NNLO splitting and coefficient functions with time-like kinematics

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We discuss recent results on the three-loop (next-to-next-to-leading order, NNLO) time-like splitting functions of QCD and the two-loop (NNLO) coefficient functions in one-particle inclusive $e^+e^-$-annihilation. These results form the basis for extracting fragmentation functions for light and heavy flavors with NNLO accuracy that will be needed at the LHC and ILC. The two-loop calculations have been performed in Mellin space based on a new method, the main features of which we also describe briefly.

1. Introduction

Observables with identified hadron(s) in the final state depend on the fragmentation function(s) for these hadron(s). A prominent example for the physics at hadron colliders is the $p_T$-spectrum of $b$-flavored mesons [1–3],

$$\frac{d\sigma_B}{dp_T} \simeq \sum_{i,j,k} f_i \otimes f_j \otimes \frac{d\hat{\sigma}_{i,j \rightarrow k}}{dp_T} \otimes D_{k/B}. \quad (1)$$

Unlike the parton distributions (pdf's) $f_i$, the scale dependence (evolution) of the fragmentation functions $D_{k/B}$ is in terms of time-like splitting functions. As is well-known [4–6], starting from two loops (i.e., NLO) the time-like and the space-like splitting functions of QCD differ.

To derive the time-like splitting functions to any order in perturbation theory, one can exploit the universal factorization property of the collinear singularities in some particular process, for instance in $e^+e^-$-annihilation to hadrons,

$$e^+e^- \rightarrow f(p) + X, \quad (2)$$

where $f(p)$ can be any massless on-shell parton. The differential cross-sections for the reaction (2) are known to two loops [7–10], permitting the extraction of the time-like NLO splitting functions and NNLO coefficient functions.

The full three-loop calculation, needed for obtaining the NNLO splitting functions is a problem of remarkable complexity due to, among other reasons, the incomplete inclusiveness of the final state in this process. In contrast to the recent calculation of deep-inelastic scattering (DIS) [11–14], one cannot apply the optical theorem here. Progress in this direction is being made [15] which will be discussed in Sec. 3. Before we present in Sec. 2 an alternative approach and first results for the time-like NNLO splitting functions.

2. Time-like NNLO splitting functions

The essence of our approach is to devise a relation between the space- and time-like splitting functions in QCD capable of predicting the quantities with time-like kinematics from the known space-like ones [11,12]. This approach is a subject with interesting history starting with the Gribov-Lipatov relation at leading order [16]. The NLO calculations [4–6] explicitly demonstrated the breaking of the Gribov-Lipatov relation beyond the leading order, see also Ref. [17]. The interest in the subject has been re-emerging throughout the years [18–20], and the space- or time-like two-loop results were independently confirmed by several groups [10,21–23]. New results beyond two loops, however, were obtained only very recently [24].

Our starting point is the factorization of mass-
less differential cross-sections. Specifically, we consider in parallel the following two reactions:

\[ \text{DIS : } f(p) + \gamma^* \rightarrow X, \quad (3) \]
\[ e^+e^- : \quad \gamma^* \rightarrow f(p) + X, \]

and the corresponding parton level observables

\[ \frac{d\sigma}{dx}, \quad x = -\frac{q^2}{2p\cdot q}, \quad q^2 < 0, \quad (4) \]
\[ \frac{d\sigma}{dz}, \quad z = \frac{2p\cdot q}{q^2}, \quad q^2 > 0 . \]

The above differential distributions contain singularities of collinear origin. These, however, completely factorize and can be absorbed into the definition of the corresponding non-perturbative parton distribution or fragmentation functions. Thus, they are completely specified in terms of the kernels of the evolution equation.

The observables in Eq. (3) (including Z-boson exchange) are expressed in terms of three structure functions. In DIS these are known as \( F_1, F_2 \) and \( F_3 \) while their counterparts in \( e^+e^- \) are denoted as \( F_T, F_L \) and \( F_A \). In the following we will consider only the relationship between the functions \( F_1, F_2 \) and \( F_T \), the others being similar.

We first take the bare (i.e. collinear singularities are not factored out) structure function \( F^b_1 \) expanded in terms of the bare strong coupling \( \alpha^b_s \):

\[ F^b_1(\alpha^b_s, Q^2) = \delta(1-x) + \sum_{l=1}^{\infty} \left( \frac{\alpha^b_s}{4\pi} \right)^l \left( \frac{Q^2}{\mu^2} \right)^{-\ell} F^b_{1,1} . \]

The terms in the above series are written as

\[ F^b_{1,1} = 2F_1 \delta(1-x) + R_1 \]
\[ F^b_{1,2} = 2F_2 \delta(1-x) + (F_1)^2 \delta(1-x) + 2F_1 R_1 + R_2 \]
\[ F^b_{1,3} = 2F_3 \delta(1-x) + 2F_1 F_2 \delta(1-x) + (2F_2 + (F_1)^2) R_1 + 2F_1 R_2 + R_3 . \]

This iterative decomposition into form-factor (\( F \)) and real-emission (\( R \)) parts is done according to the \( \epsilon \)-dependence in the soft limit, see Ref. [25]. It represent the closest approach to a full decomposition into contributions from the separate physical cuts possible on the basis of Refs. [11–14].

To predict the time-like quantities from their space-like counterparts, we subject Eq. (6) to the following analytical continuation: first, as can be easily seen from the definitions (4) of the kinematical variables in the two processes, one changes \( x \rightarrow 1/x \) and \( q^2 \rightarrow -q^2 \). Accounting for the difference in the two phase-space measures, one has to multiply the time-like expression by an overall factor of \( z^{1-2\epsilon} \) (see [10] for more details). The only subtle point in the analytic continuations is the treatment of logarithmic singularities for \( x \rightarrow 1 \), cf. Ref. [17], starting with

\[ \ln(1-x) \rightarrow \ln(1-z) - \ln z + i \pi . \]

After the continuation has been performed, we keep only the real parts of the continued functions \( R_i \) and then re-assemble the resulting expression analogously to Eq. (6). This later result is identified with the corresponding structure function \( F^b_T \) in \( e^+e^- \) which, according to the mass factorization, takes the form

\[ F_{T,1} = -\epsilon^{-1} P^{(0)} + \epsilon^{(1)} T + \epsilon a^{(1)} T + \epsilon^2 b^{(1)} T + \epsilon^3 d^{(1)} T + \ldots , \]

and correspondingly for the coefficients \( F_{T,2} \) and \( F_{T,3} \) (see Ref. [24] for their explicit expressions). The same procedure applies to the other two structure functions \( F^b_L \) and \( F^b_A \).

The above described analytic continuation can in principle be applied to any order in the strong coupling and to any order in the expansion in \( \epsilon \). Indeed, by comparing to the known expressions at two loops [4–10] for the time-like splitting functions \( P^{(1)} \) as well as the coefficient functions \( c^{(2)} \) and the new \( a^{(2)} \) terms, we observe complete agreement – which, beyond order \( \epsilon^{-1} \), depends on the inclusion of the \( i\pi \) term in Eq. (7). Moreover, all terms proportional to \( \epsilon^k, k \leq -2 \) at three loops are also correctly predicted by the analytic continuation carried out in this manner.

Despite the highly non-trivial predictions mentioned above, we would like to stress the following point. Unlike the per-diagram treatment of Refs. [4–6,17], our continuation relies on the
space-like evaluation of Refs. [11–14] based on the optical theorem. Therefore, we have incomplete information on the separate contributions from the various physical cuts, recall that Eq. (6) does not represent a full decomposition according to the number of emitted partons. Thus one has to be prepared for some problem at the third order, especially in the abelian ($C_F^3$) piece, related to $\pi^2$ contributions originating from phase space integrations over unresolved regions.

There are two checks on the predicted three-loop time-like splitting functions: their soft behavior $x \to 1$ and the vanishing of a first moment $N = 1$. The latter check shows a mismatch in a term of the type $\pi^2 C_F^3 (1 + x^2)/(1 - x) \ln^2 x$, i.e., the analytic continuation returns an incorrect coefficient for this term which has been restored by the $N = 1$ constraint.

Clearly, one needs to devise a second and independent confirmation of this corrected prediction. For this purpose we adopt the approach of Dokshitzer, Marchesini and Salam [26]. There the evolution equations for either parton distributions or fragmentation functions $f^\text{ns}_\sigma$ are rewritten in a unified manner for space-like ($\sigma = -1$) and time-like ($\sigma = +1$) kinematics,

$$\frac{d}{d \ln Q^2} f^\text{ns}_\sigma(x, Q^2) =$$

$$\int_x^1 \frac{dz}{z} P^{\text{univ}}_{\text{univ}}(z, \alpha_s(Q^2)) f^\text{ns}_\sigma\left(\frac{x}{z}, \frac{z^2}{Q^2}\right),$$

with the universal splitting functions $P^{\text{univ}}_{\text{univ}}$ assumed to describe both the time-like and space-like cases.

One can easily work out the perturbative expansion of Eq. (9). The resulting expression for the difference $P^{(1)\text{ns}}_{\sigma=1}(x) - P^{(1)\text{ns}}_{\sigma=-1}(x)$ at NLO agrees with Ref. [4], while the NNLO prediction coincides with the ($N = 1$ corrected) result from our analytical continuation. It can be cast in the following very compact form with $\otimes$ denoting the usual convolution,

$$\delta P^{(2)}(x) = 2 \left\{ [\ln x \cdot \tilde{P}^{(1)}(x)] \otimes P^{(0)} + [\ln x \cdot P^{(0)}] \otimes \tilde{P}^{(1)}(x) \right\},$$

for the non-singlet kernels ($\xi = +, - , v$) with

$$2 \tilde{P}^{(n)}_\sigma(x) = P^{(n)}_{\sigma=1}(x) + P^{(n)}_{\sigma=-1}(x).$$

Obviously Eq. (10) predicts the correct vanishing first moment for $P^{(2)}_{\sigma=1}(x)$ and, moreover, we can even make a prediction for the fourth-order ($N^3\text{LO}$) difference of the (both unknown) time-like and space-like non-singlet splitting functions on this basis. The difference can also be written in a form similar to Eq. (10), see Ref. [24] for explicit results.

3. Hadron fragmentation in $e^+e^-$ at NNLO

Let us now turn to our method used for direct calculations of higher-order QCD corrections in $e^+e^-$-annihilation (2). In contrast to the preceding section where we have discussed the analytic continuation in kinematic variables, here we describe the derivation of the two-loop corrections to the coefficient functions for light parton production. They have been first calculated in Ref. [7–9], later confirmed by the analytical continuation as outlined above and, finally, re-derived through an independent direct two-loop calculation [10]. The aim of the latter calculation was to check the results of Rijken and van Neerven and to derive the terms $a^{(2)}$ (as defined in Eq. (8)). The latter terms of $\mathcal{O}(\epsilon)$ were a useful check on predictions of the analytic continuation at two loops, and will also be needed in a future calculation of the three-loop corrections.

The calculation [10] was performed directly in Mellin space, following the method of Ref. [15], which consists of two basic steps. First, one performs the Mellin transform before any phase-space or virtual integration:

$$\sigma(N) = \int_0^1 dz z^{N-1} \frac{d\sigma}{dz}$$

$$= \int_0^1 dzz^n \int dPS^{(m)} |M|^2 \delta(z - f)$$

$$= \int dPS^{(m)} |M|^2 f^{N-1},$$

where $f$ is some function of the external and/or integration momenta that defines the variable $z$. 
If the measure $d\text{PS}^{(m)}$ contains $\delta$-functions, they can be dealt with in the standard way [27]. From Eq. (12) it is clear that the effect of the Mellin transform is to introduce a new propagator raised to an abstract power. The generalization to multiple differential distributions involving a Mellin transform in multiple variables is straightforward.

Second, one applies the reduction identities based on integration-by-parts (IBP) to simplify the right-hand side of Eq. (12) and to reduce it to master integrals. The fact that one of the propagators is not a fixed integer but an abstract parameter does not present any complications. This is because the IBP identities can be cast in the usual form (where the powers of all propagators are fixed integers) through a shift in the variable corresponding to the power of the propagator $f$. The resulting recurrence relations explicitly depend on $N$, and can be solved in a standard way like, e.g., the algorithm of Laporta [28] as implemented in the MAPLE package AIR of Ref. [29].

The master integrals resulting from the solution of the IBP identities implicitly depend on $N$, too, and one can derive for them difference equations in $N$. To solve the latter we apply techniques used previously in the context of DIS [11,22,25] and perform the required expansions in $\epsilon$ with the packages SUMMER [30] and XSUMMER [31]. By solving the difference equations one extracts the complete dependence on the Mellin variable $N$ without the need for explicit evaluations of any Feynman integral. Finally, to fully specify the solution of a difference equation of degree $\kappa$, one has to provide $\kappa$ initial conditions. Here, the simplest option, which we have used in Ref. [10], is the direct evaluation of the master integrals for $N = 1, \ldots, \kappa$.

All but one of the master integrals in Ref. [10] satisfy difference equations of first order, the other being of second order. As pointed out in Ref. [15], however, not all of the integrals specifying the initial conditions are independent, since the IBP reductions exhibit many additional relations after fixing $N$, say to $N = 1$. Typically, for the initial conditions one has to explicitly evaluate less objects than the number of master integrals. In the case of Ref. [10], we encountered six real-real and respectively five real-virtual master integrals along with seven independent initial conditions.

Finally, a particularly powerful feature of the method of Ref. [15] is the fact that the master integrals depend only on the process but are independent of the particular observable. For that reason all integrals needed for the initial conditions could be taken over from Ref. [32]. We confirmed those results and extended them to higher orders in $\epsilon$.

4. Energy spectrum of $b$-quarks in $e^+e^-$

The most important application of the time-like QCD splitting functions is the description of hadron fragmentation in processes sensitive to collinear radiation, like in Eqs. (1) or (2). For instance, the process independent fragmentation functions $D_{b/B}$ of $b$-flavored mesons are extracted from measurements in $e^+e^-$-annihilation. Along with high-quality data, a consistent NNLO description of light-flavor fragmentation requires the knowledge of the three-loop time-like splitting functions and the two-loop coefficient functions for the production of massless partons. Additionally, within the perturbative fragmentation function (PFF) formalism [33] for heavy-flavor fragmentation one also has to supply initial conditions now known to two loops [34,35]. Flavor threshold crossing conditions may also have to be taken into account [36,37].

As an application of our results we can readily predict the two-loop (NNLO) energy spectrum of massive $b$-quarks in $e^+e^-$-annihilation based on the PFF formalism [33]. Now this formalism can be applied completely and consistently at two loops, since all fermion-initiated components are presently known [34]. The only two-loop component of the PFF not required in $e^+e^-$ at the two-loop fixed-order level is the gluon-initiated one [35].

The spectrum of a massive $b$-quark in $e^+e^-$-annihilation, up to power corrections $\sim \mathcal{O}(m)$, reads:

$$\frac{d\sigma_b}{dz}(z, Q, m) = \sum_i \frac{d\hat{\sigma}_i}{dx}(x, Q, \mu) \otimes D_{i/b}(x, m, \mu),$$

(13)
where $\mu$ is the factorization scale and $Q$ represents the characteristic hard scale of the reaction.

For the case of $e^+e^-$-collisions one usually takes $Q = \sqrt{s}$ and $m$ to be the pole mass of the heavy quark. Inserting the explicit expressions for the coefficient functions and the PFF's one can verify that indeed all dependence on the factorization scale $\mu$ completely cancels.

A particular feature of Eq. (13) which we would like to point out is the characteristic dependence $\sim 1/z$ at low $z$ that appears for a first time at two loops. This is entirely due to the pure-singlet fermion emission and similar to the well-known small-$x$ behavior of structure functions in DIS [11–14].

Detailed phenomenological studies of the energy spectrum $d\sigma_b/dz$ of Eq. (13) and related observables will appear in a forthcoming publication [38].

5. Conclusions

In these proceedings we have reviewed recently derived results for the non-singlet components of the three-loop (NNLO) time-like splitting functions and the complete two-loop (NNLO) partonic cross-sections for one-particle inclusive hadro-production in $e^+e^-$-annihilation.

The former results [24] have been obtained by utilizing an analytic continuation in the proper kinematic variables in connection with the idea [26] of a universal splitting function governing the space- and time-like parton evolution equations.

The latter results [10] provided a check on earlier calculations by Rijken and van Neerven [7-9] and extended their results to include higher order terms in $\epsilon$. The derivation of these so far unknown terms of $\mathcal{O}(\epsilon)$ was essential in verifying predictions of the space-like to time-like analytical continuation and will also be required in a future direct three-loop evaluation of this process.

The derivation of the two-loop coefficient functions in $e^+e^-$ was a first application of a new method for evaluation of differential distributions directly in Mellin space [15]. This application demonstrated the anticipated efficiency of the method both, in terms of solving the IBP identities and, in the decrease of the number and the complexity of the master integrals that require separate treatment.

The above results, together with the available two-loop contributions [34] to the PFF open the possibility for studies of light and heavy hadro-production consistently at NNLO. For example, the extraction of $b$-fragmentation functions at this level of accuracy has important applications not only at a future ILC but also at the LHC, for instance in measurements of the $p_T$-spectrum of $B$-mesons or in precision determinations of the top-quark mass.

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