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# Hadroproduction of open heavy flavour for PDF analyses

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Due to the large masses of the charm and bottom quarks, their production cross sections are calculable within the perturbative QCD. This makes the heavy-quark mesons important observables in high-energy collisions of protons and nuclei. However, the available calculations for heavy-flavored-meson hadroproduction have been somewhat problematic in reliably describing the cross sections across the full kinematic range from zero to very high  $p_T$ . This has put some question marks on the robustness of LHC heavy-flavored-meson measurements in studying the partonic structure of the colliding hadrons and nuclei. Here, we introduce SACOT- $m_T$  – a novel scheme for open heavy-flavour hadroproduction within the general-mass variable-flavour-number formalism that solves this problem. The introduced scheme is an analogue of the SACOT- $\chi$  scheme often used for deeply-inelastic scattering in global analyses of PDFs.

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## 1. Introduction

The hadroproduction of open heavy flavour – D mesons in particular – has recently been advocated as a promising constraint for proton parton distribution functions (PDFs) [1, 2]. The theoretical description is typically based on the fixed flavour-number scheme (FFNS) [3], FONLL code [4], or FFNS matched to parton showers [5]. However, the use of e.g. FFNS calculation in conjunction with PDFs defined in variable flavour-number schemes (the commonly used general-purpose PDFs) may be too restrictive, and in this sense calculations within the framework of general-mass variable-flavour-number scheme (GM-VFNS) would be more natural. Here, we will discuss our novel implementation of the GM-VFNS, the so-called SACOT- $m_T$  scheme [6].

## 2. D-meson production in fixed flavour-number scheme

Within FFNS – assuming no intrinsic heavy-quark content in the proton – the massive quarks  $Q$  are always produced in pairs by the partonic processes,  $g + g \rightarrow Q\bar{Q} + X$ ,  $q + \bar{q} \rightarrow Q\bar{Q} + X$ ,  $q + g \rightarrow Q\bar{Q} + X$ . The cross section for inclusive  $Q$  production can be written as an integral of PDFs  $f_i^p(x_1, \mu_{\text{fact}}^2)$  and partonic cross sections  $d\hat{\sigma}^{ij}$ ,

$$\frac{d\sigma(p + p \rightarrow Q + X)}{dp_T dy} = \sum_{ij} \int dx_1 dx_2 f_i^p(x_1, \mu_{\text{fact}}^2) \frac{d\hat{\sigma}^{ij \rightarrow Q+X}(\tau_1, \tau_2, m^2, \mu_{\text{ren}}^2, \mu_{\text{fact}}^2)}{dp_T dy} f_j^p(x_2, \mu_{\text{fact}}^2),$$

where  $y$  and  $p_T$  denote the rapidity and transverse momentum of the produced heavy quark. The factorization and renormalization scales are marked by  $\mu_{\text{fact}}^2$  and  $\mu_{\text{ren}}^2$ . The kinematic variables  $\tau_{1,2}$  are the “massive” Mandelstam variables,

$$\tau_1 \equiv p_1 \cdot p_3 / p_1 \cdot p_2 = m_T e^{-y} / (\sqrt{s} x_2), \quad \tau_2 \equiv p_2 \cdot p_3 / p_1 \cdot p_2 = m_T e^y / (\sqrt{s} x_1), \quad m_T^2 = p_T^2 + m^2,$$

denoting the momenta of the incoming partons and outgoing heavy quark by  $p_{1,2}$  and  $p_3$ , respectively. The partonic cross sections scale as  $d\hat{\sigma}^{ij \rightarrow Q+X} \sim \tau_{1,2}^{-n}$ , and, thanks to the heavy-quark mass, remain finite even at  $p_T = 0$ . The heavy-quark cross sections can be turned into, say  $D^0$ -meson production cross sections by folding with  $Q \rightarrow D^0$  fragmentation functions (FFs)  $D_{Q \rightarrow D^0}(z)$ . The fragmentation variable  $z$  is not unique when the masses of the heavy quark and  $D^0$  meson are kept non zero. For simplicity, we define  $z \equiv E_{D^0} / E_Q$ , where  $E_{D^0}$  and  $E_Q$  are the energies of the  $D^0$  meson and heavy quark in the center-of-mass frame of the p-p collision. Assuming that the fragmentation is collinear we get,

$$\frac{d\sigma(p + p \rightarrow D^0 + X)}{dP_T dY} = \sum_{ij} \int \frac{dz}{z} dx_1 dx_2 f_i^p(x_1, \mu_{\text{fact}}^2) \frac{d\hat{\sigma}^{ij \rightarrow Q+X}}{dp_T dy} f_j^p(x_2, \mu_{\text{fact}}^2) D_{Q \rightarrow D^0}(z),$$

where the (lower case) partonic and (upper case) hadronic variables are related by

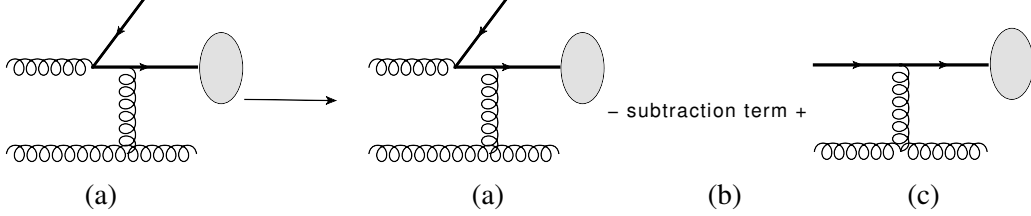
$$p_T^2 = \frac{M_T^2 \cosh^2 Y - z^2 m^2}{z^2} \left( 1 + \frac{M_T^2 \sinh^2 Y}{P_T^2} \right)^{-1} \xrightarrow{P_T \rightarrow \infty} \left( \frac{P_T}{z} \right)^2,$$

$$y = \sinh^{-1} \left( \frac{M_T \sinh Y}{P_T} \frac{P_T}{m_T} \right) \xrightarrow{P_T \rightarrow \infty} Y,$$

and  $M_T = \sqrt{P_T^2 + M_Q^2}$  marks the hadronic transverse mass. While this framework appears to work well at low  $P_T$  (see e.g. [7]), the description seems to deteriorate towards high  $P_T$ . Presumably, this can be attributed to the  $\log(p_T^2/m^2)$  behaviour of the partonic cross sections which begin to dominate and should be resummed, as we will come to conclude.

### 3. D-meson production in general-mass variable-flavour-number scheme

The GM-VFNS description can be obtained from FFNS by resumming the  $\log(p_T^2/m^2)$  terms that appear in FFNS. As an example, in Figure 1 the diagram (a) gives rise to such logarithmic behaviour when the initial-state gluon splits into a  $Q\bar{Q}$  pair. This is only the first of the whole series of diagrams that are in GM-VFNS summed into the heavy-quark PDF  $f_Q^p$ . Effectively, this



**Figure 1:** Origin of the heavy-quark initiated subprocess illustrated.

summation can be realized by including the heavy-quark initiated contribution (c) and a subtraction term (b) that avoids the double counting between diagrams (a) and (c). The contribution from  $Qg \rightarrow Q + X$  channel, represented here by the diagram (c), can be written as

$$\int \frac{dz}{z} dx_1 dx_2 f_Q^p(x_1, \mu_{\text{fact}}^2) \frac{d\hat{\sigma}^{Qg \rightarrow Q+X}(\tau_1, \tau_2)}{dp_T dy} f_g^p(x_2, \mu_{\text{fact}}^2) D_{Q \rightarrow D^0}(z).$$

The subtraction term (b) is obtained from this same expression by replacing the heavy-quark PDF with its perturbative expression,

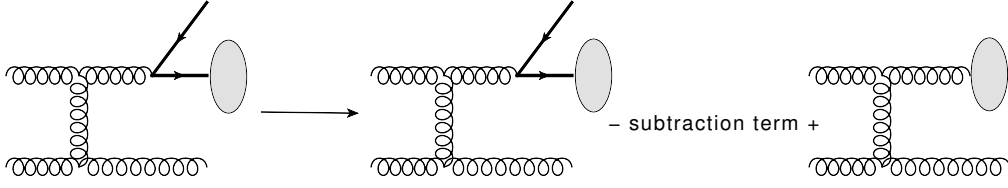
$$f_Q^p(x, \mu_{\text{fact}}^2) = \left(\frac{\alpha_s}{2\pi}\right) \log\left(\frac{\mu_{\text{fact}}^2}{m^2}\right) \int_x^1 \frac{d\ell}{\ell} P_{qg}\left(\frac{x}{\ell}\right) f_g^p(\ell, \mu_{\text{fact}}^2) + \mathcal{O}(\alpha_s^2),$$

where  $\alpha_s$  is the QCD coupling, and  $P_{qg}$  is the usual gluon-to-quark splitting function. However, the exact form of  $d\hat{\sigma}^{Qg \rightarrow Q+X}(\tau_1, \tau_2)$  in the above expressions is not unique [8]. In practice, we can only require that the zero-mass  $\overline{\text{MS}}$  expressions are recovered at high  $p_T$ ,

$$\frac{d\hat{\sigma}^{Qg \rightarrow Q+X}(\tau_1, \tau_2)}{dp_T dy} \xrightarrow{p_T \rightarrow \infty} \frac{d\hat{\sigma}^{qg \rightarrow q+X}(\tau_1^0, \tau_2^0)}{dp_T dy}, \quad \tau_{1,2}^0 = \tau_{1,2} \xrightarrow{m \rightarrow 0} p_T e^{\mp y} / (\sqrt{s} x_{2,1}).$$

The easiest option is to define  $d\hat{\sigma}^{Qg \rightarrow Q+X}(\tau_1, \tau_2) \equiv d\hat{\sigma}^{qg \rightarrow q+X}(\tau_1^0, \tau_2^0)$ , i.e. use the zero-mass expressions to begin with. This is known as the SACOT scheme [9]. The problem of this choice is that it leads to infinite cross sections towards  $p_T \rightarrow 0$  due to the  $d\hat{\sigma}^{qg \rightarrow q+X}/d^3p \sim (\tau_{1,2}^0)^{-n}$  behaviour of the partonic cross sections. In the so-called FONLL scheme [4] this is avoided by multiplying the partonic cross section by an ad-hoc damping factor  $p_T^2/(p_T^2 + c^2 m^2)$  with  $c \sim 5$ , which serves to tame the unphysical behaviour at small  $p_T$ . Alternatively, the problematic behaviour can be avoided simply by retaining the kinematics of the  $Q\bar{Q}$ -pair production which, deep down, is the underlying process we describe. With this physical picture in mind, we define  $d\hat{\sigma}^{Qg \rightarrow Q+X}(\tau_1, \tau_2) \equiv d\hat{\sigma}^{qg \rightarrow q+X}(\tau_1, \tau_2)$  taking  $\tau_{1,2} = m_T e^{\mp y} / (\sqrt{s} x_{2,1})$  as in FFNS. This leads to well-behaved cross sections in the  $p_T \rightarrow 0$  limit. We call this the SACOT- $m_T$  scheme, as it shares the same underlying idea as the SACOT- $\chi$  scheme in deeply-inelastic scattering [10].

Part of the  $\log(p_T^2/m^2)$  terms in FFNS come also from final-state splittings. As an example, Figure 2 shows a diagram in which an outgoing gluon splits into a  $Q\bar{Q}$  pair. The result-



**Figure 2:** Origin of the gluon-fragmentation subprocess illustrated.

ing  $\log(p_T^2/m^2)$  terms are absorbed into the fragmentation-scale ( $\mu_{\text{frag}}$ ) dependent gluon FFs,  $D_{g \rightarrow D^0}(z, \mu_{\text{frag}}^2)$ , giving rise to gluon-fragmentation contributions,

$$\int \frac{dz}{z} dx_1 dx_2 f_g^p(x_1, \mu_{\text{fact}}^2) \frac{d\hat{\sigma}^{gg \rightarrow g+X}(\tau_1, \tau_2)}{dp_T dy} f_g^p(x_2, \mu_{\text{fact}}^2) D_{g \rightarrow D^0}(z, \mu_{\text{frag}}^2).$$

The subtraction term avoiding the double counting is again the same expression, but replacing the gluon FF by its perturbative form,

$$D_{g \rightarrow D^0}(x, \mu_{\text{frag}}^2) = \left(\frac{\alpha_s}{2\pi}\right) \log\left(\frac{\mu_{\text{frag}}^2}{m^2}\right) \int_x^1 \frac{d\ell}{\ell} P_{qg}\left(\frac{x}{\ell}\right) D_{Q \rightarrow D^0}(\ell) + \mathcal{O}(\alpha_s^2).$$

In line with our scheme choice, the  $\overline{\text{MS}}$  zero-mass matrix elements for  $d\hat{\sigma}^{gg \rightarrow g+X}(\tau_1, \tau_2)$  with the massive expressions for  $\tau_{1,2}$ , are adopted. Even if the heavy quarks do not explicitly appear in the  $gg \rightarrow g + X$  process, the underlying process is also here the  $Q\bar{Q}$ -pair production.

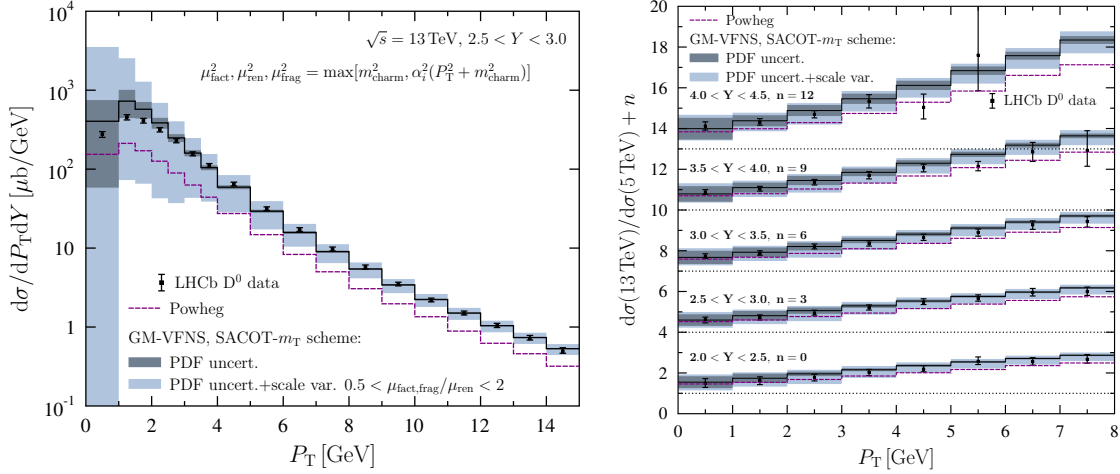
With this schematic justification, our “master formula” within GM-VFNS is,

$$\frac{d\sigma^{pp \rightarrow D^0+X}}{dp_T dY} = \sum_{ijk} \int \frac{dz}{z} dx_1 dx_2 f_i^p(x_1, \mu_{\text{fact}}^2) \frac{d\hat{\sigma}^{ij \rightarrow k}(\tau_1, \tau_2, m, \mu_{\text{ren}}^2, \mu_{\text{fact}}^2, \mu_{\text{frag}}^2)}{dp_T dy} f_j^p(x_2, \mu_{\text{fact}}^2) D_{k \rightarrow D^0}(z, \mu_{\text{frag}}^2). \quad (3.1)$$

Unlike in FFNS, all partonic subprocesses are included and the FFs are scale dependent. In the limit  $p_T \rightarrow 0$ , the partonic cross sections reduce to FFNS, but towards  $p_T \rightarrow \infty$  they tend to the zero-mass  $\overline{\text{MS}}$  expressions. Our numerical realization of SACOT- $m_T$  scheme is crafted around the Mangano-Nason-Ridolfi code [3] for heavy quarks, and the INCNLO code [11] for zero-mass partons. All terms up to  $\mathcal{O}(\alpha_s^3)$  are included.

#### 4. Description of the LHCb $D^0$ data

In Figure 3, we compare the LHCb 13 TeV  $D^0$  data [12] with our GM-VFNS theory calculation. The darker bands show the NNPDF3.1 (pch) [13] PDF uncertainty, and the lighter bands combine the scale-variation and PDF errors. We have used here the KKKS08 FFs [14]. The calculation agrees very well with the data though the scale variation leads to a significant uncertainty at small  $P_T$ . We have found that, the contribution from the three FFNS processes, including the subtraction terms, is less than 10% for  $P_T \gtrsim 3 \text{ GeV}$  and only around 3% for  $P_T \gtrsim 10 \text{ GeV}$ . This demonstrates that the  $\log(p_T^2/m^2)$  terms in FFNS become quickly the dominant ones and must be resummed as done in GM-VFNS. A comparison using FFNS + parton-shower approach (with the same PDFs) is also presented. Here, we have used the POWHEG-BOX event generator [5] matched to the PYTHIA 8 [15] parton shower. We see that the POWHEG+PYTHIA setup has a tendency to



**Figure 3:** Left: LHCb  $D^0$  data [12] in p-p collisions at  $\sqrt{s} = 13 \text{ TeV}$  compared to our GM-VFNS calculation and the POWHEG+PYTHIA framework. Right: Ratio between  $\sqrt{s} = 13 \text{ TeV}$  and  $\sqrt{s} = 5 \text{ TeV}$  data.

underpredict the experimental spectrum, and the ratio between two  $\sqrt{s}$  is clearly flatter than the GM-VFNS prediction. We deduce that the leading reason is that by starting only with  $c\bar{c}$  pairs (generated by POWHEG) one neglects the contributions in which the parton shower excites the  $c\bar{c}$  pair only later on. In GM-VFNS these are resummed to the scale-dependent FFs and, indeed, e.g. the gluon-to-D contributions can be around 50% of the total budget. The gluon fragmentation also significantly changes the  $x$  regions in which the PDFs are sampled. Thus, the use of FFNS-based computation when using D-meson data to fit GM-VFNS PDFs would inflict a potential bias.

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