Massless Parton Asymptotics within Variable Flavour Number Schemes

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Abstract

In this note we formulate and investigate theoretical uncertainties for high $Q^2$ deep inelastic heavy quark (charm, etc.) production rates which arise within collinear resummation techniques from variations of the \textit{a priori} unknown charm input scale $Q_0$ of $\mathcal{O}(\alpha_s)$ variable flavour number schemes. We show that $Q_0$ variations constitute a source of considerable theoretical uncertainty of present $\mathcal{O}(\alpha_s)$ calculations within such schemes and we suggest to consider a scale optimization from higher order corrections. We also outline how the stability of the fixed order and collinearly resummed perturbation series for heavy quark production can be comparatively investigated by variation of $Q_0$. 
The present discussion on the appropriate scheme for the perturbative treatment of the deep inelastic production of heavy quarks of mass $m \gg \Lambda_{QCD}$ can be partly traced back to the question what is the effective expansion parameter for high $Q^2$ predictions. While fixed order perturbation theory (FOPT) proceeds strictly stepwise in powers of $(\alpha_s/2\pi)^n$ at all scales, variable flavor number schemes (VFNSs) are based upon the expectation that terms $\sim (\alpha_s/2\pi \times \ln Q^2/m^2)^n$ from collinear regions in the phase space have to be resummed to all perturbative orders $n$ for high $Q^2$ when $(\alpha_s/2\pi \times \ln Q^2/m^2) \rightarrow O(1)$. Such terms are undebatedly present in the high $Q^2$ limit of the perturbative partonic coefficient functions but their impact is less clear on observable hadronic quantities like the charm component of the deep inelastic structure function $F_2^c$ where the partonic coefficient functions have to be convoluted with modern, i.e. steep, parton distribution functions $q(x, \mu_f^2)$ and dominantly $g(x, \mu_f^2)$, $\mu_f \sim m$. The question which ordering of the perturbation series optimizes its convergence can therefore not be answered a priori but only from explicit quantitative, i.e. numerical investigations: prominent tools for testing perturbative stability being $K$ factor considerations or scale variations. At present both criteria indicate a well behaved fixed order perturbation series for relevant subasymptotic but large scales $Q \gg m$. As regards scale uncertainties, mainly variations of the mass factorization scale $\mu_F$ have been considered so far despite the fact that collinear resummation techniques introduce an additional arbitrary scale in the process set by the input scale $Q_0$ for the heavy quark:

Recently proposed variable flavour number schemes for global PDF analyses are constructed upon the boundary condition

$$q^{(n_f+1)}_{uH}(x, Q_0^2)\bigg|_{Q_0=m}=0 \quad (1)$$

for a heavy sea quark density to enter the massless partonic renormalization group (RG)-evolution equations which resum collinear splitting subdiagrams to all orders at the price of neglecting mass dependent terms. In Eq. (1) $m$ is the heavy quark mass and the heavy quark input scale $Q_0$ is in more technical terms the transition (or switching) scale from a factorization scheme with $n_f$ to the one with $n_f + 1$ partonic quark degrees of freedom.
Since the scale $Q_0$ is of no physical meaning, a RG-like equation
\[
\frac{\partial \mathcal{O}}{\partial \ln Q_0^2} = 0 \tag{2}
\]
holds ideally for any heavy quark observable $\mathcal{O}$. At limited perturbative order, Eq. (2) will obviously be violated to some extent which we will investigate below for the charm contribution to the NC structure function $\mathcal{O} = F_2^c$.

At the heart of the variable flavour number schemes of [6–10] is some interpolation prescription between fixed order perturbation theory, assumed to be valid around $Q^2 = \mathcal{O}(m^2)$, and the $Q^2 \gg m^2$ massless parton (MP) asymptotics derived from the boundary condition in Eq. (1). To avoid within our rather general considerations a discussion of the peculiarities of the distinct heavy quark schemes we denote such interpolations very schematically as
\[
\text{VFNS} = w(m^2/Q^2) \times \text{FOPT} + [1 - w(m^2/Q^2)] \times \text{MP}; \quad w \rightarrow \begin{cases} 
1, & m^2/Q^2 \to 1 \\
0, & m^2/Q^2 \to 0 
\end{cases} \tag{3}
\]
where the simple weight $w$ is meant to represent all the details of some elaborate scheme prescription [6–10, 12]. The deviation of VFNS from FOPT is thus normalized to MP and the predictive power of VFNS in Eq. (3) depends on the stability of the asymptotic MP prediction which is obtained from the boundary (1) at $Q_0 = m$ via massless RG evolutions. Equation (1) emerges from the matching conditions of a factorization scheme with $n_f$ active flavours to a scheme with $n_f + 1$ active flavours at some a priori arbitrary transition (or switching) scale $Q_0$. The general transformation equations for quark ($q$) and gluon ($g$) parton densities as well as for $\alpha_s$ read up to NLO [11, 12]
\[
q_{n_f+1}^{(n_f+1)}(x, Q_0^2) = \frac{\alpha_s(Q_0^2)}{2\pi} \ln \frac{Q_0^2}{m^2} \int_x^1 \frac{d\xi}{\xi} P_{qg}^{(0)}(\xi) g^{(n_f)} \left( \frac{\xi}{Q_0^2} \right) + \mathcal{O}(\alpha_s^2)
\]
\[
g^{(n_f+1)}(x, Q_0^2) = g^{(n_f)}(x, Q_0^2) \left( 1 + \frac{\alpha_s(Q_0^2)}{6\pi} \ln \frac{m^2}{Q_0^2} \right) + \mathcal{O}(\alpha_s^2)
\]
\[
\alpha_s^{(n_f+1)}(Q_0^2) = \alpha_s^{(n_f)}(Q_0^2) \left/ \left( 1 + \frac{\alpha_s(Q_0^2)}{6\pi} \ln \frac{m^2}{Q_0^2} \right) \right. + \mathcal{O}(\alpha_s^3)
\]
\[
q^{(n_f+1)}(x, Q_0^2) = q^{(n_f)}(x, Q_0^2) + \mathcal{O}(\alpha_s^2)
\]
and obviously reduce to Eq. (1) for $Q_0 = m$:
\[
q_{n_f+1}^{(n_f+1)}(x, m^2) = 0 \ , \ g^{(n_f+1)}(x, m^2) = g^{(n_f)}(x, m^2) \ , \ \alpha_s^{(n_f+1)}(m^2) = \alpha_s^{(n_f)}(m^2) \ . \tag{5}
\]
In Eqs. (4) and (5) \( q_H \) introduces a partonic heavy quark density into the massless evolution equations and the unspecified \( \alpha_s(Q_0^2) \) may be either \( \alpha_s^{(n_f)}(Q_0^2) \) or \( \alpha_s^{(n_f+1)}(Q_0^2) \) because the difference is of the orders neglected in (4). The argument of a continuous \( g(x,Q_0^2) \) and \( \alpha_s(Q_0^2) \) has been advanced \[7, 11\] for adopting \( Q_0 = m \) in all NLO parton distribution sets constructed so far along a VFNS philosophy \[13–15\]. On the other hand, when \( Q_0 \neq m \) the discontinuity of \( \alpha_s \) is in practice as small as maximally 4% up to \( Q_0^2 \) as high as 1000 GeV\(^2\). Anyway, the recently completed NNLO transformation equations \[12, 16\] reveal that the possibility of a continuous evolution across \( Q_0 \) breaks down beyond NLO by nonlogarithmic higher order corrections to (4), (5). The restriction to \( Q_0 = m \) should hence be abandoned and effects of varying \( Q_0 \) should be taken into account on the same level as the variations of the mass factorization scale \( \mu_F^2 \) usually considered. Indeed, along

\[
\ln \frac{Q^2}{m^2} = \ln \frac{Q_0^2}{m^2} + \ln \frac{\mu_F^2}{Q_0^2} + \ln \frac{Q^2}{\mu_F^2},
\]

the two scales \( Q_0 \) and \( \mu_F \) define quite symmetrically which portion of the quasi-collinear \( \ln(Q^2/m^2) \) is actually resummed [\( \ln(\mu_F^2/Q_0^2) \)] and what amount is kept at fixed order, either in the boundary condition for \( q_H [\ln(Q_0^2/m^2)] \) or in the hard scattering coefficient function \( C_2^g \) in Eq. (7) below [\( \ln(Q^2/\mu_F^2) \)]. We will investigate the residual \( Q_0 \) dependence for the charm production contribution to the deep inelastic structure function \( F_2 \) using \( m = m_c (= 1.5 \text{ GeV}) \). To avoid complications from an interplay of several scales we will decouple the bottom and top quark from the process \( (m_{b,t} \to \infty) \) and we will fix the factorization scale at \( \mu_F = Q \).

In the asymptotic limit \( m_c^2/Q^2 \to 0 \) the schemes \[4, 7, 11\] reduce - as in Eq. (3) - to the so-called Zero Mass Variable Flavour Number Scheme, equivalent to the ‘massless parton’ scenario of Ref. \[2\] where any mass dependence is dropped except for the boundary conditions in (4). We will consider such a scenario in the following and ignore terms of \( \mathcal{O}(m_c^2/Q^2) \) because these are not handled uniformly in the individual realizations \[4, 4, 4\] of a VFNS \[4\]. For definiteness we consider an \( F_{2,c,MP}^{c,M} \) in \( \gamma^*P \) scattering which is given by

\[
\frac{1}{x} F_{2,c,MP}^{c,M}(x,Q^2) = e_c^2 \left\{ (c + \bar{c}) \left( x, Q^2 \right) + \frac{\alpha_s(Q^2)}{2\pi} \left[ g \otimes C_2^g + (c + \bar{c}) \otimes C_2^g \right] \left( x, Q^2 \right) \right\},
\]

\[1\]Indeed the charm scheme of \[10\] is explicitly constructed upon \( Q_0 = m \) and a generalization of this particular scheme for \( Q_0 \neq m \) seems nontrivial.
Figure 1: Dependence of the ‘massless parton’-type charm structure function $F^{c,MP}_2(x,Q^2)$ in Eq. (7) on the switching scale $Q_0$ in the boundary conditions in Eq. (4). The solid lines represent the central value of $Q_0 = m_c$ and $F^{c,MP}_2$ decreases monotonically with increasing $Q_0$. The underlying parton distributions below $Q_0$ are those of Ref. [13].

where the $C_{2}^{g,q}$ are the massless $\overline{\text{MS}}$ coefficient functions [17, 18]. It has already been pointed out in [2] that the ‘massless parton’ $F^{c,MP}_2$ in Eq. (6) can be rather arbitrarily suppressed if some larger effective charm mass is introduced [19] into the boundary condition (5). Our investigation here will clarify the situation if - for a fixed value of the physical charm mass $m_c$ - the unphysical switching scale $Q_0$ is varied consistently according to the NLO boundary equations (4). Fig. 1 shows the effect if the transition scale is allowed to vary over the range $m_c^2/2 < Q_0^2 < 2 m_c^2$ where the central value $Q_0 = m_c$ is represented by the solid lines and $F^{c,MP}_2$ monotonically decreases with increasing $Q_0$.²

The evolution leading to the results in Fig. 1 is based on the $n_f = 3$ valence-like NLO input of Ref. [13] using NLO (2-loop) splitting functions. Above $Q_0$ the evolution deviates from [13] because we consider general $Q_0 \neq m_c$ here and we ignore - as mentioned above - any bottom quark effects ($m_b \rightarrow \infty$). The amount of change of $F^{c,MP}_2$ under variation of $Q_0$ hints at a reasonable perturbative stability. Nevertheless, the error represented by the

² Allowing for $Q_0 < m_c$ in Eq. (5) leads obviously to $c(x, Q_0^2) < 0$ which appears somewhat counter-intuitive in probabilistic parton model language. Note, however, that a negative charm input arises even for $Q_0 = m$ from higher order corrections to Eq. (4) [20]. Anyway, the measurable cross section $F_2^c$ is certainly positive above the physical threshold $Q^2(1/x - 1) > 4m_c^2$. 
Figure 2: Dependence of the ‘massless parton’-type charm structure function $F_2^{c,MP}$ in Eq. (7) on the switching scale $Q_0$ in the boundary conditions in Eq. (4). In this Figure $Q_0$ is allowed to vary (maximally) between the input scale of [13] as a lower and the physical scale $Q^2$ as an upper limit.

The shaded bands in Fig. 1 is of the typical order of discrepancies between VFNS and FOPT calculations [10, 12] which questions the gain in predictivity if FOPT is abandoned for VFNS. Such uncertainties are critical for precise charm predictions to compare with future experimental accuracy, especially at experimentally most relevant intermediate scales and regarding the fact that $Q_0^2$ was only allowed to fluctuate by a factor of 2. This latter limitation rests on the assumption that $Q_0$ has to be very close to $m_c$ for the all-order logarithms $(\alpha_s/2\pi \times \ln Q^2/m_c^2)^n$ to be correctly resummed. One can as well adopt a very different point of view towards the choice of $Q_0$. One can easily see that inserting Eq. (4) into Eq. (7) gives

$$\lim_{Q_0 \to Q} F_2^{c,MP}(x, Q^2) = \left[ F_2^{GF} \otimes \left( 1 + \frac{\alpha_s}{2\pi} C_q q \right) \right] (x, Q^2) + \mathcal{O}(\alpha_s^2) + \mathcal{O}\left( \frac{m_c^2}{Q^2} \right)$$

(8)

which is dominated by the $\mathcal{O}[\alpha_s \ln(Q^2/m_c^2)]$ LO gluon fusion term $F_2^{GF}$ of the fixed order perturbation series. We may hence consider $Q_0 \to Q$ in a sense as a continuous path from variable flavour number to fixed order calculations. We should then consider values of $Q_0$ as high as we trust fixed order perturbation theory. In Fig. 2 we cover the maximally conceivable range for $Q_0^2$; i.e. the leftmost end of all curves is set by the low input scale of the parton distributions in [13], $Q_0^2 = 0.3$ GeV$^2$, while the rightmost ends are the ‘fixed
order limit’ in Eq. (8). The observed monotonic scale dependence has to be expected from the positivity of the collinear resummation at small $x$ which is continuously suppressed the more $Q_0$ is increased. Worrisome is, however, the steep slope $\partial F_{2,\text{MP}}^{c,c}/\partial \ln(Q_0^2/m_c^2)$ around $Q_0 \sim m_c$ for high $W^2 = Q^2(1/x - 1)$, where the charm contribution is most important. This observation restricts the predictive power of NLO collinear resummation techniques which have thus far been constructed to match the asymptotic ($Q^2 \to \infty$) $F_{2,\text{MP}}^{c,c}$ derived from $c(x, Q_0^2 = m_c^2) = 0$. The uncertainty from the residual $Q_0$ dependence, inherent to any VFNS \cite{7,8,10} worked out to NLO, seems to dominate over scheme uncertainties of $O(m_c^2/Q^2)$ between the individual schemes. The arbitrariness of $Q_0$ therefore constitutes a main limiting factor on the perturbative accuracy of VFNS heavy quark predictions at high $Q^2$. On the other hand we observe a flattening slope $\partial F_{2,\text{MP}}^{c,c}/\partial \ln(Q_0^2/m_c^2)$ towards the ‘fixed order limit’ at high $Q_0 \lesssim Q$ where perturbative NLO $\leftrightarrow$ LO stability had been found in \cite{2} by $K$ factor considerations for the full fixed order predictions, i.e. including logs and finite terms. We should reemphasize that these conclusions are based on the NLO matching conditions in Eq. (4) - which is the present state of the art for PDF sets including partonic heavy quarks \cite{13–15} - and do not take into account the higher corrections of \cite{12,13}. The terms beyond Eq. (4) represent NNLO contributions to the asymptotic VFNS prediction $F_{2,\text{MP}}^{c,c}$. Very recently the results of \cite{12} have been implemented in a $O(\alpha_s^2)$ implementation of a VFNS\footnote{A $c(x, Q^2)$ derived from the NNLO boundary conditions in \cite{12} would, however, be problematic to apply to hadroproduction calculations, since the higher terms in \cite{12} are not yet contained in, e.g., the fixed NLO $[O(\alpha_s^2)]$ hadroproduction process $pp \to c(p_T)X$ \cite{21}.} where the contribution from the unknown NNLO (3-loop) splitting functions had to be neglected. Choosing $Q_0 = m$ the results of \cite{20} seem to indicate that the impact of terms from the resummation beyond fixed NLO $[O(\alpha_s^2)]$ perturbation theory is rather moderate. As a further step in the line of the present investigation it would clearly be interesting to generalize \cite{20} to $Q_0 \neq m$. If a $Q_0 > m$ would be prefered by such an analysis the difference between VFNS and FOPT would be reduced even more. Such a result would again re-confirm the perturbative reliability of FOPT found in \cite{2} as much as it would help reduce unphysical scheme dependences of QCD predictions on charm production and thus make a comparison to experiment even

\footnote{The confusion of counting perturbative orders differently in resummed (MP) and fixed order (FOPT) calculations is treated in more detail in \cite{8,10}.}
more compelling.

To summarize, we have considered variations of the a priori arbitrary charm input scale $Q_0$, which separates a 3 from a 4 flavour scheme in variable flavour number approaches, around its usually adopted but by no means theoretically required value of $Q_0 = m_c$. From the NLO boundary conditions we found a monotonic $Q_0$ dependence and a worrisome steep slope of $F_{c,MP}^2$ in (7) with respect to $\ln Q_0^2$ just around $Q_0 \sim m_c$. This behaviour restricts the accuracy of a collinearly resummed NLO approach towards calculating high $Q^2$ charm production from matching $\mathcal{O}(\alpha_s)$ boson gluon fusion at $Q_0 = m_c$ in the MP component of Eq. (8). This uncertainty in MP from the unknown $Q_0$ feeds back onto the entire VFNS via Eq. (3) which is normalized to MP asymptotically ($Q^2 \gg m^2$). Our results imply to consider variations of $Q_0$ both as a limiting factor on the present perturbative accuracy if estimating the theoretical uncertainty of VFNS heavy quark predictions as well as in order to optimize the starting scale for the charm evolution within higher order realizations of VFNSs [12, 20, 22]. This latter higher order analysis assumes, however, that the unknown NNLO (3-loop) splitting functions can be neglected [20].

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References

[1] M.A. Shifman, A.I. Vainshtein and V.I. Zakharov, Nucl. Phys. B136 (1978) 157.

[2] M. Glück, E. Reya and M. Stratmann, Nucl. Phys. B422 (1994) 37.

[3] F.I. Olness and S.T: Riemersma, Phys. Rev. D51 (1995) 4746.

[4] M. Glück, E. Reya and A. Vogt, Eur. Phys. J. C5 (1998) 461.
[5] M. Glück, S. Kretzer and E. Reya, Astropart. Phys. 11 (1999) 327.

[6] M.A.G. Aivazis, F.I. Olness and W.- K. Tung, Phys. Rev. D50 (1994) 3085.

[7] M.A.G. Aivazis, J.C. Collins, F.I. Olness and W.- K. Tung, Phys. Rev. D50 (1994) 3102.

[8] J.C. Collins, Phys. Rev. D58 (1998) 094002.

[9] A.D. Martin, R.G. Roberts, M.G. Ryskin and W.J. Stirling, Eur. Phys. J. C2 (1998) 287.

[10] R.S. Thorne and R. G. Roberts, Phys. Rev. D57 (1998) 6871; R.S. Thorne and R. G. Roberts, Phys. Lett. B421 (1998) 303.

[11] J. C. Collins and W.- K. Tung, Nucl. Phys. B278 (1986) 934; S. Qian, Argonne preprint ANL-HEP-PR-84-72, (unpublished).

[12] M. Buza, Y. Matiounine, J. Smith, W.L. van Neerven, Eur. Phys. J. C1 (1998) 301; Phys. Lett. B411 (1997) 211.

[13] M. Glück, E. Reya and A. Vogt, Z. Phys. C53 (1992) 127.

[14] A.D. Martin, R.G. Roberts, W.J. Stirling, and R.S. Thorne, Eur. Phys. J. C4 (1998) 463.

[15] H. L. Lai et al., CTEQ Collab., hep-ph/9903282.

[16] K. G. Chetyrkin, B. A. Kniehl and M. Steinhauser, Phys. Rev. Lett. 79 (1997) 2184; W. Wetzel, Nucl. Phys. B196 (1982) 259; W. Bernreuther and W. Wetzel, Nucl. Phys. B197 (1982) 228, B513 (1998) 758 (E); W. Bernreuther, Ann. Phys. 151 (1983) 127; W. Bernreuther, Z. Phys. C20 (1983) 331; S. A. Larin, T. van Ritbergen and J. A. M. Vermaseren, Nucl. Phys. B438 (1995) 278.

[17] G. Altarelli, R. K. Ellis and G. Martinelli, Nucl. Phys. B157 (1979) 461.

[18] W. Furmanski and R. Petronzio, Z. Phys. C11 (1982) 293.
[19] A.D. Martin, R.G. Roberts and W.J. Stirling, Phys. Lett. B306 (1993) 145; B309 (1993) 492 (E).

[20] A. Chuvakin, J. Smith and W.L. van Neerven, hep-ph/9910250. J. Smith, talk at the 7th International Workshop on Deep Inelastic Scattering and QCD (DIS 99), DESY Zeuthen, April 1999, to appear in the proceedings (ps-file can be obtained at http://www.ifh.de/~dis99p/wg1.html).

[21] P. Nason, S. Dawson and R.K. Ellis, Nucl. Phys. B303 (1988) 607, B327 (1989) 49, B335 (1990) 260 (E); W. Beenakker, H. Kuif, W.L. van Neerven and J. Smith, Phys. Rev. D40 (1989) 54, W. Beenakker, W.L. van Neerven, R. Meng, G.A. Schuler and J. Smith, Nucl. Phys. B351 (1991) 507; M.L. Mangano, P. Nason and G. Ridolfi, Nucl. Phys. B373 (1992) 295; F.I. Olness, R.J. Scalise and Wu-Ki Tung, Phys. Rev. D59 (1998) 59; M. Cacciari, M. Greco and P. Nason, J. High Energy Phys. 05 (1998) 007.

[22] C. R. Schmidt, proceedings of the 5th International Workshop on Deep Inelastic Scattering and QCD (DIS 97), Chicago, IL, USA, April 1997.