Large $p_\perp$ Hadroproduction of Heavy Quarks

Matteo Cacciari$^a$ and Mario Greco$^{a,b}$

$^a$Dipartimento di Fisica Nucleare e Teorica
Università di Pavia, Pavia, Italy

$^b$INFN, Laboratori Nazionali di Frascati, Frascati, Italy

Abstract

The production of heavy quarks at large $p_\perp$ ($p_\perp \gg m$) in hadronic collisions is considered. The analysis is carried out in the framework of perturbative fragmentation functions, thereby allowing a resummation at the NLO level of final state large mass logarithms of the kind $\log(p_\perp/m)$. The case of $b$-quark production is considered in detail. The resulting theoretical uncertainty from factorization/renormalization scales at large $p_\perp$ is found to be much smaller than that shown by the full $O(\alpha_s^3)$ perturbative calculation.
1 Introduction

Much of the theoretical and experimental interest has been recently devoted to the study of the production of heavy quarks in hadronic collisions. On the theoretical side the calculation in perturbative QCD of the differential and total cross sections to order \( \alpha_s^3 \) has been performed by two groups \([1, 2, 3, 4]\), providing a firm basis for a detailed study of the properties of the bottom and charm quarks, and leading to reliable predictions for the production rate of the top quark \([5, 6]\).

These results do however present a non-negligible residual renormalization/factorization scale dependence, particularly at large \( p_\perp \). Furthermore, the validity of this next-to-leading (NLO) \( O(\alpha_s^3) \) calculation is limited when \( p_\perp \gg m, m \) being the large quark mass, by the appearance of potentially large logarithms of the type \( \log(p_\perp/m) \), which have to be resummed to all orders. The physical reason for that is quite clear. For example, terms of order \( (\alpha_s^3) \log(p_\perp/m) \) or \( (\alpha_s^4) \log(p_\perp/m)^2 \) are simply related to the mass singularities originating from collinear configurations when \( m \to 0 \) for fixed \( p_\perp \). The theoretical uncertainty associated to those corrections has been roughly estimated in \([2]\). Whereas for top quark production this uncertainty is irrelevant, this is not the case for the production of bottom and charm quarks at large \( p_\perp \), leading to relevant phenomenological consequences.

In the present paper we consider a solution to this problem, namely we study the behaviour of the differential cross section for the production of heavy quarks in the limit \( (p_\perp/m) \gg 1 \), to NLO accuracy. To this aim we follow an approach based on the properties of fragmentation of a generic parton \( p \ (p = q, g, Q) \) in the heavy quark \( Q \), after the parton has been produced inclusively in the hard collision of the two initial hadrons. The basic formula is represented by eq. (1), where the partonic cross sections \( \hat{\sigma}^{ij\to kX} \) at \( O(\alpha_s^3) \) have been given in ref. \([7]\) in the massless quark limit. \( \hat{\sigma}^{ij\to kX} \) introduces an explicit dependence on \( p_\perp \) and on renormalization/factorization mass scales. The dependence on the heavy quark mass is then obtained through the fragmentation function of the parton \( p \to Q + X \), evolved at NLO accuracy from an initial scale \( \mu_0 \sim m \) (see below) to \( \mu \sim p_\perp \). This approach explicitly resums potentially large terms of the kind \( [\alpha_s \log(p_\perp/m)]^n \), giving a better description of the theoretical predictions at large \( p_\perp \). Indeed the corresponding uncertainty is quite reduced in this region with respect to the perturbative result, due to a significantly smaller sensitivity to the relevant scales. On the other hand, because of the massless limit used for the \( O(\alpha_s^3) \) kernel cross sections \( \hat{\sigma}^{ij\to kX} \), this approach does not allow to recover in a simple way the limit \( p_\perp \ll m \) of the perturbative calculation.

In this paper we restrict our approach to \( b \)-quark production, the application to charm production will be given elsewhere. In Sect. 2 we give the general formalism. In Sect. 3 we first discuss the basic ingredients necessary to obtain our NLO cross sections and then we present our results. We compare with the perturbative calculation of ref. \([4]\) and study in detail the dependence on the various mass scales entering the problem. Our conclusions are finally given in Sect. 4.
# 2 The fragmentation function approach

According to factorization theorems the cross section for the inclusive hadroproduction of a hadron at high transverse momentum, i.e. for the process

\[ H_1 + H_2 \rightarrow H_3 + X \]

can be written as

\[
d\sigma = \sum_{i,j,k} \int dx_1 dx_2 dx_3 F_{H_1}^i(x_1, \mu_F) F_{H_2}^j(x_2, \mu_F) d\hat{\sigma}_{ij \rightarrow kX}(x_1, x_2, \mu_R, \mu_F) D_{kH_3}^H(x_3, \mu_F) \tag{1} \]

As usual, the \( F \)'s are the distribution functions of the partons in the colliding hadrons, \( \hat{\sigma} \) is the kernel cross section and \( D \) is the fragmentation function of the observed hadron. The factorization mass scales \( \mu_F \) of the structure and fragmentation functions are assumed to be equal for the sake of simplicity. \( \mu_R \) is the renormalization scale.

Due to the presence of collinear singularities both in the initial and final state this process is not fully predictable by QCD itself. We can actually calculate the kernel cross section and the evolution of the structure and fragmentation functions, but we have to rely on some phenomenological input to obtain the latter at some given initial scale.

This situation changes drastically when we come to consider the inclusive production of a heavy quark. In this case its mass, being finite and considerably greater than \( \Lambda \), makes the perturbative expansion feasible and prevents collinear singularities from appearing in the splitting vertices which involve the heavy quark.

Having this in mind two approaches can be pursued in the calculation of heavy quark production.

The first one is to directly calculate in perturbation theory the process \( d\hat{\sigma}_{ij \rightarrow QX} \), \( Q \) being the heavy quark and \( i, j \) the initial state light partons (i.e. light quarks and gluons). This kernel cross section will then be convoluted with initial state structure functions only, the final state showing no singularities of any kind. This approach has been followed in the past, providing a full perturbative \( O(\alpha_s^3) \) calculation. In the following we shall use for comparisons the results of Nason, Dawson and Ellis, and refer to them as NDE. In this perturbative approach, as stated earlier, terms of the kind \( \alpha_s \log(p_\perp/m) \) will appear. They are remnant of the collinear singularity screened by the finite quark mass. As noted in ref. they can grow quite large at high tranverse momenta, thereby spoiling the validity of the expansion in \( \alpha_s \). Therefore they have to be summed to all orders.

The alternative way is to consider that when a quark, of whichever flavour, is produced at very high transverse momentum \( p_\perp \gg m \) its mass plays almost no role at all in the scattering process. This is to say that mass effects in the kernel cross section are suppressed as power ratios of mass over the scale of the process. We can therefore devise a picture in which all quarks are produced in a massless fashion at the high scale \( \mu_F \sim p_\perp \gg m \) and only successively, as their virtuality decreases, they can fragment into a massive heavy quark. The cross section can therefore be described by a formula analogous to eq. (1), with \( H_3 = Q \). The key difference to the
hadron production case considered in eq. (1) is that initial state conditions for the heavy quark fragmentation functions are now calculable from first principles in QCD (hence the definition of “perturbative” fragmentation functions, PFF) and do not have to be taken from experiment.

Actually, the following set of next-to-leading initial state conditions can be obtained \[9\] in the \(\overline{MS}\) scheme for the fragmentation function of a heavy quark, gluon and light quark respectively, in the heavy quark \(Q\)

\[
D_Q^Q(x, \mu_0) = \delta(1-x) + \frac{\alpha_s(\mu_0)}{2\pi} C_F \left[ \frac{1 + x^2}{1 - x} \left( \log \frac{\mu_0^2}{m^2} - 2 \log(1-x) - 1 \right) \right]_+ \tag{2}
\]

\[
D_g^Q(x, \mu_0) = \frac{\alpha_s(\mu_0) T_F}{2\pi} (x^2 + (1-x)^2) \log \frac{\mu_0^2}{m^2} \tag{3}
\]

\[
D_{q,q,Q}^Q(x, \mu_0) = 0 \tag{4}
\]

where \(\mu_0\) must be taken of the order of the heavy quark mass.

Then using the usual Altarelli-Parisi evolution equations at NLO accuracy one finds the fragmentation functions set at any desired factorization scale \(\mu_F\). An important feature of this approach can now be appreciated. The “almost-singular” logarithmic term \(\log \left( \frac{p_\perp}{m} \right)\) splits into two, as follows.

A \(\log \left( \frac{p_\perp}{\mu_F} \right)\) will be found in the kernel cross section \(\hat{\sigma}\) which has no dependence on the heavy quark mass, according to the assumption that it is produced in a massless way. Moreover, by choosing \(\mu_F \sim p_\perp\) it will not contain large logarithms and its perturbative expansion will behave correctly.

The remaining part of the log will instead be lurked into the fragmentation function \(D(x_3, \mu_F)\). The large \(\log(\mu_F/\mu_0)\) is resummed to all orders by the evolution equations, and only the small \(\log(\mu_0/m)\) provided by the initial state condition is treated at fixed order in perturbation theory. Therefore one expects a better control of the theoretical uncertainty at large \(p_\perp\). On the other hand, for \(p_\perp \lesssim m\) the fragmentation approach does not allow to recover easily the perturbative result, which, of course, holds exactly.

3 NLO Cross Section Evaluation

In order to implement the “perturbative fragmentation function (PFF) approach” at a numerical level we need four ingredients, which are all available at the next-to-leading level:

i) the distribution functions of any parton (including the heavy flavour in question) in the hadrons (proton or antiproton), evolved at NLO accuracy. All modern sets satisfy this requirement. An important point must however be made clear. A heavy quark present in the initial state can be directly brought to the final state where it is fragmented to the detected heavy flavour through the \(D_Q^Q\), and therefore with high probability (see below). This means that the resulting cross section is particularly sensitive to the overall heavy flavour content of the colliding hadrons. In the Parton Distribution Functions (PDF) sets available this content is generated through perturbative gluon splitting above a given
threshold. The total yield will therefore depend on the choice made. For instance, the
HMRS set \cite{10} takes \( F_b(x, 2m_b) = 0 \) as initial condition, whereas the MT \cite{11} and the
CTEQ \cite{12} ones choose, according to ref. \cite{13}, \( F_b(x, m_b) = 0 \). The resulting different
bottom distributions are plotted in figure 1: the MT and CTEQ bottom contents are
consistently higher than the HMRS one, the discrepancy growing larger as the HMRS
threshold value is approached.

\textit{ii)} the kernel cross section for the scattering of any two massless partons into another massless
parton. This calculation is provided at the NLO in various renormalization/factorization
schemes in ref. \cite{7}. The massless limit approximation used in these \( O(\alpha_s^3) \) kernel cross
sections will not allow to evaluate the heavy quark cross section for \( p_\perp \ll m \).

\textit{iii)} the next-to-leading expression for the strong running coupling:

\[
\alpha_s(\mu^2) = \frac{1}{b \ln(\mu^2/\Lambda^2)} \left[ 1 - \frac{b'}{b} \frac{\ln \ln(\mu^2/\Lambda^2)}{\ln(\mu^2/\Lambda^2)} \right]
\]

\[
b = \frac{33 - 2N_f}{12\pi}, \quad b' = \frac{153 - 19N_f}{24\pi^2}
\]

The QCD scale \( \Lambda \) is set at the value fixed by the structure function set used and the
number of active flavours \( N_f \) is set at 5 above the appropriate threshold.

\textit{iv)} the fragmentation functions of any parton into the heavy flavour. They are obtained by
evolving the initial conditions given above (eqs. 2, 3, 4) with NLO accuracy \cite{14}. This is
done through numerical inversion of the Mellin moments of the evolved distributions\(^1\),
and a typical result for bottom fragmentation is depicted in figure 2, together with the un-
certainty given by the choice of the initial condition scale \( \mu_0 \) around \( m_b \). The implication
of these ideas to LEP hadronic data is discussed in ref. \cite{15}.

With these four ingredients at our disposal we can now evaluate the cross section for the high
\( p_\perp \) inclusive hadroproduction of a bottom quark. This will be done by performing numerically
the triple integration of eq. (1). It must be noted that this integration is not as straightforward
as the one usually performed when calculating hadron distributions. Indeed while the hadronic
fragmentation functions fall smoothly to zero as \( x \) approaches one, now the \( D_{Q^2} \) is instead
singular in the \( x \to 1 \) limit, due to unresummed Sudakov terms. This makes the most usual
integration routines to fail in calculating both the integral and the associated numerical error,
the latter being heavily underestimated.

More in detail this problem has been overcome by suitably rearranging the integration in
such a way that the numerical integration could be reliably performed. By rewriting eq. (1) in
a more compact form, and dropping all unnecessary symbols, we have

\[
\sigma = \int_{x_3}^{1} \int_{x_1}^{1} \int_{x_2}^{1} F_1 F_2 \sigma_{ijk}(x_3) D_k(x_3) =
\]

\(^1\)We thank Paolo Nason for having provided us with the FORTRAN code for this.
\[ = \int_{x_{3}^{\text{min}}}^{1} dx_{3} \int dx_{1} dx_{2} \sum_{\substack{ijk \kern 1em k \neq \text{Q}}} F_{i} F_{j} \hat{\sigma}_{ijk}(x_{3}) D_{k}(x_{3}) + \]
\[ + \int_{x_{3}^{\text{min}}}^{1-\epsilon} dx_{3} \int dx_{1} dx_{2} \sum_{ij} F_{i} F_{j} \hat{\sigma}_{ijQ}(x_{3}) D_{Q}(x_{3}) + \]
\[ + \int_{1-\epsilon}^{1} dx_{3} \left[ \frac{\int dx_{1} dx_{2} \sum_{ij} F_{i} F_{j} \hat{\sigma}_{ijQ}(x_{3})}{x_{3}} - \frac{\int dx_{1} dx_{2} \sum_{ij} F_{i} F_{j} \hat{\sigma}_{ijQ}(1)}{1} \right] x_{3} D_{Q}(x_{3}) + \]
\[ + \int dx_{1} dx_{2} \sum_{ij} F_{i} F_{j} \hat{\sigma}_{ijQ}(1) \int_{1-\epsilon}^{1} dx_{3} x_{3} D_{Q}(x_{3}) \]  
(5)

The last integral over \( x_{3} \) is then evaluated by resorting to the Mellin moments\(^2\) of the evolved fragmentation function:

\[ \int_{1-\epsilon}^{1} dx_{3} x_{3} D_{Q}(x_{3}) = \tilde{D}_{Q}(2) - \int_{0}^{1-\epsilon} dx_{3} x_{3} D_{Q}(x_{3}) \]  
(6)

The result should of course be independent of the choice of \( \epsilon \), and we have verified that this is indeed the case for \( 0.9 \leq \epsilon \leq 0.99 \).

Figure 3 shows a comparison of the perturbative result of ref. [2] with our calculations for two different PDF sets, at the Fermilab energy of 1800 GeV, for \( \mu = \sqrt{m_{b}^{2} + p_{T}^{2}} \). We can see that in the high \( p_{T} \) region the perturbative cross section is quite sensitive to the structure function set choice, the MT one giving a markedly lower result. The opposite happens in the PFF approach, which becomes very sensitive in the low \( p_{T} \) region which, as stated above, is plagued by the neglect of the heavy quark mass terms in the partonic cross sections. This pattern is due to the fact that the NDE calculation only uses the light quark content from the structure functions, since the heavy one is produced at the purely perturbative level. This introduces a mismatch (albeit of higher order) as the evolution had been performed by taking into account all flavours, which get mixed through gluon exchange. Our calculation, on the other hand, treats all quarks on the same ground and uses the full information of the PDF set. This leads to substantially identical predictions obtained in the high \( p_{T} \) region with the two PDF sets. On the contrary, at low \( p_{T} \) the different threshold behaviour of the two sets in the heavy quark content is responsible for the discrepancy between the two results.

Figure 4a,b show the same kind of comparison at 630 GeV and 16 TeV. The behaviour is practically identical, once a rescaling on the \( p_{T} \) axis has been considered to account for the different cm energies.

One further comparison can also be made between the MT-B2 and the CTEQ1M sets, which have a similar threshold behaviour for the heavy quark flavour. As can be seen in figure 3a,b the theoretical uncertainty due to the structure functions set choice is once again smaller in the fragmentation function approach.

\(^2\)We recall that the Mellin moments are defined by

\[ \tilde{D}(N) = \int_{0}^{1} dx \ x^{N-1} D(x) \]
Next we consider the dependence on the choice of the renormalization/factorization mass scale $\mu$. Figure 6a(b) shows, at 1800 GeV and with the MT-B2 (HMRS-B) set, the theoretical uncertainty resulting from the variation of the factorization and renormalization mass scales between $\mu_{\text{ref}}/2$ and $2\mu_{\text{ref}}$, where $\mu_{\text{ref}}$ is defined as $\sqrt{m_b^2 + p_{\perp}^2}$ and we have taken $\mu = \mu_F = \mu_R$. As expected the band of the perturbative NDE calculation is sensibly larger than ours, showing the improvement brought by the resummation of the large logarithms of $p_{\perp}/m_b$. The drop at low $p_{\perp}$ in the prediction of the HMRS-B set with $\mu = \mu_{\text{ref}}/2$, which considerably broadens our band in that region, is due to the very poor heavy quark content of this set at such a low scale (see Fig. 1). All these features can be better appreciated in figure 7, where the cross section at 1800 GeV with the MT-B2 set is plotted, at fixed $y$ and $p_{\perp}$, as a function of $\mu = \xi \mu_{\text{ref}}$, for $\xi$ varying between 0.25 and 4. This figure also shows a comparison with the factorized calculation with a Born (i.e. LO) cross section kernel (but with two-loop $\alpha_s$ and NLO structure and fragmentation functions). As expected, the lack of the next-to-leading terms strongly enhances the scale dependence. The similarity between the NDE result and the fragmentation function approach with Born kernel cross section is striking. The small scale sensitivity of our full NLO calculation shows that the fragmentation/renormalization scale dependence is a real $O(\alpha_s^4)$ effect, whereas in the perturbative approach (e.g. NDE) the presence of large $\log(p_{\perp}/m)$ results in an effective $O(\alpha_s^3)$ dependence.

Once again, the results at 630 GeV greatly mimic those at 1800 GeV (see figure 8).

One further theoretical uncertainty must be considered, namely the one related to the freedom in the choice of the initial condition scale $\mu_0$ in the fragmentation functions evolution. Figure 9 shows that the cross section is marginally affected by a change of $\mu_0$ in the range $m_b/2 \rightarrow 2m_b$, particularly in the high $p_{\perp}$ region. This leads to the conclusion that the PFF approach has still a smaller overall theoretical uncertainty also after this qualitatively new feature has been taken into account.

Finally, we show in figs. 10a,b the relative importance of the various partonic subprocesses contributing to the cross section for two sets of PDFs. In the case of the MT-B2 set (similar results are obtained with the CTEQ1M one) the $Qg$ scattering clearly dominates at low $p_{\perp}$, whereas at large $p_{\perp}$ it becomes comparable to other channels. Comparing with the HMRS-B set we see that the different threshold behaviour of the heavy quark structure function in this latter set, repeatedly pointed out before, is responsible for the lower contribution of the $Qg$ and $Qq$ channels.

We can now turn to quantities of more direct experimental interest and see how the advantages of our approach are reflected onto them. Namely, we will consider the total cross section for one particle inclusive heavy quark production, integrated above a given $p_{\perp}^{\text{min}}$ and within a rapidity region $|y| < y_{\text{max}}$. Only the variation of the theoretical prediction due to changes in the factorization/renormalization scale and in the PDF set used will be studied. Other possible sources of uncertainties, aside the change of $\mu_0$ which has been shown to be almost negligible, are the value of the QCD scale $\Lambda$ and of the bottom mass $m_b$. They should however be common to both the perturbative and the fragmentation function approach, and have been studied in detail in ref. [2].
Figures 11, 12 and 13 show the total cross section $\sigma(p_\perp > p_{\perp}^{\text{min}}, |y| < 1)$ at a cm energy of 1800 GeV. The HMRS-B, MT-B2 and CTEQ1M sets have been used respectively, and the curves obtained with $\mu = 2\mu_{\text{ref}}$ and $\mu = \mu_{\text{ref}}/2$ are plotted. We can see that the features of the differential cross sections previously discussed translate almost directly into the total cross section. In particular, the scale dependence of our result is once again remarkably smaller than the one of the perturbative calculation, especially in the high $p_\perp$ region. The broadening of the band in the low $p_\perp$ region than can be observed when the HMRS-B or the CTEQ1M set is used with the scale choice $\mu = \mu_{\text{ref}}/2$ is once again due to the different heavy quark content at low scales (see fig. 1).

The overall smaller theoretical uncertainty of the PFF result can finally be appreciated in fig. 14, where the highest and lowest predictions of the two approaches, out of the six curves previously considered, have been plotted. Note that we have not considered in detail the uncertainties for $p_\perp \lesssim 10$ GeV. The CDF experimental data [16] are also shown.

The same kind of result can also be produced at 630 GeV. Figure 15 compares the band of NDE to our one and to experimental data by UA1 [17]. Also in this case we find a sizeable reduction in the uncertainty of the theoretical prediction.

## 4 Conclusions

In this paper we have discussed the production of heavy quarks at large $p_\perp$ ($p_\perp \gg m$) in hadronic collisions, in order to make the theoretical predictions for the differential distributions more reliable. We have studied this problem in the framework of the perturbative fragmentation functions, which allow a NLO evaluation of the potentially large logarithms of the kind $\log(p_\perp/m)$, which are resummed to all orders.

Our analysis for the $b$-quark leads to much more stable results with respect to changes of the factorization/renormalization scales compared to what is obtained in the $O(\alpha_s^3)$ perturbative calculation. Also the theoretical uncertainty related to different choices of PDF sets is reduced. Other possible sources of uncertainties, like the scale $\mu_0$ of the initial state condition in the fragmentation functions evolutions, are negligible. A detailed discussion of the differential and integrated cross sections of experimental interest has also been presented.

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