VIRTUAL CORRECTIONS TO THE NLO SPLITTING FUNCTIONS FOR MONTE CARLO:
THE NON-SINGLET CASE*

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Construction of a QCD cascade at the NLO level requires recalculation of the splitting functions in a different manner. We describe the calculation of some of the virtual contributions to the non-singlet splitting function. In order to be compatible with the earlier calculated real contributions, the principal value prescription for regularizing the infrared singularities must be used in a new way. We illustrate this new scheme on simple examples. For the calculations, we wrote a Mathematica package called Axiloop. We describe its current status.

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1. Introduction

With the second, 14 TeV, phase of the LHC experiments approaching, the need for the precision QCD parton shower increases. To date, there are successful approaches of merging NLO hard process and LO cascade such us MC@NLO [1] or POWHEG [2, 3]. Other attempts are also taken to improve precision of parton showers [4–8]. However, in order to construct QCD parton shower that includes NNLO hard process, it will be mandatory to construct a cascade at the NLO level. Such a cascade is developed within the KRKMC project [9–11].

One of the crucial elements of this project is the recalculation and reorganization of the NLO splitting functions [12]. The real emission part of the non-singlet (NS) splitting function has been discussed at length in [13].

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The virtual $C_F^2$ NS components have been briefly discussed in [14]. Here, we concentrate on the remaining NS virtual corrections. We will also give an update on the development of the Mathematica package Axiloop [15], that is written to assist with the NLO calculations in the light-cone gauge.

Before going into details, let us comment on the real corrections. Let us consider a graph shown in Fig. 1. This interference graph contributes to the NS splitting function and is labelled (d). By comparing the results for this graph from [13] with the previous ones of [16], we note that they differ. The singular part of the graph (d) in [16] reads (Table 3.10)

\[
p_{qq}(x) \frac{1}{\epsilon^2} + 2I_0 \frac{p_{qq}(x)}{\epsilon} - \frac{1 - x}{\epsilon} + p_{qq}(x)(-2I_1 + 4I_0 + 2I_0 \ln x - 2I_0 \ln (1 - x)) - 2(1 - x)I_0
\]

and contains single and double poles in $\epsilon$ (the first line), and pure spurious poles (the second line); where $p_{qq}(x) = (1 + x^2)/(1 - x)$ is the LO quark–quark splitting function, $I_0 \sim -\ln \delta$ and $I_1 \sim -(1/2)\ln^2 \delta$ are the infrared divergent functions regulated with $\delta$, cf. Eq. (3), and dimension of the phase space is defined as $m = 4 - 2\epsilon$. In [13], for the same contribution, we find only pure spurious pole terms (Eq. 3.48)

\[
p_{qq}(x)(2I_1 + 4I_0 + 2I_0 \ln x - 2I_0 \ln (1 - x))
\]

Note, that those are semi-inclusive results which means that additional integration over one real momentum is left to be calculated. It is of the generic form $N(\epsilon) \int_0^{Q^2} d(-q^2)(-q^2)^{-1-2\epsilon}$. Such an integration introduces additional pole in $\epsilon$, so the inclusive form of Eq. (1) contains $1/\epsilon^3$ pole, whereas inclusive form of Eq. (2) contains just $1/\epsilon$ terms\(^1\).

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\(^1\) Note that in the Eq. (3.48) of [13] instead of $1/\epsilon$ pole one finds $\ln Q/q_0$, where $q_0$ is the lower limit of the integral $\int_{q_0}^{Q^2} d(-q^2)(-q^2)^{-1-2\epsilon}$, see Eq. (2.10) of [13].
Summarizing, the result (1) contains higher order poles in $\epsilon$, absent in the new result in Eq. (2). As explained in [12], the absence of higher order poles is important for the construction of the stochastic cascade, which must be done in four dimensions. Some clarifications are in order here: (i) in the standard, inclusive approach one adds real and virtual corrections and, as can be seen in [16], the higher order poles cancel out. However, from the Monte Carlo point of view real-virtual cancellations pose additional complications. (ii) The $1/\epsilon^2$ pole does not disappear in the new approach of [13] — the singularity is simply regulated differently, as $(1/\epsilon) \ln \delta$ etc., see below. (iii) Due to the presence of higher order poles, the “trivial” terms, $\ln Q^2$, $\ln 4\pi$, etc., cancel between real and virtual corrections in [16], and are absent in [13]. (iv) The complete NLO NS kernel, which is a coefficient of the single pole is also affected by the changes in higher order pole terms, however, it must be independent of the choice of the regularization. Therefore, we expect that the difference between results (1) and (2) will be compensated by an appropriate change in the virtual contributions.

Let us now discuss the mechanism responsible for this difference.

2. Regularization prescription

Besides the fact that the Lorentz structure of Feynman rules in the light-cone gauge is more complicated than in the covariant gauges, additional difficulties arise due to the specific structure of the axial denominator, $1/l_+$, where $l_+ = nl$ and $n$ is the axial vector. It leads to the spurious (non-physical) singularities when integrated over the virtual or real phase space. Therefore, one must apply some prescription to regularize them in the intermediate steps.

The common choice is a principal value (PV) prescription [13, 16–18]. It was originally used in [17] in the first calculation of the NLO splitting functions from the Feynman diagrams. The other option is the Mandelstam–Leibbrandt prescription [19, 20]. It is better founded in the QFT, but significantly more complicated in practical calculations. Further analysis and comparison of these prescriptions can be found e.g. in [16].

The idea of the PV regularization is to replace $1/l_+$ terms by

$$\frac{1}{l_+} \rightarrow \left[\frac{1}{l_+}\right]_{PV} = \frac{l_+}{l_+^2 + \delta^2 p_+^2},$$

where $\delta$ is an infinitesimal regulator, $p_+ = np$ and $p$ is some reference momentum. This prescription has to be applied to the axial propagators of the gluons [16] at the level of Feynman rules, i.e. at the very beginning of the calculation, and it leads to the results like (1).
Closer inspection of the derivations in [13] reveals that there are, however, also different sources of the $1/l_+$ terms, related to the phase space evaluation, change of variables etc. In the standard PV prescription, these terms are not regularized by $\delta$, dimensional regularization takes care of them. On the contrary, we propose, that all these singularities in plus variable are regulated also by the PV prescription. In practice, we replace

$$ l_+^{-1+\epsilon} \rightarrow \left[ \frac{1}{l_+} \right]_{\text{PV}}^\epsilon $$

in all the places, keeping track of the higher order $\epsilon$ terms, if needed. Contrary to the previous case, this has to be done at the very end of the integrations. On the technical level, it means that the usual (PV) approach, i.e.: (i) use some parametrization technique (like the Feynman or Schwinger parametrization) to combine denominators; (ii) perform momentum integration; (iii) perform integration over the Feynman/Schwinger parameters, is not suitable. Instead, one needs to perform integration over $l_+$ at the very end, after the integration over $l_-$, $l_\perp$, and $z_i$ variables

$$ \int \frac{d^ml}{(2\pi)^m} \frac{f(l_+)}{(l + k_1)^2 \cdots (l + k_n)^2} = \int dl_+ f(l_+) \int dz_1 \cdots dz_{n-1} \int \frac{dl_- d^{m-2}l_\perp}{(2\pi)^m} \frac{1}{(l^2 + lA + B^2)^n}. \tag{5} $$

For explicit formulae arranged in this way, see, for example, [18].

As a consequence, now also the non-axial integrals, initially free of axial vector $n$ (which defines the plus component, $l_+ = nl$), can develop dependence on the vector $n$. For example, let us show the three-point integral without axial denominator

$$ J^F_3 = \int \frac{d^ml}{(2\pi)^m} \frac{1}{l^2(l + q)^2(l + p)^2} \tag{6} $$

for the special kinematic configuration: $p^2 = (p - q)^2 = 0$. Standard approach leads to the following expression

$$ J^F_3 = \frac{i}{(4\pi)^2|q^2|} \left( \frac{4\pi}{|q^2|} \right)^\epsilon \Gamma(1 + \epsilon) \left( -\frac{1}{\epsilon^2} + \frac{\pi^2}{6} \right). \tag{7} $$

In contrast, our prescription gives the result

$$ J^F_3 = \frac{i}{(4\pi)^2|q^2|} \left( \frac{4\pi}{|q^2|} \right)^\epsilon \Gamma(1 + \epsilon) \left( \frac{2I_0 + \ln(1 - x)}{\epsilon} \right. $$

$$ -4I_1 + 2I_0 \ln(1 - x) + \frac{\ln^2(1 - x)}{2}, \tag{8} $$
where \( x = q_+/p_+ \) is the axial-vector-dependent parameter. As one can see, Eq. (8) is free of double poles in \( \epsilon \). Note that this singularity did not disappear, but has been replaced by \( I_1 \) and \( I_0/\epsilon \). More details will be presented elsewhere [21].

3. Results

Let us now use the new prescription in the actual calculation. We present here results for one of the virtual graphs contributing to the non-singlet splitting function, namely graph (d), \( i.e. \) the second graph in Fig. 2. The presented results have been obtained with the help of the Mathematica package Axiloop, which we developed to assist with the calculations in the light-cone gauge. Overview of the Axiloop package is provided in Appendix.

In Table I, we show inclusive results separately for the real graph (d) (Fig. 1) taken from Eq. (3.48) of [13] and virtual graph (d) (Fig. 2, second picture), calculated in the new regularization scheme. Table I is constructed in analogy to Table 1 of [17] but in addition contains a section with double pole contributions.

Let us describe these results in more detail.

First of all, the last column in Table I is in full agreement with the result of Table 1 of [17], where only the sum of real and virtual contributions is given. The virtual contribution alone can be obtained from [16] in the standard PV prescription.

The second point is that \( 1/\epsilon^3 \) pole is absent in the inclusive virtual contribution, in a similar manner as it disappeared from the inclusive real contribution, see discussion of Eq. (2). Results obtained by applying the PV prescription (see Eq. (1) for the real graph) do not have this property.

Thirdly, neither real nor virtual contribution depends on the scale \( Q \) of the hard process. This is not true for the standard prescription — in that case, only the sum of real and virtual terms is independent of \( Q \). The same happens also for the “trivial” terms, like \( \ln 4\pi \) or \( \gamma_E \). Note, however, that there are some contributions for which this property does not hold.
Contributions from real and virtual graphs (d) to inclusive splitting function and their sum, calculated in the new regularization prescription.

|                  | SUM |
|------------------|-----|
| **Double poles** |     |
| $p_{qq}$         | $-3/2$ | 0 | $-3/2$ |
| $p_{qq} I_0$     | 4 | 0 | 4 |
| $p_{qq} \ln x$   | 1 | 0 | 1 |
| $p_{qq} \ln(1 - x)$ | 2 | 0 | 2 |
| **Single poles** |     |
| $p_{qq}$         | $-7$ | $-4$ | $-11$ |
| $1 - x$          | $-5/2$ | $3/2$ | $-1$ |
| $1 + x$          | $-1/2$ | $1/2$ | 0 |
| $p_{qq} \ln x$   | 0 | $-3/2$ | $-3/2$ |
| $(1 - x) \ln x$  | 2 | 0 | 2 |
| $(1 + x) \ln x$  | 0 | $1/2$ | $1/2$ |
| $p_{qq} \ln(1 - x)$ | $-3$ | 8 | 5 |
| $(1 - x) \ln(1 - x)$ | 4 | 0 | 4 |
| $p_{qq} \ln^2 x$ | 2 | $-1$ | 1 |
| $p_{qq} \ln x \ln(1 - x)$ | 2 | 4 | 6 |
| $p_{qq} \ln^2(1 - x)$ | 4 | $-2$ | 2 |
| $p_{qq} \text{Li}_2(1 - x)$ | $-2$ | 2 | 0 |
| $p_{qq} \text{Li}_2(1)$ | 8 | $-2$ | 6 |
| $p_{qq} I_1$     | $-12$ | 4 | $-8$ |
| $p_{qq} I_0$     | 0 | 8 | 8 |
| $(1 - x) I_0$    | 8 | 0 | 8 |
| $p_{qq} I_0 \ln x$ | 4 | 4 | 8 |
| $p_{qq} I_0 \ln(1 - x)$ | 12 | $-4$ | 8 |

4. Summary and outlook

In this note, we presented some details of the recalculation of virtual graphs contributing to the NLO NS splitting function, necessary for the construction of the Monte Carlo cascade at the NLO level. We argued that in order to be compatible with the earlier calculation [13] for the real components, the PV prescription must be used in a modified way. As a result, at the inclusive level, the $1/\epsilon^3$ poles are replaced by the structures like $\ln \delta/\epsilon^2$ and no cancellations of $1/\epsilon^3$ poles between real and virtual parts is
needed. We performed calculations for the case of the NS splitting function and presented them here on the example of one diagram. As expected, our results for real and virtual contributions differ from the ones in PV prescription, but the sum of real and virtual contributions is the same\textsuperscript{2}. In the next step, we plan to apply the new prescription to the singlet virtual graphs.

In order to automatize the calculations in the light-cone gauge, we developed a \texttt{Mathematica} package \texttt{Axiloop} with the help of which a set of one-loop graphs contributing to the NS splitting functions at the next-to-leading order can be calculated in the standard and modified PV prescriptions. In the future, the package can be extended to calculate singlet one-real-one-virtual as well as two-loop and two-real corrections to the splitting functions.

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\textbf{Appendix}

\textit{Overview of the Axiloop software package}

For calculating virtual corrections to the NLO splitting functions, we built a software package for the \texttt{Wolfram Mathematica} system — \texttt{Axiloop} \cite{15}. In this section, we describe a general structure as well as some core features of the package implemented up to date.

\texttt{Axiloop} is an open-source, general-purpose package which provides a complete set of routines for calculating Feynman-diagram-based objects in light-cone gauge in analytical form. In the current version, a full set of the virtual diagrams contributing to the non-singlet NLO splitting functions (Fig. 2) is calculated using a new regularization prescription.

Functions provided by \texttt{Axiloop} may be divided into the two main groups: a set of general-purpose \textit{core routines}, which likely can be used in other packages for solving general-purpose problems and \textit{custom routines} dedicated to calculation of the splitting functions.

\textsuperscript{2} Let us note that the importance of the PV regularization on the way from the $\overline{\text{MS}}$ to the “physical” collinear factorization scheme is also underlined in the recent paper \cite{22}.
Core routines perform the following tasks: trace and vector algebra operations in arbitrary number of dimensions \cite{23}; virtual integrals in the light-cone and Feynman gauges with custom regularization schemes (including the one discussed in this paper); various simplification algorithms for loop integrals (e.g. \cite{24}); reduction of tensor integrals using the Passarino–Veltman approach \cite{25}; final-state integration. It is worth to emphasize that Axiloop provides a flexible implementation of the loop integration routines which can be modified and extended for various contexts.

One of the core routines is \texttt{IntegrateLoop} function which performs one-loop integration in $m = 4 - 2\epsilon$ dimensions. It handles the Feynman and axial two- and three-point integrals with up to a rank 3 tensor structures in the numerator. As a demonstration, we show the scalar integral of Eq. (6), which in Axiloop notation looks as follows:

\begin{verbatim}
In[1]:= IntegrateLoop[ 1/(l.l (l+k).(l+k) (l+p).(l+p)), l]
Out[1]= Q[eps] (-k.k)^(-1-eps) ((2 I0 + Log[1-x])/eir
- 4 I1 + 2 I0 Log[1-x] + Log[1-x]^2/2)
\end{verbatim}

In general, we distinguish infrared and ultraviolet singularities when dimensional regularization prescription is used. The infrared origin of the pole is indicated by the \texttt{eir} symbol. Ultraviolet poles, which appear in two- and some three-point integrals, are represented by poles in the \texttt{euv} symbol.

Custom routines in our case are dedicated to the calculation of the NLO virtual splitting functions. They produce analytical expressions for the components of the splitting functions at different stages of the calculation, as defined in \cite{14}: (i) renormalized and bare exclusive formulas, which are usually omitted by other authors — they play a key role in the construction of the parton shower Monte Carlo; (ii) inclusive results for cross-checking with previous known results; and (iii) ultraviolet counter-terms.

The routine for calculating splitting functions is \texttt{SplittingFunction}. As its input a complete description of the calculated graph in terms of the Feynman rules should be provided. The following example demonstrates invocation of \texttt{SplittingFunction} for calculating virtual contribution of the topology (d):

\begin{verbatim}
In[3]:= SplittingFunction[ G[n]/(4p.n) FP[k] FV[i1] FP[l] FV[i2]
GP[i1,i3, l+k] GP[i2,i4, l+p] GV[i3,-l-k, i4,l+p, mu,-p+k]
FPx[p] GPx[mu,nu, p-k] FV[nu] FP[k]
, IntegrateLoopPrescription -> "MPV"
]
\end{verbatim}
The **IntegrateLoopPrescription** option allows one to change regularization prescription for loop integrals. It accepts PV and MPV values for the PV prescription or its modification (described in this work) respectively. Remaining routines, *i.e.* FP (FPx), GP (GPx), FV, and GV, correspond to the Feynman rules and read as fermion/gluon propagator (suffix “x” indicates that corresponding propagator is cut) and fermion/gluon vertex respectively.

At the moment, in the **Axiloop** package, we have implemented all the NS one-real-one-virtual corrections (corresponding graphs are depicted in the Fig. 2) and the library of two- and three-point integrals in the light-cone gauge for both regularization schemes.

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