 1, 2, 3, 4, 5$, $j = 1, 2$, $f_q^5 = \Sigma(5)$ and the gluon is a five-flavor gluon.

The densities should satisfy the momentum conservation sum rule

$$\begin{aligned} \int_0^1 x \Big[& u(x,\mu^2) + d(x,\mu^2) + \bar{u}(x,\mu^2) + \bar{d}(x,\mu^2) + 2s(x,\mu^2) \\ & + 2c(x,\mu^2)\theta(\mu^2 - m_c^2) + 2b(x,\mu^2)\theta(\mu^2 - m_b^2) + g(x,\mu^2) \Big]\, dx = 1\,. \end{aligned} \tag{3.1.12}$$

As the quark constituents carry all the charge, isospin, strange, charm and bottom quantum numbers of the nucleon they should also satisfy the other standard sum rules for the conservation of these quantities.

There are several methods to solve these equations. Among them the most popular are to use Mellin moments (used by [23], [24], see full list of references in [18] and [17]) and to use the direct x-space solution (as in [21],

[17],[24], see also [18]). Also the authors in [22] describe a method involving Laguerre polynomials, that dates back to early paper of [5].

Our choice of direct x-space method is justified by the necessity to step densities across matching points using LO, NLO and NNLO boundary conditions. The procedure of doing this in the Mellin moment method would involve converting densities to and from Mellin moments several times. Using the direct x-space method is much more intuitive and straightforward. The main features of this method are linear interpolation over a grid in x and second-order interpolation over a grid in t. Let us describe the method in more detail to point out where we differ from the work in [17].

First we consider the x-variable in the evolution. Consider the right-hand-side of the evolution equation (3.1.8) for non-singlet density

$$I(x_0) = \int \frac{dz}{z} \frac{x_0}{z} P\left(\frac{x_0}{z}\right) q\left(z\right) , \tag{3.1.13}$$

where $x_0 \leq z \leq 1$ and

$$q(x) = xf(x) , \tag{3.1.14}$$

and

$$x_0 < x_1 < ... < x_n < x_{n+1} \equiv 1 , \tag{3.1.15}$$

with $q(x_{n+1}) = q(1) \equiv 0$. Between grid points x_i and x_{i+1}, x is chosen so that

$$q(x) = (1-y)q(x_i) + yq(x_{i+1}) , \tag{3.1.16}$$

with $y = (x - x_i)/(x_{i+1} - x_i)$. Using this relation we convert the integral into a sum

$$I(x_0) = \sum_{i=0}^{n+1} w(x_i, x_0) q(x_i) , \tag{3.1.17}$$

where the weights are

$$\begin{aligned} w(x_0, x_0) &= S_1(s_1, s_0) \\ w(x_i, x_0) &= S_1(s_{i+1}, s_i) - S_2(s_i, s_{i-1}) , \end{aligned} \tag{3.1.18}$$

where $s_i = x_0/x_i$ and

$$\begin{aligned} S_1(u, v) &= \frac{v}{v-u} \int_u^v (z-u) P(z) \frac{dz}{z} \\ S_2(u, v) &= \frac{u}{v-u} \int_u^v (z-v) P(z) \frac{dz}{z} . \end{aligned} \tag{3.1.19}$$

We have calculated these integrals analytically and the results are in the computer program. This leads to the final formula describing the grid for the x

variable. Note that the weights $w^{(0)}$ and $w^{(1)}$ include LO and NLO splitting functions respectively. Thus, for the singlet case, we have

$$\begin{aligned}\frac{d(x_0\Sigma(x_0))}{dt} &= \frac{\alpha_s}{2\pi}\sum\left[w_{qq}^{(0)}(x_i,x_0)+\frac{\alpha_s}{2\pi}w_{qq}^{(1)}(x_i,x_0)\right]x_i\Sigma(x_i)\\ &\quad+\left[w_{qg}^{(0)}(x_i,x_0)+\frac{\alpha_s}{2\pi}w_{qg}^{(1)}(x_i,x_0)\right]x_i g(x_i)\,. \qquad (3.1.20)\end{aligned}$$

Now consider the variation in the variable t. For each x_i we pick a grid in t labelled by distinct points t_j. Then the example the non-singlet equation becomes

$$q^{'}(x_i,t_j)=\frac{\alpha_s(t_j)}{2\pi}\sum_{k=1}^{n}\left[w_{\pm}^{(0)}(x_k,x_i)+\frac{\alpha_s(t_j)}{2\pi}w_{\pm}^{(1)}(x_k,x_i)\right]q(x_k,t_j)\,, \qquad (3.1.21)$$

where $q^{'}(x_i,t_j)$ denotes the derivative with respect to t evaluated at $t=t_j$. In compact notation this equation can be rewritten as

$$q_j^{'}=wq_j+S\,, \qquad (3.1.22)$$

with S being the sum of the terms on the right hand side of (3.1.21) excluding the j-th term.

For t between the grid points t_{j-1} and t_j we interpolate the parton density using quadratic interpolation as follows

$$q(x_i,t)=at^2+bt+c\,. \qquad (3.1.23)$$

Thus we relate the value of q at the point t_j to that of q at the point t_{j-1} by

$$q(x_i,t_j)=q(x_i,t_{j-1})+\frac{1}{2}[q^{'}(x_i,t_j)+q^{'}(x_i,t_{j-1})]\Delta t_j\,, \qquad (3.1.24)$$

where $\Delta t_j=t_j-t_{j-1}$. This equation can also be written more compactly as

$$q_j=q_{j-1}+\frac{1}{2}(q_{j-1}^{'}+q_j^{'})\Delta t_j\,. \qquad (3.1.25)$$

The resulting system of two linear equations (3.1.25) and (3.1.22) for q_j and $q_j^{'}$ has the solution

$$q_j=\frac{2q_{j-1}+(q_{j-1}^{'}+S)\Delta t_j}{2-w\Delta t_j}\,, \qquad (3.1.26)$$

and yields $q_j^{'}$ from (3.1.22). Applying the same procedure to the gluon and singlet equations Eqs.(A.10)-(A.11) involves four equations because we have to compute both the densities and their derivatives.

The evolution proceeds from the initial $\mu_0^2 = \mu_{\rm LO}^2$ (or $\mu_0^2 = \mu_{\rm NLO}^2$) to the first matching point at the scale $\mu^2 = m_c^2$. Next the charm density is introduced in the NNLO (α_s^2-order terms) and all the four-flavor densities are evolved from the boundary conditions in Ens.(5.2.8)-(5.2.10). This evolution continues up to the transition point $\mu^2 = m_b^2$, where the same procedure is applied to generate the bottom quark density. At that matching point all five-flavor densities are evolved starting from the boundary conditions in Eqs.(5.2.8)-(5.2.11) up to all higher μ^2 scales.

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Chapter 4

Comparison between variable flavor number schemes for charm quark electroproduction

4.1 Introduction

Charm quark production is one of the important reactions used to extract the gluon density $f_g(x,\mu^2)$ of the proton in deep inelastic lepton-hadron scattering, especially when the Bjorken scaling variable x is small. However this is only true when the deep inelastic process is of the neutral current type and the charm component of the proton wave function is negligible. In this case the charm quark is produced in the so-called extrinsic way. For neutral current processes with only light partons in the initial state this means that the Born approximation in perturbative QCD is given by the virtual vector-boson gluon-fusion process [1]. Notice that the light partons consist of the gluon and the three light flavors u, d, s together with their anti-particles. Furthermore if the virtuality of the exchanged vector boson in deep inelastic lepton-hadron scattering satisfies $Q^2 \ll M_Z^2$ then the vector boson is represented by the photon only and the contribution of the Z-boson is negligible. Extrinsic charm production also receives next-to-leading order (NLO) contributions from boson-quark subprocesses, which could hamper the extraction of the gluon density. Fortunately this is not the case at HERA, where the experiments [2], [3] are carried out at small x, because the gluon density overwhelms the light flavor densities completely. Moreover the NLO quark initiated processes are suppressed by at least one power of the strong coupling constant $\alpha_s(\mu^2)$ with respect to the Born contribution to the boson-gluon fusion reaction. The quantity μ in the running coupling constant and the parton densities represents both the renormalization and factorization scales respectively, because it is convenient to chose them to be equal.

In the literature one has adopted two different treatments of extrinsic charm production, which are known as the massive and massless charm descriptions. The former, advocated in [4], treats the charm quark as a heavy quark (with mass m_c) and the cross sections or coefficient functions have to be described by fixed order perturbation theory. Notice that due to the work in [5] the perturbation series is now known up to second order and the NLO massive charm approach agrees with the recent data in [2] and [3]. The latter treatment, which has been rather popular among groups which fitted parton densities to experimental data, treats the charm quark as a massless quark so that it can be represented by a parton density $f_c(x,\mu^2)$, with the boundary condition $f_c(x,\mu^2) = 0$ for $\mu \leq m_c$. Although at first sight these approaches are completely different they are actually intimately related. It was shown in [6] that the large logarithms of the type $\ln(Q^2/m_c^2)$, which appear in the perturbation series when $Q^2 \gg m_c^2$, can be resummed in all orders. The upshot of this procedure is that the charm components of the deep inelastic struc-

ture functions $F_{i,c}(x,Q^2,m_c^2)$, where $i = 2, L$, which in the first approach are written as convolutions of heavy quark coefficient functions with light parton densities, become, after resummation, convolutions of light parton coefficient functions with light parton densities which also include a charm quark density. This procedure leads to the so-called zero mass variable flavor number scheme (ZM-VFNS) for $F_{i,c}(x,Q^2)$ where the mass of the charm quark is absorbed into the new four flavor densities. To implement this scheme one has to be careful to use quantities which are collinearly finite in the limit $m_c \to 0$. From the above considerations it is clear that the first approach is better when the charm quark pair is produced near threshold because the mass of the quark is important in this region and it cannot be neglected. On the other hand far away from threshold, where also $Q^2 \gg m_c^2$, the large logarithms above dominate the structure functions so that the second approach should be more appropriate. Both approaches are characterized by the number of active flavors involved in the description of the parton densities which are given by three and four respectively. Therefore one can also speak of three and four flavor number schemes (TFNS and FFNS respectively). Each scheme has a different gluon density so that the momentum sum rule is always satisfied.

As most of the experimental data occur in the kinematical regime which is between the threshold and the region of large Q^2 a third approach has been introduced to describe the charm components of the structure functions. This is called the variable flavor number scheme (VFNS). A first discussion was given by Aivasis, Collins, Olness and Tung [7], where a VFNS prescription called ACOT was given in lowest order only. The ACOT results were compared with the NLO results in [8]. We will give our NLO version of a VFNS scheme in this paper and we call it the CSN scheme to distinguish it. A different approach, generalized to all orders, was given in the papers by Buza, Matiounine, Smith and van Neerven [6],[9], which we denote by BMSN. Finally another version of a VFNS for the charm component of the structure function was presented by Thorne and Roberts in [10], which will be called the TR scheme. Note that a proof of factorization to all orders for the total structure function, which includes charm and light parton production, was recently given in [11].

The difference between the various versions can be attributed to two ingredients entering the construction of a VFNS. The first one is the mass factorization procedure carried out before the large logarithms can be resummed. The second one is the matching condition imposed on the charm quark density, which has to vanish in the threshold region of the production process. It will be one of our goals to elucidate these differences in the next Section. Another problem, which was not clarified in the papers above is that the mass factorization cannot be carried out on the level of the charm components of the

structure functions alone, because one also needs contributions coming from the light parton components of the structure functions. The latter can be attributed to all heavy charm quark loop contributions to gluon self energies, which appear in the virtual corrections to the light parton coefficient functions. These corrections have to be combined with contributions from gluon splitting into heavy charm anti-charm quark pairs, which belong to the charm components (not the light quark components) of the structure functions. In this paper we will give a much more careful analysis than has been done previously in the literature. Another aspect of any VFNS approach is that one needs two sets of parton densities. One set only contains densities in a three flavor number scheme whereas the second one, which also includes a charm quark density, is parametrized in a four flavor number scheme. Both parameterizations have to satisfy the relations quoted in [6]. At this moment the latter set is not available in the literature and we would like to fill in this gap. Starting from a three flavor number set of parton densities recently published in [12] we will construct a four flavor number set of densities satisfying the relations in [6].

In Sec.II we give a general discussion of the CSN description for heavy quark electroproduction, and explain the problems with mass factorization, collinear singularities and threshold dependence in the heavy flavor components of the structure functions. We then specialize to charm quark electroproduction in Sec.III, working to second order in the running coupling constant $\alpha_s(\mu^2)$. We first present details about the charm quark density. Next numerical results are shown for the structure functions in the various schemes. Analytic results for the contributions from the Compton scattering reaction with an invariant mass cut are relegated to an Appendix. Finally we want to emphasize that we only consider inclusive charm quark production in this paper. Exclusive charm production which involves transverse momentum and rapidity distributions will be dealt with in another paper.

4.2 Discussion of variable flavor number schemes

In this section we discuss two different representations of the deep inelastic structure functions in variable flavor number schemes. One is proposed here (CSN). The other (BMSN) was proposed in [6] and [9]. The former starts from mass factorization of the exact heavy quark coefficient functions whereas the latter only applies this procedure to the asymptotic expressions for these functions. In both schemes the special role of the heavy quark loop contributions to the light quark coefficient functions in combination with heavy quark production via gluon splitting was overlooked. This will be repaired in this paper. Furthermore in both schemes there is a lot of freedom in the choice of matching conditions, which are needed to connect the structure functions presented for n_f and $n_f + 1$ light flavors. Different matching conditions lead to different threshold behaviors, which have consequences for the description of the structure functions at small Q^2 and large x.

Limiting ourselves to electroproduction, where deep inelastic lepton-hadron scattering is only mediated by a photon, the light parton components of the structure functions are defined by

$$\begin{aligned}
&F_i^{\rm LIGHT}(n_f, Q^2, m^2) = \\
&\sum_{k=1}^{n_f} e_k^2 \left[f_q^{\rm S}(n_f,\mu^2) \otimes \left(\tilde{\mathcal{C}}_{i,q}^{\rm PS}\left(n_f, \frac{Q^2}{\mu^2}\right) + \tilde{\mathcal{C}}_{i,q}^{\rm VIRT,PS}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right)\right)\right. \\
&+ f_g^{\rm S}(n_f,\mu^2) \otimes \left(\tilde{\mathcal{C}}_{i,g}^{\rm S}\left(n_f, \frac{Q^2}{\mu^2}\right) + \tilde{\mathcal{C}}_{i,g}^{\rm VIRT,S}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right)\right) \\
&\left. + f_{k+\bar{k}}(n_f,\mu^2) \otimes \left(\mathcal{C}_{i,q}^{\rm NS}\left(n_f, \frac{Q^2}{\mu^2}\right) + \mathcal{C}_{i,q}^{\rm VIRT,NS}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right)\right)\right] , \quad (4.2.1)
\end{aligned}$$

where $\otimes$ denotes the convolution symbol in the parton Bjorken scaling variable z. In this expression the $\mathcal{C}_{i,k}$ $(i = 2, L; k = q, g)$ denote the light parton coefficient functions and the e_k represent the charges of the light flavor quarks. The quantities $\mathcal{C}_{i,k}^{\rm VIRT}$ only contain the heavy quark loop contributions to the light parton coefficient functions. Furthermore $f_g^{\rm S}(n_f,\mu^2)$ stands for the gluon density while the singlet (S) and non-singlet (NS) light quark densities, with respect to the SU(n_f) flavor group, are defined by

$$f_{k+\bar{k}}(n_f,\mu^2) \equiv f_k(n_f,\mu^2) + f_{\bar{k}}(n_f,\mu^2)$$

$$f_q^{\rm S}(n_f,\mu^2) = \sum_{k=1}^{n_f} f_{k+\bar{k}}(n_f,\mu^2)$$

$$f_q^{\rm NS}(n_f,\mu^2) = f_{k+\bar{k}}(n_f,\mu^2) - \frac{1}{n_f} f_q^{\rm S}(n_f,\mu^2)\,. \qquad (4.2.2)$$

Finally we have set the factorization scale equal to the renormalization scale μ. The light parton coefficient functions have been calculated up to order α_s^2 in [13]. The contributions to $\mathcal{C}_{i,k}^{\rm VIRT}$ appear for the first time in second order perturbation theory and can be found in [14]. For our further discussion it will be convenient to distinguish between the numbers of external and internal flavors. The former refers to the number of light flavor densities whereas the latter denotes the number of light flavors in the quark loop contributions to the virtual corrections. They are not necessarily equal. Some of the coefficient functions have the external flavor number as an overall factor. To explicitly cancel this factor we have defined the quark and gluon coefficient functions in Eq. (5.2.1) as follows

$$\begin{aligned}
\mathcal{C}_{i,q}^{\rm S}(n_f,\frac{Q^2}{\mu^2}) &= \mathcal{C}_{i,q}^{\rm NS}(n_f,\frac{Q^2}{\mu^2}) + \mathcal{C}_{i,q}^{\rm PS}(n_f,\frac{Q^2}{\mu^2})\,, \\
\mathcal{C}_{i,q}^{\rm PS}(n_f,\frac{Q^2}{\mu^2}) &= n_f\,\tilde{\mathcal{C}}_{i,q}^{\rm PS}(n_f,\frac{Q^2}{\mu^2})\,,\ \mathcal{C}_{i,g}^{\rm S}(n_f,\frac{Q^2}{\mu^2}) = n_f\,\tilde{\mathcal{C}}_{i,g}^{\rm S}(n_f,\frac{Q^2}{\mu^2})\,, \qquad (4.2.3)
\end{aligned}$$

where PS represents the purely singlet component. Hence the remaining n_f in the argument of the coefficient functions marked with a tilde denotes the number of internal flavors. The same holds for the n_f in the parton densities. However the argument n_f in the structure functions is external and it refers to the number of parton densities appearing in their expressions. The parton densities satisfy the renormalization group equations. If we define

$$D \equiv \mu\frac{\partial}{\partial\mu} + \beta(n_f,g)\frac{\partial}{\partial g}\,, \qquad g \equiv g(n_f,\mu^2) \qquad (4.2.4)$$

then

$$\begin{aligned}
Df_q^{\rm NS}(n_f,\mu^2) &= -\gamma_{qq}^{\rm NS}(n_f,g) f_q^{\rm NS}(n_f,\mu^2) \\
Df_k^{\rm S}(n_f,\mu^2) &= -\gamma_{kl}^{\rm S}(n_f,g) f_l^{\rm S}(n_f,\mu^2) \qquad k,l = q,g \qquad (4.2.5)
\end{aligned}$$

where γ_{kl} represent the anomalous dimensions of the operators in the operator product expansion (OPE).

The heavy flavor components ($Q = \mathrm{c}, \mathrm{b}, \mathrm{t}, \bar{Q} = \bar{\mathrm{c}}, \bar{\mathrm{b}}, \bar{\mathrm{t}}$) of the structure functions F_2 and F_L arise from Feynman graphs with heavy flavors (Q and $\bar{Q}$ with mass m) in the final state and are given by

$$F_{i,Q}^{\mathrm{EXACT}}(n_f, Q^2, m^2) = \sum_{k=1}^{n_f} e_k^2 \left[f_q^{\mathrm{S}}(n_f, \mu^2) \otimes L_{i,q}^{\mathrm{PS}}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right) \right.$$

$$\left. + f_g^{\mathrm{S}}(n_f, \mu^2) \otimes L_{i,g}^{\mathrm{S}}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right) + f_{k+\bar{k}}(n_f, \mu^2) \otimes L_{i,q}^{\mathrm{NS}}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right) \right]$$

$$+ e_Q^2 \left[f_q^{\mathrm{S}}(n_f, \mu^2) \otimes H_{i,q}^{\mathrm{PS}}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right) + f_g^{\mathrm{S}}(n_f, \mu^2) \otimes H_{i,g}^{\mathrm{S}}\left(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\right) \right] , \tag{4.2.6}$$

where e_Q represents the charge of the heavy quark. Furthermore $L_{i,k}$ and $H_{i,k}$ ($i = 2, L; k = q, g$) represent the heavy-quark coefficient functions which are exactly calculated order by order in perturbation theory. In Figs. 4.1-4.5 we have shown some of the Feynman diagrams contributing to the coefficient functions up to order α_s^2. Like in the case of the light-parton coefficient functions $\mathcal{C}_{i,k}$ they can be split into (purely)-singlet and non-singlet parts. The distinction between $L_{i,k}$ and $H_{i,k}$ can be traced back to the different (virtual) photon-parton heavy-quark production mechanisms from which they originate. The functions $L_{i,k}$, $H_{i,k}$ are attributed to the reactions where the virtual photon couples to the light quarks and the heavy quark respectively. Hence $L_{i,k}$ and $H_{i,k}$ in Eq. (5.2.6) are multiplied by e_k^2 and e_Q^2 respectively. As has been mentioned in the introduction the heavy quark coefficient functions contain large logarithms of the type $\ln^i(Q^2/m^2)$ when $Q^2 \gg m^2$ which can be removed from the former by using mass factorization. To do this we first have to split the heavy quark coefficient functions $L_{i,k}$ into soft and hard parts

$$L_{i,k}(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) = L_{i,k}^{\mathrm{HARD}}(n_f, \Delta, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) + L_{i,k}^{\mathrm{SOFT}}(n_f, \Delta, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) , \tag{4.2.7}$$

where Δ is a cut on the invariant mass $s_{Q\bar{Q}}$ of the heavy quark pair. The cut can be determined by experiment. It is chosen such that in the limit $m \to 0$ all mass singularities reside in the soft parts so that the hard parts are collinearly finite. Taking Fig. 4.5 as an example we mean by hard that one detects a $Q\bar{Q}$-pair with a large invariant mass which is experimentally observable if $s_{Q\bar{Q}} > \Delta$. In the case $s_{Q\bar{Q}} < \Delta$ the $Q\bar{Q}$-pair is soft and becomes indistinguishable from other light parton final states which contain contributions from virtual heavy

quark loops. Next we add the soft parts to the other contributions to $F_i^{\rm LIGHT}$ in Eq. (5.2.1) and the mass factorization proceeds like

$$\tilde{\mathcal{C}}_{i,k}(n_f,\frac{Q^2}{\mu^2}) + \mathcal{C}_{i,k}^{\rm VIRT}(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}) + L_{i,k}^{\rm SOFT}(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}) =$$

$$A_{lk,Q}(n_f,\frac{\mu^2}{m^2}) \otimes \tilde{\mathcal{C}}_{i,l}(n_f,\frac{Q^2}{\mu^2})$$

$$+A_{lk}(n_f,\frac{\mu^2}{m^2}) \otimes \mathcal{C}_{i,l,Q}^{\rm CSN,SOFT}(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}), \quad k,l = q,g\,. \tag{4.2.8}$$

Here $\mathcal{C}_{i,l,Q}$ are those parts of the light parton coefficient functions $\mathcal{C}_{i,l}$ which contain the heavy quark loops. The hard parts of $L_{i,k}$ are left in $F_{i,Q}^{\rm EXACT}$ in Eq. (5.2.6) and do not need any mass factorization. Furthermore we have the condition that the dependence on the parameter Δ cancels in the sums so

$$\begin{aligned}\mathcal{C}_{i,k,Q}^{\rm CSN}\left(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\right) &= \mathcal{C}_{i,k,Q}^{\rm CSN,SOFT}\left(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\right) \\ &\quad +L_{i,k}^{\rm HARD}\left(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\right), \end{aligned}\tag{4.2.9}$$

where μ in the hard parts only represents the renormalization scale. The coefficient functions $H_{i,k}$ satisfy the relations [1]

$$H_{i,k}(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}) = A_{lk}(n_f,\frac{\mu^2}{m^2}) \otimes \mathcal{C}_{i,l}^{\rm CSN}(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}) \quad k,l = Q,q,g \tag{4.2.10}$$

Notice that mass factorization applied to the functions $H_{i,q}$ and $H_{i,g}$ occurring in $F_{i,Q}^{\rm EXACT}$ (5.2.6) leads to the coefficient functions $\mathcal{C}_{i,Q}^{\rm CSN}$. The latter also follow from mass factorization of the functions $H_{i,Q}$ which represent processes with a heavy quark in the initial state. The quantities $H_{i,Q}$, which do not appear in $F_{i,Q}^{\rm EXACT}$, together with the corresponding operator matrix elements (OME's) A_{QQ} are characteristic of variable flavor number schemes. The procedure above transfers the logarithms $\ln^i(\mu^2/m^2)$, appearing in $L_{i,k}^{\rm SOFT}$ and $H_{i,k}$, to the heavy quark operator matrix elements $A_{lk,Q}$ and A_{Qk}. The latter are defined by (see

[1] In order to help the reader, who is more familiar with the notation in [7], one can make the following comparison. For instance Eq. (7) in the latter reference $f_g^{Q(1)}$ is equal to our $A_{Qg}^{(1)}$. Similarly in Eq. (8) $\sum_\lambda \omega_{Bg}^{\lambda(1)} = H_{i,g}^{(1)}$ and $\sum_\lambda \omega_{BQ}^{\lambda(0)} = H_{i,Q}^{(0)}$.

[6] for details of renormalization and mass factorization)

$$A_{lk,Q} = \langle k \mid O_l(0) \mid k \rangle \qquad k,l = q,g\,,$$
$$A_{Qk} = \langle k \mid O_Q(0) \mid k \rangle \qquad k = Q,q,g\,. \tag{4.2.11}$$

Note that the O_l are the light quark and gluon operators and in $A_{lk,Q}$ we only retain contributions from subgraphs which contain heavy quark (Q) loops. The quantity O_Q represents the heavy quark operator. Here we want to stress that the operators are sandwiched between quark and gluon states. This will cause mass singularities of the type $\ln^i(\mu^2/m^2)$ to appear in a similar way as they appear in partonic cross sections.

The heavy quark coefficient functions defined in the CSN scheme in Eqs. (5.2.8)-(5.2.10) are collinearly finite and tend asymptotically to the massless parton coefficient functions presented in Eq. (5.2.1) i.e.

$$\lim_{Q^2\to\infty} \mathcal{C}_{i,k}^{\rm CSN}(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) = \mathcal{C}_{i,k}(n_f, \frac{Q^2}{\mu^2})\,, \qquad k = Q,q,g\,. \tag{4.2.12}$$

In particular we have

$$\mathcal{C}_{i,k}(n_f, \frac{Q^2}{\mu^2}) + \lim_{Q^2\gg m^2} \mathcal{C}_{i,k,Q}^{\rm CSN}(n_f, \frac{Q^2}{m^2}, \frac{\mu^2}{m^2}) = \mathcal{C}_{i,k}(n_f+1, \frac{Q^2}{\mu^2})\,, \tag{4.2.13}$$

so that the number of internal flavors is enhanced by one unit.

The CSN scheme above has similarities with the VFNS schemes proposed in [7], [10]. The decomposition of the $L_{i,k}$ into soft and hard parts has not been discussed previously. However one must address this issue because the mass singularities in $L_{i,k}$ and $\mathcal{C}_{i,k}^{\rm VIRT}$ separately have such high powers in $\ln(Q^2/m^2)$ that they cannot be removed via mass factorization. Another feature is that in the limit $m \to 0$ the final state invariant energies in the reactions which contribute to these two types of coefficient functions become equal. Hence $L_{i,k}$ and $\mathcal{C}_{i,k}^{\rm VIRT}$ have to be added so that the leading singularities cancel and the remaining ones are then removed by mass factorization according to Eq. (5.2.8). Notice that the the total coefficient functions $L_{i,k}$ cannot be moved to $F_i^{\rm LIGHT}$ because this would contradict the definitions of the latter structure functions where only light partons are observed in the final states. Therefore it is sufficient to transfer the $L_{i,k}^{\rm SOFT}$ to the $F_i^{\rm LIGHT}$ since they contain the same mass singularities as the $L_{i,k}$. If Δ is chosen small enough, the heavy quarks are unobservable in a measurement of $F_i^{\rm LIGHT}$. Note that the problem of the separation of $L_{i,k}$ into soft and hard parts is not needed for the total structure

function $F_i^{\rm LIGHT} + F_{i,Q}^{\rm EXACT}$. The all order mass factorization of the latter is shown in [11].

To illustrate the procedure above we carry it out up to order α_s^2. The coefficients in the series expansion are defined as follows

$$\begin{aligned} \mathcal{C}_{i,k} &= \sum_{n=0}^{\infty} a_s^n \mathcal{C}_{i,k}^{(n)} \quad , \quad H_{i,k} = \sum_{n=0}^{\infty} a_s^n H_{i,k}^{(n)} \quad , \quad L_{i,k} = \sum_{n=2}^{\infty} a_s^n L_{i,k}^{(n)} \, , \\ A_{kl} &= \sum_{n=0}^{\infty} a_s^n A_{kl}^{(n)} \quad , \quad \text{with} \quad a_s \equiv \frac{\alpha_s}{4\pi} \, . \end{aligned} \tag{4.2.14}$$

Up to second order the mass factorization relations become

$$\begin{aligned} &\mathcal{C}_{i,q}^{\rm VIRT,NS,(2)}(\frac{Q^2}{m^2}) + L_{i,q}^{\rm SOFT,NS,(2)}\Big(\Delta, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\Big) = A_{qq,Q}^{\rm NS,(2)}\Big(\frac{\mu^2}{m^2}\Big)\mathcal{C}_{i,q}^{\rm NS,(0)} \\ &-\beta_{0,Q} \ln\left(\frac{\mu^2}{m^2}\right) \mathcal{C}_{i,q}^{\rm NS,(1)}\Big(\frac{Q^2}{\mu^2}\Big) + \mathcal{C}_{i,q,Q}^{\rm CSN,SOFT,NS,(2)}\Big(\Delta, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\Big) \, , \end{aligned} \tag{4.2.15}$$

with

$$\mathcal{C}_{i,q}^{\rm VIRT,NS,(2)}(\frac{Q^2}{m^2}) = F^{(2)}(\frac{Q^2}{m^2})\, \mathcal{C}_{i,q}^{(0)} \, . \tag{4.2.16}$$

Here $F^{(2)}(Q^2/m^2)$ denotes the two-loop vertex correction in Fig. 4.6. This function satisfies the decoupling theorem which implies that it vanishes in the limit $m \to \infty$. The heavy quark coefficient functions $L_{i,k}^{\rm NS,(2)}$ have been calculated in [15] and, after their convolution with the partonic densities, yield contributions to the structure functions which behave asymptotically like $\ln^3(Q^2/m^2)$. These logarithms are canceled after adding $F^{(2)}(Q^2/m^2)$ in Ref. [14] to $L_{i,k}^{\rm NS,SOFT,(2)}$ which contains the same mass singularities as $L_{i,k}^{\rm NS,(2)}$ (see the remark below Eq. (5.2.7)). To obtain the hard and soft parts we divide the integral over $s_{Q\bar{Q}}$ in the graphs of Fig. 4.5 in two regions i.e. $s > s_{Q\bar{Q}} > \Delta$ and $\Delta > s_{Q\bar{Q}} > 4\, m^2$ which we denote by HARD and SOFT respectively. Here $s_{Q\bar{Q}}$ and s denote the CM energies squared of the $Q\bar{Q}$ system and the incoming photon-parton state respectively. The hard and soft parts are presented in the Appendix. Finally $\beta_{0,Q} = -2/3$ denotes the heavy quark contribution to the lowest order coefficient of the β-function in Eq. (2.4). We must change the running coupling constant when we change schemes.

The mass factorization of the heavy quark coefficient functions $H_{i,k}$ is simpler. Here we get

$$H_{i,q}^{\rm PS,(2)}\Big(\frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\Big) = A_{Qq}^{\rm PS,(2)}\Big(\frac{\mu^2}{m^2}\Big)\mathcal{C}_{i,Q}^{\rm CSN,NS,(0)}\Big(\frac{Q^2}{m^2}\Big) + \mathcal{C}_{i,q}^{\rm CSN,PS,(2)}\Big(\frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\Big) \, ,$$

(4.2.17)

$$H_{i,Q}^{\mathrm{NS},(1)}\Big(\frac{Q^2}{m^2}\Big) = A_{QQ}^{\mathrm{NS},(1)}\Big(\frac{\mu^2}{m^2}\Big)\mathcal{C}_{i,Q}^{\mathrm{CSN},\mathrm{NS},(0)}\Big(\frac{Q^2}{m^2}\Big) + \mathcal{C}_{i,Q}^{\mathrm{CSN},\mathrm{NS},(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\,,$$

(4.2.18)

$$H_{i,g}^{\mathrm{S},(1)}\Big(\frac{Q^2}{m^2}\Big) = A_{Qg}^{\mathrm{S},(1)}\Big(\frac{\mu^2}{m^2}\Big)\mathcal{C}_{i,Q}^{\mathrm{CSN},\mathrm{NS},(0)}\Big(\frac{Q^2}{m^2}\Big) + \mathcal{C}_{i,g}^{\mathrm{CSN},\mathrm{S},(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\,,$$

(4.2.19)

$$\begin{aligned} H_{i,g}^{\mathrm{S},(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) &= A_{Qg}^{\mathrm{S},(2)}\Big(\frac{\mu^2}{m^2}\Big)\mathcal{C}_{i,Q}^{\mathrm{CSN},\mathrm{NS},(0)}\Big(\frac{Q^2}{m^2}\Big) + \mathcal{C}_{i,g}^{\mathrm{CSN},\mathrm{S},(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \\ &\quad + A_{Qg}^{\mathrm{S},(1)}\Big(\frac{\mu^2}{m^2}\Big) \otimes \mathcal{C}_{i,Q}^{\mathrm{CSN},\mathrm{NS},(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\,. \end{aligned} \tag{4.2.20}$$

In the expressions above we have only given the arguments on which the coefficient functions and operator matrix elements depend, like n_f, Q^2/m^2, or Q^2/μ^2 (at least up to that order in perturbation theory). Furthermore we have dropped the convolution symbol when the corresponding coefficient function behaves as a δ-function of the type $\delta(1-z)$. The heavy quark coefficient functions correspond to the following processes

$$\begin{aligned} H_{i,g}^{\mathrm{S},(1)} &: \gamma^* + g \to Q + \bar{Q} \quad \text{Fig. 4.1} \\ H_{i,g}^{\mathrm{S},(2)} &: \gamma^* + g \to Q + \bar{Q} + g \quad \text{Figs. 4.2, 4.3} \\ H_{i,q}^{\mathrm{PS},(2)} &: \gamma^* + q(\bar{q}) \to Q + \bar{Q} + q(\bar{q}) \quad \text{Fig. 4.4} \\ L_{i,q}^{\mathrm{NS},(2)} &: \gamma^* + q(\bar{q}) \to Q + \bar{Q} + q(\bar{q}) \quad \text{Fig. 4.5} \\ H_{i,Q}^{\mathrm{NS},(0)} &: \gamma^* + Q \to Q \\ H_{i,Q}^{\mathrm{NS},(1)} &: \gamma^* + Q \to Q + g \quad \text{Fig. 4.7}\,. \end{aligned} \tag{4.2.21}$$

In the reactions above the virtual corrections to the lowest order processes are implicitly understood. The coefficient functions $L_{i,q}^{\mathrm{NS},(2)}$, $H_{i,q}^{\mathrm{PS},(2)}$ and $H_{i,g}^{\mathrm{S},(2)}$,

computed in the $\overline{MS}$-scheme, can be found in [5] whereas the $H_{i,Q}^{\rm NS,(1)}$ are computed in the context of QED in [16]. The $\overline{\rm MS}$-scheme is also chosen for the OME's in Eqs. (4.2.15)-(4.2.20) which are computed up to order α_s^2 in [6] and [15]. This also holds for $A_{QQ}^{\rm NS,(1)}$ in Eq. (4.2.18) which is presented in the context of QED in [17]. Furthermore the running coupling constant appearing in the quantities above contains n_f active flavors.

The mass singular logarithms of the type $\ln(\mu^2/m^2)$, appearing in the OME's above, are absorbed by the light parton densities. This procedure leads to parton densities which are represented in the n_f+1 light flavor scheme. For the light parton densities one obtains

$$f_{k+\bar{k}}(n_f+1,\mu^2) = A_{qq,Q}^{\rm NS}\Big(n_f,\frac{\mu^2}{m^2}\Big) \otimes f_{k+\bar{k}}(n_f,\mu^2) + \tilde{A}_{qq,Q}^{\rm PS}\Big(n_f,\frac{\mu^2}{m^2}\Big)$$
$$\otimes f_q^{\rm S}(n_f,\mu^2) + \tilde{A}_{qg,Q}^{\rm S}\Big(n_f,\frac{\mu^2}{m^2}\Big) \otimes f_g^{\rm S}(n_f,\mu^2)\,,\; k = 1\cdots n_f\,. \qquad (4.2.22)$$

The parton density representing the heavy quark in the n_f+1 flavor scheme is

$$f_{Q+\bar{Q}}(n_f+1,\mu^2) = \tilde{A}_{Qq}^{\rm PS}\Big(n_f,\frac{\mu^2}{m^2}\Big) \otimes f_q^{\rm S}(n_f,\mu^2)$$
$$+\tilde{A}_{Qg}^{\rm S}\Big(n_f,\frac{\mu^2}{m^2}\Big) \otimes f_g^{\rm S}(n_f,\mu^2)\,. \qquad (4.2.23)$$

Finally the gluon density in the n_f+1 flavor scheme is

$$f_g^{\rm S}(n_f+1,\mu^2) = A_{gq,Q}^{\rm S}(n_f,\frac{\mu^2}{m^2}) \otimes f_q^{\rm S}(n_f,\mu^2)$$
$$+A_{gg,Q}^{\rm S}(n_f,\frac{\mu^2}{m^2}) \otimes f_g^{\rm S}(n_f,\mu^2)\,. \qquad (4.2.24)$$

One can check (see [6]) that the new parton densities satisfy the renormalization group equations in Eq. (5.2.5) wherein all quantities n_f are replaced by n_f+1. Up to order a_s^2 the above relations become

$$f_{k+\bar{k}}(n_f+1,\mu^2) = f_{k+\bar{k}}(n_f,\mu^2)$$
$$+a_s^2(n_f,\mu^2)A_{qq,Q}^{\rm NS,(2)}\Big(\frac{\mu^2}{m^2}\Big) \otimes f_{k+\bar{k}}(n_f,\mu^2)\,, \qquad (4.2.25)$$

$$f_{Q+\bar{Q}}(n_f+1,\mu^2) = a_s(n_f,\mu^2)\tilde{A}_{Qg}^{\rm S,(1)}\Big(\frac{\mu^2}{m^2}\Big) \otimes f_g^{\rm S}(n_f,\mu^2)$$

$$+a_s^2(n_f,\mu^2)\Big[\tilde{A}_{Qq}^{\mathrm{PS},(2)}\Big(\frac{\mu^2}{m^2}\Big)\otimes f_q^{\mathrm{S}}(n_f,\mu^2)+\tilde{A}_{Qg}^{\mathrm{S},(2)}\Big(\frac{\mu^2}{m^2}\Big)\otimes f_g^{\mathrm{S}}(n_f,\mu^2)\Big]\,, \tag{4.2.26}$$

$$f_g^{\mathrm{S}}(n_f+1,\mu^2)=f_g^{\mathrm{S}}(n_f,\mu^2)+a_s(n_f,\mu^2)A_{gg,Q}^{\mathrm{S},(1)}(\frac{\mu^2}{m^2})\otimes f_g^{\mathrm{S}}(n_f,\mu^2)$$

$$+a_s^2(n_f,\mu^2)\Big[A_{gq,Q}^{\mathrm{S},(2)}(\frac{\mu^2}{m^2})\otimes f_q^{\mathrm{S}}(n_f,\mu^2)+A_{gg,Q}^{\mathrm{S},(2)}(\frac{\mu^2}{m^2})\otimes f_g^{\mathrm{S}}(n_f,\mu^2)\Big]\,. \tag{4.2.27}$$

Notice that in passing from an n_f-flavor to an n_f+1-flavor scheme the running coupling constant becomes

$$a_s(n_f+1,\mu^2) \;=\; a_s(n_f,\mu^2)\Big[1-a_s(n_f,\mu^2)\beta_{0,Q}\ln(\frac{\mu^2}{m^2})\Big]\,, \tag{4.2.28}$$

which has to be used in all expressions for the structure functions in the CSN scheme. Using the mass factorization relations in Eqs. (5.2.8), (5.2.10) and the redefinitions of the parton densities in Eqs. (4.2.22)-(2.24) we obtain from Eq. (5.2.6) the heavy quark components of the structure functions in the CSN scheme are

$$F_{i,Q}^{\mathrm{CSN}}(n_f+1,\Delta,Q^2,m^2)=$$

$$e_Q^2\Bigg[f_{Q+\bar{Q}}(n_f+1,\mu^2)\otimes\Bigg\{\mathcal{C}_{i,Q}^{\mathrm{CSN,NS}}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+\mathcal{C}_{i,Q}^{\mathrm{CSN,PS}}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg\}$$

$$+\sum_{l=1}^{n_f}f_{l+\bar{l}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,q}^{\mathrm{CSN,PS}}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+f_g^{\mathrm{S}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,g}^{\mathrm{CSN,S}}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg]$$

$$+\sum_{k=1}^{n_f}e_k^2\Bigg[\sum_{l=1}^{n_f}f_{l+\bar{l}}(n_f+1,\mu^2)\otimes L_{i,q}^{\mathrm{HARD,PS}}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+f_g^{\mathrm{S}}(n_f+1,\mu^2)\otimes L_{i,g}^{\mathrm{HARD,S}}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+f_{k+\bar{k}}(n_f+1,\mu^2)\otimes L_{i,q}^{\rm HARD,NS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg]\,. \tag{4.2.29}$$

In a similar way one obtains from Eq. (5.2.1) the light parton components of the structure functions in the CSN scheme are

$$\begin{aligned}
F_i^{\rm CSN,LIGHT}(n_f,\Delta,Q^2,m^2) = \sum_{k=1}^{n_f} e_k^2\Bigg[& \\
\sum_{l=1}^{n_f} f_{l+\bar{l}}(n_f+1,\mu^2)\otimes\Bigg(\tilde{\mathcal{C}}_{i,q}^{\rm PS}\Big(n_f,\frac{Q^2}{\mu^2}\Big)+\mathcal{C}_{i,q,Q}^{\rm CSN,SOFT,PS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg) & \\
+f_g^{\rm S}(n_f+1,\mu^2)\otimes\Bigg(\tilde{\mathcal{C}}_{i,g}^{\rm S}\Big(n_f,\frac{Q^2}{\mu^2}\Big)+\mathcal{C}_{i,g,Q}^{\rm CSN,SOFT,S}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg) & \\
+f_{k+\bar{k}}(n_f+1,\mu^2)\otimes\Bigg(\mathcal{C}_{i,q}^{\rm NS}\Big(n_f,\frac{Q^2}{\mu^2}\Big)+\mathcal{C}_{i,q,Q}^{\rm CSN,SOFT,NS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg)\Bigg]\,. &
\end{aligned} \tag{4.2.30}$$

Up to a given order Eqs. (4.2.29) and (4.2.30) do not differ from the structure functions presented in Eqs. (5.2.6) and (5.2.1) respectively as long as one uses fixed order perturbation theory. This can be checked up to second order when the coefficient functions in Eqs. (4.2.29) and (4.2.30) are substituted using the mass factorization relations in (4.2.15)-(4.2.20). The difference arises if the logarithms of the type $\ln^i(\mu^2/m^2)$, which show up in the parton densities, are resummed using the renormalization group equations in Eq. (5.2.5). This resummation induces corrections beyond fixed order perturbation theory which become noticeable for $\mu^2 \gg m^2$. On the other hand we do not want that the resummation bedevils the threshold behavior of the structure functions. In this region the best representation is still given by Eqs. (5.2.1) and (5.2.6). Therefore one has to look for a scale at which expressions (4.2.29) and (4.2.30) coincide with those given by fixed order perturbation theory in (5.2.6) and (5.2.1) respectively. Finding this scale is the most important issue in CSN as we will show below. Both expressions $F_{i,Q}^{\rm CSN}$ and $F_i^{\rm CSN,LIGHT}$ are renormalization group invariants. Hence they satisfy the renormalization group equations (see Eq. (5.2.4))

$$D\,F_{i,Q}^{\rm CSN}=0\,,\qquad D\,F_i^{\rm CSN,LIGHT}=0\,. \tag{4.2.31}$$

The same holds for the total structure function in the variable flavor number scheme which is defined as

$$F_i^{\rm CSN}(n_f+1,Q^2,m^2)=F_i^{\rm CSN,LIGHT}(n_f,\Delta,Q^2,m^2)$$

$$+F_{i,Q}^{\rm CSN}(n_f+1,\Delta,Q^2,m^2)\,. \qquad (4.2.32)$$

One can now show that for large Q^2, $F_i^{\rm CSN}(n_f+1,Q^2,m^2)$ turns into the same expression as Eq. (5.2.1) where n_f in the light parton coefficient functions $\mathcal{C}_{i,k}$ is replaced by n_f+1 and $\mathcal{C}_{i,k}^{\rm VIRT}=0$ for the n_f+1 heavy flavor piece.

After having discussed the general procedure to construct CSN scheme structure functions we now turn to the practical issues. For asymptotic values of Q^2, far above the heavy $Q\bar{Q}$ threshold at $(1-x)Q^2/x = 4m^2$, all coefficient functions $\mathcal{C}_{i,k}^{\rm CSN}$ in Eq. (4.2.29) can be replaced by the light parton coefficient functions so that, after having removed $L_{i,k}^{\rm HARD}$, one gets the heavy quark components of the structure functions in the so-called zero mass variable flavor number scheme (ZM-CSN). However near threshold at low Q^2 and large x there is a problem, which has not been solved satisfactorily in the literature. In this region one would like the $F_{i,Q}^{\rm CSN}$ to vanish in the same way that the $F_{i,Q}^{\rm EXACT}$ vanish. Unfortunately the coefficient functions $\mathcal{C}_{i,Q}^{\rm CSN}$ do not vanish in the threshold region due to the presence of the OME's $A_{Qk}^{\rm S}$ and the functions $H_{i,Q}^{\rm NS}$ which describe processes with ONE heavy quark in the final state (see Eq. (4.2.21)) contrary to $H_{i,g}$ and $H_{i,q}$ which originate from reactions with at least TWO heavy quarks (Q and $\bar{\rm Q}$) in the final state. Only the latter functions have the correct threshold behavior. In the literature two ways have been proposed to obtain reasonable threshold behaviors. The first one was given in a paper by Aivasis, Collins, Olness and Tung [7], which will be denoted as the ACOT boundary conditions. The second one was proposed in a paper by Thorne and Roberts [10], which we shall call the TR boundary conditions. In both approaches the structure functions have the properties

$$F_{i,Q}(Q^2,m^2) = F_{i,Q}^{\rm EXACT}(n_f,Q^2,m^2) \quad \text{for} \quad Q^2 < m^2\,,$$

$$F_{i,Q}(Q^2,m^2) = F_{i,Q}^{\rm CSN}(n_f+1,Q^2,m^2) \quad \text{for} \quad Q^2 \geq m^2\,, \qquad (4.2.33)$$

where the parton densities satisfy the boundary conditions at $\mu^2=m^2$

$$\begin{aligned} f_{k+\bar{k}}(n_f+1,x,\mu^2) &= f_{k+\bar{k}}(n_f,x,\mu^2)\,,\\ f_{Q+\bar{Q}}(n_f+1,x,\mu^2) &= 0 \quad {}^2\,,\\ f_g(n_f+1,x,\mu^2) &= f_g(n_f,x,\mu^2)\,. \end{aligned} \qquad (4.2.34)$$

Notice that there is no relation between the scale μ, chosen in these boundary conditions, and the production threshold of heavy quarks $(1-x)\,Q^2/x \geq 4\,m^2$.

[1]Note that in the existing parton density sets $f_{Q+\bar{Q}}(n_f+1,x,\mu^2)$ also vanishes for $\mu^2 < m^2$.

If one e.g. takes $\mu^2 = Q^2$ and $Q^2 \leq m^2$ all terms in Eq. (4.2.29), where the heavy quark density is multiplied with $\mathcal{C}_{i,Q}^{\rm CSN}$, vanish in spite of the fact that heavy flavors are still produced as long as $x < Q^2/(Q^2 + 4\ m^2)$. On the other hand it is possible that $Q^2 > m^2$ and $x \geq Q^2/(Q^2 + 4\ m^2)$ which implies a non-vanishing heavy quark density with no heavy quark pair production. Therefore the value for Q^2 chosen in Eq. (4.2.33) is a little arbitrary and no condition is imposed on x. Since we do not have any alternative we shall choose the same value of Q^2 as in Eq. (4.2.33) above which $F_{i,Q}^{\rm EXACT}$ turns into $F_{i,Q}^{\rm CSN}$. Another problem is is that the boundary conditions in Eq. (4.2.34) do not agree with the relations in Eqs. (4.2.22)-(4.2.24) if the computations are extended beyond order a_s^2 which happens in the $\overline{\rm MS}$-scheme. In this case the continuity at $\mu^2 = m^2$ is changed into a discontinuity. Finally there is a problem with the heavy quark density if we choose an arbitrary value for μ^2 in $f_{Q+\bar{Q}}(n_f + 1, x, \mu^2)$. In deep inelastic scattering one very often chooses $\mu^2 = Q^2$. If $Q^2 < m^2$ one has to know $f_{Q+\bar{Q}}(n_f + 1, x, \mu^2)$ for values $\mu^2 < m^2$ which are not specified in Eq. (4.2.34). Furthermore the OME's do not vanish for $\mu^2 < m^2$ so that $C_{i,k}^{\rm CSN} \neq H_{i,k}$. (see Eqs. (4.2.17)-(4.2.20)). Hence in Eq. (4.2.33) $F_{i,Q} \neq F_{i,Q}^{\rm EXACT}$ for $Q^2 < m^2$ so that the threshold behavior will be spoiled. Therefore one has to avoid chosing $\mu^2 < m^2$ which can be achieved by the prescription given by ACOT in [7]

$$\begin{aligned} \mu^2 &= m^2 + kQ^2 \left(1 - \frac{m^2}{Q^2}\right)^n \quad \text{for} \quad Q^2 > m^2\,, \\ \mu^2 &= m^2 \qquad\qquad\qquad\qquad\quad \text{for} \quad Q^2 \leq m^2\,, \end{aligned} \tag{4.2.35}$$

with $k = 1/2$ and $n = 2$. In this way one gets $C_{i,k}^{\rm CSN} = H_{i,k}$ for $Q^2 < m^2$ at least up to order a_s. For higher orders one has to use the relations in Eqs. (4.2.22)-(4.2.24) instead of those given in Eq. (4.2.34) as the latter only hold up to order a_s. The new conditions are presented up to order a_s^2 in Eqs. (4.2.25)-(2.27).

In the TR prescription one first chooses $\mu^2 = Q^2$ and then requires

$$\begin{aligned} F_i^{\rm CSN}(n_f + 1, Q^2, m^2)\,|_{Q^2=m^2} &= F_i^{\rm EXACT}(n_f, Q^2, m^2)\,|_{Q^2=m^2}\,, \\ \frac{d\,F_i^{\rm CSN}(n_f + 1, Q^2, m^2)}{d\,\ln(Q^2/m^2)}\,|_{Q^2=m^2} &= \frac{d\,F_i^{\rm EXACT}(n_f, Q^2, m^2)}{d\,\ln(Q^2/m^2)}\,|_{Q^2=m^2}\,. \end{aligned} \tag{4.2.36}$$

Using the mass factorization relations in Eqs. (4.2.17)-(4.2.20) the TR boundary conditions lead to new heavy quark coefficient functions $\mathcal{C}_{i,Q}^{\rm CSN}$ which have

nothing to do with the reactions in Eq. (4.2.21). For instance the lowest order coefficient functions in the TR prescription corresponding to the reaction $\gamma^* + Q \to Q$ in Eq. (4.2.21) vanish at the $Q\bar{Q}$ threshold although this process only contains one heavy quark in the final state. Moreover, as already admitted by the authors in [10], this procedure breaks down beyond order a_s because there are more coefficient functions than relations between them. Another problem is that it is unclear in which subtraction scheme one is working since the subtraction terms in [10] have nothing to do with the usual OME's except in the limit $Q^2 \gg m^2$. For example in order a_s the subtraction term needed for $H_{i,Q}^{\mathrm{NS},(1)}$ in Eq. (4.2.18) is not given by $A_{QQ}^{\mathrm{NS},(1)}$. The same holds for $H_{i,g}^{\mathrm{S},(1)}$ in Eq. (4.2.19), which gets another subtraction than given by $A_{Qg}^{\mathrm{S},(1)}$. From the theoretical viewpoint the boundary conditions in Eq. (4.2.36) seem very unattractive to us because the relations between the coefficient functions $\mathcal{C}_{i,k}^{\mathrm{CSN}}$ $(k = Q, q, g)$ and the actual parton reactions are broken and the scheme is unknown. Notice that the parton densities in [10] are still presented in the $\overline{\mathrm{MS}}$-scheme.

A different VFNS from that discussed above has been proposed by Buza, Matiounine, Smith and van Neerven in [6], [9], which we call the BMSN scheme. In the latter it was advocated that only when the large logarithms dominate the heavy quark coefficient functions do they have to be removed via mass factorization so that they can be resummed via the renormalization group equations. In the BMSN scheme we need the asymptotic heavy quark coefficient functions defined by

$$\lim_{Q^2 \gg m^2} H_{i,k}(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) = H_{i,k}^{\mathrm{ASYMP}}(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}), \tag{4.2.37}$$

which behave like

$$H^{\mathrm{ASYMP},(l)}(n_f, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) \sim a_s^l \sum_{n+j \le l} a_{nj} \ln^n \left(\frac{Q^2}{m^2}\right) \ln^j \left(\frac{Q^2}{\mu^2}\right), \tag{4.2.38}$$

with a similar behavior for $L_{i,k}^{\mathrm{ASYMP}}$. In the BMSN scheme $F_{i,Q}^{\mathrm{EXACT}}$ is given by Eq. (5.2.6) except that $L_{i,k} \to L_{i,k}^{\mathrm{HARD}}$ analogous to the CSN. The asymptotic heavy quark structure functions, denoted by $F_{i,Q}^{\mathrm{ASYMP}}$, are given by the same expressions as presented for $F_{i,Q}^{\mathrm{EXACT}}$ where now all exact heavy quark functions are replaced by their asymptotic ones. Up to second order the latter can be found in [15]. The functions $L_{i,q}^{\mathrm{SOFT,ASYMP,NS},(2)}$ and $L_{i,q}^{\mathrm{HARD,ASYMP,NS},(2)}$ are given in Appendix A. In the BMSN scheme the charm components of the structure functions are defined as

$$F_{i,Q}^{\mathrm{BMSN}}(n_f + 1, \Delta, Q^2, m^2) = F_{i,Q}^{\mathrm{EXACT}}(n_f, \Delta, Q^2, m^2)$$

$$-F_{i,Q}^{\rm ASYMP}(n_f,\Delta,Q^2,m^2)+F_{i,Q}^{\rm PDF}(n_f+1,\Delta,Q^2,m^2)\,, \quad (4.2.39)$$

with

$$F_{i,Q}^{\rm PDF}(n_f+1,\Delta,Q^2,m^2) =$$

$$e_Q^2\left[f_q^{\rm S}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}_{i,q}^{\rm PS}\Big(n_f+1,\frac{Q^2}{\mu^2}\Big)+f_g^{\rm S}(n_f+1,\mu^2)\right.$$

$$\left.\otimes\tilde{\mathcal{C}}_{i,g}^{\rm S}\Big(n_f+1,\frac{Q^2}{\mu^2}\Big)+f_{Q+\bar{Q}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,q}^{\rm NS}\Big(n_f+1,\frac{Q^2}{\mu^2}\Big)\right]$$

$$+\sum_{k=1}^{n_f}e_k^2\left[\sum_{l=1}^{n_f}f_{l+\bar{l}}(n_f+1,\mu^2)\otimes L_{i,q}^{\rm HARD,ASYMP,PS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right.$$

$$+f_g^{\rm S}(n_f+1,\mu^2)\otimes L_{i,g}^{\rm HARD,ASYMP,S}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$\left.+f_{k+\bar{k}}(n_f+1,\mu^2)\otimes L_{i,q}^{\rm HARD,ASYMP,NS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right]\,. \quad (4.2.40)$$

The structure functions $F_{i,Q}^{\rm PDF}$ are obtained from the $F_{i,Q}^{\rm ASYMP}$ via the mass factorization relations in Eqs. (5.2.7), (5.2.10) by making the replacements $H_{i,k}\to H_{i,k}^{\rm ASYMP}$, $L_{i,k}\to L_{i,k}^{\rm ASYMP}$ and $\mathcal{C}_{i,k}^{\rm CSN}\to\tilde{\mathcal{C}}_{i,k}$ on the left and right-hand sides respectively. Furthermore we have used the definitions for the parton densities in Eqs. (4.2.22)- (4.2.24). Notice that if the coefficient functions, indicated by $L_{i,k}^{\rm HARD,ASYMP}$, are removed from $F_{i,Q}^{\rm PDF}$ one obtains the structure functions in the ZM-CSN. The light parton components of the structure functions become

$$F_i^{\rm BMSN,LIGHT}(n_f,\Delta,Q^2,m^2) =$$

$$\sum_{k=1}^{n_f}e_k^2\left[\sum_{l=1}^{n_f}f_{l+\bar{l}}(n_f+1,\mu^2)\otimes\delta\,\mathcal{C}_{i,q}^{\rm PS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right.$$

$$+f_g^{\rm S}(n_f+1,\mu^2)\otimes\delta\,\mathcal{C}_{i,g}^{\rm S}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$\left.+f_{k+\bar{k}}(n_f+1,\mu^2)\otimes\delta\,\mathcal{C}_{i,q}^{\rm NS}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right]\,, \quad (4.2.41)$$

with

$$\delta\,\mathcal{C}_{i,k}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)=\tilde{\mathcal{C}}_{i,k}\Big(n_f+1,\frac{Q^2}{\mu^2}\Big)+\tilde{\mathcal{C}}^{\rm VIRT}_{i,k}\Big(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+L^{\rm SOFT}_{i,k}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)-\tilde{\mathcal{C}}^{\rm VIRT,ASYMP}_{i,k}\Big(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$-L^{\rm ASYMP}_{i,k}\Big(n_f,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\,. \tag{4.2.42}$$

The coefficient functions above satisfy the property that

$$\lim_{Q^2\gg m^2}\delta\,\mathcal{C}_{i,k}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)=$$

$$\tilde{\mathcal{C}}_{i,k}\Big(n_f+1,\frac{Q^2}{\mu^2}\Big)-L^{\rm HARD,ASYMP}_{i,k}\Big(n_f,\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\,. \tag{4.2.43}$$

Using the relations in Eqs. (5.2.9), (4.2.12) one can make a comparison between the CSN and the BMSN schemes. In the asymptotic limit the heavy quark components satisfy (see Eqs. (4.2.29), (4.2.39), (4.2.40))

$$\lim_{Q^2\gg m^2}F^{\rm BMSN}_{i,Q}(n_f+1,\Delta,Q^2,m^2)=\lim_{Q^2\gg m^2}F^{\rm CSN}_{i,Q}(n_f+1,\Delta,Q^2,m^2)$$

$$=\lim_{Q^2\gg m^2}F^{\rm PDF}_{i,Q}(n_f+1,\Delta,Q^2,m^2)\,, \tag{4.2.44}$$

and the light parton components satisfy (see Eqs. (4.2.30), (4.2.41))

$$\lim_{Q^2\gg m^2}F^{\rm BMSN,LIGHT}_{i}(n_f,\Delta,Q^2,m^2)=\lim_{Q^2\gg m^2}F^{\rm CSN,LIGHT}_{i}(n_f,\Delta,Q^2,m^2)\,, \tag{4.2.45}$$

provided we impose the same boundary conditions on both schemes. From the discussion above we infer that the only difference between the CSN and the BMSN schemes can be attributed to the m^2/Q^2-terms which are present in $\mathcal{C}^{\rm CSN}_{i,Q}$. Such terms do not occur in the $\mathcal{C}_{i,q}$ appearing in $F^{\rm PDF}_{i,Q}$ if one chooses the BMSN-scheme. In the next Section we will make a study where in Q^2 these differences are noticeable.

4.3 Comparison between the CSN and the BMSN scheme

In this Section we will make a comparison in the case of charm production between the above CSN scheme and the BMSN scheme proposed in [6], [9]. For that purpose we construct a parton density set with four active flavors from an existing three flavor set in the literature following Eqs. (2.22)-(2.24). The charm quark density of our set will be compared with those in other sets with four active flavors presented in [18] (MRST98, central gluon) and [19] (CTEQ5HQ). Using our set we will study the differences between the charm components of the structure functions $F_{i,c}^{\rm CSN}(n_f+1)$ in Eq. (4.2.29) and $F_{i,c}^{\rm BMSN}(n_f+1)$ in Eq. (4.2.39) in particular in the threshold region.

Since all coefficient functions are computed in the $\overline{\rm MS}$-scheme we choose the leading order (LO) and next-to-leading order (NLO) parton density sets presented in [12] which contain three active flavors only (i.e. u,d,s). This implies that one has chosen $n_f = 3$ for the anomalous dimensions. In order to make this paper self contained we give some details here. In LO where the input scale μ_0 is chosen to be $\mu_0^2 = \mu_{\rm LO}^2 = 0.26$ (GeV/c)^2 the input parton densities are

$$\begin{aligned}
x u_v(3,x,\mu_{\rm LO}^2) &= 1.239\ x^{0.48}(1-x)^{2.72}(1-1.8\sqrt{x}+9.5x)\\
x d_v(3,x,\mu_{\rm LO}^2) &= 0.614\ (1-x)^{0.9}\ x u_v(3,x,\mu_{\rm LO}^2)\\
x\Delta(3,x,\mu_{\rm LO}^2) &= 0.23\ x^{0.48}(1-x)^{11.3}(1-12.0\sqrt{x}+50.9x)\\
x(\bar u+\bar d)(3,x,\mu_{\rm LO}^2) &= 1.52\ x^{0.15}(1-x)^{9.1}(1-3.6\sqrt{x}+7.8x)\\
x g(3,x,\mu_{\rm LO}^2) &= 17.47\ x^{1.6}(1-x)^{3.8}\\
x s(3,x,\mu_{\rm LO}^2) &= x\bar s(x,\mu_{\rm LO}^2) = 0
\end{aligned} \tag{4.3.1}$$

In NLO where the input scale equals $\mu_{\rm NLO}^2 = 0.40$ (GeV/c)^2 we have

$$\begin{aligned}
x u_v(3,x,\mu_{\rm NLO}^2) &= 0.632\ x^{0.43}(1-x)^{3.09}(1+18.2x)\\
x d_v(3,x,\mu_{\rm NLO}^2) &= 0.624\ (1-x)^{1.0}\ x u_v(3,x,\mu_{\rm NLO}^2)\\
x\Delta(3,x,\mu_{\rm NLO}^2) &= 0.20\ x^{0.43}(1-x)^{12.4}(1-13.3\sqrt{x}+60.0x)\\
x(\bar u+\bar d)(3,x,\mu_{\rm NLO}^2) &= 1.24\ x^{0.20}(1-x)^{8.5}(1-2.3\sqrt{x}+5.7x)\\
x g(3,x,\mu_{\rm NLO}^2) &= 20.80\ x^{1.6}(1-x)^{4.1}\\
x s(3,x,\mu_{\rm NLO}^2) &= x\bar s(x,\mu_{\rm NLO}^2) = 0.
\end{aligned} \tag{4.3.2}$$

where $\Delta \equiv \bar d - \bar u$. Furthermore in [12] the heavy quark masses are $m_c = 1.4$ GeV/c^2, $m_b = 4.5$ GeV/c. In both sets the densities are evolved from

a very low starting scale, where it is necessary to use the exact numerical solution for the running coupling constant $\alpha_s(\mu^2)$. The latter follows from the implicit equation

$$\ln \frac{Q^2}{\Lambda^{\overline{\rm MS}}_{n_f}} = \frac{4\pi}{\beta_0 \alpha_s(\mu^2)} - \frac{\beta_1}{\beta_0^2} \ln \left[\frac{4\pi}{\beta_0 \alpha_s(\mu^2)} + \frac{\beta_1}{\beta_0^2} \right] ,$$

$$\beta_0 = 11 - \frac{2}{3} n_f \,, \qquad \beta_1 = 102 - \frac{38}{3} n_f \,, \tag{4.3.3}$$

and will be used in all the following formulae. Furthermore we adopt the values $\Lambda^{\overline{\rm MS}}_{3,4,5,6} = 299.4, 246, 167.7, 67.8$ MeV which yield $\alpha_s(5, M_Z^2) = 0.114$. Notice that the values for Λ_{n_f} follow from the matching conditions

$$\alpha_s(n_f, \Lambda_{n_f}, m^2) = \alpha_s(n_f + 1, \Lambda_{n_f+1}, m^2) \,. \tag{4.3.4}$$

where for $n_f = 3$ and $n_f = 4$ one has to choose $m = m_c$ and $m = m_b$ respectively. For the computation of $F_{i,c}^{\rm EXACT}$ (5.2.6) and $F_{i,c}^{\rm ASYMP}$ ((4.2.39) we take $n_f = 3$ for the parton densities and the running coupling constant in Eq. (4.3.3). However for $F_{i,c}^{\rm CSN}$ (4.2.29), $F_{i,c}^{\rm BMSN}$ (4.2.39) and $F_{i,c}^{\rm PDF}$ (4.2.40) we need $n_f = 4$ for the coupling constant in Eq. (4.3.3) and a parton density set with four active flavors (i.e. u,d,s,c) when the scale μ becomes larger or equal to the heavy flavor mass m. For reasons which will be explained below our computations are performed with parton densities represented in LO, NLO and NNLO (next-to-next-to leading order). The LO densities are convoluted with the order α_s^2 contributions to the coefficient functions. The NLO densities are convoluted with the order α_s parts of the coefficient functions. The zeroth order contributions to the latter have to be multiplied with the NNLO densities. Notice that for $n_f = 3$ we only need LO and NLO densities here since the heavy quark coefficient functions in $F_{i,c}^{\rm EXACT}$ and $F_{i,c}^{\rm ASYMP}$ start in order α_s. Our sets with four active flavors are derived from the ones with three active flavors by putting $n_f = 3$ in Eqs. (4.2.25)-(4.2.27) starting at a specific scale which we choose as $\mu^2 = m^2$. Hence it follows that in LO or in zeroth order α_s one gets

$$\begin{aligned} f_{k+\bar{k}}^{\rm LO}(4, x, m^2) &= f_{k+\bar{k}}^{\rm LO}(3, x, m^2) \,, \\ f_{c+\bar{c}}^{\rm LO}(4, x, m^2) &= 0 \,, \\ f_g^{\rm S,LO}(4, x, m^2) &= f_g^{\rm S,LO}(3, x, m^2) \,, \end{aligned} \tag{4.3.5}$$

whereas in NLO or in first order α_s one obtains

$$f_{k+\bar{k}}^{\rm NLO}(4, x, m^2) = f_{k+\bar{k}}^{\rm NLO}(3, x, m^2) \,,$$

$$
\begin{aligned}
f_{c+\bar{c}}^{\rm NLO}(4,x,m^2) &= 0\,, \\
f_g^{\rm S,NLO}(4,x,m^2) &= f_g^{\rm S,NLO}(3,x,m^2)\,. \qquad (4.3.6)
\end{aligned}
$$

Since the two-loop OME's $A_{Qk}^{(2)}$, $A_{kl,Q}^{(2)}$ in Eqs. (4.2.25)-(4.2.27) do not vanish at $\mu^2 = m^2$ in the $\overline{\rm MS}$-scheme we find that in NNLO or in order α_s^2 the parton densities are discontinuous at $\mu^2 = m^2$ while going from three to four flavors i.e.

$$
\begin{aligned}
f_{k+\bar{k}}^{\rm NNLO}(4,x,m^2) &\neq f_{k+\bar{k}}^{\rm NNLO}(3,x,m^2)\,, \\
f_{c+\bar{c}}^{\rm NNLO}(4,x,m^2) &\neq 0\,, \\
f_g^{\rm S,NNLO}(4,x,m^2) &\neq f_g^{\rm S,NNLO}(3,x,m^2)\,. \qquad (4.3.7)
\end{aligned}
$$

Note that if we would drop the terms independent of $\ln \mu^2/m^2$ in the two-loop operator matrix elements the inequalities in Eq. (4.3.7) would become equalities. Above $\mu = m_c$ all four flavor number densities evolve with $n_f = 4$ (we have not yet included a bottom quark density above $\mu = m_b$). The evolution of the parton densities, given by the renormalization group equations in Eq. (5.2.5), is determined by the anomalous dimensions $\gamma_{ij}^{(0)}$ (LO), $\gamma_{ij}^{(1)}$ (NLO) and $\gamma_{ij}^{(2)}$ (NNLO). Unfortunately the three-loop anomalous dimensions $\gamma_{ij}^{(2)}$ are not known yet except for the moments $N = 2, 4, 6, 8$ (see [20]). However an analysis of the light parton structure function in Eq. (5.2.1) [21] reveals that the contribution from $\gamma_{ij}^{(2)}$ is less important numerically than the contribution due to the two-loop coefficient functions computed in [13]. Hence our ignorance about the three-loop anomalous dimension will not appreciably alter our results. Therefore our NNLO analysis is only determined by the boundary conditions in Eq. (4.3.7) which only affects the charm density appearing in $F_{i,c}^{\rm CSN}$, $F_{i,c}^{\rm BMSN}$ and $F_{i,c}^{\rm PDF}$. The evolution of the parton densities above $\mu^2 = m_c^2$, presented in [22], was performed using a computer program which implements the direct x-space method (similar to that of [23]). The code is written in C++ and has the options to evolve densities in LO and NLO whereas the NNLO option presently only uses the NLO anomalous dimensions. We have checked that the evolution of the parton densities is in agreement with the results in [24].

Before substituting the parton densities into the structure functions we encounter a problem caused by the inequalities in Eq. (4.3.7). This happens in the threshold region which, according to the ACOT boundary conditions in Eq. (4.2.35), is defined by $Q^2 < m^2$. In this region one has to choose $\mu^2 = m^2$

so that $F_{i,c}^{\rm CSN}(n_f=4)$ and $F_{i,c}^{\rm BMSN}(n_f=4)$ are equal to $F_{i,c}^{\rm EXACT}(n_f=3)$. Notice that the latter has to be understood in the sense mentioned below Eq. (4.2.38) where $L_{i,k} \to L_{i,k}^{\rm HARD}$. However since $\alpha_s(m^2)$ is rather large we have to truncate the perturbation series for the structure functions to the desired order otherwise the threshold behavior of all the $F_{i,c}^{\rm CSN}(n_f=4)$ and $F_{i,c}^{\rm BMSN}(n_f=4)$ will be destroyed. Let us explain this for the BMSN scheme in Eq. (4.2.39). The arguments for the CSN scheme proceed in an analogous way. The conditions that the $F_{i,c}^{\rm BMSN}(n_f=4) = F_{i,c}^{\rm EXACT}(n_f=3)$ for $\mu^2=m^2$ implies that the $F_{i,c}^{\rm ASYMP}(n_f=3)$ in Eq. (4.2.39) are canceled by the $F_{i,c}^{\rm PDF}(n_f=4)$. Further we have to bear in mind that the $F_{i,c}^{\rm EXACT}(n_f=3)$ and $F_{i,c}^{\rm ASYMP}(n_f=3)$ are determined by the parton densities in the three flavor number scheme whereas the $F_{i,c}^{\rm PDF}(n_f=4)$ are constructed out of the four flavor number scheme parton densities. The latter have the form

$$\begin{aligned}
f_k(4,x,m^2)^{\rm NNLO} &= f_k(3,x,m^2)^{\rm NNLO}[1+O(\alpha_s^2)] \\
f_g^{\rm S}(4,x,m^2)^{\rm NNLO} &= f_g^{\rm S}(3,x,m^2)^{\rm NNLO}[1+O(\alpha_s^2)] \\
c(4,x,m^2)^{\rm NNLO} &= f_g^{\rm S}(3,x,m^2)^{\rm NNLO}O(\alpha_s^2) + f_q^{\rm S}(3,x,m^2)^{\rm NNLO}O(\alpha_s^2)\,.
\end{aligned} \tag{4.3.8}$$

If these densities are substituted in $F_{i,c}^{\rm PDF}(n_f=4)$ in Eq. (4.2.40) one obtains additional terms of order α_s^3 and α_s^4 in the perturbation series which are not canceled by $F_{i,c}^{\rm ASYMP}(n_f=3)$. Notice that the latter are only computed up to order α_s^2. This effect is caused by multiplying the four flavor number densities with the coefficient functions $\mathcal{C}_{i,k}$ corrected beyond zeroth order in α_s. To avoid these higher order terms we propose the following formulae for the structure functions in the CSN scheme

$$\begin{aligned}
F_{i,Q}^{\rm CSN}(n_f+1,\Delta,Q^2,m^2) = e_Q^2 \Bigg[& f_{Q+\bar{Q}}^{\rm NNLO}(n_f+1,\mu^2)\mathcal{C}_{i,Q}^{\rm CSN,NS,(0)}\Big(\frac{Q^2}{m^2}\Big) \\
& + a_s(n_f+1,\mu^2)\Bigg\{ f_{Q+\bar{Q}}^{\rm NLO}(n_f+1,\mu^2) \otimes \mathcal{C}_{i,Q}^{\rm CSN,NS,(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \\
& + f_g^{\rm S,NLO}(n_f+1,\mu^2) \otimes \mathcal{C}_{i,g}^{\rm CSN,S,(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg\} \\
& + a_s^2(n_f+1,\mu^2)\Bigg\{ f_{Q+\bar{Q}}^{\rm LO}(n_f+1,\mu^2) \otimes \Bigg(\mathcal{C}_{i,Q}^{\rm CSN,NS,(2)}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)
\end{aligned}$$

$$+\mathcal{C}_{i,Q}^{\mathrm{CSN,PS,(2)}}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Big)+\sum_{l=1}^{n_f} f_{l+\bar{l}}^{\mathrm{LO}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,q}^{\mathrm{CSN,PS,(2)}}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+f_g^{\mathrm{S,LO}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,g}^{\mathrm{CSN,S,(2)}}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Big\}\Big]$$

$$+a_s^2(n_f+1,\mu^2)\sum_{k=1}^{n_f} e_k^2\, f_{k+\bar{k}}^{\mathrm{LO}}(n_f+1,\mu^2)\otimes L_{i,q}^{\mathrm{HARD,NS,(2)}}\Big(\Delta,\frac{Q^2}{m^2}\Big)\,. \quad (4.3.9)$$

Notice that from the perturbative point of view the heavy quark density $f_{Q+\bar{Q}}^{\mathrm{LO}}$ starts in order $\alpha_s(\mu^2)$ so that after multiplication with $\mathcal{C}_{i,Q}^{\mathrm{CSN,NS,(2)}}$ and $\mathcal{C}_{i,Q}^{\mathrm{CSN,PS,(2)}}$ the product becomes of order $\alpha_s^3(\mu^2)$. Hence these coefficient functions did not appear in the mass factorization relations (4.2.17)-(4.2.20) since the latter are carried out up to order $\alpha_s^2(\mu^2)$. Since the heavy quark density in CSN has to be treated on the same footing as the light flavor densities, in particular after resummation of the terms in $\ln^i(\mu^2/m^2)$, all densities are considered to start in zeroth order in perturbation theory. This explains the form of of the above expression. Furthermore the coefficient functions $\mathcal{C}_{i,Q}^{\mathrm{CSN,NS,(2)}}$ and $\mathcal{C}_{i,Q}^{\mathrm{CSN,PS,(2)}}$ which originate from parton processes with an heavy quark in the initial state have not been calculated yet. Therefore we have to approximate them by the replacements

$$\mathcal{C}_{i,Q}^{\mathrm{CSN,NS,(2)}}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\to\mathcal{C}_{i,q}^{\mathrm{NS,(2)}}\Big(n_f+1,\frac{Q^2}{\mu^2}\Big)\,,$$

$$\mathcal{C}_{i,Q}^{\mathrm{CSN,PS,(2)}}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\to\mathcal{C}_{i,q}^{\mathrm{CSN,PS,(2)}}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\,, \quad (4.3.10)$$

respectively. The remaining CSN scheme coefficient functions can be computed via the relations in Eqs. (4.2.17)-(4.2.20), which are defined in terms of the known H's and A's. The light partonic parts of the CNS structure functions up to second order are given by

$$F_i^{\mathrm{CSN,LIGHT}}(n_f,\Delta,Q^2)=\sum_{k=1}^{n_f} e_k^2\Big[f_{k+\bar{k}}^{\mathrm{NNLO}}(n_f+1,\mu^2)\mathcal{C}_{i,q}^{\mathrm{NS,(0)}}$$

$$+a_s(n_f+1,\mu^2)\Big\{f_{k+\bar{k}}^{\mathrm{NLO}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,q}^{\mathrm{NS,(1)}}(\frac{Q^2}{\mu^2})+f_g^{\mathrm{S,NLO}}(n_f+1,\mu^2)$$

$$\otimes\tilde{\mathcal{C}}_{i,g}^{\mathrm{S,(1)}}(\frac{Q^2}{\mu^2})\Big\}+a_s^2(n_f+1,\mu^2)\Big\{f_{k+\bar{k}}^{\mathrm{LO}}(n_f+1,\mu^2)\otimes\Big(\mathcal{C}_{i,q}^{\mathrm{NS,(2)}}\Big(n_f,\frac{Q^2}{\mu^2}\Big)$$

$$+\mathcal{C}^{\rm SOFT,NS,(2)}_{i,q,Q}\Big(\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Big)+\sum_{l=1}^{n_f} f^{\rm LO}_{l+\bar{l}}(n_f+1,\mu^2)\otimes\hat{\mathcal{C}}^{\rm PS,(2)}_{i,q}\Big(\frac{Q^2}{\mu^2}\Big)$$

$$+f^{\rm S,LO}_g(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}^{\rm S,(2)}_{i,g}\Big(\frac{Q^2}{\mu^2}\Big)\Big\}\Big], \tag{4.3.11}$$

with

$$\mathcal{C}^{\rm SOFT,NS,(2)}_{i,q,Q}\Big(\Delta,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)=L^{\rm SOFT,NS,(2)}_{i,q,Q}\Big(\Delta,\frac{Q^2}{m^2}\Big)+\Big(F^{(2)}(Q^2,m^2)$$

$$-A^{\rm NS,(2)}_{qq,Q}\Big(\frac{\mu^2}{m^2})\Big)\,\mathcal{C}^{\rm NS,(0)}_{i,q}+\beta_{0,Q}\ln\left(\frac{\mu^2}{m^2}\right)\mathcal{C}^{\rm NS,(1)}_{i,q}\Big(\frac{Q^2}{\mu^2}\Big) \tag{4.3.12}$$

For the BMSN scheme we need the expression for $F^{\rm EXACT}_{i,Q}$ as defined above Eq. (4.2.39)

$$F^{\rm EXACT}_{i,Q}(n_f,\Delta,Q^2,m^2)=e_Q^2\left[a_s(n_f,\mu^2)f^{\rm S,NLO}_g(n_f,\mu^2)\otimes H^{\rm S,(1)}_{i,g}\Big(\frac{Q^2}{m^2}\Big)\right.$$

$$+a_s^2(n_f,\mu^2)\left\{\sum_{k=1}^{n_f} f^{\rm LO}_{k+\bar{k}}(n_f,\mu^2)\otimes H^{\rm PS,(2)}_{i,q}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right.$$

$$\left.\left.+f^{\rm S,LO}_g(n_f,\mu^2)\otimes H^{\rm S,(2)}_{i,g}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right\}\right]$$

$$+a_s^2(n_f,\mu^2)\sum_{k=1}^{n_f} e_k^2 f^{\rm LO}_{k+\bar{k}}(n_f,\mu^2)\otimes L^{\rm HARD,NS,(2)}_{i,q}\Big(\Delta,\frac{Q^2}{m^2}\Big). \tag{4.3.13}$$

If we choose the maximum $\Delta=s$ (defined in the figure caption for Fig. 4.5), we get $L^{\rm HARD,NS,(2)}_{i,q}=0$. On the other hand if the minimum value is adopted i.e. $\Delta=4m^2$ one gets $L^{\rm HARD,NS,(2)}_{i,q}=L^{\rm NS,(2)}_{i,q}$ and $F^{\rm EXACT}_{i,Q}$ becomes equal to the conventional expression given in Eq. (5.2.6). The structure function $F^{\rm ASYMP}_{i,Q}$ is obtained from the expression above by replacing the exact coefficient functions by their asymptotic analogues. Furthermore to calculate $F^{\rm BMSN}_{i,Q}$ in Eq. (4.2.39) we need

$$F^{\rm PDF}_{i,Q}(n_f+1,\Delta,Q^2,m^2)=e_Q^2\Big[f^{\rm NNLO}_{Q+\bar{Q}}(n_f+1,\mu^2)\mathcal{C}^{\rm NS,(0)}_{i,q}$$

$$+a_s(n_f+1,\mu^2)\left\{f^{\rm NLO}_{Q+\bar{Q}}(n_f+1,\mu^2)\otimes\mathcal{C}^{\rm NS,(1)}_{i,q}(\frac{Q^2}{\mu^2})\right.$$

$$+f_g^{\mathrm{S,NLO}}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}_{i,g}^{\mathrm{S},(1)}(\frac{Q^2}{\mu^2})\Big\}$$

$$+a_s^2(n_f+1,\mu^2)\Big\{f_{Q+\bar{Q}}^{\mathrm{LO}}(n_f+1,\mu^2)\otimes\Big(\mathcal{C}_{i,q}^{\mathrm{NS},(2)}(n_f+1,\frac{Q^2}{\mu^2})$$

$$+\tilde{\mathcal{C}}_{i,q}^{\mathrm{PS},(2)}\Big(\frac{Q^2}{\mu^2}\Big)\Big)+\sum_{l=1}^{n_f}f_{l+\bar{l}}^{\mathrm{LO}}(n_f+1,\mu^2)\Big)\otimes\tilde{\mathcal{C}}_{i,q}^{\mathrm{PS},(2)}\Big(\frac{Q^2}{\mu^2}\Big)$$

$$+f_g^{\mathrm{S,LO}}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}_{i,g}^{\mathrm{S},(2)}(\frac{Q^2}{\mu^2})\Big\}\Big]$$

$$+a_s^2(n_f+1,\mu^2)\sum_{k=1}^{n_f}e_k^2 f_{k+\bar{k}}^{\mathrm{LO}}(n_f,\mu^2)\otimes L_{i,q}^{\mathrm{HARD,ASYMP,NS},(2)}\Big(\Delta,\frac{Q^2}{m^2}\Big)\,. \tag{4.3.14}$$

Finally up to order α_s^2, Eq. (4.2.41) becomes

$$F_i^{\mathrm{BMSN,LIGHT}}(n_f+1,\Delta,Q^2)=\sum_{k=1}^{n_f}e_k^2\Big[f_{k+\bar{k}}^{\mathrm{NNLO}}(n_f+1,\mu^2)\mathcal{C}_{i,q}^{\mathrm{NS},(0)}$$

$$+a_s(n_f+1,\mu^2)\Big\{f_{k+\bar{k}}^{\mathrm{NLO}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,q}^{\mathrm{NS},(1)}(\frac{Q^2}{\mu^2})+f_g^{\mathrm{S,NLO}}(n_f+1,\mu^2)$$

$$\otimes\tilde{\mathcal{C}}_{i,g}^{\mathrm{S},(1)}(\frac{Q^2}{\mu^2})\Big\}+a_s^2(n_f+1,\mu^2)\Big\{f_{k+\bar{k}}^{\mathrm{LO}}(n_f+1,\mu^2)\otimes\mathcal{C}_{i,q}^{\mathrm{NS},(2)}(n_f+1,\frac{Q^2}{\mu^2})$$

$$+\sum_{l=1}^{n_f}f_{l+\bar{l}}^{\mathrm{LO}}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}_{i,q}^{\mathrm{PS},(2)}(\frac{Q^2}{\mu^2})+f_g^{\mathrm{S,LO}}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}_{i,g}^{\mathrm{S},(2)}(\frac{Q^2}{\mu^2})\Big\}\Big]$$

$$+a_s^2(n_f+1,\mu^2)\sum_{k=1}^{n_f}e_k^2 f_{k+\bar{k}}^{\mathrm{LO}}(n_f,\mu^2)\otimes\Big[L_{i,q}^{\mathrm{SOFT,NS},(2)}\Big(\Delta,\frac{Q^2}{m^2}\Big)$$

$$-L_{i,q}^{\mathrm{ASYMP,NS},(2)}\Big(\frac{Q^2}{m^2}\Big)+\Big(F^{(2)}(Q^2,m^2)-F^{\mathrm{ASYMP},(2)}(Q^2,m^2)\Big)\mathcal{C}_{i,q}^{\mathrm{NS},(0)}\Big]\,. \tag{4.3.15}$$

Notice that we have the relations

$$\mathcal{C}_{i,q}^{\mathrm{NS},(2)}(n_f+1,\frac{Q^2}{\mu^2}) = \mathcal{C}_{i,q}^{\mathrm{NS},(2)}(n_f,\frac{Q^2}{\mu^2}) + \mathcal{C}_{i,q,Q}^{\mathrm{NS},(2)}(\frac{Q^2}{\mu^2})\,, \tag{4.3.16}$$

with

$$\mathcal{C}_{i,q,Q}^{\mathrm{NS},(2)}(\frac{Q^2}{\mu^2}) = L_{i,q}^{\mathrm{ASYMP,NS},(2)}(\frac{Q^2}{m^2}) + \Big(F^{\mathrm{ASYMP},(2)}(Q^2,m^2)$$

$$-A_{qq,Q}^{\mathrm{NS},(2)}(\frac{\mu^2}{m^2})\Big)\,\mathcal{C}_{i,q}^{\mathrm{NS},(0)} + \beta_{0,Q}\,\ln(\frac{\mu^2}{m^2})\mathcal{C}_{i,q}^{\mathrm{NS},(1)}(\frac{Q^2}{\mu^2})\,. \tag{4.3.17}$$

The first and second terms in the expression above cancel the third last and final term in Eq. (4.3.15). The result is then equal to $\mathcal{C}_{i,q,Q}^{\mathrm{SOFT,NS},(2)}$ in Eq. (4.3.11) in the limit $Q^2 \gg m^2$. The form of the above structure functions also suppresses higher order terms beyond α_s^2 arising from the three flavor number parton densities since the latter also contain terms proportional to α_s and higher. This becomes apparent if one takes the Nth moments of the densities. For instance we observe the following behavior up to NNLO in the non-singlet case

$$\begin{aligned}
f_q^{\mathrm{LO},(\mathrm{N})}(\mu^2) &\sim \left[\frac{\alpha_s(\mu^2)}{\alpha_s(\mu_0^2)}\right]^{\gamma_{qq}^{(0)}/2\beta_0} f_q^{\mathrm{LO},(\mathrm{N})}(\mu_0^2)\,,\\
f_q^{\mathrm{NLO},(\mathrm{N})}(\mu^2) &\sim \left[1+\alpha_s(\mu^2)A_q^{(1)}\right]\left[\frac{\alpha_s(\mu^2)}{\alpha_s(\mu_0^2)}\right]^{\gamma_{qq}^{(0)}/2\beta_0} f_q^{\mathrm{NLO},(\mathrm{N})}(\mu_0^2)\,,\\
f_q^{\mathrm{NNLO},(\mathrm{N})}(\mu^2) &\sim \left[1+\alpha_s(\mu^2)A_q^{(1)}+\alpha_s^2(\mu^2)A_q^{(2)}\right]\left[\frac{\alpha_s(\mu^2)}{\alpha_s(\mu_0^2)}\right]^{\gamma_{qq}^{(0)}/2\beta_0}\\
&\quad\times f_q^{\mathrm{NNLO},(\mathrm{N})}(\mu_0^2)\,.
\end{aligned} \tag{4.3.18}$$

The choice of the multiplication rules above avoids the appearance of scheme dependent terms beyond the order in which we want to compute the structure functions. The above prescription guarantees that for $Q^2 < m^2$ we satisfy the condition $F_{i,c} = F_{i,c}^{\mathrm{EXACT}}(n_f)$ in both schemes.

In the subsequent part of this section we will only discuss the case where the heavy quark is the charm quark, i.e. $Q = c$. Hence in all expressions above we have to choose $n_f = 3$. Further we have to make a choice for the cut off Δ appearing in the coefficient functions $L_{k,q}^{\mathrm{SOFT,NS},(2)}$ $(k = 2, L)$. The $\delta = (\Delta - 4m^2)/(s - 4m^2)$ dependence of $xL_{2,q}^{\mathrm{SOFT,NS},(2)}$ is shown in Fig. 4.8,

where one notes that it peaks at large x, i.e., near threshold. (The plot for $xL_{L,q}^{\mathrm{SOFT,NS},(2)}$ has a similar shape). After convoluting this function with the parton densities its contribution to the structure function F_2^{LIGHT} only amounts to a few percent at $Q^2 = 10^3$ (GeV/c)^2. At decreasing Q^2 the contribution becomes even smaller. The same holds for $L_{2,q}^{\mathrm{HARD}}$ contributing to $F_{2,c}$. Hence the dependence of the structure functions on the value of Δ will be very small. Therefore in the subsequent analysis we choose $\Delta = 10$ GeV^2. Other choices hardly affect the plots so that our conclusions will be unaltered.

Next we present the x-dependence of the NNLO charm density (see Eq. (4.3.7)) for various values of μ^2 in Figs. 4.9a,b. The latter plot emphasizes the region $0.01 < x < 1$. At $\mu = m$ it becomes negative for $x < 0.007$ which is due to the boundary condition in Eq. (4.2.23) and the momentum sum rule. When $\mu > m$ the density becomes positive over the whole x range. In Figs. 4.9c and 4.9d we have shown the charm densities in NLO which are obtained from [18] and [19] respectively, with an offset scale so that they can easily be compared with Fig. 4.9a. The former is constructed in the TR scheme whereas the latter follows the prescription of ACOT. Both are positive over the whole x range. Our LO and NLO parameterizations, which are not shown in the figures, are also positive for all values of x. This property can be traced back to the boundary conditions which yield in LO and NLO $c(x, m^2) = 0$. Note that a direct comparison between the charm densities from different groups is not meaningful because each group fits different data to determine their respective input three flavor number gluon densities. However it seems that our charm density, at small μ^2, does not rise as steeply as that of the CTEQ5HQ [19] at small x. It is more similar to the MRST98 (central gluon) [18] density. In Fig. 4.10 we make a comparison between our charm density which evolves according to the renormalization group equation and the one computed in fixed order perturbation theory (FOPT) via Eq. (4.2.23). To that order we have plotted

$$R(x, \mu^2) = \frac{c^{\mathrm{EVOLVED}}(x, \mu^2)}{c^{\mathrm{FOPT}}(x, \mu^2)} \,. \tag{4.3.19}$$

The density c^{FOPT} is computed up to order α_s^2 since the OME's in Eq. (4.2.26) are only known up to that order. In Fig. 4.10a we have shown the ratio in LO. The latter implies that we have only kept the leading logarithms in $\ln \mu^2/m^2$ in the OME's which are resummed in all orders in c^{EVOLVED}. The deviation of R from unity shows the effect of the resummation. The same ratio is shown in NLO in Fig. 4.10b where we also included the subleading terms in the OME's. Finally if we take into account the non-logarithmic terms in the two-loop OME's $A_{Qg}^{\mathrm{S},(2)}$ and $A_{Qq}^{\mathrm{PS},(2)}$ (4.2.26) one obtains the NNLO ratio (see Fig.

4.10c). The figures reveal that in LO and NLO the effect of the resummation is very small except near $x = 1$. This picture changes if we go to NNLO where the deviation of R from one becomes appreciable when x tends to zero. Here R can even become negative which happens for $\mu^2 \approx 3$ (GeV/c)^2. This effect is wholly due to the boundary condition $c(x, m^2) \neq 0$ which occurs beyond NLO. Furthermore the figures reveal that $R > 1$ at large x whereas $R < 1$ at small x. Notice that in Fig. 4.10c $c^{\rm FOPT}(x, \mu^2) = 0$ for $x = 0.007$ at $\mu^2 = 2$ (GeV/c)^2 so that $R = \infty$ which explains the bump in the figure. Figure 4.10c is important because it shows that $c^{\rm EVOLVED}(x, \mu^2) < c^{\rm FOPT}(x, \mu^2)$ at small x. The consequence is that $F_{i,c}^{\rm BMSN}(x, Q^2)$ and $F_{i,c}^{\rm CSN}(x, Q^2)$ will become smaller than $F_{i,c}^{\rm EXACT}(x, Q^2)$ when Q^2 becomes slightly larger than m^2 due to the choice made for the factorization scale in Eq. (4.2.35). This can even lead to a negative structure function as will happen for $F_{L,c}^{\rm CSN}$ which we will see later on.

Now we present results for the various structure functions. In Fig.4.11 we show the charm quark structure functions in NNLO given by $F_{2,c}^{\rm CSN}(n_f = 4)$, $F_{2,c}^{\rm BMSN}(n_f = 4)$, $F_{2,c}^{\rm PDF}(n_f = 4)$ and $F_{2,c}^{\rm EXACT}(n_f = 3)$ plotted in the region $1 < Q^2 < 10^3$ (GeV/c)^2 for $x = 0.05$. The figure reveals that there is hardly any difference between the BMSN and CSN prescriptions. The curves in both prescriptions lie between the ones representing $F_{2,c}^{\rm PDF}(n_f = 4)$ and $F_{2,c}^{\rm EXACT}(n_f = 3)$ except for low Q^2. In this region the latter is a little bit larger than the other ones which is expected from the discussion of the charm density given above. Notice that in the low Q^2 region $F_{2,c}^{\rm PDF}(n_f = 4)$ becomes negative which means that charm quark electroproduction cannot be described by this quantity anymore. In Fig. 4.12 we present the same plots for $x = 0.005$. Again one cannot distinguish between $F_{2,c}^{\rm BMSN}(n_f = 4)$ and $F_{2,c}^{\rm CSN}(n_f = 4)$ but now both are smaller than $F_{2,c}^{\rm EXACT}(n_f = 3)$ over the whole Q^2 range. The latter is even larger than $F_{2,c}^{\rm PDF}(n_f = 4)$ in particular for $Q^2 > 50$ (GeV/c)^2. Further we want to emphasize that due to our careful treatment of the threshold region there is an excellent cancellation (to three significant places) between $F_{2,c}^{\rm PDF}(n_f = 4)$ and and $F_{2,c}^{\rm ASYMP}(n_f = 3)$ at very small Q^2 so that both $F_{2,c}^{\rm CSN}(n_f = 4)$ and $F_{2,c}^{\rm BMSN}(n_f = 4)$ tend to $F_{2,c}^{\rm EXACT}(n_f = 3)$. Also at large Q^2 we have an excellent cancellation between $F_{2,c}^{\rm ASYMP}(n_f = 3)$ and $F_{2,c}^{\rm EXACT}(n_f = 3)$ so that both $F_{2,c}^{\rm CSN}(n_f = 4)$ and $F_{2,c}^{\rm BMSN}(n_f = 4)$ tend to $F_{2,c}^{\rm PDF}(n_f = 4)$ (see Eq. (4.2.44)).

In Fig. 4.13 we show similar plots as in Fig. 4.11 but now for the charm quark longitudinal structure functions. Here we observe a difference between the plots for $F_{L,c}^{\rm CSN}(n_f = 4)$ and $F_{L,c}^{\rm BMSN}(n_f = 4)$ in the region $m_c^2 < Q^2 < 40$ (GeV/c)^2. In particular the latter tends to $F_{L,c}^{\rm EXACT}(n_f = 3)$ while the former is larger. Furthermore $F_{L,c}^{\rm PDF}(n_f = 3)$ is considerably larger than

the other three structure functions, which differs from the behavior seen in Fig. 4.11. This can be mainly attributed to the gluon density which plays a more prominant role in $F_{L,c}$ than in $F_{2,c}$. For $x = 0.005$ (see Fig. 4.14) the difference between the BMSN and the CSN descriptions becomes even more conspicuous. In this case $F_{L,c}^{\rm CSN}(n_f = 4)$ becomes negative in the region $m_c^2 < Q^2 < 7\ ({\rm GeV/c})^2$ which is unphysical. This effect can be attributed to the zeroth order longitudinal coefficient function in Eq. (4.3.9), which behaves like $\mathcal{C}_{L,Q}^{\rm CSN,NS,(0)} = 4m^2/Q^2$ (see [16]), and the non-vanishing charm density at $\mu^2 = m^2$. In the case of BMSN the longitudinal coefficient function is equal to zero in lowest order so that $F_{L,c}^{\rm BMSN}(n_f = 4)$ does not become negative.

In Figs. 4.15 and 4.16 we make a comparison between the NLO and the NNLO structure functions $F_{2,c}^{\rm CSN}(n_f = 4)$ and $F_{2,c}^{\rm BMSN}(n_f = 4)$. Both prescriptions i.e. CSN and BMSN lead to the same result in NNLO. However while going from NLO to NNLO the the structure function $F_{2,c}^{\rm CSN}(n_f = 4)$ decreases whereas $F_{2,c}^{\rm BMSN}(n_f = 4)$ increases a little bit. The differences in the case of $x = 0.005$ are even smaller than those observed for $x = 0.05$. The same comparison between NLO and NNLO is made for the longitudinal structure functions in Figs. 4.17 and 4.18. Here the differences between NLO and NNLO are much larger than in the case of $F_{2,c}$ in Figs. 4.15, 4.16. In NLO $F_{L,c}^{\rm BMSN}(n_f = 4)$ is smaller than the one plotted for NNLO. However for $F_{L,c}^{\rm CSN}(n_f = 4)$ we see a decrease in the small Q^2-region while going from NLO to NNLO whereas for large Q^2 we observe the opposite. In particular the valley in the region $m_c^2 < Q^2 < 7\ ({\rm GeV/c})^2$ observed for $F_{L,c}^{\rm CSN}(n_f = 4)$ at $x = 0.005$ in NNLO turns into a bump. This is due the boundary condition on the charm density which in NLO vanishes at $\mu = m_c$ whereas in NNLO it is negative at small x-values (see Fig. 4.10c). From the observations above one can conclude that the CSN prescription bedevils the threshold (low Q^2) behavior for $F_{L,c}$ due to the non-vanishing zeroth order longitudinal coefficient function $\mathcal{C}_{L,Q}^{\rm CSN,NS,(0)}$. This problem is avoided by TR in [10] by imposing a condition on the structure functions as indicated in Eq. (4.2.36). Hence our results for $F_{i,c}^{\rm BMSN}$ agree reasonably well for $i = 2$ and $i = L$ with those presented in NLO by TR in [10]. This is mainly due to the fact that there is only a small difference between the NLO and NNLO approximations in the BMSN scheme. It also reveals that the condition in Eq. (4.2.36) for $i = L$ can be mimicked by a vanishing zeroth order longitudinal coefficient function. Note that results for the x-values presented above are representative for the whole range $5 \times 10^{-5} < x < 0.5$.

To summarize the main points of this paper we have discussed two variable flavor number schemes for charm quark electroproduction in NNLO. They

are distinguished by the way mass factorization is implemented. In the CSN scheme this is done with respect to the full heavy and light quark structure functions at finite Q^2. In the BMSN scheme the mass factorization is only applied to the coefficient functions in the large Q^2 limit. Both schemes require three flavor and four flavor number parton densities which satisfy NNLO matching conditions at a scale $\mu^2 = m^2$. We have constructed these densities using our own evolution code. The schemes also require matching conditions on the coefficient functions which are implemented in this paper. We have also made a careful analysis of the removal of dangerous terms in $\ln(Q^2/m^2)$ from the Compton contributions so that both $F_{i,c}^{\rm CSN}(n_f+1)$ and $F_{i,c}^{\rm BMSN}(n_f+1)$ are collinearly safe. We have done this in a way which is simplest from the theoretical point of view, by implementing a cut Δ on the mass of the $c-\bar{c}$ pair which has to be determined by experiment. This cut is not required in the fixed order perturbation theory approach given by $F_{i,c}^{\rm EXACT}$ in [5] for moderate Q^2-values.

Finally we made a careful analysis of the threshold behaviors of $F_{i,c}^{\rm CSN}(n_f+1)$ and $F_{i,c}^{\rm BMSN}(n_f+1)$. In order to achieve the required cancellations near threshold so that they both become equal to $F_{i,c}^{\rm EXACT}(n_f)$ one must be very careful to combine terms with the same order in the expansion in the running coupling constant α_s. Therefore technically we require six sets of parton densities, namely the LO, NLO and NNLO three flavor number sets and the LO, NLO and NNLO four flavor number sets. However not all the necessary theoretical inputs are available to us to finish this task. The approximations we made in this paper were sufficient to provide very clear answers. We successfully implemented the required cancellations near threshold and the corresponding limits at large scales came out naturally. Inconsistent sets of parton densities automatically spoil these cancelations. We did not have to use matching conditions on derivatives of structure functions as proposed in [10], which seem very artificial. The numerical results do however end up quite similar. We have also shown that the CSN scheme defined above leads to an unnatural behavior of the longitudinal structure function in the threshold region which is due to a non-vanishing zeroth order coefficient function. Since there are no other differences between the CSN and BMSN schemes we recommend the latter because it is less complicated than the former. In particular it does not need additional coefficient functions other than the existing heavy quark and light parton coefficient functions available in the literature.

ACKNOWLEDGMENTS

The work of A. Chuvakin and J. Smith was partially supported by the National Science Foundation grant PHY-9722101. The work of W.L. van Neerven was supported by the EC network 'QCD and Particle Structure' under contract

No. FMRX–CT98–0194.

4.4 Appendix A

In this appendix we present the exact expressions for the heavy quark coefficient functions $L_{i,q}^{(2)}$ corresponding to the Compton process in Fig. 4.5 when there is a cut Δ on the invariant mass $s_{Q\bar{Q}}$ of the heavy quark pair. As explained in [15] the calculation is straightforward because one can first integrate over the heavy quark momenta in the final state without affecting the momentum of the remaining light quark. The phase space integrals are the same as the ones obtained for the process $\gamma(q) + q(k_1) \to g^* + q$ ($g^* \to Q + \bar{Q}$) where the gluon becomes virtual. In the expressions for the complete integration over the virtual mass $s_{Q\bar{Q}}$ of the gluon (see Fig. 4.5) one integrates over the range $4\,m^2 \le s_{Q\bar{Q}} \le s$ with $s = (q + k_1)^2$. The resulting expressions, called $L_{i,q}^{\mathrm{r},(2)}$ with $r = \mathrm{NS,S}$ and $i = 2, L$ are presented in appendix A of [15]. Notice that up to order α_s^2 there is no difference between singlet and non-singlet so that $L_{i,q}^{\mathrm{NS},(2)} = L_{i,q}^{\mathrm{S},(2)}$. If we limit the range of integration to $4\,m^2 \le s_{Q\bar{Q}} \le \Delta$ one obtains

$$
\begin{aligned}
L_{L,q}^{\mathrm{SOFT,NS},(2)}(z,\Delta,\frac{Q^2}{m^2}) &= C_F T_f \Big\{ 96 a^2(s) z (1-z)^2 \Big[L_1 (L_2 + L_4 + L_5) \\
&-2(DIL_1 - DIL_2 - DIL_3 + DIL_4) \Big] - 32 a^2(s) [1 + 3(1-z) \\
&-6(1-z)^2] L_1 + \frac{16}{3} z \Big[1 - 26 a(s)(1-z) + 88 a^2(s)(1-z)^2 \Big] \frac{L_3}{sq_2} \\
&-\frac{256}{3} b(\Delta) a(s) z (1-z)(1-d(\Delta)) L_6 + \frac{64}{3} b(\Delta) a(s) \Big[2 + 10(1-z) \\
&-14(1-z)^2 - d(\Delta) \Big(2 - (1-z) - 3(1-z)^2 \Big) \Big] \\
&-128 b(\Delta) d(\Delta) a^2(s) z (1-z)^2 (1 + 2d(\Delta)) L_6 \\
&+\frac{64}{3} b(\Delta) d(\Delta) a^2(s) \Big(1 + 2d(\Delta) \Big) \Big[1 + 3(1-z) - 6(1-z)^2 \Big] \\
&-\frac{32}{3} b(\Delta) z + \frac{16}{9} b^3(\Delta) z \Big\} \,, \qquad (4.1.1)
\end{aligned}
$$

$$
\begin{aligned}
L_{2,q}^{\mathrm{SOFT,NS},(2)}(z,\Delta,\frac{Q^2}{m^2}) &= C_F T_f \Big\{ \Big(\frac{4}{3} \frac{1+z^2}{1-z} - 16 a^2(s)(1-z)[1 \\
&-9(1-z) + 9(1-z)^2] \Big) [L_1 (L_2 + L_4 + L_5) - 2(DIL_1 - DIL_2 \\
&-DIL_3 + DIL_4)] - \Big(\frac{8}{3} - \frac{4}{1-z} + 8 a^2(s) [2 + 18(1-z) \\
&-36(1-z)^2 + \frac{1}{1-z}] \Big) L_1 + \Big(\frac{8}{9} [28 - 17(1-z) - \frac{19}{1-z}]
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{16}{9}a(s)[61-160(1-z)+128(1-z)^2] \\
&-\frac{64}{9}a^2(s)(1-z)[23-104(1-z)+94(1-z)^2]\Big)\frac{L_3}{sq_2} \\
&+\frac{64}{3}b(\Delta)a(s)\Big[\Big[2-7(1-z)+6(1-z)^2\Big](1-d(\Delta)) \\
&+d(\Delta)a(s)(1-z)[1-9(1-z)+9(1-z)^2](1+2d(\Delta))\Big]L_6 \\
&+\frac{8}{9}b(\Delta)\Big(6-b^2(\Delta)\Big)\Big[2-(1-z)-\frac{2}{1-z}\Big]L_6 \\
&-\frac{32}{3}b(\Delta)d(\Delta)a(s)\Big[7-3(1-z)-9(1-z)^2-\frac{1}{1-z}\Big] \\
&-\frac{32}{9}b(\Delta)a(s)\Big[2-95(1-z)+121(1-z)^2+\frac{3}{1-z}\Big] \\
&+\frac{16}{3}b(\Delta)d(\Delta)a^2(s)\Big(1+2d(\Delta)\Big)\Big[2+18(1-z) \\
&-36(1-z)^2+\frac{1}{1-z}\Big]-\frac{8}{9}b(\Delta)\Big[50-34(1-z)-\frac{29}{1-z}\Big] \\
&+\frac{4}{27}b^3(\Delta)\Big[38-28(1-z)-\frac{17}{1-z}\Big]\Big\}\,, \qquad (4.1.2)
\end{aligned}
$$

where the partonic scaling variable is equal to $z = Q^2/(2q\cdot k_1) = Q^2/(s+Q^2)$, Further we have defined

$$
\begin{aligned}
&\xi = \frac{Q^2}{m^2} \quad , \quad sq_1 = \sqrt{1-4\frac{z}{(1-z)\xi}} \quad , \qquad sq_2 = \sqrt{1-4\frac{z}{\xi}}\,, \\
&a(s) = \frac{m^2}{s} = \frac{z}{(1-z)\xi} \quad , \quad b(\Delta) = \sqrt{1-4\frac{m^2}{\Delta}} \quad , \quad d(\Delta) = \frac{\Delta}{4\ m^2} \\
&L_1 = \ln\Big(\frac{1+b(\Delta)}{1-b(\Delta)}\Big) \quad , \quad L_2 = \ln\Big(\frac{1+sq_2}{1-sq_2}\Big) \quad , \quad L_3 = \ln\Big(\frac{sq_2+b(\Delta)}{sq_2-b(\Delta)}\Big)\,, \\
&L_4 = \ln\Big(\frac{1-z}{z^2}\Big) \quad , \quad L_5 = \ln\Big(\frac{1-b^2(\Delta)}{1-sq_1^2}\Big) \quad , \quad L_6 = \ln\Big(\frac{sq_2^2-b^2(\Delta)}{z(1-sq_1^2)}\Big)\,, \\
&DIL_1 = \mathrm{Li}_2\Big(\frac{(1-sq_2^2)(1+b(\Delta))}{(1+sq_2)(1-b^2(\Delta))}\Big) \quad , \quad DIL_2 = \mathrm{Li}_2\Big(\frac{1-sq_2}{1+b(\Delta)}\Big) \quad , \\
&DIL_3 = \mathrm{Li}_2\Big(\frac{1-b(\Delta)}{1+sq_2}\Big) \quad , \quad DIL_4 = \mathrm{Li}_2\Big(\frac{1+b(\Delta)}{1+sq_2}\Big)\,. \qquad (4.1.3)
\end{aligned}
$$

The variable Δ, which allows us to distinguish between soft and hard (observable) heavy quark anti-quark pairs, is in the range $4m^2 \le \Delta \le s$. The variable z is in the range $0 \le z \le \xi/(\xi+4)$.

Note that when $\Delta = s$ one obtains $L_{L,q}^{\rm SOFT,r,(2)} \to L_{i,q}^{\rm r,(2)}$ which are reported in [15]. When the integration range is given by $\Delta \leq s_{Q\bar{Q}} \leq s$ we get $L_{i,q}^{\rm HARD,r,(2)}$ which are given by

$$L_{i,q}^{\rm HARD,NS,(2)}(z,\Delta,\frac{Q^2}{m^2}) = L_{i,q}^{\rm NS,(2)}(z,\frac{Q^2}{m^2}) - L_{i,q}^{\rm SOFT,NS,(2)}(z,\Delta,\frac{Q^2}{m^2})\,. \quad (4.1.4)$$

Notice that $L_{i,q}^{\rm HARD,NS,(2)}$ is finite in the limit $m \to 0$ so that it does not contain collinear divergences. The latter can be wholly attributed to $L_{i,q}^{\rm SOFT,NS,(2)}$ as is revealed if one takes the limit $Q^2 \to \infty$. In this case the expressions (A.1) and (A.2) reduce to

$$\begin{aligned}
L_{L,q}^{\rm SOFT,ASYMP,NS,(2)}(z,\Delta,\frac{Q^2}{m^2}) &= C_F T_f \Big[\frac{16}{3} z \ln\frac{Q^2}{m^2} - \frac{16}{3} z \ln\Big(\frac{Q^2}{\Delta} - z\Big) \\
&+ \frac{32}{3} z \ln\frac{1+b(\Delta)}{2} - \frac{80}{9} z - \frac{80}{9}(b(\Delta)-1)z + \frac{16}{9} b(\Delta)\Big(b^2(\Delta)-1\Big)z \\
&+ b(\Delta)\Bigg\{\Big(\frac{64}{3}\frac{\Delta}{Q^2} z^2 - 16\frac{\Delta^2}{Q^4} z^3\Big) \ln\Big[\Big(\frac{Q^2}{\Delta} - z\Big)\frac{(1-z)}{z^2}\Big] \\
&- \frac{16}{3}\frac{\Delta}{Q^2} z\Big(\frac{2}{1-z} - 4 + 3z\Big) + \frac{8}{3}\frac{\Delta^2}{Q^4} z^2\Big(\frac{1}{(1-z)^2} + \frac{3}{1-z} - 6\Big)\Bigg\}\Big] \quad (4.1.5)
\end{aligned}$$

and

$$\begin{aligned}
L_{2,q}^{\rm SOFT,ASYMP,NS,(2)}(z,\Delta,\frac{Q^2}{m^2}) &= C_F T_f \Big[\Big(\frac{1+z^2}{1-z}\Big)\Big\{\frac{8}{3}\ln\frac{Q^2}{m^2}\ln\Big(\frac{1-z}{z^2}\Big) \\
&+ \Big(\frac{8}{3}\ln\frac{Q^2}{m^2} + \frac{16}{3}\ln\Big(\frac{1-z}{z^2}\Big) + \frac{8}{3}\ln\frac{Q^2}{\Delta} - \frac{116}{9}\Big)\ln\Big(\frac{1+b(\Delta)}{2}\Big) \\
&+ \frac{4}{3}\ln^2\frac{Q^2}{m^2} - \frac{4}{3}\ln^2\frac{Q^2}{\Delta} - \frac{8}{3}\ln\frac{Q^2}{\Delta}\ln\Big(\frac{1-z}{z^2}\Big) - \frac{8}{3}{\rm Li}_2\Big(\frac{\Delta z(1+b(\Delta))}{2Q^2}\Big) \\
&- \frac{8}{3}{\rm Li}_2\Big(\frac{1+b(\Delta)}{2}\Big) + \frac{8}{3}{\rm Li}_2\Big(\frac{2m^2}{\Delta(1+b(\Delta))}\Big) - \frac{58}{9}\ln\frac{Q^2}{m^2} - 2\ln\frac{Q^2}{\Delta} \\
&+ 4\ln\Big(\frac{Q^2}{\Delta} - z\Big) - \frac{40}{9}\ln\Big(\frac{1-z}{z^2}\Big) + \frac{314}{27}\Big\} + \Big(\frac{2}{3} + \frac{26}{3}z\Big)\ln\frac{Q^2}{m^2} \\
&+ \Big(\frac{2}{3} - 2z\Big)\ln\frac{Q^2}{\Delta} - \Big(\frac{4}{3} + \frac{20}{3}z\Big)\ln(\frac{Q^2}{\Delta} - z) + \Big(\frac{4}{3} + \frac{52}{3}z\Big)\ln\frac{1+b(\Delta)}{2} \\
&- \frac{10}{9} - \frac{130}{9}z + b(\Delta)\Bigg\{\Big[-\frac{16}{3}\frac{\Delta}{Q^2}z\Big(\frac{2}{1-z} - 1 - 6z\Big) + \frac{8}{3}\frac{\Delta^2}{Q^4}z^2\Big(\frac{1}{1-z} \\
&- 9z\Big)\Big]\ln\Big[\Big(\frac{Q^2}{\Delta} - z\Big)\frac{(1-z)}{z^2}\Big] - \frac{8}{3}\frac{\Delta}{Q^2}z\Big(\frac{7}{1-z} - 12 + 9z - \frac{1}{(1-z)^2}\Big)
\end{aligned}$$

$$+\frac{2}{3}\frac{\Delta^2}{Q^4}z^2\Big(\frac{2}{(1-z)^2}+\frac{18}{1-z}-36+\frac{1}{(1-z)^3}\Big)\Big\}+\Big(\frac{8}{9}b(\Delta)(1-b^2(\Delta))$$
$$+\frac{40}{9}\Big(b(\Delta)-1\Big)\Big(1+z-\frac{2}{1-z}\Big)\ln\left(\Big(\frac{Q^2}{\Delta}-z\Big)\frac{(1-z)}{z^2}\right)$$
$$+\frac{4}{27}b(\Delta)\Big(b^2(\Delta)-1\Big)\Big(10+28z-\frac{17}{1-z}\Big)+(b(\Delta)-1)\Big(-\frac{344}{27}$$
$$-\frac{704}{27}z+\frac{628}{27}\frac{1}{1-z}\Big)\Big] \tag{4.1.6}$$

respectively. In the limit $m \to 0$ the results above show the same logarithmic terms in $\ln^i(Q^2/m^2)$ $(i = 1, 2)$ as the asymptotic expressions for $L_{i,q}^{\mathrm{r},(2)}$ given in Eqs. (D.7) and (D.8) of [15]. Hence the differences between the results there and the asymptotic expressions above are free of any terms in $\ln(Q^2/m^2)$. The asymptotic expressions of $L_{i,q}^{\mathrm{HARD,r},(2)}$ for $Q^2 \to \infty$ are given by

$$L_{L,q}^{\mathrm{HARD,ASYMP,NS},(2)}(z,\Delta,\frac{Q^2}{m^2}) = C_F T_f\left[\frac{16}{3}z\ln\frac{1-z}{z^2}+\frac{16}{3}z\ln\Big(\frac{Q^2}{\Delta}-z\Big)\right.$$
$$-\frac{32}{3}z\ln\frac{1+b(\Delta)}{2}+\frac{16}{3}-\frac{40}{3}z+\frac{80}{9}(b(\Delta)-1)z+\frac{16}{9}b(\Delta)\Big(1$$
$$-b^2(\Delta)\Big)z-b(\Delta)\left\{\Big(\frac{64}{3}\frac{\Delta}{Q^2}z^2-16\frac{\Delta^2}{Q^4}z^3\Big)\ln\left(\Big(\frac{Q^2}{\Delta}-z\Big)\frac{(1-z)}{z^2}\right)\right.$$
$$\left.\left.-\frac{16}{3}\frac{\Delta}{Q^2}z\Big(\frac{2}{1-z}-4+3z\Big)+\frac{8}{3}\frac{\Delta^2}{Q^4}z^2\Big(\frac{1}{(1-z)^2}+\frac{3}{1-z}-6\Big)\right\}\right], \tag{4.1.7}$$

and

$$L_{2,q}^{\mathrm{HARD,ASYMP,},(2)}(z,\Delta,\frac{Q^2}{m^2}) = C_F T_f\left[\Big(\frac{1+z^2}{1-z}\Big)\left\{\frac{4}{3}\ln^2(1-z)\right.\right.$$
$$-2\ln\Big(\frac{1-z}{z^2}\Big)-\frac{16}{3}\ln z\ln(1-z)+6\ln z+\frac{5}{3}+\frac{4}{3}\ln^2\frac{Q^2}{\Delta}$$
$$+\frac{8}{3}\ln\frac{Q^2}{\Delta}\ln\Big(\frac{1-z}{z^2}\Big)+\Big(\frac{116}{9}-\frac{8}{3}\ln\frac{Q^2}{m^2}-\frac{16}{3}\ln\Big(\frac{1-z}{z^2}\Big)-\frac{8}{3}\ln\frac{Q^2}{\Delta}\Big)$$
$$\times\ln\Big(\frac{1+b(\Delta)}{2}\Big)+\frac{8}{3}\mathrm{Li}_2\Big(\frac{\Delta z(1+b(\Delta))}{2Q^2}\Big)+\frac{8}{3}\mathrm{Li}_2\Big(\frac{1+b(\Delta)}{2}\Big)-\frac{8}{3}\zeta(2)$$
$$\left.-\frac{8}{3}\mathrm{Li}_2(1-z)-\frac{8}{3}\mathrm{Li}_2\Big(\frac{2m^2}{\Delta(1+b(\Delta))}\Big)+2\ln\frac{Q^2}{\Delta}-4\ln\Big(\frac{Q^2}{\Delta}-z\Big)\right\}$$
$$-\Big(\frac{2}{3}-2z\Big)\ln\frac{Q^2}{\Delta}+\Big(\frac{4}{3}+\frac{20}{3}z\Big)\ln(\frac{Q^2}{\Delta}-z)-\Big(\frac{4}{3}+\frac{52}{3}z\Big)\ln\Big(\frac{1+b(\Delta)}{2}\Big)$$

$$+\Big(\frac{2}{3}+\frac{26}{3}z\Big)\ln(1-z)-\Big(2+\frac{46}{3}z\Big)\ln z+\frac{13}{3}-\frac{55}{3}z+b(\Delta)\Big\{\Big[\frac{16}{3}\frac{\Delta}{Q^2}z$$
$$\times\Big(\frac{2}{1-z}-1-6z\Big)-\frac{8}{3}\frac{\Delta^2}{Q^4}z^2\Big(\frac{1}{1-z}-9z)\Big)\Big]\ln\Big[\Big(\frac{Q^2}{\Delta}-z\Big)\frac{(1-z)}{z^2}\Big]$$
$$+\frac{8}{3}\frac{\Delta}{Q^2}z\Big(\frac{7}{1-z}-12+9z-\frac{1}{(1-z)^2}\Big)-\frac{2}{3}\frac{\Delta^2}{Q^4}z^2\Big(\frac{2}{(1-z)^2}+\frac{18}{1-z}$$
$$-36+\frac{1}{(1-z)^3}\Big)\Big\}+\Big(\frac{8}{9}b(\Delta)(b^2(\Delta)-1)+\frac{40}{9}(1-b)\Big)\Big(1+z-\frac{2}{1-z}\Big)$$
$$\times\ln\Big[\Big(\frac{Q^2}{\Delta}-z\Big)\frac{(1-z)}{z^2}\Big]+\frac{4}{27}b(\Delta)(1-b^2(\Delta))\Big(10+28z-\frac{17}{1-z}\Big)$$
$$+(1-b(\Delta))\Big(-\frac{344}{27}-\frac{704}{27}z+\frac{628}{27}\frac{1}{1-z}\Big)\Big] \qquad (4.1.8)$$

respectively. As has been mentioned below Eq. (4.4) the expressions above are finite in the limit $m \to 0$ ($b \to 1$) so that they do not contain collinear divergences.

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Chapter 5

Bottom quark electroproduction in variable flavor number schemes

5.1 Introduction

The H1 and ZEUS experiments at HERA now have enough integrated luminosity to study bottom quark deep inelastic electroproduction. Therefore it is an appropriate time to present up-to-date predictions for the bottom quark components of the deep inelastic structure functions $F_i(x,Q^2)$ where $i = 2, L$. We assume that the bottom quark is produced in an extrinsic fashion and that the neutral current reaction dominates over the charged current one. This means that in fixed order perturbative QCD the heavy quark structure functions $F_{i,b}(x,Q^2,m_b^2)$, $i = 2, L$ are given by the virtual-photon gluon-fusion processes and their higher order corrections with only light partons in the initial state. Notice that in the case of bottom quark production the light partons are represented by the gluon and the four light flavors u, d, s, c together with their anti-particles.

In the literature one has adopted two different treatments of extrinsic bottom quark production, which are known as the massive and massless descriptions. The former treats the bottom quark as a heavy quark (with mass m_b) and the partonic cross sections (or heavy quark coefficient functions) are described by fixed order perturbation theory (FOPT) as mentioned above. Notice that due to the work in [1] the perturbation series is now known up to second order. The latter treatment, which has been rather popular among groups which fit parton densities to experimental data, treats the bottom quark as a massless quark so that it can be represented by a scale dependent parton density $f_b(x,\mu^2)$. Although at first sight these approaches are completely different they are actually intimately related. It was shown in [2] that the large logarithms of the type $\ln(Q^2/m_b^2)$, which appear in FOPT when $Q^2 \gg m_b^2$, can be resummed in all orders. The upshot of this procedure is that the bottom components of the deep inelastic structure functions $F_{i,b}(x,Q^2,m_b^2)$, where $i = 2, L$, which in the FOPT approach are written as convolutions of heavy quark coefficient functions with four-flavor light-mass (u,d,s,c) parton densities, become, after resummation, convolutions of light-mass parton coefficient functions with five-flavor light-mass parton densities which also include a bottom quark density. This procedure leads to the so-called zero mass variable flavor number scheme (ZM-VFNS) for $F_{i,b}(x,Q^2)$ where the mass of the bottom quark is absorbed into the new five flavor densities. To implement this scheme one has to be careful to use quantities which are collinearly finite in the limit $m_b \to 0$. From the above considerations it is clear that the FOPT approach is better when the bottom quark pair is produced near threshold (where $Q^2(x^{-1}-1) \geq 4m_b^2$) because terms in m_b are important in this kinematic region. On the other hand far above threshold, where also $Q^2 \gg m_b^2$, the

large logarithms mentioned above dominate the structure functions so that the ZM-VFNS approach should be more appropriate. Both approaches are characterized by the number of active flavors involved in the description of the parton densities which are given by four and five respectively. Each scheme has different densities but the momentum sum rule either gets contributions from four-flavor densities or five-flavor densities and is always satisfied.

As most of the experimental data will be in the kinematical regime which is between the threshold and the large Q^2 region, a third approach, called the variable flavour number scheme (VFNS), has been introduced to describe the heavy quark components $F_{i,b}(x,Q^2)$ of the deep inelastic structure functions. Actually there are several such schemes. They include the Aivasis, Collins, Olness, Tung (ACOT) [3], scheme, the Buza, Matiounine, Smith, van Neerven (BMSN) [2], [4] scheme, the Thorne, Roberts (TR) [5] scheme and the Chuvakin, Smith, van Neerven (CSN) [6] scheme. A discussion of them is given in the last reference. The difference between the schemes can be attributed to two ingredients entering in their construction. The first one is the mass factorization procedure carried out before the large logarithms can be resummed. The second one is the matching condition imposed on the heavy quark density, which has to vanish in the threshold region of the production process. Another aspect of these approaches is that one needs two sets of parton densities. For bottom quark production one set only contains densities in a four-flavor number scheme whereas the second one, which also includes a bottom quark density, is parametrized in a five-flavor number scheme. Both parameterizations have to satisfy the matching relations quoted in [2]. Up to next-to-leading order (NLO) they are continuous at the scale $\mu = m_b$ whereas in next-to-next-to leading order (NNLO) the parton densities become discontinuous while going from a four to a five flavor scheme. Starting from a three-flavor set of parton densities given in [7] we have recently constructed in [8] a four-flavor set of densities which satisfied the matching relations in [2] at the scale $\mu = m_c$. Then we evolved these densities with LO or NLO splitting functions up to the scale $\mu = m_b$ and constructed a five-flavor set which also satisfied the matching relations in [2]. This set was further evolved with LO and NLO splitting functions up to high scales. Notice that since the NNLO splitting functions are unknown the only difference between the NLO and NNLO parton densities can be attributed to the boundary conditions at $\mu = m_c$ and $\mu = m_b$ where the latter densities become discontinuous contrary to the LO and NLO ones. We can now use these densities to discuss VFNS for bottom quark deep inelastic electroproduction, in particular in the CSN and BMSN schemes. The previous discussions in [6] were focussed on applications to charm quark electroproduction.

Since any description for bottom quarks follows closely that for charm quarks we refer the interested reader to [6] for most of the details and simply specialize to bottom quark electroproduction in Sec.II. We work to second order in the running coupling constant $\alpha_s(\mu^2)$. Numerical results are shown for the structure functions $F_{2,b}$ and $F_{L,b}$ in the CSN and BMSN schemes.

5.2 Bottom quark structure functions

In this Section we consider bottom quark deep inelastic electroproduction in two variable flavor number schemes, namely the BMSN scheme as proposed in [2], [4] and in the CSN scheme as proposed in [6]. For that purpose we have constructed in [8] a five-flavor parton density set from a four-flavor parton density set. Using our densities we will study the differences between the bottom components of the deep inelastic structure functions $F_{i,b}^{\rm CSN}(n_f+1)$ and $F_{i,b}^{\rm BMSN}(n_f+1)$, where the number of light flavors is $n_f = 4$.

To keep the discussion short we simply refer the reader to Sec.III of [6] for a discussion of the $\overline{\rm MS}$ parton densities, the exact solution for the running coupling constant and the scale choice. All references to three-flavour (four-flavor) densities should be replaced by four-flavor (five-flavor) densities respectively. All our calculations of next-to-leading (NLO) and next-to-next-leading order (NNLO) quantities use $\Lambda_{3,4,5,6}^{\overline{\rm MS}} = 299.4, 246, 167.7, 67.8$ MeV, which yields $\alpha_s(5, M_Z^2) = 0.114$. The structure functions are defined in Eqs.(3.9)-(3.17) of [6], where now $n_f = 4$ and m_c is replaced by $m_b = 4.5$ GeV/c^2. To make this paper reasonably self-contained we now reproduce the final formulae we use for the structure functions. For $i = 2, L$ the CSN scheme uses

$$
\begin{aligned}
F_{i,Q}^{\rm CSN}(n_f+1,\Delta,Q^2,m^2) = e_Q^2 \Bigg[& f_{Q+\bar{Q}}^{\rm NNLO}(n_f+1,\mu^2) \mathcal{C}_{i,Q}^{\rm CSN,NS,(0)}\Big(\frac{Q^2}{m^2}\Big) \\
& + a_s(n_f+1,\mu^2) \Bigg\{ f_{Q+\bar{Q}}^{\rm NLO}(n_f+1,\mu^2) \otimes \mathcal{C}_{i,Q}^{\rm CSN,NS,(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \\
& + f_g^{\rm S,NLO}(n_f+1,\mu^2) \otimes \mathcal{C}_{i,g}^{\rm CSN,S,(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \Bigg\} \\
& + a_s^2(n_f+1,\mu^2) \Bigg\{ f_{Q+\bar{Q}}^{\rm LO}(n_f+1,\mu^2) \otimes \Bigg(\mathcal{C}_{i,q}^{\rm NS,(2)}\Big(n_f+1,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \\
& + \mathcal{C}_{i,q}^{\rm PS,(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \Bigg) + \sum_{l=1}^{n_f} f_{l+\bar{l}}^{\rm LO}(n_f+1,\mu^2) \otimes \mathcal{C}_{i,q}^{\rm CSN,PS,(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \\
& + f_g^{\rm S,LO}(n_f+1,\mu^2) \otimes \mathcal{C}_{i,g}^{\rm CSN,S,(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big) \Bigg\} \Bigg] \\
& + a_s^2(n_f+1,\mu^2) \sum_{k=1}^{n_f} e_k^2\, f_{k+\bar{k}}^{\rm LO}(n_f+1,\mu^2) \otimes L_{i,q}^{\rm HARD,NS,(2)}\Big(\Delta,\frac{Q^2}{m^2}\Big) \,. \qquad (5.2.1)
\end{aligned}
$$

where we choose the heavy quark Q to be the bottom quark, so that the number of light flavors is $n_f = 4$. The charge of the bottom quark is $e_Q = -1/3$ and its mass is $m = m_b$. The coefficient function $L_{i,q}^{\rm HARD}$ depends on a parameter Δ which refers to the invariant mass of the $Q\ \bar{Q}$-pair. For bottom quark production we choose $\Delta = 100\ ({\rm GeV}/c)^2$. The coefficient functions labelled by $C^{\rm CSN}$ depend on the heavy quark mass but are finite in the limit $m \to 0$. They are defined in Eqs.(2.8)-(2.20) in [6]. To simplify the notation we will refer to the above structure functions as $F_{i,b}^{\rm CSN}(n_f = 5)$, indicating that they depend on five-flavor parton densities.

The same parameters e_Q, m_b, Δ etc., also show up in the expressions for the bottom quark structure functions in the BMSN scheme. Here we have the representations

$$F_{i,Q}^{\rm BMSN}(n_f+1,\Delta,Q^2,m^2) = F_{i,Q}^{\rm EXACT}(n_f,\Delta,Q^2,m^2)$$

$$-F_{i,Q}^{\rm ASYMP}(n_f,\Delta,Q^2,m^2) + F_{i,Q}^{\rm PDF}(n_f+1,\Delta,Q^2,m^2)\,. \qquad (5.2.2)$$

The pieces in this formulae represent first the results in FOPT, given by

$$F_{i,Q}^{\rm EXACT}(n_f,\Delta,Q^2,m^2) = e_Q^2\left[a_s(n_f,\mu^2) f_g^{\rm S,NLO}(n_f,\mu^2) \otimes H_{i,g}^{\rm S,(1)}\Big(\frac{Q^2}{m^2}\Big)\right.$$

$$+a_s^2(n_f,\mu^2)\left\{\sum_{k=1}^{n_f} f_{k+\bar{k}}^{\rm LO}(n_f,\mu^2)\otimes H_{i,q}^{\rm PS,(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right.$$

$$\left.\left.+f_g^{\rm S,LO}(n_f,\mu^2)\otimes H_{i,g}^{\rm S,(2)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\right\}\right]$$

$$+a_s^2(n_f,\mu^2)\sum_{k=1}^{n_f} e_k^2 f_{k+\bar{k}}^{\rm LO}(n_f,\mu^2)\otimes L_{i,q}^{\rm HARD,NS,(2)}\Big(\Delta,\frac{Q^2}{m^2}\Big)\,. \qquad (5.2.3)$$

The next pieces are the structure functions $F_{i,Q}^{\rm ASYMP}(n_f)$ which can be obtained from $F_{i,Q}^{\rm EXACT}(n_f)$ by replacing all exact heavy quark coefficient functions $H_{i,k}$ and $L_{i,k}$ $(k = q,g)$ by their asymptotic analogues which are defined by

$$H_{i,k}^{\rm ASYMP} = \lim_{Q^2\gg m^2} H_{i,k} \quad , \quad L_{i,k}^{\rm ASYMP} = \lim_{Q^2\gg m^2} L_{i,k}\,. \qquad (5.2.4)$$

Finally the structure functions $F_{i,Q}^{\rm PDF}(n_f+1)$ which are very often called the ZM-VFNS representations are defined by

$$F_{i,Q}^{\rm PDF}(n_f+1,\Delta,Q^2,m^2) = e_Q^2\Big[f_{Q+\bar{Q}}^{\rm NNLO}(n_f+1,\mu^2)\mathcal{C}_{i,q}^{\rm NS,(0)}$$

$$
\begin{aligned}
&+a_s(n_f+1,\mu^2)\left\{f^{\rm NLO}_{Q+\bar{Q}}(n_f+1,\mu^2)\otimes\mathcal{C}^{\rm NS,(1)}_{i,q}(\frac{Q^2}{\mu^2})\right.\\
&\left.+f^{\rm S,NLO}_{g}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}^{\rm S,(1)}_{i,g}(\frac{Q^2}{\mu^2})\right\}\\
&+a_s^2(n_f+1,\mu^2)\left\{f^{\rm LO}_{Q+\bar{Q}}(n_f+1,\mu^2)\otimes\left(\mathcal{C}^{\rm NS,(2)}_{i,q}(n_f+1,\frac{Q^2}{\mu^2})\right.\right.\\
&\left.\left.+\tilde{\mathcal{C}}^{\rm PS,(2)}_{i,q}\Big(\frac{Q^2}{\mu^2}\Big)\right)+\sum_{l=1}^{n_f}f^{\rm LO}_{l+\bar{l}}(n_f+1,\mu^2)\Big)\otimes\tilde{\mathcal{C}}^{\rm PS,(2)}_{i,q}\Big(\frac{Q^2}{\mu^2}\Big)\right.\\
&\left.+f^{\rm S,LO}_{g}(n_f+1,\mu^2)\otimes\tilde{\mathcal{C}}^{\rm S,(2)}_{i,g}(\frac{Q^2}{\mu^2})\right\}\Big]\\
&+a_s^2(n_f+1,\mu^2)\sum_{k=1}^{n_f}e_k^2 f^{\rm LO}_{k+\bar{k}}(n_f,\mu^2)\otimes L^{\rm HARD,ASYMP,NS,(2)}_{i,q}\Big(\Delta,\frac{Q^2}{m^2}\Big)\,.
\end{aligned}
\tag{5.2.5}
$$

In all these results the heavy quark Q refers to the bottom quark and the other parameters are defined above. For simplicity we will refer to these structure functions as $F^{\rm EXACT}_{i,b}(n_f=4)$, $F^{\rm ASYMP}_{i,b}(n_f=4)$, and $F^{\rm PDF}_{i,b}(n_f=5)$ respectively, which indicates that the first two structure functions depend on four-flavor densities and the last one depends on five-flavor densities. The parton densities f_k in the above formulae are represented in leading order (LO), next-to-leading order (NLO) and next-to-next-to-leading order (NNLO). The NNLO case refers to the boundary conditions imposed in [6] since the three-loop splitting functions are not known yet. These parton densities have been constructed in [8] starting from a three-flavor parametrization in [7]. The multiplication of the densities with the heavy and light parton coefficient functions is done in such a way that the perturbation series is strictly truncated at order α_s^2. This is necessary to avoid scheme dependent terms which would otherwise arise beyond order α_s^2. Therefore the following requirement is satisfied

$$
F^{\rm CSN}_{i,Q}(n_f=5)=F^{\rm BMSN}_{i,Q}(n_f=5)=F^{\rm EXACT}_{i,Q}(n_f=4)\quad\text{for}\quad Q^2\le m^2\,. \tag{5.2.6}
$$

Since $f_Q(m^2)^{\rm NNLO}\neq 0$ (see [2]) this condition can be only satisfied when we truncate the perturbation series at the same order. Furthermore because of

Eq. (5.2.4) and the property

$$\lim_{Q^2 \gg m^2} \mathcal{C}_{i,k}^{\mathrm{CSN},(\mathrm{l})}(n_f+1, \frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}) = \mathcal{C}_{i,k}^{(l)}(n_f+1, \frac{Q^2}{\mu^2}) \,, \tag{5.2.7}$$

we have the asymptotic relation

$$\lim_{Q^2 \gg m^2} F_{i,Q}^{\mathrm{BMSN}}(n_f+1, \Delta, Q^2, m^2) = \lim_{Q^2 \gg m^2} F_{i,Q}^{\mathrm{CSN}}(n_f+1, \Delta, Q^2, m^2)$$

$$= F_{i,Q}^{\mathrm{PDF}}(n_f+1, \Delta, Q^2, m^2) \,. \tag{5.2.8}$$

At first sight the form of the expression for $F_{i,Q}^{\mathrm{BMSN}}$ in Eq. (5.2.2) looks quite different from the one presented for $F_{i,Q}^{\mathrm{CSN}}$ in Eq. (5.2.1). However this is not true. Using the mass factorization relations for the asymptotic heavy quark coefficient functions in [2] one can cast $F_{i,Q}^{\mathrm{BMSN}}$ into the same form as presented for $F_{i,Q}^{\mathrm{CSN}}$ where all quark coefficient functions of the type $\mathcal{C}_{i,Q}^{\mathrm{CSN}}$ are replaced by their light quark analogues $\mathcal{C}_{i,q}$ appearing in Eq. (5.2.5). This replacement also applies to the $\mathcal{C}_{i,Q}^{\mathrm{CSN}}$ occurring in the mass factorization relations for $\mathcal{C}_{i,g}^{\mathrm{CSN,S}}$ and $\mathcal{C}_{i,q}^{\mathrm{CSN,PS}}$ presented in [6]. Therefore the difference between the CSN and BMSN schemes can be attributed to the powers $(m^2/Q^2)^j$ showing up in $\mathcal{C}_{i,Q}^{\mathrm{CSN}}$ but absent in $\mathcal{C}_{i,q}$. This effect is only noticeable in the threshold region where $Q^2 \sim m^2$ as we will show below.

The heavy quark coefficient functions $\mathcal{C}_{i,k}^{\mathrm{CSN}}$, $H_{i,k}$, $L_{i,k}$ $(k = Q, q, g)$ and the light partonic coefficient functions $\mathcal{C}_{i,k}$ $(k = q, g)$ can be traced back to the following processes

$$\mathcal{C}_{i,g}^{\mathrm{CSN,S},(1)}, H_{i,g}^{\mathrm{S},(1)} \;:\; \gamma^* + g \to Q + \bar{Q} \quad \text{[6] (CSN), [1] (EXACT), [11] (ASYMP)}$$

$$\mathcal{C}_{i,g}^{\mathrm{CSN,S},(2)}, H_{i,g}^{\mathrm{S},(2)} \;:\; \gamma^* + g \to Q + \bar{Q} + g \quad \text{[6] (CSN), [1] (EXACT), [11] (ASYMP)}$$

$$\mathcal{C}_{i,q}^{\mathrm{CSN,PS},(2)}, H_{i,q}^{\mathrm{PS},(2)} \;:\; \gamma^* + q \to Q + \bar{Q} + q \quad \text{Bethe-Heitler reaction; [6] (CSN), [1] (EXACT), [11] (ASYMP)}$$

$$L_{i,q}^{\mathrm{HARD,NS},(2)} \;:\; \gamma^* + q \to Q + \bar{Q} + q \quad \text{Compton reaction; [6] (EXACT and ASYMP)}$$

$$\mathcal{C}_{i,Q}^{\mathrm{CSN,NS},(0)}, H_{i,Q}^{\mathrm{NS},(0)} \;:\; \gamma^* + Q \to Q$$

$$
\begin{aligned}
\mathcal{C}_{i,Q}^{\mathrm{CSN,NS,(1)}}, H_{i,Q}^{\mathrm{NS,(1)}} &: \gamma^* + Q \to Q + g \quad [12] \\
\mathcal{C}_{i,q}^{\mathrm{NS,(0)}} &: \gamma^* + q \to q \\
\mathcal{C}_{i,q}^{\mathrm{NS,(1)}} &: \gamma^* + q \to q + g \quad [13] \\
\mathcal{C}_{i,q}^{\mathrm{NS,(2)}} &: \gamma^* + q \to q + g + g \quad [13] \\
\mathcal{C}_{i,q}^{\mathrm{NS,(2)}} &: \gamma^* + q \to q + \bar{q} + q \quad [13] \\
\tilde{\mathcal{C}}_{i,q}^{\mathrm{PS,(2)}} &: \gamma^* + q \to q + \bar{q} + q \quad [13] \\
\tilde{\mathcal{C}}_{i,g}^{\mathrm{S,(1)}} &: \gamma^* + g \to q + \bar{q} \quad [13] \\
\tilde{\mathcal{C}}_{i,g}^{\mathrm{S,(2)}} &: \gamma^* + g \to q + \bar{q} + g \quad [13]. \qquad (5.2.9)
\end{aligned}
$$

Behind the reactions we have quoted the references in which the corresponding coefficient functions can be found. Note that the heavy quark coefficient functions $H_{i,k}$ are mass singular when $m \to 0$. This can be observed immediately when one looks at $H_{i,k}^{\mathrm{ASYMP}}$ which behaves like $\ln^m(\mu^2/m^2)\ \ln^n(Q^2/m^2)$ (see [11]). After the logarithms are removed one obtains the quantities $\mathcal{C}_{i,k}^{\mathrm{CNS}}$ which, even though they depend on m, are finite in the limit $m \to 0$. The coefficient function $L_{i,k}^{\mathrm{HARD}}$ is finite by itself because as we mentioned above we have imposed a lower cut off $\Delta = 100\ (\mathrm{GeV}/c)^2$ on the invariant mass of the $Q\ \bar{Q}$-pair. Finally notice that all parton densities, coefficient functions and the running coupling constant are presented in the $\overline{\mathrm{MS}}$-scheme.

Now we present results for the various structure functions. We are interested in the bottom quark structure functions $F_{i,b}^{\mathrm{CSN}}(n_f = 5)$ and $F_{i,b}^{\mathrm{BMSN}}(n_f = 5)$ for $i = 2, L$ in NNLO for the CSN [6] and BMSN [2] schemes respectively. In Fig. 5.1 we have plotted the structure functions $F_{2,b}^{\mathrm{CSN}}(n_f = 5)$, $F_{2,b}^{\mathrm{BMSN}}(n_f = 5)$, $F_{2,b}^{\mathrm{PDF}}(n_f = 5)$ and $F_{2,b}^{\mathrm{EXACT}}(n_f = 4)$ in the region $20 < Q^2 < 10^3$ in units of $(\mathrm{GeV/c})^2$ for $x = 0.05$. This figure reveals that there is hardly any difference between the BMSN and CSN prescriptions. The curves in both prescriptions are essentially identical to that for $F_{2,b}^{\mathrm{EXACT}}(n_f = 4)$. In this region $F_{2,b}^{\mathrm{PDF}}(n_f = 5)$ is larger than the other results which is expected from the discussion of the bottom quark density given in [8]. There is still an appreciable difference at the highest plotted Q^2 demonstrating that mass effects are important up to very large scales. Notice that for $Q^2 \leq 35\ (\mathrm{GeV/c})^2$ $F_{2,b}^{\mathrm{PDF}}(n_f = 5)$ becomes negative which means that bottom quark electroproduction cannot

be described by this quantity anymore. In Fig. 5.2 we present the same plots for $x = 0.005$. Again one cannot distinguish between $F_{2,b}^{\rm BMSN}(n_f = 5)$ and $F_{2,c}^{\rm CSN}(n_f = 5)$ but now both are smaller than $F_{2,b}^{\rm EXACT}(n_f = 4)$ over the whole Q^2 range. The latter is smaller than $F_{2,b}^{\rm PDF}(n_f = 5)$ in particular for $Q^2 > 35$ (GeV/c)^2. Further we want to emphasize that due to our careful treatment of the threshold region there is an excellent cancellation between $F_{2,b}^{\rm PDF}(n_f = 5)$ and $F_{2,b}^{\rm ASYMP}(n_f = 4)$ so that both $F_{2,b}^{\rm CSN}(n_f = 5)$ and $F_{2,b}^{\rm BMSN}(n_f = 5)$ tend to $F_{2,b}^{\rm EXACT}(n_f = 4)$ at $Q^2 = m_b^2$. At large Q^2 we have a cancellation between $F_{2,b}^{\rm ASYMP}(n_f = 4)$ and $F_{2,b}^{\rm EXACT}(n_f = 4)$ so that both $F_{2,b}^{\rm CSN}(n_f = 5)$ and $F_{2,b}^{\rm BMSN}(n_f = 5)$ slowly tend to $F_{2,b}^{\rm PDF}(n_f = 5)$. They are only identical at extremely large Q^2 demonstrating that mass effects are still important over a wide range in x and Q^2.

In Fig. 5.3 we show similar plots as in Fig. 5.1 for the bottom quark longitudinal structure functions. Here we observe a small difference between the plots for $F_{L,b}^{\rm CSN}(n_f = 5)$ and $F_{L,b}^{\rm BMSN}(n_f = 5)$ in the region $20 < Q^2 < 10^3$ (GeV/c)^2. Furthermore $F_{L,b}^{\rm PDF}(n_f = 5)$ is considerably larger than the other three structure functions, which differs from the behavior seen in Fig. 5.1. This can be mainly attributed to the gluon density which plays a more prominant role in $F_{L,b}$ than in $F_{2,b}$. For $x = 0.005$ (see Fig. 5.4) the small difference between the BMSN and the CSN descriptions becomes more conspicuous for low Q^2.

In Figs. 5.5 and 5.6 we make a comparison between the NLO and the NNLO structure functions $F_{2,b}^{\rm CSN}(n_f = 5)$ and $F_{2,b}^{\rm BMSN}(n_f = 5)$. Both the CSN and and BMSN descriptions lead to the same results in both NLO and NNLO. However while going from NLO to NNLO the the structure functions $F_{2,b}^{\rm CSN}(n_f = 5)$ and $F_{2,b}^{\rm BMSN}(n_f = 5)$ increase a little bit. The differences in the case of $x = 0.005$ in Fig. 5.6 are even smaller than those observed for $x = 0.05$ in Fig. 5.5. The same comparison between NLO and NNLO results is made for the longitudinal structure functions in Figs. 5.7 and 5.8. Here the differences between NLO and NNLO cases are much larger than in the case of $F_{2,b}$ in Figs.5,6. In NLO both $F_{L,b}^{\rm BMSN}(n_f = 5)$ and $F_{L,b}^{\rm CSN}(n_f = 5)$ are smaller than the NNLO results.

Previous results for $F_{i,b}^{\rm EXACT}(x, Q^2, m_b^2)$ and have been presented in Figs. 5.20a, 5.20b in [1] for a now obsolete set of parton densities, so the values quoted there are too small. To show these changes we add in Figs. 5.9 and 5.10 plots for the x dependence of $F_{2,b}^{\rm CSN}(n_f = 5)$, $F_{2,b}^{\rm BMSN}(n_f = 5)$, $F_{2,b}^{\rm PDF}(n_f = 5)$ and $F_{2,b}^{\rm EXACT}(n_f = 4)$ at fixed $Q^2 = 30$ and $Q^2 = 100$ in units of (GeV/c)^2 respectively. Finally we also show in Figs. 5.11 and 5.12 plots for the x dependence of $F_{L,b}^{\rm CSN}(n_f = 5)$, $F_{L,b}^{\rm BMSN}(n_f = 5)$, $F_{L,b}^{\rm PDF}(n_f = 5)$ and $F_{L,b}^{\rm EXACT}(n_f = 4)$ at fixed $Q^2 = 30$ and $Q^2 = 100$ in units of (GeV/c)^2 respectively. Note that

there are also some recent results for $F_{2,b}$ in [5] in the TR scheme and in [14] for FOPT.

The plots for $F_{L,b}^{\rm CSN}(n_f = 5)$ in Figs. 5.7,5.8 do not show a negative region at small Q^2 which could have been expected by analogy with the results for $F_{L,c}^{\rm CSN}(n_f = 4)$ in [6]. In the case of bottom quark production the negative regions do occur but at even smaller values of x. In Figs. 5.13, 5.14 we show the same plots as in Figs. 5.1, 5.3 respectively but for $x = 5 \times 10^{-5}$. Now the structure function $F_{L,b}^{\rm CSN}$ is negative in the region $Q^2 \approx 30$ (GeV/c)^2. In Figs. 5.15,5.16 we show the same plots as in Figs. 5.5,5.7 respectively but for $x = 5 \times 10^{-5}$. Fig. 5.16 shows that the longitudinal structure functions for the case of bottom production also have negative regions at small Q^2 values in both NLO and NNLO. This phenomenon also occurs for the charm quark structure functions in [6]. In the NLO case this arises because the term $f_g^{\rm S,NLO}(n_f + 1, \mu^2) \otimes \mathcal{C}_{L,g}^{\rm CSN,S,(1)}\Big(Q^2/m^2, Q^2/\mu^2\Big)$ in Eq. (5.2.1) is negative due to the definition of the gluon coefficient function in the CSN scheme (see Eq.(2.19)) in [6]) which is given by

$$\begin{aligned} \mathcal{C}_{L,g}^{\rm CSN,S,(1)}\Big(\frac{Q^2}{m^2}, \frac{Q^2}{\mu^2}\Big) &= H_{L,g}^{\rm S,(1)}\Big(\frac{Q^2}{m^2}\Big) - A_{Qg}^{\rm S,(1)}\Big(\frac{\mu^2}{m^2}\Big)\, \mathcal{C}_{L,Q}^{\rm CSN,NS,(0)}\Big(\frac{Q^2}{m^2}\Big), \\ \text{with} \quad \mathcal{C}_{L,Q}^{\rm CSN,NS,(0)} &= \frac{4m^2}{Q^2}, \end{aligned} \tag{5.2.10}$$

where $A_{Qg}^{\rm S,(1)}$ denotes the one-loop operator matrix element computed in [11]. Notice that the latter and the lowest order exact coefficient function $H_{L,g}^{\rm S,(1)}$ are always positive. Because of the minus sign in Eq. (5.2.10) it appears that the coefficient function $\mathcal{C}_{L,g}^{\rm CSN,S,(1)}$ can become negative in particular at low Q^2 values. In the NNLO case one obtains more negative contributions due to the term $f_{Q+\bar{Q}}^{\rm NNLO}(n_f + 1, \mu^2)\mathcal{C}_{L,Q}^{\rm CSN,NS,(0)}$ in formula (5.2.1). It turns out that $f_{Q+\bar{Q}}^{\rm NNLO}(n_f + 1, x, \mu^2)$ is negative at small x and $\mu^2 = Q^2 \geq m^2$. Notice that at the latter scale $f_{Q+\bar{Q}}^{\rm LO}(n_f + 1, x, \mu^2)$ and $f_{Q+\bar{Q}}^{\rm NLO}(n_f + 1, x, \mu^2)$ are very small because they vanish at $\mu = m$ in contrast to $f_{Q+\bar{Q}}^{\rm NNLO}(n_f+1, x, \mu^2)$. The behavior of the structure function above is characteristic of the CSN scheme since it does not appear in the case of BMSN. This is because in the latter scheme the longitudinal coefficient function, represented by $\mathcal{C}_{L,q}^{\rm CSN,NS,(0)}$, is identical to zero so that the zeroth order contribution to $F_{L,b}^{\rm BMSN}(n_f = 5)$ vanishes and the first order correction is given by $\mathcal{C}_{L,g}^{\rm BMSN,S,(1)} = H_{L,g}^{\rm S,(1)}$. The latter leads to a positive structure function over the whole kinematical region. To further demonstrate

this point we plot in Fig. 5.17 pieces of the NLO result

$$F_{L,b}^{\rm CSN}(n_f+1,Q^2,m^2) = e_b^2\Bigg[f_{b+\bar{b}}^{\rm NLO}(n_f+1,\mu^2)\mathcal{C}_{L,b}^{\rm CSN,NS,(0)}(\frac{Q^2}{m^2})$$

$$+a_s(n_f+1,\mu^2)\Bigg\{f_{b+\bar{b}}^{\rm LO}(n_f+1,\mu^2)\otimes\mathcal{C}_{L,b}^{\rm CSN,NS,(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)$$

$$+f_g^{\rm S,LO}(n_f+1,\mu^2)\otimes\mathcal{C}_{L,g}^{\rm CSN,S,(1)}\Big(\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\Big)\Bigg\}\ . \qquad (5.2.11)$$

The sum of the b-quark contributions, labelled Term1, is always positive. The gluonic contribution, labelled Term2, is clearly negative over a wide range in Q^2 and large enough that the sum $F_{L,b}^{\rm CSN}$ is also negative for $30 \le Q^2 \le 150$ GeV^2, as in Fig. 5.16. This behavior is due to the gluonic coefficient function $\mathcal{C}_{L,g}^{\rm CSN,S,(1)}$ which is explained below Eq. (5.2.10). However the magnitude of the gluonic contribution depends on the choice of the gluon density. If we use an NLO gluon density in the order α_s contribution to the structure function in Eq. (5.2.11) rather than a LO gluon density then the sum of the first two terms is unchanged but the gluonic part is now smaller in magnitude. These contributions are shown in Fig.5.18 where now |Term2| $\le$ Term1 so that the total result for $F_{L,b}^{\rm CSN}$ is everywhere positive. However this procedure violates our prescription for the computation of the structure functions in both the CSN and the BMSN schemes. In this prescription the LO densities are multiplied by the highest order coefficient function whereas the NLO densities are combined with lower order coefficient functions (see formulae (5.2.1), (5.2.3) and (5.2.5)). In this way the perturbation series is truncated up to the order we want to compute the structure functions. Hence we avoid terms, arising beyond that order, which introduce a scheme dependence and spoils the threshold behavior (see [6]). The latter happens if one follows the usual procedure where one multiplies the highest order densities by the highest order coefficient functions. The difference between the usual procedure and our prescription is not only shown by our parton density set but is also observed for other sets presented in the literature. Examples are recent sets such as MRST98 [9] (with $m_b = 4.3$ GeV, $m_c = 1.35$ GeV), MRST99 [15] (with $m_b = 4.3$ GeV, $m_c = 1.43$ GeV), and CTEQ5 [10] (with $m_b = 4.5$ GeV, $m_c = 1.3$ GeV). Note that the MRST99 set does not provide LO densities. Using their NLO densities they yield positive values for the Q^2 dependence of $F_{L,b}^{\rm CSN}$ at $x = 5\times10^{-5}$. There are both LO (CTEQ5L) and NLO (CTEQ5M) densities in the CTEQ5 set and we have checked that, for the same x, Q^2 values $F_{L,b}^{\rm CSN}$ is positive with purely NLO densities but has a negative region when the LO and NLO densities are

used according to our prescription. The observations made above leads to the conclusion that the $4m^2/Q^2$ term in the non-singlet CSN longitudinal coefficient function in Eq. (5.2.10) leads to a negative gluonic coefficient function. When the latter is used together with the latest LO and NLO parton density sets $F_{L,b}^{\rm CSN}(n_f = 5)$ becomes negative in the low Q^2-region at small x. We speculate that the CSN scheme would always yield positive structure functions if we could use parton density sets which fitted data with convolutions of LO densities with $O(\alpha_s)$ coefficient functions and NLO densities with zeroth order coefficient functions. Unfortunately such densities are not available.

To summarize the main points we have implemented two variable flavor number schemes for bottom quark electroproduction in NNLO and compared them with NLO FOPT results. The schemes differ in the way mass factorization is implemented. In the CSN scheme this is done with respect to the full heavy and light quark structure functions at finite Q^2. In the BMSN scheme the mass factorization is only applied to the coefficient functions in the large Q^2 limit. Both schemes require four-flavor and five-flavor parton densities which satisfy discontinuous NNLO matching conditions at a scale $\mu = m_b$. We have constructed these densities using our own evolution code [8]. The schemes also require matching conditions on the coefficient functions which are implemented in this paper. Note that we have also removed the dangerous terms in $\ln^3(Q^2/m_b^2)$ from the Compton contributions so that both $F_{i,b}^{\rm CSN}(n_f = 5)$ and $F_{i,b}^{\rm BMSN}(n_f = 5)$ are collinear safe. As in [6] we have done this in a way which is consistent with our study of inclusive quantities by implementing a cut Δ on the mass of the $b-\bar{b}$ pair. We stress that any ZM-VFNS bottom quark density description of $F_{i,b}$ must use collinear safe definitions. This is not required in the fixed order perturbation theory approach given by $F_{i,b}^{\rm EXACT}(n_f = 4)$ in [1] for moderate Q^2-values.

Finally we made a careful analysis of the threshold behaviors of $F_{i,b}^{\rm CSN}(n_f = 5)$ and $F_{i,b}^{\rm BMSN}(n_f = 5)$. In order to achieve the required cancellations at the scale $\mu = m_b$ so that they both become equal to $F_{i,b}^{\rm EXACT}(n_f = 4)$ one must be very careful to combine terms with the same order in the expansion in α_s. The approximation we made in this paper, of using NLO splitting functions in place of NNLO splitting functions, was sufficient for our purposes. We successfully implemented the required cancellations near threshold and the corresponding limits at large scales came out naturally. Inconsistent sets of parton densities automatically spoil these cancelations. Since there are only minor differences between the CSN, BMSN and NLO FOPT predictions it is clear that the use of variable flavor number schemes for bottom quark production is not required for the analysis of HERA data. However the ZM-VFNS description is clearly inadequate at small Q^2.

ACKNOWLEDGMENTS

The work of A. Chuvakin and J. Smith was partially supported by the National Science Foundation grant PHY-9722101. The work of W.L. van Neerven was supported by the EC network 'QCD and Particle Structure' under contract No. FMRX–CT98–0194.

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Chapter 6

Variable flavor number schemes versus fixed order perturbation theory for charm quark electroproduction

6.1 Introduction

Electromagnetic interactions have long been used to study both hadronic structure and strong interaction dynamics. Examples include deep inelastic lepton-nucleon scattering, hadroproduction of lepton pairs, the production of photons with large transverse momenta, and various photoproduction processes involving scattering of real or very low mass virtual photons from hadrons. In particular, heavy quark production in deep inelastic electron-proton scattering is calculable in QCD and provides information on the gluonic content of the proton which is complementary to that obtained in direct photon production or structure function scaling violation measurements. In addition, the scale of the hard scattering may be large relative to the mass of the charm quark, thus allowing one to study whether and when to treat the charm quark as a massless parton. It is this second aspect we wish to examine further in this paper.

The photon-gluon fusion mechanism is the simplest description of charmed quark electroproduction so that their production is assumed extrinsic, and their mass m_c is retained throughout. We call this description fixed order perturbation theory (FOPT). It depends on a three-flavor set of parton densities for the u, d, and s quarks together with a corresponding gluon density. Calculations for rates and single particle inclusive distributions are available to next-to-leading order (NLO) in [1]. These calculations were later redone to cover fully differential production [2], and decays into hadronic or semileptonic final states [3]. This framework generally provides a very good description of the ZEUS [4] and H1 data [5] on the differential distributions for $D^{*\pm}(2010)$ electroproduction. Updated analyses now exist from H1 [6] and ZEUS [7]. The ZEUS data [7] now extend up to $Q^2 \approx 1000$ GeV^2. Since the FOPT results in NLO are very stable under scale changes it has been advocated that a three-flavor description should be the best one to fit the data [8, 9]. This is the reason that the GRV98 leading order (LO) and NLO density sets [10] only contain three flavors.

Other descriptions of charm quark electroproduction have been used. One, which describes the charm quark as a massless parton density $c(x,\mu^2)$, with the boundary condition $c(x,\mu^2) = 0$ for $\mu \leq m_c$, is expected to be more appropriate at large Q^2. This scheme has generally been used by groups which fitted parton densities to data and is called the zero-mass variable flavor number scheme (ZM-VFNS). The transition from a three-flavor parton density set to a four-flavor set can be made on purely theoretical grounds by evaluating appropriate massive and massless operator matrix elements containing heavy quark loops in the operator product expansion and then absorbing the

terms containing $\ln^i(Q^2/m_c^2)$ into the definition of four-flavor parton densities [11], [12]. The resummation of the above logarithms is incorporated into the boundary conditions on the $c-$quark density as well as the other four-flavor quark and gluon densities. In particular if one does this at the scale where $\mu^2 = Q^2 = m_c^2$ then all the logarithmic terms in the operator matrix elements vanish and only the non-logarithmic terms are included in the boundary conditions. Since a charm quark density is a parton model concept the QCD perturbation series then starts with α_s^0 coefficient functions. The lowest order photon-gluon fusion reaction then has $O(\alpha_s)$ coefficient functions. The NLO corrections contain $O(\alpha_s^2)$ coefficient functions. When the resulting four-flavor parton densities are convolved with the massless coefficient functions in [13] one obtains predictions for the charm content in the deep inelastic structure functions. One expects this four-flavor ZM-VFNS description to be better than the FOPT one at large scales since it resums the terms in $\ln^i(Q^2/m_c^2)$.

Another approach, which is even more ambitious, is a scheme designed to interpolate between the FOPT result at low scales and the ZM-VFNS result at large scales. In these variable flavor number schemes (VFNS) one hopes to provide a unified framework for all scales. Unfortunately there is no unique prescription for a VFNS and several have been constructed. The differences between them are due to two inputs. The first is the mass factorization procedure carried out before the large logarithms can be resummed, namely should one retain massive or massless charmed quarks in the coefficient functions, which are convolved with either the three-flavor or four-flavor parton densities. The second is the matching condition imposed on the charmed quark density, namely how does it vanish in the threshold region of the electroproduction process, where the partonic subenergy is approximately $4m_c^2$. Variable flavor number schemes are presently available to $O(\alpha_s)$ in [14, 15, 16, 17] and to $O(\alpha_s^2)$ in [18, 19], called BMSN and CSN, respectively, in this paper. The latter schemes require the parton densities provided in [12]. Review articles and discussions about VFNS schemes are available in [20, 21, 22, 23].

In Sec. II we give a short discussion of the BMSN and CSN descriptions for charmed quark electroproduction and then compare theoretical predictions with differential distribution data from H1 [6] and ZEUS [4, 7].

6.2 Comparison

The reaction under consideration is heavy quark Q production via neutral-current electron-proton scattering

$$e^-(l) + P(p) \to e^-(l') + Q(p_1) + X. \tag{6.2.1}$$

We concentrate on the case where Q is a charm quark with mass $m_c = 1.4$ GeV. When the momentum transfer squared $Q^2 = -q^2 > 0$ ($q = l - l'$) is not too large, $Q^2 \ll M_Z^2$, the contribution from virtual Z-boson exchange is small compared to that of virtual-photon exchange. For example, using the leading order Monte Carlo program AROMA [24], at $Q^2 = 1000$ GeV^2 we find the Z-boson exchange contribution is a factor of 100 smaller than the photon exchange contribution.

The charm quark cross section can be written in terms of the structure functions $F_2^c(x, Q^2, m_c^2)$ and $F_L^c(x, Q^2, m_c^2)$ as follows:

$$\frac{d^2\sigma}{dydQ^2} = \frac{2\pi\alpha^2}{yQ^4}\{[1 + (1-y)^2]F_2^c(x, Q^2, m_c^2) - y^2 F_L^c(x, Q^2, m_c^2)\}\,, \tag{6.2.2}$$

where $x = Q^2/2p \cdot q$ and $y = p \cdot q/p \cdot l$ are the usual Bjorken scaling variables and α is the electromagnetic coupling. The scaling variables are related to the square of the center-of-momentum energy of the electron-proton system $S = (l + p)^2$ *via* $xyS = Q^2$. The total cross section is given by [25]

$$\sigma = \int_{4m_c^2/S}^{1} dy \int_{m_e^2 y^2/(1-y)}^{yS - 4m_c^2} dQ^2 \left(\frac{d^2\sigma}{dydQ^2}\right)\,, \tag{6.2.3}$$

where m_e is the electron mass. In deriving Eq. (2.2) one integrates over the azimuthal angle between the plane containing the incoming and outgoing electrons and the plane containing the incoming proton and the outgoing charm quark.

Experimentally it is the decay products of charmed hadrons that are observed. The H1 and ZEUS groups measure $D^{*\pm}(2010)$ production. We assume a Peterson *et al.* [26] fragmentation function to model the nonperturbative transition from charmed quark to hadron. The cross section for D^* production is then obtained by convolving the charm quark cross section Eq. (2.3) with the fragmentation function

$$D(z) = \frac{N}{z[1 - 1/z - \epsilon/(1-z)]^2} \tag{6.2.4}$$

where N is fixed such that $D(z)$ is normalized to unity once the parameter $\epsilon = 0.035$ [27] is fixed. The normalization of the cross section is then given by the charm fragmentation probability which we take as $P(c \to D^*) = 0.235$ [28].

The H1 collaboration has recently [6] measured $D^{*\pm}$ production for $1 < Q^2 < 100$ GeV^2 and $0.05 < y < 0.7$ and quote a cross section in the region $1.5 < p_T(D^*) < 15$ GeV and $|\eta(D^*)| < 1.5$ of

$$\sigma(e^+p \to e^+D^{*\pm}X) = 8.37 \pm 0.41(\text{stat.})^{+1.11}_{-0.82}(\text{syst.})\ \text{nb}\,. \tag{6.2.5}$$

The data came from the 1996-97 run with proton energy 820 GeV and positron energy 27.5 GeV (18.6 pb^{-1}).

The ZEUS collaboration has recently [7] measured $D^{*\pm}$ production for $Q^2 > 10$ GeV^2 and $0.04 < y < 0.95$ and quote a cross section in the region $1.5 < p_T(D^*) < 15$ GeV and $|\eta(D^*)| < 1.5$ of

$$\sigma(e^+p \to e^+D^{*\pm}X) = 2.33 \pm 0.12(\text{stat.})^{+0.14}_{-0.07}(\text{syst.})\ \text{nb}\,. \tag{6.2.6}$$

The data came partly from the 1999-2000 run with proton energy 920 GeV (45.0 pb^{-1}) and partly from the 1995-1997 run with proton energy 820 GeV (37.6 pb^{-1}). In both cases the positron beam energy was 27.6 GeV. They demonstrated [7] that the predictions from HVQDIS [3], which is based on FOPT, agree with their $D^{*\pm}$ electroproduction data up to the highest measured value of $Q^2 \approx 1350$ GeV^2.

Previously in [4] they presented the 1996-1997 positron production data (37 pb^{-1}) for $D^{*\pm}$ in the range $1 < Q^2 < 600$ GeV^2 and $0.02 < y < 0.7$ in the same kinematic range $1.5 < p_T(D^*) < 15$ GeV and $|\eta(D^*)| < 1.5$ with the cross section

$$\sigma(e^+p \to e^+D^{*\pm}X) = 8.31 \pm 0.31(\text{stat.})^{+0.30}_{-0.50}(\text{syst.})\ \text{nb}\,. \tag{6.2.7}$$

Therein [4] they also concluded that the HVQDIS [3] results agree with their data, apart from a distortion of the pseudo-rapidity distribution. This was attributed to a beam drag effect [29], which was estimated by Monte Carlo [30]. Still FOPT seemed to be the best model to fit their data.

The BMSN [18] and CSN [19] variable flavor number schemes were constructed so that the charm quark structure functions $F_2^c(x, Q^2, m_c^2, \mu^2)$ and $F_L^c(x, Q^2, m_c^2, \mu^2)$ are numerically equal to the corresponding FOPT results at the scale $\mu^2 = m_c^2 = Q^2 = 1.96$ GeV^2, so the differences between the them could be monitored at higher scales. For this reason we chose the scale $\mu^2 = m_c^2 + \frac{1}{2}Q^2(1 - m_c^2/Q^2)^2$ and set the charm density to zero when $\mu^2 < m_c^2$.

Also we used the exact solution of the differential equation for the QCD running coupling (α_s) as well as an electromagnetic running coupling (α). The QCD expansion was truncated at α_s^2. Therefore we were careful to construct the structure functions in the FOPT, BMSN and CSN schemes according to the symbolic formula

$$\begin{aligned} F(x,Q^2,m_c^2) &= f(LO)\otimes C(LO) \\ &+ \alpha_s[f(NLO)\otimes C(LO) + f(LO)\otimes C(NLO)] \\ &+ \alpha_s^2[f(LO)\otimes C(NNLO) + f(NLO)\otimes C(NLO) \\ &+ f(NNLO)\otimes C(LO)]\,, \end{aligned} \tag{6.2.8}$$

where the $\otimes$ symbol refers to the convolution integral and the parton densities f and coefficient functions C are taken in either LO, NLO or next-to-next-to-leading order (NNLO) perturbation theory. Note that this result is different from the usual FOPT prescription which is based on expressions like

$$\begin{aligned} F(x,Q^2,m_c^2) &= [f(LO) + \alpha_s f(NLO) + \alpha_s^2 f(NNLO)] \\ &\otimes [C(LO) + \alpha_s C(NLO) + \alpha_s^2 C(NNLO)]\,. \end{aligned} \tag{6.2.9}$$

These prescriptions retain terms which are even higher order in α_s. Normally it does not matter if such terms are retained because they are numerically unimportant at large Q^2. However such terms are numerically significant at small Q^2 and ruin the cancellations among the various terms in our formulae for the structure functions in the three schemes with the result that they do not agree numerically at $Q^2 = \mu^2 = m_c^2$. Therefore we have to use Eq. (2.8) and not Eq. (2.9). Even our FOPT (extrinsic) expression, called EXACT in this paper, only retains the second and third sets of terms in Eq. (2.8) and agrees with the corresponding results from the (appropriately modified) HVQDIS code.

The difference between the BMSN and CSN schemes is that the former has $m_c = 0$ in the heavy quark coefficient functions while the latter retains terms containing m_c. We refer the reader to [19] for more details, in particular the definition of the collinear safe inclusive structure functions and the contributions which are incorporated into the light mass (u, d, s) contributions to the coefficient functions. Our previous theoretical results showed that differences between the EXACT, BMSN and CSN schemes in LO perturbation theory diminish substantially in NLO perturbation theory. Such differences are more apparent for b-quark electroproduction in [31] but there are no events yet.

The aim of this paper is to compare our results with the data. Since there are no VFNS schemes available for differential distributions in the transverse

momentum and rapidity of the D^* meson in $O(\alpha_s^2)$ we make the assumption that the experimental acceptances do not differ much between these schemes and FOPT. We have therefore recalculated the experimental acceptances from the HVQDIS program with the above scale choice, running coupling constant and GRV98 [10] three-flavor parton density set. This is appropriate for the FOPT result, which we called EXACT in our papers on the BMSN and CSN schemes. Our acceptances in Q^2 are slightly modified from those used by the Collaborations. The acceptances in Q^2, from integrating Eq. (2.2) over $0.04 < y < 0.95$, $0.05 < y < 0.7$, or $0.02 < y < 0.7$ are nearly identical, so we do not distinguish between them. The corresponding acceptances in x, however, from integrating Eq. (2.2) over $10 < Q^2 < 1350$ or $1 < Q^2 < 600$ and the corresponding y ranges are different and we distinguish between them. We start with the recent data from the Osaka meeting [6, 7]. The results for the ratio $\sigma(\text{cuts})/\sigma(\text{no cuts})$ are presented in Figs. 6.1 and 6.2 plotted versus $\log_{10}Q^2$ and $\log_{10}x$ respectively. These plots demonstrate the large corrections necessary to include the experimental acceptances. The corrections were applied to the corresponding differential cross sections calculated from the structure functions given in the CSN [19] and BMSN [18] papers. Here we used our own set of densities [12] which are based on the three-flavor GRV98 densities at scales below $\mu = m_c$, but which incorporate the discontinuity across the $c-$flavor threshold at $\mu = m_c$ to define a four-flavor set both in $O(\alpha_s)$ and in $O(\alpha_s^2)$ together with their subsequent evolution to higher scales with NLO splitting functions.

The resulting differential cross sections in $\log_{10}Q^2$ are compared with the H1 and ZEUS data in Figs. 6.3 and 6.4. We see from Fig. 6.3 that the FOPT is a good fit to the data at large Q^2. This is in agreement with the conclusions of the ZEUS collaboration in [7]. It is difficult to distinguish the BMSN and CSN results from the FOPT ones because there is only a 4% difference even at this large Q^2. Clearly it will take a substantial increase in the number of events to distinguish between the schemes at large Q^2. All we can say at present is that the terms containing powers of $\ln(Q^2/m_c^2)$ do not seem to lead to different predictions.

One can see from the semi-logarithmic plot in Fig. 6.4 that all curves meet at $Q^2 = m_c^2 = 1.96$ GeV^2, which is expected from the construction of the BMSN and CSN schemes. There are differences between the three schemes in the region of small Q^2, however the currently available data is unable to resolve them. We understand that the events with $Q^2 < 10$ GeV^2 and with $Q^2 > 10$ GeV^2 are measured in different regions of the ZEUS detector and the events accumulated in 1999-2000 in the former region have not been analyzed. Note also that the bin widths in this region are not the same. More data for

small Q^2 would clearly be very useful.

The resulting differential cross sections in $\log_{10}x$ are compared with the new ZEUS data [7] in Figs. 6.5 and 6.6. We see from Fig. 6.5 that there is good agreement over a wide range in x. The semi-logarithmic plot in Fig. 6.6 shows a small disagreement between the FOPT theory result and the data in the region $x \approx 10^{-3}$. However the normalization is determined mainly by the magnitude of differential cross section at the lowest measured point in Q^2, which is precisely where additional data is required.

Integrations over the theoretical results displayed in Figs. 6.3 - 6.6 for $10 < Q^2 < 1350$ GeV^2 and $0.04 < y < 0.95$ yield 2.86 nb, 2.51 nb and 2.48 nb for the FOPT, BMSN and CSN schemes respectively. The latter two results are within the error bars of the experimental result in Eq. (2.6) while the FOPT result is slightly higher.

The previous published ZEUS data in [4] had different cuts in Q^2 and y, namely $1 < Q^2 < 600$ GeV^2 and $0.02 < y < 0.7$ which affect the normalization of the corresponding x distribution. Therefore we reran the acceptance in $\log_{10}x$ from the HVQDIS program and it is shown in Fig. 6.7. We then applied the same acceptance to the other programs. The BMSN and CSN results between $1 < Q^2 < 1.96$ GeV^2 are set equal to the EXACT result. Our results are compared to the data in Figs. 6.8 and 6.9. The overall shape and normalization are well described. Integration over the results in Fig. 6.8 yield 9.29 nb, 8.43 nb and 8.55 nb for the FOPT, BMSN and CSN schemes respectively compared to the experimental results in Eq. (2.5) and (2.7).

We have run our computer codes in other ranges of the variables $\log_{10}Q^2$ and $\log_{10}x$ to find where differences between the three schemes might be measurable. As an illustration we show in Fig. 6.10 a contour plot of the ratio of the BMSN double differential cross section divided by the FOPT double differential cross section plotted versus these variables. Contour lines are drawn where this ratio is 1, 1.5, 2, 2.5 and 3. The ratio increases as Q^2 increases for fixed x. Note that no acceptance corrections in p_T or η have been applied to the ratio in this figure. One sees that the region of large Q^2 and large x must be probed to find significant differences between FOPT and the variable flavor number schemes. Roughly speaking one needs $x > 0.2$ and $Q^2 > 100$ GeV^2. In fact Fig. 6.5 in [32], which only shows the Q^2 dependence of the structure function $F_2^c(x, Q^2, m_c^2)$ at fixed values of x, already illustrates the kind of differences one can expect in this region.

Finally we remark that as far as the FOPT result is concerned the standard version of HVQDIS uses the scale $\mu^2 = Q^2 + 4m_c^2$. This increases the scale in the running coupling. Also it uses the second and third lines of Eq. (2.9) with all parton densities set to their three flavor NLO values. These

standard settings alter slightly the above acceptance curves. The net effect of both changes is approximately a ten percent reduction of the FOPT results (usgin GRV98) for the differential distribution in $\log_{10}Q^2$ at the smallest Q^2, which is within the present experimental errors.

To summarize we have made a first comparison between the FOPT, BMSN and CSN descriptions for $D^{*\pm}$ electroproduction. We have observed that the three schemes give nearly identical predictions up to the highest Q^2 measured. It is therefore difficult to distinguish between the various schemes on the basis of a data comparison. The small scale dependence of the FOPT result indicates that there is no sign that the terms containing powers of $\ln(Q^2/m_c^2)$ destroy the convergence of the QCD perturbation expansion and that one is forced to switch to a variable flavor number scheme like the BMSN or CSN. In fact they all provide a good description of the data for the differential distributions in Q^2 and x. At small Q^2 there is a chance to distinguish between the schemes (say for $2 < Q^2 < 20$ in GeV^2). The comparisons in the case of the x-distributions are not conclusive due to the correlations with the points in small Q^2. It will be interesting to see what happens when more events are collected so that the error bars are reduced.

We would like to acknowledge discussions with W. L. van Neerven on the results presented above, and thank José Repond for discussions about the ZEUS data and comments on the text. The work of A. Chuvakin and J. Smith was supported in part by the National Science Foundation Contract PHY-9722101. The work of B. Harris was supported by the U.S. Department of Energy, High Energy Physics Division, under contract W-31-109-Eng-38.

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Chapter 7

Conclusions

In this dissertation we illustrated the importance of constructing variable flavor number schemes for a consistent theoretical analysis of DIS data on both inclusive production and single-particle charm production. VFNS descriptions for charm electroproduction should turn out to be more accurate than fixed flavor scheme descriptions for moderately high values of Q^2 and for a wide range in x.

While there is still no conclusive evidence which particular VFNS scheme provides the most accurate description of experimental data it seems evident that adding higher order terms to the perturbative expansion increases the accuracy and stability of the theoretical results. Hence it is clear that the VFNS descriptions described in this thesis are based on stronger theoretical foundations than other VFNS schemes presently available. Our schemes are constructed in higher order that the others so they have less dependence on arbitrary parameters, such as factorization and renormalization scales and heavy quark masses. They use all currently available higher order corrections to both splitting functions and coefficient functions. They have a compatible set of numerical programs for evolving the PDFs and calculating the structure functions. The computer programs developed as part of my dissertation research provide simple and user-friendly methods to compute cross-sections for DIS processes.