UH-511-1078-05
DESY 05-212

The Heavy Quark Fragmentation Function at NNLO *

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arXiv:hep-ph/0510263 v1 20 Oct 2005

We present a general discussion of collider processes with not-completely inclusive production of heavy flavors. We review the Perturbative Fragmentation Functions formalism as the appropriate tool for studying such processes and detail the extension of this formalism at Next-to-Next-to-Leading order. We conclude that the prospects for the future in this field are bright and at present are limited by the available experimental data. Hopefully, the future ILC will be able to fill this gap.

I. INTRODUCTION: PRODUCTION OF HEAVY FLAVORS

Production of heavy flavors presents special challenges to theory. There are two reasons for that. The first one is technical and is related to the appearance of an additional parameter (the quark mass) in the integrals. This is a complication that could lead to a manifold increase in the computational effort. The second reason is, however, more subtle and is the subject of the present discussion.

Let us consider some not-completely inclusive differential observable. A typical example would be a one particle inclusive cross-section like the energy spectrum of a quark q in the reaction $e^+e^- \to q\overline{q}$. If the observed parton is massless the differential distribution is divergent once the radiative corrections to the process are included. These collinear divergences arise from configurations where two or more partons become collinear. To deal with the collinear singularities one first introduces a suitable regulator. The most convenient and popular method is the dimensional regularization which simultaneously regularizes all UV divergences. After the usual UV renormalization is performed, one arrives at the following result for the desired massless differential cross-section:

$$\frac{d\sigma_a}{dz}(z,Q,\epsilon) = \sum_b \frac{d\tilde{\sigma}_b}{dz}(z,Q,\mu) \otimes \Gamma_{ba}(z,\mu,\epsilon), \tag{1}$$

where b runs over the relevant quark flavors and the gluon, and $\otimes$ stands for the usual integral convolution.

Eq.(1) demonstrates that the collinear divergences in *any* differential distribution completely factorize, i.e. they are solely contained in the function Γ. Of course, the explicit form of this function depends on the regularization method chosen and on the convention for the non-divergent pieces that Γ contains. It has become standard practise to factorize the collinear divergences in the so-called $\overline{\rm MS}$ scheme. The most important property of the collinear "counterterm" Γ is its universality, i.e. its form is independent of the process $d\sigma$. The physical meaning of the collinear divergences appearing in differential distributions like Eq.(1) is well understood; they are related to long distance effects and should be absorbed into the fragmentation function of the experimentally observed hadronic state.

* Based on talks given at the Linear Collider meeting LCWS05 at Stanford University in April 2005, at the Workshop on LHC/ILC Synergies at SLAC in April 2005 and at the DIS 2005 Workshop in Wisconsin, Madison in April 2005.

The simple picture described above does not work if the produced quark is massive (a relevant example is the process $e^+e^- \to b\bar{b}$). Naively, one observes that the corresponding energy distribution is no longer divergent. The finiteness of the result, however, has little to do with its applicability. A closer inspection shows that the spectrum contains terms of the type $\sim \ln(Q/m)$ at all orders in the perturbative expansion. Here, Q stands for the typical hard scale of the process and m is the mass of the "observed' final quark. For example, in $e^+e^- \to b\bar{b}$, the scale Q is identified with the center of mass energy $\sqrt{s}$ and m with the pole mass of the b-quark.

In QCD, the six quark flavors are typically divided in light and heavy according to the size of their mass relative to $\Lambda_{\rm QCD}$: if $m \lesssim \Lambda_{\rm QCD}$ then the flavor is light, while for $m \gg \Lambda_{\rm QCD}$ it is heavy. In applications c,b and t quarks are considered heavy. The relevant for our discussion reason for such separation is the fact that light and heavy quarks hadronize very differently: the former hadronize at scales of the order of the typical hadronic scale, while the later hadronize at a scale set by the mass of the heavy quark. Clearly, at a scale of the order of the mass of the heavy quark perturbation theory is still valid since $\alpha_s(m)$ is sufficiently small to be within the perturbative domain.

At the same time it is intuitively clear that heavy flavors can behave as massless in reactions where the typical hard scale Q is much larger than the mass $Q >> m$. To illustrate the point, one can imagine taking formally the limit $m/Q \to 0$; then the corresponding differential distribution diverges due to logarithmic terms $\sim \ln(m/Q)$, i.e. we get situation similar to the one in the pure massless case discussed above but with the collinear divergences regulated with small quark mass rather than dimensionally.

It is now easy to understand the reasons leading to the above mentioned complications in the case of heavy quark production: one cannot neglect the quark mass altogether since it sets the very important hadronization scale. Yet, in presence of very large hard scales, the mass becomes "irrelevant" and plays merely the role of a regulator for the collinear divergences. In such situation one may wish to find a way to compute hard cross-sections with massless quarks (because it is simpler) and at the same time to keep the relevant information on the mass in the differential distribution.

II. THE PERTURBATIVE FRAGMENTATION FUNCTION

The method that combines the convenience of massless, dimensionally regularized calculations while keeping the relevant information about the mass of the heavy quark was proposed by Mele and Nason [1] and is known as the Perturbative Fragmentation Function (PFF) formalism. The method relies on the factorization of long and short distance effects in QCD by making use of the DGLAP evolution equation to resum the above mentioned large logs $\sim \ln^k(m/Q)$ to all orders in the strong coupling constant.

Before we describe in detail how the PFF method works, lets us explain the need for resummation of the quasi-collinear logs. In practical applications one can never achieve the strict limit $m/Q \to 0$ since the hard scale Q is always "finite", i.e. we work with finite quantities at each perturbative level. The large (though finite) difference between m and Q shows up in a somewhat disguised way - through the convergence of the perturbative expansion. Even if $\alpha_s(m)$ is sufficiently small and one can expect reasonable convergence of the perturbative series, the presence of large number like $\ln(m/Q)$ at each order of the coupling effectively alters the expansion parameter from α_s to $\ln^k(m/Q)\alpha_s$, $k \geq 0$, which may not be small anymore. To circumvent this problem one has to sum up the whole perturbation series.

The resummation of classes of terms $\sim \ln^k(m/Q)\alpha_s^n$ is possible. This follows from the fact that the logs $\sim \ln^k(m/Q)$ are of universal collinear origin and can all be predicted with the help of the QCD evolution equations.

Let us consider the production of a heavy quark of flavor $\mathcal{Q}$ with mass m and a definite value of energy $E_{\mathcal{Q}}$ in a hard scattering process. According to the QCD factorization theorems the heavy quark energy spectrum can be computed as a convolution of the energy distribution of massless partons produced in the hard process, and the fragmentation function that describes the probability that the massless parton fragments into a massive quark with a definite energy. If the energy fraction $E_{\mathcal{Q}}/E_{\mathcal{Q},max}$ of the heavy quark is denoted by z, then the energy distribution

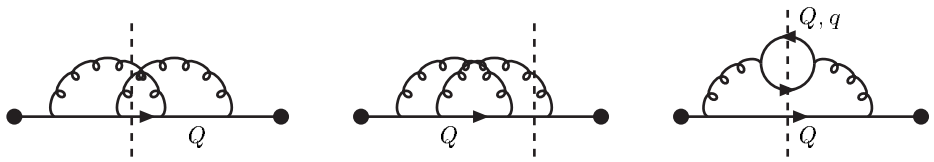

FIG. 1: Examples of diagrams that contribute to perturbative fragmentation of a heavy quark $Q \to Q + X$ at $\mathcal{O}(\alpha_s^2)$. The dashed vertical line indicates the intermediate (i.e. real emission) state that has to be considered; q denotes light quark flavor.

of that quark can be written as:

$$\frac{d\sigma_{\mathcal{Q}}}{dz}(z,Q,m) = \sum_a \int_z^1 \frac{dx}{x} \frac{d\hat{\sigma}_a}{dx}(x,Q,\mu) D_{a/\mathcal{Q}}\left(\frac{z}{x},\frac{\mu}{m}\right) + \mathcal{O}\left(\frac{m}{Q}\right)^p . \tag{2}$$

Here, the sum runs over all partons (i.e. quarks, antiquarks and gluons) that can be produced in the hard process and μ denotes the factorization scale. The coefficient function $d\hat{\sigma}_a/dx$ is the differential cross-section for producing a massless parton a as in Eq.(1) and with collinear singularities subtracted in the $\overline{\rm MS}$ scheme (recall that Γ_{ab} are universal collinear subtraction terms that depend only on the QCD time-like splitting functions). Important feature of Eq.(2) is that power corrections $(m/Q)^p$, i.e. all terms vanishing in the strict limit $m/Q \to 0$, are neglected. We next explain what is the effect of these terms and why we may want to neglect them.

There are basically two reasons why such power corrections are omitted. The first one is that the non-logarithmic terms do not have universal origin and are therefore not controlled by a Renormalization Group (RG) equation. They are instead process dependent and must be calculated perturbatively in any particular process. The second reason has to do with the size of these terms. Clearly, when $Q >> m$, such terms will have negligible numerical effect. Of importance will be only the logarithmic terms that are resumed with the help of Eq.(2) and terms that are finite in the limit $m/Q \to 0$ (often referred to as constant term). A very important implication of the PFF formalism is that while the constant term cannot be predicted and must be obtained from a process-dependent, fixed order calculation, it is sufficient to do that calculation in a massless fashion, i.e. by setting $m = 0$ from the outset. Of course, it is also possible to encounter situation where the condition $Q >> m$ does not really hold. In such situations one may want to consider a "mix" of resummation and fixed order calculation of the power suppressed term. We will come back to that point in Section (IV).

The functions $D_{a/\mathcal{Q}}(x,\mu/m)$ in Eq.(2) are the perturbative fragmentation functions [1]. They satisfy the DGLAP evolution equation and can be fully reconstructed from it, if the initial condition at a scale $\mu = \mu_0$ is known. When we take $\mu_0 \sim m$ the initial condition $D_a^{\rm ini}$ cannot contain large logarithms and can be derived from fixed order perturbative calculations. Next we describe their derivation.

III. DERIVATION OF THE INITIAL CONDITION

The most obvious way for the evaluation of the initial condition for the PFF is by de-convoluting Eq.(2). In such approach one needs to calculate separately the corresponding differential distributions for massless and massive quark production to fixed perturbative order in some process. Historically, such approach was used in [1] to derive the initial condition at NLO in α_s:

$$D_{a/\mathcal{Q}}^{\rm ini}\left(z,\frac{\mu_0}{m}\right) = \sum_{n=0} \left(\frac{\alpha_s(\mu_0)}{2\pi}\right)^n d_a^{(n)}\left(z,\frac{\mu_0}{m}\right) . \tag{3}$$

with:

$$d_a^{(0)}(z) = \delta_{a\mathcal{Q}}\,\delta(1-z),$$
$$d_{a=\mathcal{Q}}^{(1)}\left(z,\frac{\mu_0}{m}\right) = C_F\left[\frac{1+z^2}{1-z}\left(\ln\left(\frac{\mu_0^2}{m^2(1-z)^2}\right)-1\right)\right]_+ ,$$

$$d^{(1)}_{a=g}\left(z,\frac{\mu_0}{m}\right) = T_R\left(z^2+(1-z)^2\right)\ln\left(\frac{\mu_0^2}{m^2}\right),$$
$$d^{(1)}_{a\neq\mathcal{Q},g}\left(z,\frac{\mu_0}{m}\right) = 0, \tag{4}$$

Such approach is however too impractical beyond NLO. Next we describe a better, process independent approach for the derivation of the initial condition. This approach was first proposed in [2] and further elaborated upon in [3] where it was also applied for the derivation of all components of the PFF at order α_s^2.

The method is based on the observation that in any process, collinearly enhanced terms are produced only from diagrams with real radiation in the external legs. Applying this observation together with power counting arguments and using the factorization of phase-space and matrix elements in the collinear limit, one can derive an explicit expression for the fragmentation function in Eq.(2). For example, the contributions at NNLO from real gluon radiation or quark-antiquark pair emission take the form [3]:

$$\widetilde{D}(z) = \frac{1}{z}\int [dq_1][dq_2]\; W\;\delta\left(1-z-\frac{(nq_1)}{(pn)}-\frac{(nq_2)}{(pn)}\right). \tag{5}$$

Here, $[dq]$ is the phase space for each of the two emitted particles with momenta q_1 and q_2 and W stands for the appropriately projected square of the matrix element for the "process" $q(p)\to q+a(q1)+b(q2)$ with the decaying particle having off-shell momentum p. The "splitting" function W is given by $\sim \mathrm{Tr}\left[\not{p}V^{\mathrm{coll}}(p,q_1,q_2,n;m)\right]$ in the case when the decaying parton is a quark and by $\sim g^{\mu\nu}V^{\mathrm{coll}}_{\mu\nu}(p,q_1,q_2,n;m)$ for decaying gluon. Note that in the calculation of the matrix V^{coll} we assign to the decaying particle not the usual spinor or polarization vector but a propagator as appropriate for particle with momentum p, $p^2\neq m^2$ and mass zero or m depending on its flavor and spin. An important ingredient to the factorization program is that one works in a physical gauge defined with the help of an auxiliary light-like vector n. This vector is arbitrary with the only requirement that its dot product with the hard momentum p is non-zero i.e. $p.n\neq 0$. The delta function appearing in Eq.(5) simply represents the constraint defining the observed fraction of the energy. Its argument can be easily understood in terms of the usual Sudakov parametrization.

Similar expression exists for the virtual corrections as well. In this case the only change with respect to Eq.(5) is in the argument of the delta function and in the phase-space for real emission for one of the particles. Examples for the two types of contributions to the heavy quark $\mathcal{Q}$ initiated component of PFF are given on Fig.1, and for the gluon initiated component are shown on Fig.2.

Another unusual feature of this construction (compared to the usual single particle decay kinematics) is that the contributions $\sim\delta(1-z)$ that contain the pure virtual corrections arise from diagrams with a cut through a single line (compared to two lines in the heavy particle decay case). We do not have to consider such diagrams in our derivation since all contributions $\sim\delta(1-z)$ can be completely fixed from the flavor conservation condition:

$$\int_0^1 dz\left(D^{\mathrm{ini}}_{\mathcal{Q}/\mathcal{Q}}(z)-D^{\mathrm{ini}}_{\overline{\mathcal{Q}}/Q}\right)=1. \tag{6}$$

Because the integration range of all integrals covers the full one- or two-particle real emission phase space, we can exploit for their evaluation methods and techniques that have become by now standard. We apply the IBP identities [4] constructed from the vectors p and n and the integration momenta along the lines of the approach in [5]. We apply the Laporta algorithm [6] implemented in the program AIR [7]. We have reduced the problem to the evaluation of about 40 master integrals. For their evaluation we have made use of differential equation derived from the IBP identities.

IV. APPLICATIONS

The formalism described in the previous Sections is indispensable in not-completely inclusive observables where heavy flavored hadrons (typically mesons) are measured. Such observables are more complicated and at the same

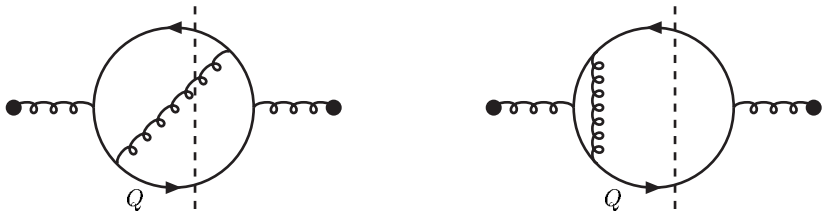

FIG. 2: Examples of diagrams for the gluon decay process $g \to Q + X$ at $\mathcal{O}(\alpha_s^2)$ that contribute to the function W. The dashed vertical line again indicates the intermediate state.

time very interesting because they are sensitive to the non-perturbative structure of the observed hadrons. The usual way of treating such processes is the following: one assumes that a heavy flavored meson is produced at a scale of the order of the mass of the heavy quark from the non-perturbative hadronization of a heavy quark with the corresponding flavor. In hard reactions where the hard scale Q is much larger than the quark's mass one can split the production of the heavy flavor in a convolution of perturbative and non-perturbative parts. The perturbative part describes the production of heavy quark and correctly accounts for all the radiation at scales down to $\sim m$. Naturally, that function is correct up to power corrections $\sim (m/Q)^p$. If necessary, these corrections can be incorporated from a fixed order calculation (examples are the p_T spectrum of hadrons in hadronic collisions [8], [9] and the study of B and D fragmentation in e^+e^- [10]).

The non-perturbative part of the production of the observed meson is described by the so-called non-perturbative fragmentation function $D^{n.p.}(z)$. At the fragmentation stage the fragmenting quark can radiate only small, of the order of the hadronic scale, transverse energy. Therefore, it is natural to identify z with the fraction of the large component of the momentum of the observed hadron. For example, that can be its longitudinal momentum fraction $p_H^{||} = z p_{\mathcal{Q}}^{||}$.

Similarly to the parton distributions, the non-perturbative heavy quark fragmentation function has to be extracted from experiment. The cleanest process studied so far is the energy spectrum of heavy flavors in e^+e^-. The most important property of the function $D^{n.p.}(z)$ is its process independence i.e. it can be applied to any other process subject only to the restriction $\mathcal{O}(m/Q)^p$.

There are many processes where this formalism can be successfully applied, like the high p_T spectrum of hadrons in hadron collisions, photoproduction, b-fragmentation in t-decay etc. The later process, for example, presents an interesting method for the precise determination of the top-quark mass at the LHC. The knowledge of the initial condition for the PFF through order $\mathcal{O}(\alpha_s^2)$ permits resummation of quasi-collinear logs with NNLL accuracy. That will, however, be possible only after the time-like splitting kernels of the DGLAP equation have been evaluated.

It seems that after the perturbative part has been promoted to the NNLO/NNLL level, the dominant uncertainty will be associated with the extracted non-perturbative function. The presently available data on heavy flavor fragmentation, and particularly on b-fragmentation, from LEP has been already analyzed and no significant further improvements can be expected (for charm fragmentation see also [11]). Therefore, the viable source of improvement in the quality of the extracted non-perturbative component lies with the future International Linear Collider. A Giga-Z option can supply new data with much higher quality that will permit new level of precision in the extraction of the non-perturbative fragmentation function.

V. SUMMARY

Production of heavy flavors is becoming an integral part of the precision physics program of the present and future colliders. Although the presence of masses leads to theoretical complications, it is by now well understood how to deal with them in a systematic fashion. Putting larger effort into the study of processes of heavy flavor production at colliders will be rewarding since differential distributions are sensitive to the non-perturbative hadronization effects.

The successful realization of such program depends crucially on two factors: improvement of the quality of the perturbative corrections and precise and systematic extraction and application of the non-perturbative fragmentation component. On the perturbative side the future is bright. Many important ingredients are already known at the

NNLO level and the advances in the higher order perturbative calculations makes plausible the calculation of all relevant pieces (the most important being the three-loop time-like splitting functions).

The present state of the non-perturbative components is not as exciting. Particularly for b-fragmentation, the knowledge of that function is based on analyzes of LEP data which results in relatively large uncertainty. The situation is somewhat better for the lowest few moments of the non-perturbative fragmentation function (for b-mesons); the first moment is measured with $\sim 1\%$ accuracy [12]. However, future prospects for making significant progress in this direction exist. They are based on the Giga-Z option of the International Linear Collider. In view of the impressive state of the perturbative side, improvement in the quality of the extracted non-perturbative component is mandatory. Achieving such precision can bring to a qualitatively new level our understanding of the processes involving heavy flavors. Our community can make this happen.

Acknowledgments

It is my pleasure to thank Kirill Melnikov for fruitful collaboration on this project. Research supported by the US DOE under contract DE-FG03-94ER-40833 and by the start up funds of the University of Hawaii.

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[1] B. Mele and P. Nason, Nucl. Phys. **B 361** (1991) 626.
[2] S. Keller and E. Laenen, Phys. Rev. **D 59** (1999) 114004; M. Cacciari and S. Catani, Nucl. Phys. **B 617** (2001) 253.
[3] K. Melnikov and A. Mitov, Phys. Rev. D **70**, 034027 (2004) (hep-ph/0404143); A. Mitov, Phys. Rev. D **71**, 054021 (2005) (hep-ph/0410205).
[4] F. V. Tkachov, Phys.Lett. **B 100** (1981) 65. K. G. Chetyrkin and F. V. Tkachov, Nucl. Phys. **B 192** (1981) 345.
[5] C. Anastasiou and K. Melnikov, Nucl. Phys. **B 646** (2002) 220; C. Anastasiou, L. Dixon and K. Melnikov, Nucl. Phys. Proc. Suppl. **116** (2003) 193.
[6] S. Laporta, Int. J. Mod. Phys. **A 15** (2000) 5087.
[7] C. Anastasiou and A. Lazopoulos, JHEP **07** (2004) 046.
[8] B. A. Kniehl, G. Kramer, I. Schienbein and H. Spiesberger, Phys. Rev. **D 71** (2005) 014018 (hep-ph/0410289).
[9] M. Cacciari, M. Greco and P. Nason, JHEP **9805** (1998) 007 (hep-ph/9803400).
[10] P. Nason and C. Oleari, Nucl.Phys. **B 565** (2000) 245 (hep-ph/9903541).
[11] Belle Collaboration (R. Seuster et al.), BELLE-PREPRINT-2005-23, KEK-PREPRINT-2005-34 (hep-ex/0506068).
[12] DELPHI Collaboration, ICHEP 2002 Note, DELPHI 2002-069 CONF 603.