

# AUTOMATIC CALCULATIONS OF NLO SPLITTING FUNCTIONS WITH LOOPS FOR EXCLUSIVE PARTON SHOWER MONTE CARLO\*

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We describe a status of the software package `Axiloop` for symbolic calculations in the axial gauge. The package is dedicated to computations of the virtual components of the QCD NLO splitting functions in the collinear factorization scheme and its exclusive extension. We present some aspects of the employed technique, the structure of the package and results for the  $C_F^2$  part of the non-singlet case.

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## 1. Introduction

The LHC collaborations recently presented strong indications that the particle discovered at the LHC in the year 2012 is indeed the Higgs boson. This result opens the era of precision measurements of the properties of the Higgs boson. High precision measurements at hadron colliders are a theoretical challenge. The basic theoretical tools for the data analysis, the Monte Carlo programs, are still not on par neither with the analytical calculations nor with the foreseen experimental precision of LHC experiments. The popular QCD parton shower Monte Carlo programs `PYTHIA` [1, 2] and `HERWIG` [3, 4] are based on the improved LO accuracy. The NLO corrections in the hard process have been accounted for in the `MC@NLO` [5, 6] and `POWHEG` [7] projects. Among other approaches, one should mention the `GR@PPA` [8, 9] project with some NLO effects included in the cascade and the `SHERPA` [10] project combining the tree-level QCD matrix elements with the LO parton shower. The recent interesting developments include `MEPS@NLO` —

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a technique of combining next-to-leading order parton-level calculations of varying jet multiplicity and parton showers within the SHERPA project [11], the GENEVA project [12] which combines higher-order resummation of large Sudakov logarithms with next-to-leading order matrix-element corrections and parton showers, and the MINLO concept with multi-scale improved NLO effects [13].

A different, novel approach to the QCD parton showers has been proposed within the KRKMC project [14–16]. It aims at including the NLO corrections in both the hard process and ladder in a fully exclusive way. It is based on the collinear factorization theorem [17, 18] but requires its reformulation in a fully exclusive way, recalculation of the evolution kernels, construction of the kinematic mappings and designing of an efficient reweighting procedure. Some of these goals have already been achieved. In particular, the non-singlet real emission kernels have been recalculated and the structure of their singularities has been studied. This task has to be continued to the virtual non-singlet contributions as well as to the singlet case. The experience shows that it is essential to automatize these calculations.

To this end, we develop a software package, named `Axiloop`, written in Wolfram Mathematica. The calculations are done in the axial gauge. In this gauge, thanks to the internal cancellations, the factorization theorem has a remarkably simple form based on two-particle-irreducible objects. On the other hand, the axial gauge generates unphysical, spurious, singularities which complicate the analytical structure of expressions and make this gauge unpopular in actual calculations. We follow the methodology of the original paper [18] further developed in [19, 20]. The developed `Axiloop` package will provide various intermediate formulae not available in the literature, for all the non-singlet and singlet kernels and selected hard processes.

## 2. Calculation technique

Let us begin by discussing some aspects of the splitting functions calculation method [18, 20]. Though our intention is to calculate a complete set of NLO splitting functions, in this paper we consider only non-singlet virtual contributions, see Fig. 1. Despite of such a limitation, described technique will be appropriate for the calculation of remain topologies as well.

As a master formula, we use a definition of the *parton density* from [18, Eq. 2.27d]

$$\hat{G}\left(x, \alpha_s, \frac{1}{\epsilon}\right) = \delta(1-x) + \text{PP} \int \frac{d^m k}{(2\pi)^m} \delta\left(x - \frac{k \cdot n}{p \cdot n}\right) \left[ \frac{\not{n}}{4 p \cdot n} \frac{K}{1 - \mathbb{P}K} \not{p} \right], \quad (2.1)$$

where (a)  $p$  is the incoming quark's momentum; (b)  $q = p - k$  is a momentum of the outgoing gluon; (c) the constant vector  $n$  defines a gauge condition for

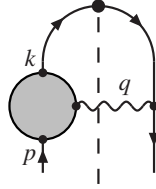


Fig. 1. A general form of the 2PI kernel for the NLO non-singlet virtual splitting functions.

the light-cone gauge, *i.e.*  $n^2 = 0$ ; (d) the dimensional regulator  $\epsilon$  regulates ultra-violet (UV) and infra-red (IR) singularities; (e) the square brackets denote contractions of the spinor indices as defined in [18, Eq. 2.2]; and (f) the operator  $\mathbb{P}$  denotes the pole part of the  $d^m k$  integral.

In addition, the following expansion is assumed

$$\frac{K}{1 - \mathbb{P}K} = K + K \otimes (\mathbb{P}K) + K \otimes (\mathbb{P}K) \otimes (\mathbb{P}K) + \dots, \quad (2.2)$$

where (a) the two-particle-irreducible (2PI) kernel  $K$  is a cut-graph expressed in terms of the Feynman rules; (b) the projector  $\mathbb{P}$  extracts a singular part of the kernel; and (c) the product of two kernels, *e.g.*  $K \otimes (\mathbb{P}K)$ , denotes a convolution in a sense of [18, Eq. 2.1].

### 2.1. Exclusive splitting functions

Our first step is to contract spinor indices in the integrand of Eq. (2.1), which we define as

$$\tilde{T}^{(\text{NLO})}(k, p, l, \epsilon) \equiv \left[ \frac{\not{k}}{4 p \cdot n} K \not{p} \right]. \quad (2.3)$$

In practice, that leads to the computation of a trace of the gamma matrices. Since a dimensional regularization technique is used in our calculations, we set a number of dimensions  $m = 4 - 2\epsilon$ , as in [20]. In [18], the authors work in  $m = 4 + \epsilon$  dimensions. The final results are identical anyway since analytical continuation to  $m = 4 + 2\epsilon$  dimensions is performed after the renormalization step.

We provide some examples of how to construct the kernels  $K$  in Sec. 3. The reader will find more examples in papers [18, 20] or in the Axiloop source code at the project's web page [21].

The next step is to proceed with the calculation of the **exclusive bare**<sup>1</sup> **splitting functions**. They are obtained by integrating expression (2.3) over the loop momentum in  $m = 4 - 2\epsilon$  dimensions

<sup>1</sup> Those that contain UV singularities.

$$T_B^{(\text{NLO})}(k, p, \epsilon, \delta) \equiv \int \frac{d^m l}{(2\pi)^m} \tilde{T}^{(\text{NLO})}(k, p, l, \epsilon). \tag{2.4}$$

Such an integration introduces two kinds of singularities: the infra-red and ultra-violet ones. They appear as single (IR, UV) or double (IR) poles in  $\epsilon$  during explicit calculations. In order to distinguish the origin of those poles, we tag them with corresponding labels, *i.e.*  $\epsilon_{\text{IR}}$  or  $\epsilon_{\text{UV}}$ . We stress that these are not new regulators, but a single one,  $\epsilon$ , with different labels. Technically speaking, their numerical values are equal, *i.e.*  $\epsilon = \epsilon_{\text{IR}} = \epsilon_{\text{UV}}$ . In addition, cancellations like  $\frac{1}{\epsilon_{\text{IR}}} - \frac{1}{\epsilon_{\text{UV}}} = 0$  are not allowed, but  $\frac{\epsilon}{\epsilon_{\text{IR}}} = 1$  or  $\frac{\epsilon}{\epsilon_{\text{UV}}} = 1$  may be used.

Another type of divergences which arise during the loop-momentum integration are *spurious singularities*. They are specific to the axial gauge only, thus should be considered as unphysical. There are several approaches to regularize this kind of singularities [20]. We use a *principal value prescription* as described in [18, 20]. This prescription introduces a new regulator  $\delta$ , which appears in the final results as the  $I_0$  or  $I_1$  singular functions.

The general form of the NLO exclusive bare splitting function is as follows

$$T_B^{(\text{NLO})}(k, p, \epsilon, \delta) = \alpha_s^2 (4\pi)^\epsilon \Gamma(1 + \epsilon) (k^2)^{-1} \left( \frac{T_{\text{IR}}^k(x, \delta) k^{-2\epsilon}}{\epsilon_{\text{IR}}} + \frac{T_{\text{UV}}^k(x, \delta) k^{-2\epsilon} + T_{\text{UV}}^p(x, \delta) p^{-2\epsilon} + T_{\text{UV}}^q(x, \delta) q^{-2\epsilon}}{\epsilon_{\text{UV}}} + T_0^k(x, \delta) k^{-2\epsilon} + O(\epsilon) \right). \tag{2.5}$$

We would like to stress several important points here. Firstly, terms proportional to  $p^{-2\epsilon}$  and  $q^{-2\epsilon}$  are kept only for  $\epsilon_{\text{UV}}$  poles. In the IR limit, *i.e.*  $p^2 = q^2 = 0$ , they disappear and, therefore, do not contribute to the final results. Secondly, the right-hand side of Eq. (2.5) may contain double poles in  $\epsilon_{\text{IR}}$ , which should cancel with the corresponding real contributions. For that reason, we ignore terms proportional to  $1/\epsilon_{\text{IR}}^2$  in that expression. Lastly, double poles are absent in the examples we discuss in this paper (see Fig. 3).

Before we continue with renormalization of expression (2.5), let us define the **NLO ultra-violet counter-term**,  $T_{\text{UV}}^{(\text{NLO})}$ , as proposed in [18, 20]. At first, we extract a pole part (residue) of (2.5) in  $\epsilon_{\text{UV}}$  regulator. It turns out to be proportional to the leading part,  $T_{\text{R}}^{(\text{LO},0)}(x)$ , of the **LO exclusive splitting function** in  $4 - 2\epsilon$  dimensions defined as follows (see [20])

$$\begin{aligned} T_{\text{R}}^{(\text{LO})}(k, p, \epsilon) &= \frac{\alpha_s}{2\pi} (k^2)^{-1} \left( T_{\text{R}}^{(\text{LO},0)}(x) - \epsilon T_{\text{R}}^{(\text{LO},1)}(x) \right) \\ &= \frac{\alpha_s}{2\pi} (k^2)^{-1} \left( \frac{1+x^2}{1-x} - \epsilon(1-x) \right). \end{aligned} \tag{2.6}$$

Instead of such a dependence, we require the UV counter-term to be proportional to the complete, with all  $\epsilon$ -terms preserved,  $T_R^{(LO)}$  function (2.6). That leads to the following definition

$$T_{UV}^{(NLO)}(k, p, \epsilon, \delta) \equiv \alpha_s^2 (4\pi)^\epsilon \Gamma(1 + \epsilon) (k^2)^{-1} \times \frac{T_{UV}^k(x, \delta) + T_{UV}^p(x, \delta) + T_{UV}^q(x, \delta)}{\epsilon_{UV}} \frac{T_R^{(LO,0)}(x) - \epsilon T_R^{(LO,1)}(x)}{T_R^{(LO,0)}(x)}. \tag{2.7}$$

At this point, we are ready to discuss the central expression of this paper, the **exclusive (renormalized) splitting function**, which is free of the UV singularities and is defined as follows (note the analytical continuation to  $m = 4 + 2\epsilon$  dimensions)

$$T_R(k, p, \epsilon, \delta) \equiv \lim_{p^2, q^2 \rightarrow 0} ((T_B(k, p, \epsilon, \delta) - T_{UV}(k, p, \epsilon, \delta))_{\epsilon \rightarrow -\epsilon}). \tag{2.8}$$

Let us see explicitly a cancellation mechanism of the UV divergences at the next-to-leading order

$$T_B^{(NLO)}(k, p, \epsilon, \delta) - T_{UV}^{(NLO)}(k, p, \epsilon, \delta) = \alpha_s^2 (4\pi)^\epsilon \Gamma(1 + \epsilon) (k^2)^{-1} \times \left( - \frac{T_{UV}^k(x, \delta) (1 - k^{-2\epsilon}) + T_{UV}^p(x, \delta) (1 - p^{-2\epsilon}) + T_{UV}^q(x, \delta) (1 - q^{-2\epsilon})}{\epsilon_{UV}} + \frac{T_{IR}^k(x, \delta) k^{-2\epsilon}}{\epsilon_{IR}} + T_0^k(x, \delta) k^{-2\epsilon} + \left( T_{UV}^k(x, \delta) + T_{UV}^p(x, \delta) + T_{UV}^q(x, \delta) \right) \frac{T_R^{(LO,1)}(x)}{T_R^{(LO,0)}(x)} + O(\epsilon) \right). \tag{2.9}$$

This expression has no UV singularities in the  $\epsilon_{UV} \rightarrow 0$  limit since the first term vanishes.

Finally, we need to analytically continue the above expression to  $m = 4 + 2\epsilon$  dimensions and take the IR limit. At this point, two types of the IR singularities are still left: (a) the poles in  $\epsilon_{IR}$ , which contribute directly to the inclusive splitting functions; and (b) the on-shell momenta terms,  $p^{-2\epsilon}$  and  $q^{-2\epsilon}$  ( $\epsilon > 0$ ), which become singular in the IR limit. In order to regularize the latter, we perform analytical continuation to  $m = 4 + 2\epsilon$  dimensions, that leads to the following expression

$$\begin{aligned}
 & \left( T_B^{(\text{NLO})}(k, p, \epsilon, \delta) - T_{\text{UV}}^{(\text{NLO})}(k, p, \epsilon, \delta) \right)_{\epsilon \rightarrow -\epsilon} \\
 &= \alpha_s^2 (4\pi)^{-\epsilon} \Gamma(1 - \epsilon) (k^2)^{-1} \left( \frac{T_{\text{UV}}^k(x, \delta) (1 - k^{2\epsilon}) - T_{\text{IR}}^k(x, \delta) k^{2\epsilon}}{\epsilon} \right. \\
 &+ \frac{T_{\text{UV}}^p(x, \delta) (1 - p^{2\epsilon}) + T_{\text{UV}}^q(x, \delta) (1 - q^{2\epsilon})}{\epsilon} + T_0^k(x, \delta) k^{2\epsilon} \\
 &+ \left. \left( T_{\text{UV}}^k(x, \delta) + T_{\text{UV}}^p(x, \delta) + T_{\text{UV}}^q(x, \delta) \right) \frac{T_{\text{R}}^{(\text{LO},1)}(x)}{T_{\text{R}}^{(\text{LO},0)}(x)} + \mathcal{O}(\epsilon) \right). \quad (2.10)
 \end{aligned}$$

Now, we are safe to put  $p$  and  $q$  on shell, that gives us expression for the NLO exclusive splitting function

$$\begin{aligned}
 T_{\text{R}}^{(\text{NLO})}(k, p, \epsilon, \delta) &= \alpha_s^2 (4\pi)^{-\epsilon} \Gamma(1 - \epsilon) (k^2)^{-1} \\
 &\times \left( \frac{T_{\text{UV}}^k(x, \delta) + T_{\text{UV}}^p(x, \delta) + T_{\text{UV}}^q(x, \delta)}{\epsilon} - \frac{T_{\text{UV}}^k(x, \delta) + T_{\text{IR}}^k(x, \delta)}{\epsilon} k^{2\epsilon} \right. \\
 &+ \left. T_0^k(x, \delta) k^{2\epsilon} + \left( T_{\text{UV}}^k(x, \delta) + T_{\text{UV}}^p(x, \delta) + T_{\text{UV}}^q(x, \delta) \right) \frac{T_{\text{R}}^{(\text{LO},1)}(x)}{T_{\text{R}}^{(\text{LO},0)}(x)} + \mathcal{O}(\epsilon) \right). \quad (2.11)
 \end{aligned}$$

We stress that remaining poles in  $\epsilon$  should be treated as IR, despite that  $T_{\text{UV}}(x, \delta)$  terms originally come from the UV singularities.

### 2.2. Inclusive splitting functions

In order to cross-check the calculation technique, we compare our results with already-known inclusive splitting functions [18, 20]. They are obtained by integrating the exclusive splitting functions (2.11) over the final-state momentum

$$\hat{\Gamma}^{(\text{NLO})}(x, \delta) \equiv \text{PP} \int \frac{d^m k}{(2\pi)^m} 2\pi \delta^+((p - k)^2) \delta\left(x - \frac{k \cdot n}{p \cdot n}\right) T_{\text{R}}^{(\text{NLO})}(k, p, \epsilon, \delta), \quad (2.12)$$

where (a) PP is the pole part operator (or residue) in the  $\epsilon$  regulator; and (b) the number of dimensions  $m = 4 + 2\epsilon$ . After performing these operations,

we obtain an explicit expression for the inclusive splitting functions

$$\hat{I}^{(\text{NLO})}(x, \delta) = \frac{1}{2} \left( \frac{\alpha_s}{2\pi} \right)^2 \left( \left( \ln(1-x) + 2 \frac{T_{\text{R}}^{(\text{LO},1)}(x)}{T_{\text{R}}^{(\text{LO},0)}(x)} \right) \times \left( T_{\text{UV}}^k(x, \delta) + T_{\text{UV}}^p(x, \delta) + T_{\text{UV}}^q(x, \delta) \right) + T_0^k(x, \delta) \right). \quad (2.13)$$

### 3. Axiloop software package

In the previous section, we have presented some key details of the technique for calculating the NLO splitting functions. This section describes implementation of that technique as a fully automated software package, *Axiloop*, written for the Wolfram Mathematica system.

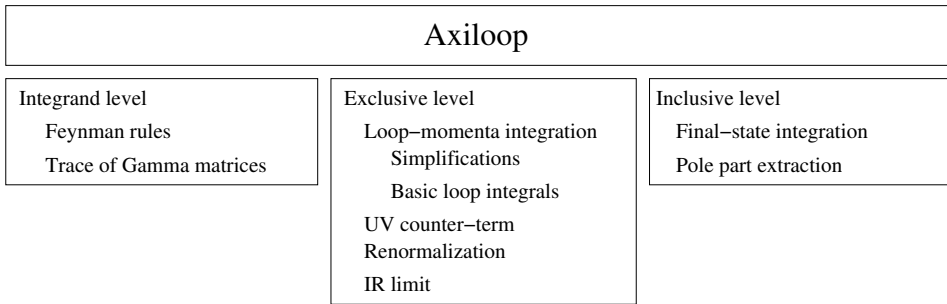


Fig. 2. General structure of the *Axiloop* package.

The idea is to make *Axiloop* able to analytically perform described computational steps for any NLO splitting function. Such a method has various advantages in the calculation process comparing to the on-paper approach. The most valuable one is the ability to modify the computational technique itself in order to obtain splitting functions in modified prescriptions. For example, the need of having such a modified prescription could be seen by looking at the expression for the exclusive splitting function (2.11). Being defined in  $4 + 2\epsilon$  dimensions makes it impossible to be used in parton shower Monte Carlo simulations in 4 dimensions. For that purpose, one needs to modify the prescription [18].

*Axiloop* is designed to automate calculations as much as possible. In particular, it means that it is enough to provide just a product of Feynman rules, as written in (3.1)–(3.2), and all final expressions are calculated automatically. Those are: (a) the integrand (2.3); (b) the exclusive bare splitting function (2.4); (c) the ultra-violet counter-term (2.7); (d) the exclusive splitting function (2.8); and (e) the inclusive splitting function (2.12).

Let us demonstrate what the calculations described in the previous section look like in `Axiloop` package. For that purpose, we choose two NLO kernels that contribute to the  $C_F^2$  color structure (Fig. 3).

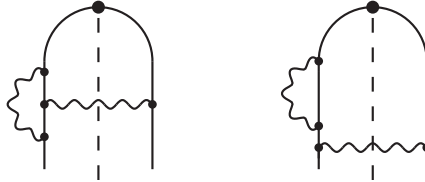


Fig. 3. NLO kernels (c) and (e) contributing to the  $C_F^2$  color structure, see Eqs. (3.1)–(3.2).

### 3.1. Integrand level

In `Axiloop` a set of high-level routines is provided for user's disposition, which are used to describe input information and to produce final results:

- `FP`, `FV`, `GP`, and `GV` are used to describe a topology of the calculated splitting function. They represent a set of Feynman rules in a light-cone gauge. In particular, `FV` and `GV` represent fermion and gluon vertices, while `FP` and `GP` are fermion and gluon propagators, respectively. The suffix `x`, like in `GPx`, indicates that the corresponding propagator is crossed by a cut line, thus it is on-shell.
- `SplittingFunction` calculates various expressions for the splitting functions. It needs a description of the kernel to be provided as an input in terms of the above functions representing the Feynman rules.

Let us write down the explicit expressions for the NLO kernels depicted in Fig. 3 in form they are put into the `SplittingFunction` routine

$$\begin{aligned}
 T_c &= \frac{\not{n}}{4p \cdot n} \text{FP}(k) \text{FV}^{i_1} \text{FP}(l-k) \text{FV}^\mu \text{FP}(l-p) \text{FV}^{i_2} \\
 &\quad \times \text{GP}_{i_1 i_2}(l) \text{FPx}(p) \text{FV}^\nu \text{FP}(k) \text{GPx}_{\mu\nu}(p-k), \quad (3.1)
 \end{aligned}$$

$$\begin{aligned}
 T_e &= \frac{\not{n}}{4p \cdot n} \text{FP}(k) \text{FV}^{i_1} \text{FP}(l-k) \text{FV}^{i_2} \text{FP}(k) \text{FV}^\mu \\
 &\quad \times \text{GP}_{i_1 i_2}(l) \text{FPx}(p) \text{FV}^\nu \text{FP}(k) \text{GPx}_{\mu\nu}(p-k). \quad (3.2)
 \end{aligned}$$

By analogy, the user may write down input expressions for other kernels. The point is that further computation happens in a completely automated way, so that no user intervention is needed.



3.2. Exclusive splitting functions

The most difficult task in calculating exclusive quantities is the loop-momenta integration. The expressions in the form (3.1)–(3.2) are not suitable to be directly integrated over the loop-momenta. For that reason, we perform a series of simplifications on the unintegrated expression; only after that we perform loop-momenta integrals. The simplifications are based on (a) the Passarino–Veltman rules; (b) kinematic rules; (c) on-shell rules; and (d) translation rules. Such rules allow us to express the incoming expression as a linear combination of a known set of integrals which are substituted later on.

After the loop-momenta integration, the UV counter-term and the exclusive splitting function are calculated as described in Sec. 2.1. In Table I, we show the form factors which define the exclusive and inclusive splitting functions (2.11) and (2.13) for the topologies (c) and (e) depicted in Fig. 3.

TABLE I

Form factors for the (c) and (e) topologies.

	$T_{UV}^k(x, \delta)$	$T_{UV}^p$	$T_{UV}^q$	$T_{IR}^k$	$T_0^k$
Topology (c)					
$\frac{1}{1-x}$	$1 + 3x - x^2$	$x^2$	$2 - 3x + 3x^2$	$2 - 3x + 4x^2$	$4 + 5x + 5x^2$
$\frac{1+x^2}{1-x} \ln x$	-3	0	1	1	0
$\frac{1+x^2}{1-x} I_0$	-3	-1	0	-1	0
$(1-x) I_0$	0	0	0	0	4
$\frac{1+x^2}{1-x} I_0 \ln x$	0	0	0	0	-4
$\frac{1+x^2}{1-x} I_1$	0	0	0	0	4
$(1-x) \ln x$	0	0	0	0	2
$\frac{1+x^2}{1-x} \ln^2 x$	0	0	0	0	-2
$\frac{1+x^2}{1-x} \text{Li}_2(1-x)$	0	0	0	0	-2
$\frac{1+x^2}{1-x} \text{Li}_2(1)$	0	0	0	0	-4
Topology (e)					
$\frac{1}{1-x}$	$-3(1+x^2)$	0	0	0	$-4 - 6x - 4x^2$
$\frac{1+x^2}{1-x} \ln x$	4	0	0	0	0
$\frac{1+x^2}{1-x} I_0$	4	0	0	0	0
$\frac{1+x^2}{1-x} I_1$	0	0	0	0	-4
$(1-x) I_0$	0	0	0	0	-4
$\frac{1+x^2}{1-x} I_0 \ln x$	0	0	0	0	4
$(1-x) \ln x$	0	0	0	0	-4
$\frac{1+x^2}{1-x} \ln^2 x$	0	0	0	0	2
$\frac{1+x^2}{1-x} \text{Li}_2(1)$	0	0	0	0	4

Let us notice the interesting relation between the terms aroused from the IR and UV phase-space regions for the diagrams depicted in Fig. 3

$$T_{UV}^p(x, \delta) + T_{UV}^q(x, \delta) - T_{IR}^k(x, \delta) = 0. \quad (3.3)$$

Though it seems not to be the general rule, this relation is quite important since the sum (3.3) is proportional to the  $\ln Q^2$  term in the final result for the inclusive quantity and its vanishing guaranties that this contribution to the result does not depend on  $Q^2$ .

### 3.3. Inclusive splitting functions

This step is performed mainly to ensure correctness of the provided calculations and of the final results. The inclusive quantities were already calculated in [18] and [20], thus form a reliable set of tests for our calculations. We have found the full agreement with the mentioned papers. This forms a strong test of the correctness of our algorithm.

## 4. Summary

We have presented some details of the ongoing work on the **Axiloop** package. This package is designed for symbolic computation of the NLO splitting functions, as described in [18]. It may also be used to perform general-purpose tasks, *e.g.* the trace of the gamma matrices, the loop- and final-momenta integration, *etc.* At the moment, **Axiloop** is able to calculate the virtual splitting functions for the  $C_F^2$  color structure. The implementation of a complete set of virtual non-singlet topologies is well advanced. There are several possible features to be added to **Axiloop** in the future: (a) the two-particle final-state integration; (b) the two-loop integration; (c) the coefficient functions computation; (d) implementation of alternative factorization approaches; *etc.* The singlet topologies will be added in the next step. We have also briefly described some aspects of the technique for calculating the NLO splitting functions in the exclusive form, based in the formalism of [18]. In particular, much attention has been paid to the mechanism of renormalization of the UV singularities in virtual topologies.

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