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Antenna subtraction at NNLO with identified hadrons

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Abstract: We extend the antenna subtraction method to include hadron fragmentation processes up to next-to-next-to-leading order (NNLO) in QCD in e^+e^- collisions. To handle collinear singularities associated with the fragmentation process, we introduce fragmentation antenna functions in final-final kinematics with associated phase space mappings. These antenna functions are integrated over the relevant phase spaces, retaining their dependence on the momentum fraction of the fragmenting parton. The integrated antenna functions are cross-checked against the known NNLO coefficient functions for identified hadron production from $\gamma^*/Z^* \to q\bar{q}$ and $H \to gg$ processes.

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1 Introduction

The production of identified hadrons in high-energy particle collisions has been among the very first observables studied in experimental particle physics. These measurements were usually performed in a single-particle inclusive manner, i.e. differential in the kinematics of the identified hadron but fully inclusive over all hadronic activity in the event. Very extensive measurements of single-inclusive hadron production were performed at e^+e^- colliders [1]. The resulting legacy data sets provide important information on the transition from partons to hadrons and are used to tune the parameters of empirical hadronisation models [2, 3] that form the basis of modern Monte Carlo event simulation.

In QCD, single-inclusive hadron production can be described by convoluting single-inclusive parton production, which is calculable in perturbation theory, with fragmentation functions (FF, [4, 5]) that parametrise the parton-to-hadron transition as a function of the fractional momentum transfer. The factorisation behaviour of FFs closely resembles that of parton distribution functions (PDF), and they also fulfil Altarelli-Parisi evolution equations [6] in their associated resolution scale. In contrast to a description based on empirical hadronisation models, the FF framework can be systematically expanded [7] in perturbative QCD by computing higher-order corrections to the partonic coefficient functions and the FF evolution kernels. The coefficient functions for single-inclusive hadron production are known to next-to-leading order (NLO) for electron-proton [7–9] and proton-proton [10] collisions and to next-to-next-to-leading order (NNLO) for electron-positron annihilation [11, 12]. The FF evolution kernels are also known to NLO [13] and NNLO [14]. The initial conditions to the FF evolution equations reflect the non-perturbative dynamics of the parton-to-hadron transition. They can not be computed from first principles in perturbative QCD, and are typically determined by global fits to experimental data on single-inclusive hadron cross sections [15–23] for various hadron species.

The fragmentation function formalism was initially developed for light quarks, where the initial conditions to the evolution equations are purely non-perturbative. In the case of heavy quarks, the quark mass acts as an infrared regulator that prevents exactly collinear emissions in the fragmentation process (dead-cone effect, [24, 25]). By introducing a perturbative contribution to the heavy-quark fragmentation functions [26], it is possible to incorporate the heavy quark mass effects for observables including identified heavy hadrons (or identified heavy quark jets, [27]) into otherwise fully massless calculations at higher orders, and resum large logarithms of collinear origin [28]. The perturbative heavy-quark FFs were computed up to NNLO [29, 30] and augmented by soft-gluon resummation [31]. They were used especially in NLO calculations of identified heavy hadron production.

Identified hadrons play an increasingly important role in precision measurements at the LHC, for example in cross sections in association with a vector boson or a photon, where they are relevant to determining the flavour decomposition of PDFs, or in the study of hadron production in jet substructure studies [32–34] or hadron-in-jet production [35–37].

These collider measurements do however not fall into the class of single-inclusive hadron production observables, since their final state definition involves a set of criteria that is applied not only to the identified hadron momentum but to the full final state of the event. These criteria can be fiducial cuts on other particles, or more generally any type of infrared-safe event classification criterion, such as the application of a jet algorithm or of an event shape requirement. While FFs for the hadron species under consideration may well be known from a global fit, their application to these less inclusive observables is prevented by the incomplete understanding of the parton-level cross sections for identified hadrons in the presence of generic event-based fiducial selection criteria. Instead, data on these processes is typically compared only to Monte Carlo event simulation using empirical hadronisation models, which offer a considerably larger degree of flexibility in adapting to specific final state definitions than the FF framework, however with the drawback of considerably lower theory precision.

Higher order corrections to single-inclusive coefficient functions are typically obtained by analytical integration of the relevant parton-level subprocesses from real and virtual contributions. For fully exclusive fiducial cross sections, this approach is not viable due to the complexity of the final state definition. Instead, one employs a subtraction method to extract infrared singular real radiation contributions and to recombine them with virtual contributions to obtain infrared-finite predictions. The subtracted real and virtual subprocesses are individually finite and can be integrated numerically, taking into account the fiducial cuts defining the observable under consideration. Generic subtraction methods for NLO [38, 39] and NNLO [40–49] calculations are available and have been used widely for jet cross sections. For processes involving hadron fragmentation, any subtraction method requires an extension in order to keep track of parton momentum fractions in unresolved emissions, which are usually integrated over. Such an extension is available at NLO for dipole subtraction [38]. At NNLO, recent work towards fragmentation processes yielded results for heavy hadron production in top quark decays [50] in the residue subtraction method [45] and photon fragmentation [51, 52] in the antenna subtraction method [43, 44].

It is the objective of this paper to extend the antenna subtraction formalism to incorporate hadron fragmentation processes up to NNLO. In section 2, we establish the relevant notation for hadron fragmentation processes. Sections 3 and 4 develop the antenna subtraction for identified hadrons at NLO and NNLO, respectively, by introducing the fragmentation antenna functions and describing the structure of the subtraction terms. The integration of the fragmentation antenna functions in final-final kinematics is described in section 5, where we also investigate their relation to inclusive antenna functions in initial-final kinematics. Our results are validated by re-deriving existing results for single-inclusive NNLO coefficient functions in vector boson and Higgs boson decay in section 6. As an illustration of the method, in section 7 we describe the subtraction for hadron-in-jet fragmentation in three-jet final states in e^+e^- annihilation. Finally, in section 8 we summarise our results and provide an outlook on future applications and extensions.

2 Hadron fragmentation processes in the antenna formalism

Processes with identified hadrons require the introduction of a fragmentation function to describe the fragmentation of the high-energy quark or gluon into the actually detected hadron. In this paper, we focus on one hadron (plus jets) production at e^+e^- colliders:

$$e^+ + e^- \to H(K_H) + X\,(+\text{jets}) \tag{2.1}$$

where we identify a hadron H with momentum K_H and possibly some jets, which may or not contain the identified hadron. The restriction to e^+e^- initial states is largely for notational simplicity, allowing us the develop the essential aspects of the antenna subtraction formalism for identified hadron cross sections in a clear and concise manner. Its extension to hadron-hadron collisions is straightforward and will be discussed in section 8.

The fully differential cross section can be written as

$$\mathrm{d}\sigma^H = \sum_p \int \mathrm{d}\eta\, D_p^H\left(\eta, \mu_a^2\right)\, \mathrm{d}\hat{\sigma}_p\left(\eta, \mu_a^2\right)\,, \tag{2.2}$$

where the index p runs over all possible partons in the process, D_p^H is the physical (mass-factorised) fragmentation function describing the collinear fragmentation process of the parton p into the hadron H, and μ_a^2 is the fragmentation scale (which may differ from the renormalisation scale). Note that a single-hadron cross section in QCD is usually written as differential in the three-momentum of the detected hadron [10, 38, 53] as

$$K_H^0 \frac{\mathrm{d}\sigma^H}{\mathrm{d}^3 K_H} = \sum_p \int \frac{\mathrm{d}\eta}{\eta^2} D_p^H(\eta)\, k_p^0 \left.\frac{\mathrm{d}\hat{\sigma}_p}{\mathrm{d}^3 k_p}\right|_{\vec{k}_p = \vec{K}_H/\eta}, \tag{2.3}$$

where k_p is the momentum of the fragmenting parton, carrying $1/\eta$ of the momentum of the detected hadron K_H. Such a definition is not suitable for a parton-level generator. However, as shown in [54], (2.2) and (2.3) are indeed equivalent for one-particle inclusive cross sections. Hence we will adopt the former as our master equation, which is necessary to deal with the additional presence of jets in the final state.

The short-distance one-parton exclusive cross section appearing in (2.2) admits a perturbative expansion in the renormalised strong coupling constant α_s,

$$\mathrm{d}\hat{\sigma}_p(\eta) = \mathrm{d}\hat{\sigma}_p^{\mathrm{LO}}(\eta) + \left(\frac{\alpha_s}{2\pi}\right) \mathrm{d}\hat{\sigma}_p^{\mathrm{NLO}}(\eta) + \left(\frac{\alpha_s}{2\pi}\right)^2 \mathrm{d}\hat{\sigma}_p^{\mathrm{NNLO}}(\eta)\,. \tag{2.4}$$

For instance, the LO cross section is defined as the integration over the n particle phase space of the tree-level Born partonic cross section:

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{LO}}(\eta) = \int_n \mathrm{d}\hat{\sigma}_p^{\mathrm{B}}(\eta)\,, \tag{2.5}$$

with

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{B}}(\eta) = \mathcal{N}_{\mathrm{B}}\, \mathrm{d}\Phi_n(k_1, \ldots, k_n; \mathcal{Q})\, \frac{1}{S_n}\, M_n^0(k_1, \ldots, k_n)\, J(\{k_1, \ldots, k_n\}_n, \eta k_p)\,, \tag{2.6}$$

with $\mathcal{N}_{\mathrm{B}}$ the Born-level normalisation factor, S_n a symmetry factor for final-state particles, M_n^0 the squared tree-level n-particle matrix element and $\mathrm{d}\Phi_n$ the usual phase space for a n-parton final state with total four-momentum $\mathcal{Q}^\mu$ in $d = 4 - 2\epsilon$ space-time dimensions. Compared to the standard jet cross sections, the element of novelty here is the modified jet function J, which retains a dependence on the momentum fraction η, similarly to what was done in the photon fragmentation case in [51]. The purpose of the modified jet function is to define jet observables and/or any additional observable depending on the momentum k_p of the identified parton. In the framework of collinear factorisation encoded in (2.2), the momentum k_p of the identified parton is proportional to the momentum K_H of the identified hadron according to the simple relation $K_H = \eta k_p$.

Beyond leading order, it is well known that infrared divergences of soft and collinear origin appear in the short-distance cross section. They are guaranteed to cancel between real and virtual contributions in sufficiently inclusive observables, but a subtraction method is required in order to deal with such divergences in the intermediate steps of the calculation. In the antenna subtraction formalism [43, 44], the singularities associated to single or double unresolved particles in real emission matrix elements are locally subtracted by means of counterterms built out of antenna functions [55–57]. Each antenna function encodes the radiation pattern between a pair of hard radiators, thus reproducing the behaviour of the matrix element in the singular limits, but being simple enough to be analytically integrated over the unresolved degrees of freedom. The integrated subtraction terms are then added back at the virtual level, so as to cancel the explicit poles appearing in the virtual matrix elements.

Most of the elements introduced in [43], necessary to deal with jet cross sections in e^+e^- collisions, can be used for exclusive one-particle cross sections as well. However, whenever we identify a parton, we spoil the cancellation of collinear divergences. The physical reason is that by identifying for example a quark we are in the position to distinguish a quark from a collinear quark-gluon pair. These collinear divergences are subtracted from the short-distance cross sections by means of mass factorisation counterterms and absorbed in the bare fragmentation functions, which eventually result in mass-factorised fragmentation functions, the ones appearing in (2.2). In order to allow for a proper subtraction of final-state collinear divergences, we need to keep track of the momentum fraction of the fragmenting parton in the intermediate layers of the calculation. We do so by introducing fragmentation antenna functions which explicitly depend on the momentum fraction of the fragmenting parton. After integrating over all kinematical variables except the momentum fraction, these fragmentation antenna functions have the proper structure to be combined with the mass factorisation counterterms and result in a cancellation of final-state collinear divergence at the integrand level, *before* performing the convolution with the fragmentation function. In the following sections, we describe how the subtraction has to be modified to account for the presence of identified hadrons at NLO and NNLO.

3 Subtraction at NLO

The NLO corrections to the one-parton exclusive cross section in (2.4) contain contributions from real emission of one extra parton and virtual corrections. As it is customary in antenna subtraction, we introduce a real subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{S}}$ and a virtual subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{T}}$, to be subtracted from the real cross section $\mathrm{d}\hat{\sigma}_p^{\mathrm{R}}$ and the virtual cross section $\mathrm{d}\hat{\sigma}_p^{\mathrm{V}}$, respectively. The NLO short-distance cross section can then be written as

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{NLO}}(\eta) = \int_{n+1} \left[\mathrm{d}\hat{\sigma}_p^{\mathrm{R}}(\eta) - \mathrm{d}\hat{\sigma}_p^{\mathrm{S}}(\eta)\right] + \int_n \left[\mathrm{d}\hat{\sigma}_p^{\mathrm{V}}(\eta) - \mathrm{d}\hat{\sigma}_p^{\mathrm{T}}(\eta)\right] . \tag{3.1}$$

Each term in square brackets in (3.1) is free of infrared divergences and suitable for a numerical implementation. Note the subscript in (3.1), indicating that each term retains a dependence on the parton which is undergoing the fragmentation process.

The real partonic cross section $\mathrm{d}\hat{\sigma}_p^{\mathrm{R}}$ is given by (2.6) with an additional parton. It is decomposed according to its colour orderings. As for the real subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{S}}$, it will be given by the sum of several terms, summing over all possible single unresolved partons:

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{S}} = \sum_j \mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S}} . \tag{3.2}$$

The $\mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S}}$ are obtained by summing over all colour connections in which the parton j can become unresolved. They are further decomposed in two types of contributions as

$$\mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S}} = \mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S,non-id.}p} + \mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S,id.}p}, \tag{3.3}$$

where the first term contains all configurations where the identified parton p is not colour-connected to the unresolved parton j, such that we can use the standard NLO subtraction term with final-final kinematics, with p appearing unmodified in the respective reduced matrix element.

In order to subtract the infrared limits involving the unresolved parton j colour-connected to the identified p and a second hard parton k, we newly introduce the following subtraction term

$$\begin{aligned} \mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S,id}.p} = &\mathcal{N}_{\mathrm{R}} \mathrm{d}\Phi_{n+1}\left(k_1,\ldots,k_p,\ldots,k_{n+1};\mathcal{Q}\right) \frac{1}{S_{n+1}} \\ &\times X_3^0\left(k_p,k_j,k_k\right) M_n^0\left(k_1,\ldots,\tilde{K},\tilde{k}_p,\ldots,k_{n+1}\right) J\left(\left\{\ldots,\tilde{K},\tilde{k}_p,\ldots\right\}_n,\eta\, z\,\tilde{k}_p\right), \end{aligned} \tag{3.4}$$

where $\mathcal{N}_{\mathrm{R}} = \mathcal{N}_{\mathrm{B}}\,\overline{C}(\epsilon)/C(\epsilon)$, with

$$C(\epsilon) = \frac{(4\pi e^{-\gamma_E})^\epsilon}{8\pi^2}, \quad \overline{C}(\epsilon) = (4\pi e^{-\gamma_E})^\epsilon, \tag{3.5}$$

which are customary normalisation factors in the antenna subtraction formalism, and $\mathcal{N}_{\mathrm{B}}$ the Born-level normalisation factor of the process under consideration. The X_3^0 function is just the standard three-particle tree-level antenna function in the final-final kinematics, depending on the final state momenta which sum up to $q = k_j + k_k + k_p$ with $\mathcal{Q}^2 \geq q^2 > 0$. The phase space mapping involves the reconstruction of the momentum fraction z, used to define $\tilde{k}_p = k_p/z$, and of a recoil momentum $\tilde{K}$. The momentum fraction z is defined by projecting the momentum of the fragmenting parton and the momentum of its parent parton pair onto a specific reference four-vector that can be chosen freely. In our case, we choose q as reference direction, resulting in

$$\begin{aligned} z &= \frac{s_{pj}+s_{pk}}{s_{pj}+s_{pk}+s_{jk}}, \\ \tilde{K} &= k_j + k_k - (1-z)\frac{k_p}{z}, \end{aligned} \tag{3.6}$$

which satisfies all the required properties. In particular, in the collinear limit $k_p \parallel k_j$, z approaches the momentum fraction of k_p along the common collinear direction. Hence the overall momentum fraction entering the jet function is the product of η and z. It should be noted that the definition of z used here differs from the choice made in [51] for photon fragmentation antenna functions, where in the final-final kinematics k_k was used as reference in the definition of z. As a consequence, the integrated NLO fragmentation antenna functions differ from the ones listed in [51]. The different choice of reference momentum was appropriate in the photon case (where emitter and recoil could always be identified in an unambiguous manner), but generalises only poorly to the hadron fragmentation case.

In order to reach the factorisation of the phase space, we follow closely [58] by inserting

$$1 = \int \mathrm{d}^d q\, \delta\left(q - k_p - k_j - k_k\right), \tag{3.7}$$

and

$$1 = \frac{q^2}{2\pi} \int \frac{\mathrm{d}z}{z} \int \left[\mathrm{d}\tilde{K}\right] (2\pi)^d \, \delta \left(q - \frac{k_p}{z} - \tilde{K} \right) . \tag{3.8}$$

Since in (3.4) we are integrating over k_p, we need to introduce the one-particle phase space for $\tilde{k}_p$. They are related by

$$\left[\mathrm{d}\tilde{k}_p\right] = [\mathrm{d}k_p] \; z^{2-d} = [\mathrm{d}k_p] \; z^{-2+2\epsilon} , \tag{3.9}$$

which is due to the fact that $[\mathrm{d}p] \propto E^{d-3}\mathrm{d}E$. Hence, by integrating over q, we get

$$\begin{aligned} \mathrm{d}\Phi_{n+1}\left(k_1, \ldots, k_p, k_j, k_k, \ldots, k_{n+1}; \mathcal{Q}\right) = \mathrm{d}\Phi_n &\left(k_1, \ldots, \tilde{k}_p, \tilde{K}, \ldots, k_{n+1}; \mathcal{Q}\right) \\ &\times \frac{q^2}{2\pi} \mathrm{d}\Phi_2\left(k_j, k_k; q - k_p\right) \, z^{1-2\epsilon} \, \mathrm{d}z . \end{aligned} \tag{3.10}$$

We define the integrated version of the fragmentation antenna function over the two particle phase space as

$$\mathcal{X}_3^{0,\mathrm{id}.p}(z) = \frac{1}{C(\epsilon)} \int \mathrm{d}\Phi_2 \frac{q^2}{2\pi} \, z^{1-2\epsilon} \, X_3^0 \left(k_p^{\mathrm{id.}}, k_j, k_k\right) . \tag{3.11}$$

The (simple) integration is discussed in section 5.1, and explicit expressions for the $\mathcal{X}_3^{0,\mathrm{id}.p}$ can be found in appendix B. The integrated form of the subtraction term is then

$$\begin{aligned} \int_1 \mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S,id}.p} = \mathcal{N}_{\mathrm{V}} \int &\mathrm{d}z \, \mathrm{d}\Phi_n \left(k_1, \ldots, \tilde{k}_p, \tilde{K}, \ldots, k_{n+1}; \mathcal{Q}\right) \frac{1}{S_n} \\ &\times \mathcal{X}_3^{0,\mathrm{id}.p}(z) \; M_n^0\left(k_1, \ldots, \tilde{k}_p, \tilde{K}, \ldots, k_{n+1}\right) \, J\left(\left\{\ldots, \tilde{k}_p, \tilde{K}, \ldots\right\}_n, \eta \, z \, \tilde{k}_p\right) , \end{aligned} \tag{3.12}$$

with $\mathcal{N}_{\mathrm{V}} = \mathcal{N}_{\mathrm{R}} C(\epsilon) = \mathcal{N}_{\mathrm{B}} \, \overline{C}(\epsilon)$. The above expression contains the infrared poles required to cancel explicit poles of the virtual matrix element associated with the colour-connections involving the identified parton momentum p as well as collinear poles proportional to the Altarelli-Parisi splitting functions, which need to be properly subtracted by means of a NLO mass factorisation counterterm $\mathrm{d}\hat{\sigma}_p^{\mathrm{MF,NLO}}$, defined as

$$\begin{aligned} \mathrm{d}\hat{\sigma}_p^{\mathrm{MF,NLO}}(\eta) = -\mathcal{N}_{\mathrm{V}} \sum_h \int &\mathrm{d}z \, \mathrm{d}\Phi_n\left(k_1, \ldots, k_h, \ldots, k_n; \mathcal{Q}\right) \, \mu_a^{-2\epsilon} \Gamma_{p\leftarrow h}^{(1)}(z) \\ &\times \frac{1}{S_n} M_n^0\left(k_1, \ldots, k_h, \ldots, k_n\right) \, J\left(\{k_1, \ldots, k_h, \ldots, k_n\}_n, \eta \, z \, k_h\right) , \end{aligned} \tag{3.13}$$

with μ_a^2 the mass factorisation scale and $\Gamma_{p\leftarrow h}^{(1)}$ the leading order mass factorisation kernel (see appendix A). The full virtual subtraction term is then given by

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{T}}(\eta) = -\sum_j \int_1 \mathrm{d}\hat{\sigma}_{p,j}^{\mathrm{S}} - \mathrm{d}\hat{\sigma}_p^{\mathrm{MF,NLO}} . \tag{3.14}$$

Note that the integrated antenna functions and the mass factorisation kernels can be eventually combined into fragmentation dipoles, analogous to the initial-state dipoles introduced for hadron-collider processes [44].

An explicit example of subtraction at NLO is given in section 7, where we study identified hadron production inside jets in $e^+e^- \to 3$ jets final states.

4 Subtraction at NNLO

Predictions at NNLO require the calculation of three different contributions, namely double-real (RR), real-virtual (RV) and double-virtual (VV) contributions relative to the Born process. Each of these pieces is separately infrared divergent, whereas their sum is guaranteed to be finite. In order to handle the implicit divergences and explicit poles that arise in the intermediate steps of the calculation, three subtraction terms are introduced: a RR subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{S}}$, a RV subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{T}}$ and a VV subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{U}}$, such that the analogue of (3.1) at NNLO reads

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{NNLO}}(\eta) = \int_{n+2} \left[\mathrm{d}\hat{\sigma}_p^{\mathrm{RR}} - \mathrm{d}\hat{\sigma}_p^{\mathrm{S}}\right] + \int_{n+1} \left[\mathrm{d}\hat{\sigma}_p^{\mathrm{RV}} - \mathrm{d}\hat{\sigma}_p^{\mathrm{T}}\right] + \int_{n} \left[\mathrm{d}\hat{\sigma}_p^{\mathrm{VV}} - \mathrm{d}\hat{\sigma}_p^{\mathrm{U}}\right], \tag{4.1}$$

where a dependence on η in the integrands is understood. The structure of the $\mathrm{d}\hat{\sigma}_p^{\mathrm{S}}$, $\mathrm{d}\hat{\sigma}_p^{\mathrm{T}}$ and $\mathrm{d}\hat{\sigma}_p^{\mathrm{U}}$ subtraction terms has been discussed extensively in previous works: when the hard radiators are both in the final state (final-final kinematics) [43], one radiator in the final state and one in the initial state (initial-final kinematics) [58, 59] or both radiators in the initial state (initial-initial kinematics) [58, 60, 61]. A comprehensive review of the formalism in hadron-hadron collisions is given in [44]. In this section, we limit ourselves to explain where the subtraction terms have to been modified in order to account for the presence of the identified particle. Since an identified particle in the final state is conceptually similar to an initial state particle, the structure of the subtraction terms is close to the one provided in the initial-final case in [59].

The real-real subtraction term $\mathrm{d}\hat{\sigma}_p^{\mathrm{S}}$ is built out of several pieces, each of which accounts for a particular type of unresolved configuration. The first piece, $\mathrm{d}\hat{\sigma}_p^{\mathrm{S},a}$ deals with the single unresolved limits of the double real matrix elements. Its structure is similar to the NLO real subtraction term, already introduced in (3.2). The second piece, $\mathrm{d}\hat{\sigma}_p^{\mathrm{S},b}$ accounts for the double unresolved limits of the RR matrix element. We can distinguish configurations with the identified parton p colour-connected or not to the pair of unresolved partons j and k. In the latter case, we can use the standard NNLO subtraction term. In the former case, we introduce the subtraction term

$$\begin{aligned}
&\mathrm{d}\hat{\sigma}_{p,jk}^{\mathrm{S},b,\mathrm{id}.p} = \\
&\mathcal{N}_{\mathrm{RR}}\, \mathrm{d}\Phi_{n+2}(k_1,\ldots,k_{n+2};\mathcal{Q})\, \frac{1}{S_{n+2}} \\
&\times \Big[X_4^0(k_p,k_j,k_k,k_l)\, M_n^0\left(k_1,\ldots,\tilde{k}_p,\tilde{K},\ldots,k_{n+2}\right) J\left(\left\{\ldots,\tilde{k}_p,\tilde{K},\ldots\right\}_n,\eta\, z\, \tilde{k}_p\right) \\
&-X_3^0(k_p,k_j,k_k)\, X_3^0\left(\tilde{k}_p,\tilde{K},k_l\right) M_n^0\left(k_1,\ldots,\tilde{\tilde{k}}_p,\tilde{\tilde{K}},\ldots,k_{n+2}\right) J\left(\left\{\ldots,\tilde{\tilde{k}}_p,\tilde{\tilde{K}},\ldots\right\}_n,\eta\, z\, \tilde{\tilde{k}}_p\right) \\
&-X_3^0(k_j,k_k,k_l)\, X_3^0\left(k_p,\tilde{k}_{jk},\tilde{k}_{kl}\right) M_n^0\left(k_1,\ldots,\tilde{\tilde{k}}_p,\tilde{\tilde{K}},\ldots,k_{n+2}\right) J\left(\left\{\ldots,\tilde{\tilde{k}}_p,\tilde{\tilde{K}},\ldots\right\}_n,\eta\, z\, \tilde{\tilde{k}}_p\right)\Big],
\end{aligned} \tag{4.2}$$

with $\mathcal{N}_{\mathrm{RR}} = \mathcal{N}_{\mathrm{B}}\, \overline{C}(\epsilon)^2/C(\epsilon)^2$. The two products of three-parton antenna function are necessary to subtract the single unresolved limits of the four-parton antenna function, such that $d\hat{\sigma}_{p,jk}^{S,b,\mathrm{id}.p}$ is active only in the double unresolved limits. They each involve two consecutive NLO phase space mappings, whose results are abbreviated as $(\tilde{\tilde{k}}_p, \tilde{\tilde{K}})$ and where the intermediate momenta $(\tilde{k}_{jk}, \tilde{k}_{kl})$ indicate a standard final-final NLO mapping. The genuine NNLO mapping to $(\tilde{k}_p = k_p/z, \tilde{K})$ in the first term is a generalisation of (3.6) with more than one parton becoming unresolved. Explicitly, it reads:

$$
\begin{aligned}
z &= \frac{s_{pj} + s_{pk} + s_{pl}}{s_{pj} + s_{pk} + s_{jk} + s_{pl} + s_{jl} + s_{kl}}\,, \\
\tilde{K} &= k_j + k_k + k_l - (1-z)\frac{k_p}{z}\,.
\end{aligned}
\tag{4.3}
$$

with p the fragmenting parton, j and k the two unresolved partons, and l the other final state radiator. Such a mapping satisfies the appropriate limits in all double singular configurations. Moreover, it turns into an NLO phase space mapping in its single unresolved limits, as required in order to cancel the single unresolved limits of the X_4^0 antenna function. The integral of the tree-level four-particle antenna function over the three-particle phase space

$$
\mathcal{X}_4^{0,\mathrm{id}.p}(z) = \frac{1}{[C(\epsilon)]^2} \int \mathrm{d}\Phi_3 \frac{q^2}{2\pi}\, z^{1-2\epsilon}\, X_4^0\left(k_p^{\mathrm{id}.}, k_j, k_k, k_l\right)\,,
\tag{4.4}
$$

reappears at the virtual-virtual level; its integration is discussed in section 5.2.

The subtraction terms with two unresolved partons almost colour-unconnected ($\mathrm{d}\hat{\sigma}^{S,c}$) or colour-unconnected ($\mathrm{d}\hat{\sigma}^{S,d}$) do not require new ingredients: they contain products of tree-level three-parton antenna functions or fragmentation antenna functions in the final-final kinematics. They appear, after integration, at the real-virtual or at the virtual-virtual level, as the product of an integrated antenna function $\mathcal{X}_3^0$ with an unintegrated antenna function X_3^0 or as a product of two $\mathcal{X}_3^0$, respectively. In order to avoid oversubtraction of large-angle soft gluon radiation, additional soft antenna functions S_{ajc} [62] are used to construct $\mathrm{d}\hat{\sigma}^{S,e}$; in such soft antenna functions, the hard momenta a and c can be arbitrary on-shell momenta in the initial or final state. The integral of the soft antenna function in the final-final kinematics is given in [62], whereas in the initial-final kinematics in [44, 59]. Given the freedom we have in the choice of the hard momenta of the soft antenna function, we can use the known results in processes with fragmentation as well.

At the real-virtual level, we need to remove the explicit infrared poles of the one-loop matrix element and to also subtract its single unresolved limit. The former purpose is accomplished by the integral of $\mathrm{d}\hat{\sigma}_p^{S,a}$, which combined with mass factorisation terms (see below), results in $\mathrm{d}\hat{\sigma}_p^{T,a}$. The latter purpose requires the introduction of a new subtraction term:

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}_{p,j}^{T,b,\mathrm{id}.p} = \mathcal{N}_{\mathrm{RV}}\, \mathrm{d}\Phi_{n+1}\left(k_1,\ldots,k_{n+1};\mathcal{Q}\right) \frac{1}{S_{n+1}} J\left(\left\{\ldots,\tilde{k}_p,\tilde{K},\ldots\right\}_n, \eta\, z\, \tilde{k}_p\right) \\
\times\Bigg[X_3^0\left(k_p,k_j,k_k\right)\, M_n^1\left(k_1,\ldots,\tilde{k}_p,\tilde{K},\ldots,k_{n+1}\right) \\
+ X_3^1\left(k_p,k_j,k_k\right)\, M_n^0\left(k_1,\ldots,\tilde{k}_p,\tilde{K},\ldots,k_{n+1}\right)\Bigg]\,,
\end{aligned}
\tag{4.5}
$$

with $\mathcal{N}_{\mathrm{RV}} = \mathcal{N}_{\mathrm{B}}\,\overline{C}(\epsilon)^2/C(\epsilon)$, and where we have used the NLO momentum mapping (3.6). In here, M_n^1 is the one-loop reduced matrix element and X_3^1 is the one-loop three-parton antenna function in the final-final kinematics, whose integral over the two-particle phase space is denoted as

$$\mathcal{X}_3^{1,\mathrm{id}.p}(z) = \frac{1}{C(\epsilon)} \int \mathrm{d}\Phi_2 \frac{q^2}{2\pi}\, z^{1-2\epsilon}\, X_3^1\left(k_p^{\mathrm{id}.}, k_j, k_k\right)\;; \tag{4.6}$$

it is reintroduced at the virtual-virtual level. Its integration is presented in section 5.3. In order to assemble $\mathrm{d}\hat{\sigma}_p^{\mathrm{T},a}$ and $\mathrm{d}\hat{\sigma}_p^{\mathrm{T},b}$, one also needs the real-virtual mass factorisation term:

$$\mathrm{d}\hat{\sigma}_p^{\mathrm{MF,RV}}(\eta) = -\mathcal{N}_{\mathrm{RV}} \sum_h \int \mathrm{d}z\, \mu_a^{-2\epsilon} \Gamma^{(1)}_{p\leftarrow h}(z) \left(\mathrm{d}\hat{\sigma}_h^{\mathrm{R}}(\eta\, z) - \mathrm{d}\hat{\sigma}_h^{\mathrm{S}}(\eta\, z)\right)\,, \tag{4.7}$$

which contributes both to $\mathrm{d}\hat{\sigma}_p^{\mathrm{T},a}$ and $\mathrm{d}\hat{\sigma}_p^{\mathrm{T},b}$. The last piece needed for the subtraction at the real-virtual level is $\mathrm{d}\hat{\sigma}^{\mathrm{T},c}$, which results from the integration of $\mathrm{d}\hat{\sigma}^{\mathrm{S},c}$ and $\mathrm{d}\hat{\sigma}^{\mathrm{S},e}$, plus additional terms to ensure an IR finite contribution, which are added back at the double virtual level.

At the virtual-virtual level, there are no implicit infrared divergences; the explicit poles of the two-loop matrix element are canceled by the integrated form of the appropriate subtraction terms, together with the double virtual mass factorisation term:

$$\begin{aligned}\mathrm{d}\hat{\sigma}_p^{\mathrm{MF,VV}}(\eta) \;=\; -\mathcal{N}_{\mathrm{VV}} \sum_h \int \mathrm{d}z\, \mu_a^{-2\epsilon} \Big[&\Gamma^{(2)}_{p\leftarrow h}(z)\, \mathrm{d}\hat{\sigma}_h^{\mathrm{B}}(\eta\, z) \\ &+ \Gamma^{(1)}_{p\leftarrow h}(z) \left(\mathrm{d}\hat{\sigma}_h^{\mathrm{V}}(\eta\, z) - \mathrm{d}\hat{\sigma}_h^{\mathrm{T}}(\eta\, z)\right)\Big]\,, \end{aligned} \tag{4.8}$$

with $\mathcal{N}_{\mathrm{VV}} = \mathcal{N}_{\mathrm{B}}\,\overline{C}(\epsilon)^2$, to result in $\mathrm{d}\hat{\sigma}_p^{\mathrm{U}}$, and $\Gamma^{(2)}_{p\leftarrow h}$ are the colour-stripped version of the next-to-leading order splitting kernels defined in (A.8).

5 Integration of fragmentation antenna functions

The integration of the X_3^0, X_4^0 and X_3^1 fragmentation antenna functions is closely related to the integration of the corresponding initial-final antenna functions described in [58, 59].

5.1 Integration of NLO antenna functions

According to the definition of the $\mathcal{X}_3^{0,\mathrm{id}.p}$ given in (3.11), we integrate the antenna function over the two-particle phase space with kinematics

$$q + (-k_p) \to k_1 + k_2\,, \tag{5.1}$$

with $s_{12} = (q - k_p)^2 = q^2(1 - z)$ and

$$z = \frac{2\,k_p \cdot q}{q^2}\,. \tag{5.2}$$

The fragmenting parton k_p may be regarded as an initial state parton with negative four-momentum, and we are then looking at the $1 \to 3$ process with one identified parton as a $2 \to 2$ scattering process with rescaled invariant mass. By inserting the explicit expression for the two-particle phase space, (3.11) reduces to a simple one-dimensional integral

$$\mathcal{X}_3^{0,\mathrm{id}.p}(z) = z^{1-2\epsilon}(1-z)^{-\epsilon}\left(\frac{q^2}{4}\right)^{1-\epsilon}\frac{e^{\gamma\epsilon}}{\Gamma(1-\epsilon)}\int_{-1}^{+1}\mathrm{d}v\,\left(1-v^2\right)^{-\epsilon} X_3^0(s_{12}, s_{1p}, s_{2p}) \tag{5.3}$$

where

$$s_{1p} = \frac{q^2}{2}z(1-v)\,, \qquad s_{2p} = \frac{q^2}{2}z(1+v)\,. \tag{5.4}$$

After integration, the $(1-z)^{-\epsilon}$ factor, which regulates end-point soft divergences, can be safely expanded in term of distributions, according to

$$(1-z)^{-1+k\epsilon} = -\frac{1}{k\epsilon}\delta(1-z) + \sum_n \frac{(-k\epsilon)^n}{n!}\mathcal{D}_n(1-z) \tag{5.5}$$

with

$$\mathcal{D}_n(1-z) = \left(\frac{\log^n(1-z)}{1-z}\right)_+\,. \tag{5.6}$$

Explicit expressions for the integrated $\mathcal{X}_3^{0,\mathrm{id}.p}$ antenna functions are provided in appendix B. We note that they can be related to the inclusively integrated initial-final antenna functions derived in [58] by replacing

$$Q^2 \to -q^2\,, \qquad x \to 1/z\,, \tag{5.7}$$

as can be evidenced form (5.1).

5.2 Integration of NNLO real-real antenna functions

Similarly to the steps preformed in the previous section, we integrate the X_4^0 over a three-particle phase space with $2 \to 3$ kinematics

$$q + (-k_p) \to k_1 + k_2 + k_3\,. \tag{5.8}$$

The integration is performed with well-known techniques, based on multi-loop calculation technology. Namely, we rewrite the three-particle phase space in terms of cut propagators, in order to express it as a cut through a three-loop vacuum polarisation diagram. Then, we reduce the occurring integrals as linear combinations of a smaller set of master integrals, with the help of Reduze2 [63]. We managed to reduce to the same set of 9 master integrals which appears in the initial-final case, see section 4 of [59]. This is ultimately due to the fact that the processes

$$q + (-k_p) \to k_1 + k_2 + k_3\,, \qquad q^2 > 0\,, \qquad (q-k_p)^2 = (1-z)\,q^2 \tag{5.9}$$

and

$$q + k_i \to k_1 + k_2 + k_3\,, \qquad q^2 = -Q^2 < 0\,, \qquad (q+k_i)^2 = (1-x)/x\,Q^2 \tag{5.10}$$

feature the same kinematics with a different definition of invariants.

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The master integrals have been calculated by exploiting the differential equations method [64]. We first use EPSILON [65] to find the canonical form [66, 67] of the differential equations. Once expressed in the canonical form, the differential equations can be iteratively solved in term of the harmonic polylogarithms (HPLs) [68], with unknown boundary conditions. In order to impose the boundary conditions, and at the same time check the structure of the master integrals, we can fully exploit the similarity between (5.9) and (5.10): the master integrals for real-real fragmentation antenna functions are related to the master integrals for initial-final antenna functions, reported in appendix A.1 of [59], by means of the replacement (5.7), which amounts to an analytic continuation. In particular, HPLs of argument $1/z$ are expressed as HPLs of argument z by means of an iterative procedure (see for instance section 6 of [68]), which is implemented in the Mathematica package HPL [69, 70]. Full consistency has been found with the master integrals found by means of the differential equation approach, after adjustment of some typographical mistakes, in particular in (A.9) of [59] the endpoint term should be corrected as

$$\epsilon\left(256\,\zeta_3 - \frac{43}{18}\pi^4\right) \to \epsilon\left(-\frac{74}{45}\pi^4\right).$$

Once the explicit expressions for the master integrals have been found, they can be substituted inside the antenna functions. At this point, the factor $(1-z)^{-2\epsilon}$ can be safely expanded in distributions according to (5.5). The whole workflow of the calculation has been implemented in FORM [71].

In table 1 we list all the integrated tree-level four-parton antenna functions; they differ by the nature of the identified particle and the hard radiators they collapse to. Some momentum permutations of identified particles in $\mathcal{A}_4^{0,\mathrm{id}.p}$, $\mathcal{B}_4^{0,\mathrm{id}.p}$, $\mathcal{D}_4^{0,\mathrm{id}.p}$, $\tilde{\mathcal{E}}_4^{0,\mathrm{id}.p}$ and in all gluon-gluon antenna functions are not shown in table 1, because the integrated antenna functions turn out to be the same: this is ultimately due to the symmetries present in the unintegrated antenna functions under permutation of partons of the same flavour. Instead in the case of $\mathcal{C}_4^{0,\mathrm{id}.p}$ and $\mathcal{E}_4^{0,\mathrm{id}.p}$ different identified particles lead to different results at the integrated level: hence they are distinguished by a label indicating the fragmenting parton. Explicit expressions for the integrated $\mathcal{X}_4^{0,\mathrm{id}.p}$ antenna functions are provided as supplementary material attached to this paper.

5.3 Integration of NNLO real-virtual antenna functions

The integration of the X_3^1 fragmentation antenna is performed over a two-particle phase space with $2 \to 2$ kinematics, as in section 5.1. The X_3^1 antenna functions are expressed in terms of rational functions of invariants multiplying one-loop bubble and box integrals. In order to use the same techniques of section 5.2, we rewrite the one-loop integrals in terms of propagators, and then we write the two-particle phase space integral of the one-loop antenna functions as a three-loop integral with two cut propagators. By doing so, we reduce to the same set of 6 master integrals of the initial-final case [59]. The master integrals are determined with the differential equation method, with boundary conditions obtained by internal consistency of the set of equations, or by a direct calculation at $z = 1$. Three of them contain as subdiagram a one-loop bubble, one of them a one-loop triangle (that can be expressed in terms of one-loop bubbles), and two of them a one-loop box.

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Hard radiators	Notation	Integral of	In the supplementary material
Quark-quark	$\mathcal{A}_4^{0,\text{id}.q}$	$A_4^0(1_q^{\text{id.}}, 3_g, 4_g, 2_{\bar{q}})$	`qA40`
	$\mathcal{A}_4^{0,\text{id}.g}$	$A_4^0(1_q, 3_g^{\text{id.}}, 4_g, 2_{\bar{q}})$	`gA40`
	$\tilde{\mathcal{A}}_4^{0,\text{id}.q}$	$\tilde{A}_4^0(1_q^{\text{id.}}, 3_g, 4_g, 2_{\bar{q}})$	`qA40t`
	$\tilde{\mathcal{A}}_4^{0,\text{id}.g}$	$\tilde{A}_4^0(1_q, 3_g^{\text{id.}}, 4_g, 2_{\bar{q}})$	`gA40t`
	$\mathcal{B}_4^{0,\text{id}.q}$	$B_4^0(1_q^{\text{id.}}, 3_{q'}, 4_{\bar{q}'}, 2_{\bar{q}})$	`qB40`
	$\mathcal{B}_4^{0,\text{id}.q'}$	$B_4^0(1_q, 3_{q'}^{\text{id.}}, 4_{\bar{q}'}, 2_{\bar{q}})$	`qpB40`
	$\mathcal{C}_4^{0,\text{id}.\bar{q}}$	$C_4^0(1_q, 3_q, 4_{\bar{q}}, 2_{\bar{q}}^{\text{id.}})$	`qbC40`
	$\mathcal{C}_4^{0,\text{id}.q1}$	$C_4^0(1_q^{\text{id.}}, 3_q, 4_{\bar{q}}, 2_{\bar{q}})$	`q1C40`
	$\mathcal{C}_4^{0,\text{id}.q3}$	$C_4^0(1_q, 3_q^{\text{id.}}, 4_{\bar{q}}, 2_{\bar{q}})$	`q3C40`
Quark-gluon	$\mathcal{D}_4^{0,\text{id}.q}$	$D_4^0(1_q^{\text{id.}}, 2_g, 3_g, 4_g)$	`qD40`
	$\mathcal{D}_4^{0,\text{id}.g2}$	$D_4^0(1_q, 2_g^{\text{id.}}, 3_g, 4_g)$	`g2D40`
	$\mathcal{D}_4^{0,\text{id}.g3}$	$D_4^0(1_q, 2_g, 3_g^{\text{id.}}, 4_g)$	`g3D40`
	$\mathcal{E}_4^{0,\text{id}.g}$	$E_4^0(1_q, 2_{q'}, 3_{\bar{q}'}, 4_g^{\text{id.}})$	`gE40`
	$\mathcal{E}_4^{0,\text{id}.q1}$	$E_4^0(1_q^{\text{id.}}, 2_{q'}, 3_{\bar{q}'}, 4_g)$	`q1E40`
	$\mathcal{E}_4^{0,\text{id}.q2}$	$E_4^0(1_q, 2_{q'}^{\text{id.}}, 3_{\bar{q}'}, 4_g)$	`q2E40`
	$\mathcal{E}_4^{0,\text{id}.q3}$	$E_4^0(1_q, 2_{q'}, 3_{\bar{q}'}^{\text{id.}}, 4_g)$	`q3E40`
	$\tilde{\mathcal{E}}_4^{0,\text{id}.g}$	$\tilde{E}_4^0(1_q, 2_{q'}, 3_{\bar{q}'}, 4_g^{\text{id.}})$	`gE40t`
	$\tilde{\mathcal{E}}_4^{0,\text{id}.q1}$	$\tilde{E}_4^0(1_q^{\text{id.}}, 2_{q'}, 3_{\bar{q}'}, 4_g)$	`q1E40t`
	$\tilde{\mathcal{E}}_4^{0,\text{id}.q2}$	$\tilde{E}_4^0(1_q, 2_{q'}^{\text{id.}}, 3_{\bar{q}'}, 4_g)$	`q2E40t`
Gluon-gluon	$\mathcal{F}_4^{0,\text{id}.g}$	$F_4^0(1_g, 3_g^{\text{id.}}, 4_g, 2_g)$	`gF40`
	$\mathcal{G}_4^{0,\text{id}.g}$	$G_4^0(1_g^{\text{id.}}, 3_q, 4_{q'}, 2_g)$	`gG40`
	$\mathcal{G}_4^{0,\text{id}.q}$	$G_4^0(1_g, 3_q^{\text{id.}}, 4_{q'}, 2_g)$	`qG40`
	$\tilde{\mathcal{G}}_4^{0,\text{id}.g}$	$\tilde{G}_4^0(1_g^{\text{id.}}, 3_q, 4_{q'}, 2_g)$	`gG40t`
	$\tilde{\mathcal{G}}_4^{0,\text{id}.q}$	$\tilde{G}_4^0(1_g, 3_q^{\text{id.}}, 4_{q'}, 2_g)$	`qG40t`
	$\mathcal{H}_4^{0,\text{id}.q}$	$\hat{H}_4^0(1_q^{\text{id.}}, 3_{\bar{q}}, 4_{q'}, 2_{\bar{q}'})$	`qH40`

Table 1. Integrated tree-level four-parton antenna functions $\mathcal{X}_4^{0,\text{id}.p}$.

In the real-virtual case, the master integrals for fragmentation antenna functions cannot be inferred from the master integrals for initial-final antenna functions, reported in appendix A.2 of [59], since the analytic continuation from (5.10) to (5.9) acts differently on the different bubble and box integrals and must be performed prior to the phase space integration. Consequently, a simple relationship between space-like and time-like real-virtual master integrals can not be established.

The integrated one-loop squared matrix elements are subsequently renormalised, as described in detail in section 4.2 of [59]: the strong coupling constant renormalisation is carried out in the $\overline{\text{MS}}$ scheme at fixed scale $\mu^2 = q^2$; in the case of quark-gluon and

Hard radiators	Notation	Integral of	In the supplementary material
Quark-quark	$\mathcal{A}_3^{1,\mathrm{id}.q}$	$A_3^1(1_q^{\mathrm{id.}}, 3_g, 2_{\bar{q}})$	`qA31`
	$\mathcal{A}_3^{1,\mathrm{id}.g}$	$A_3^1(1_q, 3_g^{\mathrm{id.}}, 2_{\bar{q}})$	`gA31`
	$\tilde{\mathcal{A}}_3^{1,\mathrm{id}.q}$	$\tilde{A}_3^1(1_q^{\mathrm{id.}}, 3_g, 2_{\bar{q}})$	`qA31t`
	$\tilde{\mathcal{A}}_3^{1,\mathrm{id}.g}$	$\tilde{A}_3^1(1_q, 3_g^{\mathrm{id.}}, 2_{\bar{q}})$	`gA31t`
	$\hat{\mathcal{A}}_3^{1,\mathrm{id}.q}$	$\hat{A}_3^1(1_q^{\mathrm{id.}}, 3_g, 2_{\bar{q}})$	`qA31h`
	$\hat{\mathcal{A}}_3^{1,\mathrm{id}.g}$	$\hat{A}_3^1(1_q, 3_g^{\mathrm{id.}}, 2_{\bar{q}})$	`gA31h`
Quark-gluon	$\mathcal{D}_3^{1,\mathrm{id}.q}$	$D_3^1(1_q^{\mathrm{id.}}, 3_g, 2_g)$	`qD31`
	$\mathcal{D}_3^{1,\mathrm{id}.g}$	$D_3^1(1_q, 3_g^{\mathrm{id.}}, 2_g)$	`gD31`
	$\hat{\mathcal{D}}_3^{1,\mathrm{id}.q}$	$\hat{D}_3^1(1_q^{\mathrm{id.}}, 3_g, 2_g)$	`qD31h`
	$\hat{\mathcal{D}}_3^{1,\mathrm{id}.g}$	$\hat{D}_3^1(1_q, 3_g^{\mathrm{id.}}, 2_g)$	`gD31h`
	$\mathcal{E}_3^{1,\mathrm{id}.q}$	$E_3^1(1_q^{\mathrm{id.}}, 3_{q'}, 2_{\bar{q}'})$	`qE31`
	$\mathcal{E}_3^{1,\mathrm{id}.q'}$	$E_3^1(1_q, 3_{q'}^{\mathrm{id.}}, 2_{\bar{q}'})$	`qpE31`
	$\tilde{\mathcal{E}}_3^{1,\mathrm{id}.q}$	$\tilde{E}_3^1(1_q^{\mathrm{id.}}, 3_{q'}, 2_{\bar{q}'})$	`qE31t`
	$\tilde{\mathcal{E}}_3^{1,\mathrm{id}.q'}$	$\tilde{E}_3^1(1_q, 3_{q'}^{\mathrm{id.}}, 2_{\bar{q}'})$	`qpE31t`
	$\hat{\mathcal{E}}_3^{1,\mathrm{id}.q}$	$\hat{E}_3^1(1_q^{\mathrm{id.}}, 3_{q'}, 2_{\bar{q}'})$	`qE31h`
	$\hat{\mathcal{E}}_3^{1,\mathrm{id}.q'}$	$\hat{E}_3^1(1_q, 3_{q'}^{\mathrm{id.}}, 2_{\bar{q}'})$	`qpE31h`
Gluon-gluon	$\mathcal{F}_3^{1,\mathrm{id}.g}$	$F_3^1(1_g, 3_g^{\mathrm{id.}}, 2_g)$	`gF31`
	$\hat{\mathcal{F}}_3^{1,\mathrm{id}.g}$	$\hat{F}_3^1(1_g, 3_g^{\mathrm{id.}}, 2_g)$	`gF31h`
	$\mathcal{G}_3^{1,\mathrm{id}.g}$	$G_3^1(1_g^{\mathrm{id.}}, 3_q, 2_{q'})$	`gG31`
	$\mathcal{G}_3^{1,\mathrm{id}.q}$	$G_3^1(1_g, 3_q^{\mathrm{id.}}, 2_{q'})$	`qG31`
	$\tilde{\mathcal{G}}_3^{1,\mathrm{id}.g}$	$\tilde{G}_3^1(1_g^{\mathrm{id.}}, 3_q, 2_{q'})$	`gG31t`
	$\tilde{\mathcal{G}}_3^{1,\mathrm{id}.q}$	$\tilde{G}_3^1(1_g, 3_q^{\mathrm{id.}}, 2_{q'})$	`qG31t`
	$\hat{\mathcal{G}}_3^{1,\mathrm{id}.g}$	$\hat{G}_3^1(1_g^{\mathrm{id.}}, 3_q, 2_{q'})$	`gG31h`
	$\hat{\mathcal{G}}_3^{1,\mathrm{id}.q}$	$\hat{G}_3^1(1_g, 3_q^{\mathrm{id.}}, 2_{q'})$	`qG31h`

Table 2. Integrated one-loop three-parton antenna functions $\mathcal{X}_3^{1,\mathrm{id}.p}$.

gluon-gluon antenna functions, the effective operators used to couple an external current to the parton radiators are also renormalised. Finally, in order to obtain the integrated one-loop antenna functions, we subtract from the renormalised one-loop squared matrix elements the corresponding integrated tree-level antenna function multiplied with the virtual one-loop correction to the hard radiator vertex.

In table 2 we list all the integrated one-loop three-parton antenna functions; they differ by the nature of the identified particle and the hard radiators they collapse to. Explicit expressions for the integrated $\mathcal{X}_3^{1,\mathrm{id}.p}$ antenna functions are provided as supplementary material attached to this paper.

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6 Coefficient functions for hadron production at e^+e^- colliders

6.1 Identified hadrons in γ/Z boson decay

Next-to-next-to-leading order corrections to the coefficient functions contributing to the longitudinal and transverse one-hadron energy spectrum in e^+e^- annihilation have been first derived in [11, 72] and independently rederived in [12]. Since the antenna functions are extracted from double-real and real-virtual matrix elements for $\gamma^* \to q\bar{q}$ decay [55], by combining integrated antenna functions with quark form factors, we are in the position to calculate these coefficient functions in an independent manner. This comparison provides a strong check on the correctness of our integrated $\mathcal{A}$-type, $\mathcal{B}$-type and $\mathcal{C}$-type fragmentation antenna functions, and indirectly on our whole procedure.

The cross section differential in the energy fraction $x = 2E_p/\sqrt{s}$ of the identified hadron is usually written as

$$\frac{\mathrm{d}\sigma^H}{\mathrm{d}x} = \int_x^1 \frac{\mathrm{d}z}{z} \sum_{p=1}^{N_F} \sigma_p^{(0)} \left[D_{\mathrm{S}}^H\left(\frac{x}{z}\right) \mathbb{C}_q^{\mathrm{S}}(z) + D_g^H\left(\frac{x}{z}\right) \mathbb{C}_g^{\mathrm{S}}(z) + D_{\mathrm{NS},p}^H\left(\frac{x}{z}\right) \mathbb{C}_q^{\mathrm{NS}}(z) \right], \tag{6.1}$$

where we have introduced the singlet (S) and non-singlet (NS) combination of fragmentation densities, defined as

$$D_{\mathrm{S}}^H = \frac{1}{N_F} \sum_{p=1}^{N_F} \left(D_p^H + D_{\bar{p}}^H \right), \qquad D_{\mathrm{NS},p}^H = D_p^H + D_{\bar{p}}^H - D_{\mathrm{S}}^H . \tag{6.2}$$

It is customary to also define the purely singlet (PS) coefficient function $\mathbb{C}_q^{\mathrm{PS}} = \mathbb{C}_q^{\mathrm{S}} - \mathbb{C}_q^{\mathrm{NS}}$.

Higher order QCD corrections to the $\mathbb{C}$ coefficient functions originate from radiation in the final state. All electroweak effects factor out of the coefficient functions, and are included in the pointlike total cross section $\sigma_p^{(0)}$ for the process $e^+ + e^- \to p + \bar{p}$, which in the simple QED-only case is equal to the well-known $e_p^2 N 4\pi\alpha^2/(3s)$.

The coefficient functions $\mathbb{C}$ are the mass-factorised and UV-renormalised version of the parton fragmentation functions $\hat{\mathcal{F}}$, whose expansion in the (unrenormalised) strong coupling constant reads

$$\hat{\mathcal{F}} = \hat{\mathcal{F}}^{(0)} + \left(\frac{\hat{\alpha}_s}{4\pi}\right) S_\epsilon \left(\frac{\mu_0^2}{Q^2}\right)^{\epsilon} \hat{\mathcal{F}}^{(1)} + \left(\frac{\hat{\alpha}_s}{4\pi}\right)^2 S_\epsilon^2 \left(\frac{\mu_0^2}{Q^2}\right)^{2\epsilon} \hat{\mathcal{F}}^{(2)} + \mathcal{O}\left(\hat{\alpha}_s^3\right), \tag{6.3}$$

where $\hat{\alpha}_s$ is the bare coupling, $S_\epsilon = (4\pi e^{-\gamma_E})^\epsilon$ and μ_0^2 is the mass parameter of dimensional regularisation. The parton fragmentation functions are obtained as projections of the parton structure tensor $\hat{W}_{\mu\nu}$ onto its longitudinal ($\hat{\mathcal{F}}_L$), transverse ($\hat{\mathcal{F}}_T$) and asymmetric ($\hat{\mathcal{F}}_A$) components. They are in one-to-one correspondence with the homonymous contributions in the angular distribution of the detected hadron,

$$\frac{\mathrm{d}^2\sigma^H}{\mathrm{d}x\,\mathrm{d}\cos\theta} = \frac{3}{8}\left(1+\cos^2\theta\right)\frac{\mathrm{d}\sigma_T^H}{\mathrm{d}x} + \frac{3}{4}\sin^2\theta\frac{\mathrm{d}\sigma_L^H}{\mathrm{d}x} + \frac{3}{4}\cos\theta\frac{\mathrm{d}\sigma_A^H}{\mathrm{d}x}. \tag{6.4}$$

Since we are fully inclusive over the angle of emission of the detected hadron, we consider the trace $\hat{W}_\mu^\mu$, which is related to the combination

$$-\frac{z}{d-2}\hat{W}_\mu^\mu = \hat{\mathcal{F}}_T + \frac{2}{d-2}\hat{\mathcal{F}}_L \equiv \hat{\mathcal{F}}_U . \tag{6.5}$$

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The chosen normalisation is such that, at leading order, we have

$$\hat{\mathcal{F}}^{(0)}_{U,q} = \hat{\mathcal{F}}^{(0)}_{T,q} = \delta(1-z)\,, \qquad \hat{\mathcal{F}}^{(0)}_{L,q} = 0\,, \qquad \hat{\mathcal{F}}^{(0)}_{U,g} = \hat{\mathcal{F}}^{(0)}_{T,g} = \hat{\mathcal{F}}^{(0)}_{L,g} = 0\,. \tag{6.6}$$

The relationships we observe between the parton fragmentation functions and the integrated fragmentation antenna functions read at NLO

$$\frac{1}{C_F}\hat{\mathcal{F}}^{(1)}_{U,q} = 4\,\mathcal{A}_3^{0,\mathrm{id}.q} + 8\,\delta(1-z)V_q^{(1)}|_N\,, \tag{6.7}$$

$$\frac{1}{C_F}\hat{\mathcal{F}}^{(1)}_{U,g} = 4\,\mathcal{A}_3^{0,\mathrm{id}.g}\,, \tag{6.8}$$

and at NNLO

$$\frac{1}{C_F}\hat{\mathcal{F}}^{\mathrm{NS},(2)}_{U,q}|_N = 2\,\mathcal{A}_4^{0,\mathrm{id}.q} + 8\,\mathcal{A}_3^{1U,\mathrm{id}.q} + \delta(1-z)V_q^{(2)}|_N\,, \tag{6.9}$$

$$\frac{1}{C_F}\hat{\mathcal{F}}^{\mathrm{NS},(2)}_{U,q}|_{N_F} = 2\,\mathcal{B}_4^{0,\mathrm{id}.q} + \delta(1-z)V_q^{(2)}|_{N_F}\,, \tag{6.10}$$

$$\begin{aligned}\frac{1}{C_F}\hat{\mathcal{F}}^{\mathrm{NS},(2)}_{U,q}|_{1/N} = &-\tilde{\mathcal{A}}_4^{0,\mathrm{id}.q} - 8\,\tilde{\mathcal{A}}_3^{1U,\mathrm{id}.q} - 4\,\mathcal{C}_4^{0,\mathrm{id}.\bar{q}}\\ &-2\,\mathcal{C}_4^{0,\mathrm{id}.q_1} - 2\,\mathcal{C}_4^{0,\mathrm{id}.q_3} + \delta(1-z)V_q^{(2)}|_{1/N}\,,\end{aligned} \tag{6.11}$$

$$\frac{1}{C_F N_F}\hat{\mathcal{F}}^{\mathrm{PS},(2)}_{U,q} = 2\,\mathcal{B}_4^{0,\mathrm{id}.q'}\,, \tag{6.12}$$

for an identified quark and

$$\frac{1}{C_F N_F}\hat{\mathcal{F}}^{(2)}_{U,g}|_N = 4\,\mathcal{A}_4^{0,\mathrm{id}.g} + 8\,\mathcal{A}_3^{1U,\mathrm{id}.g}\,, \tag{6.13}$$

$$\frac{1}{C_F N_F}\hat{\mathcal{F}}^{(2)}_{U,g}|_{1/N} = -2\,\tilde{\mathcal{A}}_4^{0,\mathrm{id}.g} - 8\,\tilde{\mathcal{A}}_3^{1U,\mathrm{id}.g}\,, \tag{6.14}$$

for an identified gluon, respectively. The notation is such that $X|_Y$ denotes the part of X proportional to Y. The superscript U denotes the unrenormalised one-loop squared matrix elements, see section 5.3. Finally, the $V_q^{(1)}$ and $V_q^{(2)}$ terms are given by

$$V_q^{(1)} = \Re\left[\Delta\left(q^2,1\right)\right]\,F^{(1)}_{U,q}\,, \tag{6.15}$$

$$V_q^{(2)} = \left(F^{(1)}_{U,q}\right)^2 + 2\,\Re\left[\Delta\left(q^2,2\right)\right]\,F^{(2)}_{U,q}\,, \tag{6.16}$$

where $F^{(1)}_{U,q}$ and $F^{(2)}_{U,q}$ are the unrenormalised first and second order coefficients of the quark form factor respectively, with the normalisation fixed by (6.3) and by requiring that $F^{(0)}_{U,q} = 1$, and

$$\Delta\left(q^2,\kappa\right) = \left(-\mathrm{sgn}\left(q^2\right) - i0\right)^{-\kappa\epsilon}\,. \tag{6.17}$$

Explicit expressions for $F^{(1)}_{U,q}$ and $F^{(2)}_{U,q}$ can be found in [73, 74].

In order to compare against the results of [11, 72], several convolutions between splitting functions and coefficient functions needed to be computed; the Mathematica package MT [75] has been extensively used. Eqs. (6.7)–(6.14) are in full agreement with the results of [11, 72] at NLO and NNLO at all colour levels.

6.2 Identified hadrons in Higgs boson decay to gluons

The gluon-gluon antenna functions $\mathcal{F}$, $\mathcal{G}$ and $\mathcal{H}$ have been derived [57] from the decay process $H \to gg$ at NLO and NNLO, in the effective theory where the Higgs couples directly to gluons, which is valid in the limit of infinitely massive quarks. The second-order coefficient functions for the one-hadron inclusive Higgs decay in such an effective theory were first obtained in [14]. Here we are in the position to compare suitable combinations of integrated antenna functions against the results of [14], in a very similar way to what we have done in section 6.1 for the $\gamma^*/Z \to q\bar{q}$ decay.

Since the Higgs boson is a scalar, the parton fragmentation functions have only one component, $\hat{\mathcal{T}}_i$, where a quark ($i = q$) or a gluon ($i = g$) is identified. $\hat{\mathcal{T}}_i$ admits an expansion similar to (6.3),

$$\hat{\mathcal{T}}_i = \hat{\mathcal{T}}_i^{(0)} + \left(\frac{\alpha_s}{4\pi}\right)\left(\frac{\mu_R^2}{Q^2}\right)^{\epsilon}\hat{\mathcal{T}}_i^{(1)} + \left(\frac{\alpha_s}{4\pi}\right)^2\left(\frac{\mu_R^2}{Q^2}\right)^{2\epsilon}\hat{\mathcal{T}}_i^{(2)} + \mathcal{O}\left(\alpha_s^3\right), \tag{6.18}$$

where we choose to adopt an expansion in terms of the renormalised coupling constant α_s, with μ_R^2 the renormalisation scale, for ease of comparison against [14]. The normalisation is such that

$$\hat{\mathcal{T}}_q^{(0)} = 0\,, \qquad \hat{\mathcal{T}}_g^{(0)} = \delta(1-z)\,. \tag{6.19}$$

At NLO we find the following relationships:

$$\frac{1}{T_F}\hat{\mathcal{T}}_q^{(1)} = 8\,\mathcal{G}_3^{0,\mathrm{id}.q}\,, \tag{6.20}$$

$$\hat{\mathcal{T}}_g^{(1)}|_N = 2\,\mathcal{F}_3^{0,\mathrm{id}.g} + 4\,\delta(1-z)V_g^{(1)}|_N\,, \tag{6.21}$$

$$\hat{\mathcal{T}}_g^{(1)}|_{N_F} = 2\,\mathcal{G}_3^{0,\mathrm{id}.g} + 4\,\delta(1-z)V_g^{(1)}|_{N_F}\,, \tag{6.22}$$

whereas at NNLO we obtain

$$\frac{1}{T_F}\hat{\mathcal{T}}_q^{(2)}|_N = 4\,\mathcal{G}_4^{0,\mathrm{id}.q} + 16\,\mathcal{G}_3^{1R,\mathrm{id}.q}\,, \tag{6.23}$$

$$\frac{1}{T_F}\hat{\mathcal{T}}_q^{(2)}|_{1/N} = -2\,\tilde{\mathcal{G}}_4^{0,\mathrm{id}.q} - 16\,\tilde{\mathcal{G}}_3^{1R,\mathrm{id}.q} + 4\tilde{\mathcal{J}}_4^{0,\mathrm{id}.q}\,, \tag{6.24}$$

$$\frac{1}{T_F}\hat{\mathcal{T}}_q^{(2)}|_{N_F} = 4\,\mathcal{H}_4^{0,\mathrm{id}.q} + 16\,\hat{\mathcal{G}}_3^{1R,\mathrm{id}.q}\,, \tag{6.25}$$

for the quark fragmentation function and

$$\hat{\mathcal{T}}_g^{(2)}|_{N^2} = \mathcal{F}_4^{0,\mathrm{id}.g} + 4\,\mathcal{F}_3^{1R,\mathrm{id}.g} + 4\,\delta(1-z)V_g^{(2)}|_{N^2}\,, \tag{6.26}$$

$$\hat{\mathcal{T}}_g^{(2)}|_{NN_F} = 2\,\mathcal{G}_4^{0,\mathrm{id}.g} + 4\,\mathcal{G}_3^{1R,\mathrm{id}.g} + 4\,\hat{\mathcal{F}}_3^{1R,\mathrm{id}.g} + 4\,\delta(1-z)V_g^{(2)}|_{NN_F}\,, \tag{6.27}$$

$$\hat{\mathcal{T}}_g^{(2)}|_{N_F/N} = -\tilde{\mathcal{G}}_4^{0,\mathrm{id}.g} - 4\,\tilde{\mathcal{G}}_3^{1R,\mathrm{id}.g} + 4\,\delta(1-z)V_g^{(2)}|_{N_F/N}\,, \tag{6.28}$$

$$\hat{\mathcal{T}}_g^{(2)}|_{N_F^2} = 4\,\hat{\mathcal{G}}_3^{1R,\mathrm{id}.g} + 4\,\delta(1-z)V_g^{(2)}|_{N_F^2}\,, \tag{6.29}$$

for the gluon fragmentation function, respectively. The superscript R denotes the renormalised one-loop squared matrix elements, i.e. the integrated one-loop three-particle antenna

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functions before the subtraction of the integrated tree-level antenna function multiplied with the virtual one-loop correction to the hard radiator vertex, see section 5.3. $V_g^{(1)}$ and $V_g^{(2)}$ are related to the gluon form factor, and they are defined in full analogy with the quark case (see (6.15) and (6.16), respectively). Finally, the antenna function $\tilde{\mathcal{J}}_4^{0,\text{id}.q}$, which appears in (6.24), comes from the infrared-finite interference of four quark final states with identical quark flavour (see [59]). Its expression is:

$$\tilde{\mathcal{J}}_4^{0,\text{id}.q} = \left(-\frac{9}{4} + \frac{7}{2}z - \frac{7}{2}z^2 + \left(2 - 4z + 4z^2\right)\zeta_3\right) + \mathcal{O}(\epsilon)\,. \tag{6.30}$$

As it is finite in all limits, it does not appear in table 1.

Eqs. (6.20)–(6.29) are in full agreement with the results of [14] at NLO and NNLO at all colour levels.

7 Infrared structure of $e^+e^- \to 3$ jets with fragmentation at NLO

As an example of the formalism, in this section we present explicit expressions for the antenna subtraction terms for one identified hadron in the $e^+e^- \to 3$ jets process, as studied by OPAL [35], at NLO. We keep the notation as close as possible to [62], where the subtraction terms for the $e^+e^- \to 3$ jets process without fragmentation can be found.

The short-distance cross sections with one identified parton $p = q, g, \bar{q}$ for three-jet production at the leading order are given by:

$$\mathrm{d}\hat{\sigma}_q^{\mathrm{B}} = N_3\,\mathrm{d}\Phi_3\left(p_1,p_2,p_3;\mathcal{Q}\right)\,A_3^0\left(1_q^{\text{id.}},3_g,2_{\bar{q}}\right)\,J_3^{(3)}\left(\{p_1,p_2,p_3\}\,;\eta p_1\right)\,, \tag{7.1}$$

$$\mathrm{d}\hat{\sigma}_{\bar{q}}^{\mathrm{B}} = N_3\,\mathrm{d}\Phi_3\left(p_1,p_2,p_3;\mathcal{Q}\right)\,A_3^0\left(1_q,3_g,2_{\bar{q}}^{\text{id.}}\right)\,J_3^{(3)}\left(\{p_1,p_2,p_3\}\,;\eta p_2\right)\,, \tag{7.2}$$

$$\mathrm{d}\hat{\sigma}_g^{\mathrm{B}} = N_3\,\mathrm{d}\Phi_3\left(p_1,p_2,p_3;\mathcal{Q}\right)\,A_3^0\left(1_q,3_g^{\text{id.}},2_{\bar{q}}\right)\,J_3^{(3)}(\{p_1,p_2,p_3\};\eta p_3)\,, \tag{7.3}$$

with N_3 a normalisation factor and A_3^0 the tree-level matrix element squared (which coincides with the antenna function denoted with the same symbol). For ease of readability, we denote the identified particle with a superscript (id.), even though it is also indicated explicitly as argument in the jet function. We consider the NLO corrections to eqs. (7.1)–(7.3) by assuming the flavour of q as fixed. New quark flavours appearing at NLO are denoted as q', by also allowing for the possibility $q = q'$. At the end we can get the full NLO cross section for $e^+e^- \to 3$ jets by summing over all possible tree-level quark flavours.

7.1 Real level

At NLO, we can have three different four-parton final states: $q\bar{q}gg$, $q\bar{q}q'\bar{q}'$ (non-identical quarks) and $q\bar{q}q\bar{q}$ (identical quarks). The four-parton real radiation contribution to the

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NLO cross section when the quark q is identified is

$$\begin{aligned}
\mathrm{d}\hat{\sigma}_q^R = \Bigg\{ \Bigg[\frac{N}{2} \Big(& A_4^0\left(1_q^{\mathrm{id.}}, 3_g, 4_g, 2_{\bar{q}}\right) + A_4^0\left(1_q^{\mathrm{id.}}, 4_g, 3_g, 2_{\bar{q}}\right)\Big) \\
& - \frac{1}{2N}\tilde{A}_4^0\left(1_q^{\mathrm{id.}}, 3_g, 4_g, 2_{\bar{q}}\right) + N_F B_4^0\left(1_q^{\mathrm{id.}}, 3_{q'}, 4_{\bar{q}'}, 2_{\bar{q}}\right) \\
& - \frac{1}{N}\left(C_4^0\left(1_q^{\mathrm{id.}}, 3_q, 4_{\bar{q}}, 2_{\bar{q}}\right) + C_4^0\left(2_{\bar{q}}, 4_{\bar{q}}, 3_q, 1_q^{\mathrm{id.}}\right)\right)\Bigg] J_3^{(4)}(\{p_1,\ldots,p_4\};\eta p_1) \\
& + \left[B_4^0\left(1_q, 3_q^{\mathrm{id.}}, 4_{\bar{q}}, 2_{\bar{q}}\right) - \frac{1}{N}\left(C_4^0\left(1_q, 3_q^{\mathrm{id.}}, 4_{\bar{q}}, 2_{\bar{q}}\right) + C_4^0\left(2_{\bar{q}}, 4_{\bar{q}}, 3_q^{\mathrm{id.}}, 1_q\right)\right)\right] \\
& \times J_3^{(4)}\left(\{p_1,\ldots,p_4\};\eta p_3\right)\Bigg\} N_4\,\mathrm{d}\Phi_4(p_1,\ldots,p_4;\mathcal{Q}) \,,
\end{aligned} \tag{7.4}$$

whereas the contribution when q' is identified is given by

$$\mathrm{d}\hat{\sigma}_{q'}^R = \left\{B_4^0\left(1_q, 3_{q'}^{\mathrm{id.}}, 4_{\bar{q}'}, 2_{\bar{q}}\right) J_3^{(4)}\left(\{p_1,\ldots,p_4\};\eta p_3\right)\right\} N_4\,\mathrm{d}\Phi_4\left(p_1,\ldots,p_4;\mathcal{Q}\right) . \tag{7.5}$$

The contributions when the anti-quark $\bar{q}$ or $\bar{q}'$ are identified are similar to (7.4) and (7.5), respectively. Finally, the contribution with a gluon identified reads

$$\begin{aligned}
\mathrm{d}\hat{\sigma}_g^R = \Bigg\{ \sum_{(i,j)\in P(3,4)} & \left[\frac{N}{2}\left(A_4^0\left(1_q, i_g^{\mathrm{id.}}, j_g, 2_{\bar{q}}\right) + A_4^0\left(1_q, j_g, i_g^{\mathrm{id.}}, 2_{\bar{q}}\right)\right) - \frac{1}{2N}\tilde{A}_4^0\left(1_q, i_g^{\mathrm{id.}}, j_g, 2_{\bar{q}}\right)\right] \\
& \times J_3^{(4)}\left(\{p_1,\ldots,p_4\};\eta p_i\right)\Bigg\} N_4\,\mathrm{d}\Phi_4\left(p_1,\ldots,p_4;\mathcal{Q}\right) .
\end{aligned} \tag{7.6}$$

The subtraction terms for the contribution when the quark q is identified reads

$$\mathrm{d}\hat{\sigma}_q^S = \mathrm{d}\hat{\sigma}_{q(q)}^S + \mathrm{d}\hat{\sigma}_{g(q)}^S \,, \tag{7.7}$$

where in the subtraction term $\mathrm{d}\hat{\sigma}_{q(q)}^S$ the mapped particle in the reduced matrix element has the same flavour as the identified particle, whereas in the subtraction term $\mathrm{d}\hat{\sigma}_{g(q)}^S$ the flavour of the parton in the reduced matrix element is different from the flavour of the particle in the antenna, called identity changing (IC) term. Explicit expressions for the two

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subtraction terms are

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q(q)} = & N_4\,\mathrm{d}\Phi_4(p_1,\dots,p_4;\mathcal{Q}) \\
& \times \Bigg\{ \sum_{(i,j)\in P(3,4)} \Bigg[\frac{N}{2}\, d_3^0\left(1_q^{\text{id.}}, i_g, j_g\right) A_3^0\left(\widetilde{1}_q, \widetilde{(ij)}_g, 2_{\bar{q}}\right) J_3^{(3)}(\{\widetilde{1}_q, \widetilde{(ij)}_g, 2_{\bar{q}}\};\eta p_1) \\
& \qquad + \frac{N}{2}\, d_3^0\left(2_{\bar{q}}, i_g, j_g\right) A_3^0\left(1_q^{\text{id.}}, \widetilde{(ji)}_g, \widetilde{(2i)}_{\bar{q}}\right) J_3^{(3)}\left(\left\{1_q, \widetilde{(ji)}_g, \widetilde{(2i)}_{\bar{q}}\right\};\eta p_1\right) \\
& \qquad - \frac{1}{2N}\, A_3^0\left(1_q^{\text{id.}}, i_g, 2_{\bar{q}}\right) A_3^0\left(\widetilde{1}_q, j_g, \widetilde{(2i)}_{\bar{q}}\right) J_3^{(3)}\left(\{\widetilde{1}_q, j_g, \widetilde{(2i)}_{\bar{q}}\};\eta p_1\right) \Bigg] \\
& + N_F \Bigg[E_3^0\left(1_q^{\text{id.}}, 3_{q'}, 4_{\bar{q}'}\right) A_3^0\left(\widetilde{1}_q, \widetilde{(34)}_g, 2_{\bar{q}}\right) J_3^{(3)}(\{\widetilde{1}_q, \widetilde{(34)}_g, 2_{\bar{q}}\};\eta p_1) \\
& \qquad + E_3^0\left(2_{\bar{q}}, 3_{q'}, 4_{\bar{q}'}\right) A_3^0\left(1_q^{\text{id.}}, \widetilde{(34)}_g, \widetilde{(24)}_{\bar{q}}\right) J_3^{(3)}\left(\left\{1_q, \widetilde{(34)}_g, \widetilde{(24)}_{\bar{q}}\right\};\eta p_1\right) \Bigg] \Bigg\},
\end{aligned} \tag{7.8}$$

and

$$\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{g(q)} = & N_4\,\mathrm{d}\Phi_4\left(p_1,\dots,p_4;\mathcal{Q}\right) \\
& \times \left[E_3^0\left(1_q, 3_q^{\text{id.}}, 4_{\bar{q}}\right) A_3^0\left(\widetilde{(14)}_q, \widetilde{3}_g, 2_{\bar{q}}\right) J_3^{(3)}\left(\left\{\widetilde{(14)}_q, \widetilde{3}_g, 2_{\bar{q}}\right\};\eta p_3\right)\right].
\end{aligned} \tag{7.9}$$

In eqs. (7.8)–(7.9) we have denoted the mapped momenta in the reduced matrix element in two different ways, according to the type of mapping we are applying. Given three particles i,j and k, when none of them is undergoing fragmentation, we adopt the standard NLO final-final mapping, indicated as $\widetilde{(ij)}$ and $\widetilde{(jk)}$ e.g. in the second line of (7.8); when one of them is fragmenting, say i, we use the NLO fragmentation mapping of (3.6), indicated as $\widetilde{i}$ and $\widetilde{(jk)}$ e.g. in the first line of (7.8). The subtraction terms for the contribution when the quark q' is purely identity-changing (since there is no q' at the Born level), and has the same structure as (7.9):

$$\begin{aligned}
\mathrm{d}\hat{\sigma}_{q'} \equiv \mathrm{d}\hat{\sigma}^S_{g(q')} = & N_4\,\mathrm{d}\Phi_4(p_1,\dots,p_4;\mathcal{Q}) \\
& \times \left[E_3^0\left(1_q, 3_{q'}^{\text{id.}}, 4_{\bar{q}'}\right) A_3^0\left(\widetilde{(14)}_q, \widetilde{3}_g, 2_{\bar{q}}\right) J_3^{(3)}\left(\left\{\widetilde{(14)}_q, \widetilde{3}_g, 2_{\bar{q}}\right\};\eta p_3\right)\right].
\end{aligned} \tag{7.10}$$

Notice that, since the antenna function E_3^0 contains only the $3 \parallel 4$ collinear limit, we are free to choose as third momentum in the antenna either the particle 1 or 2.

Finally, the subtraction term for the contribution where the gluon is identified is given by the sum of three contributions

$$\mathrm{d}\hat{\sigma}^S_g = \mathrm{d}\hat{\sigma}^S_{g(g)} + \mathrm{d}\hat{\sigma}^S_{q(g)} + \mathrm{d}\hat{\sigma}^S_{\bar{q}(g)}\,, \tag{7.11}$$

where

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{g(g)} = {} & N_4\,\mathrm{d}\Phi_4(p_1,\ldots,p_4;\mathcal{Q}) \\
& \times \sum_{(i,j)\in P(3,4)} \Bigg\{ \frac{N}{2}\, d^0_{3,g\to g}\left(1_q, j_g, i_g^{\mathrm{id.}}\right) A^0_3\left(\widetilde{(1j)}_q, \widetilde{i}_g, 2_{\bar q}\right) J_3^{(3)}\left(\left\{\widetilde{(1j)}_q, \widetilde{i}_g, 2_{\bar q}\right\}; \eta p_i\right) \\
& \qquad + \frac{N}{2}\, d^0_{3,g\to g}\left(2_{\bar q}, j_g, i_g^{\mathrm{id.}}\right) A^0_3\left(1_q, \widetilde{i}_g, \widetilde{(2j)}_{\bar q}\right) J_3^{(3)}\left(\left\{1_q, \widetilde{i}_g, \widetilde{(2j)}_{\bar q}\right\}; \eta p_i\right) \\
& \qquad - \frac{1}{2N} A^0_3(1_q, j_g, 2_{\bar q})\, A^0_3\left(\widetilde{(1j)}_q, i_g^{\mathrm{id.}}, \widetilde{(2j)}_{\bar q}\right) J_3^{(3)}\left(\left\{\widetilde{(1j)}_q, i_g, \widetilde{(2j)}_{\bar q}\right\}; \eta p_i\right) \Bigg]\Bigg\},
\end{aligned}
\tag{7.12}
$$

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{q(g)} = {} & N_4\,\mathrm{d}\Phi_4(p_1,\ldots,p_4;\mathcal{Q}) \\
& \times \sum_{(i,j)\in P(3,4)} \Bigg\{ \frac{N}{2}\, d^0_{3,q\to g}\left(1_q, i_g^{\mathrm{id.}}, j_g\right) A^0_3\left(\widetilde{i}_q, \widetilde{(1j)}_g, 2_{\bar q}\right) J_3^{(3)}\left(\left\{\widetilde{i}_q, \widetilde{(1j)}_g, 2_{\bar q}\right\}; \eta p_i\right) \\
& \qquad - \frac{1}{2N}\, d^0_{3,q\to g}\left(1_q, i_g^{\mathrm{id.}}, j_g\right) \tilde{A}^0_3\left(\widetilde{i}_q, \widetilde{(1j)}_g, 2_{\bar q}\right) J_3^{(3)}\left(\left\{\widetilde{i}_q, \widetilde{(1j)}_g, 2_{\bar q}\right\}; \eta p_i\right) \Bigg]\Bigg\},
\end{aligned}
\tag{7.13}
$$

and

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^S_{\bar q(g)} = {} & N_4\,\mathrm{d}\Phi_4(p_1,\ldots,p_4;\mathcal{Q}) \\
& \times \sum_{(i,j)\in P(3,4)} \Bigg\{ \frac{N}{2}\, d^0_{3,q\to g}\left(2_{\bar q}, i_g^{\mathrm{id.}}, j_g\right) A^0_3\left(1_q, \widetilde{(2j)}_g, \widetilde{i}_{\bar q}\right) J_3^{(3)}\left(\left\{1_q, \widetilde{(2j)}_g, \widetilde{i}_{\bar q}\right\}; \eta p_i\right) \\
& \qquad - \frac{1}{2N}\, d^0_{3,q\to g}\left(2_{\bar q}, i_g^{\mathrm{id.}}, j_g\right) \tilde{A}^0_3\left(1_q, \widetilde{(2j)}_g, \widetilde{i}_{\bar q}\right) J_3^{(3)}\left(\left\{1_q, \widetilde{(2j)}_g, \widetilde{i}_{\bar q}\right\}; \eta p_i\right) \Bigg]\Bigg\}.
\end{aligned}
\tag{7.14}
$$

Note that in eqs. (7.13)–(7.14), in order to remove the quark-gluon collinear divergence in the photon-like matrix element $\tilde{A}^0_4$, we have used the sub-antenna $d^0_{3,q\to g}(k_q, i_g^{\mathrm{id.}}, j_j)$, which contains only the collinear limit $i \parallel k$ (see comment after (B.9)).

7.2 Virtual level

The virtual one-loop contribution to $\gamma^* \to q\bar{q}g$ is

$$
\begin{aligned}
\mathrm{d}\hat{\sigma}^V = {} & N_3\,\mathrm{d}\Phi_3\left(p_1,\ldots,p_3;\mathcal{Q}\right) J_3^{(3)}(p_1,p_2,p_3) \\
& \times \Bigg(N\left[A^1_3(1_q,3_g,2_{\bar q}) + \mathcal{A}^1_2(s_{123}) A^0_3(1_q,3_g,2_{\bar q})\right] \\
& \qquad - \frac{1}{N}\left[\tilde{A}^1_3(1_q,3_g,2_{\bar q}) + \mathcal{A}^1_2(s_{123}) A^0_3(1_q,3_g,2_{\bar q})\right] + N_F \hat{A}^1_3(1_q,3_g,2_{\bar q}) \Bigg),
\end{aligned}
\tag{7.15}
$$

where any of the three particles can be identified, thus generating the three terms $\mathrm{d}\hat{\sigma}^V_q$, $\mathrm{d}\hat{\sigma}^V_{\bar q}$ and $\mathrm{d}\hat{\sigma}^V_g$. The infrared behaviour of the virtual matrix elements reads

$$
\mathrm{Poles}\left(A^1_3\left(1_q,3_g,2_{\bar q}\right)\right) = 2\left(\mathbf{I}^{(1)}_{qg}\left(\epsilon,s_{13}\right) + \mathbf{I}^{(1)}_{qg}\left(\epsilon,s_{23}\right) - \mathbf{I}^{(1)}_{q\bar q}\left(\epsilon,s_{123}\right)\right) A^0_3\left(1,3,2\right), \tag{7.16}
$$

$$\text{Poles}\left(\tilde{A}_3^1\left(1_q,3_g,2_{\bar{q}}\right)\right)=2\left(\mathbf{I}_{q\bar{q}}^{(1)}\left(\epsilon,s_{12}\right)-\mathbf{I}_{q\bar{q}}^{(1)}\left(\epsilon,s_{123}\right)\right)A_3^0\left(1,3,2\right)\,, \tag{7.17}$$

$$\text{Poles}\left(\hat{A}_3^1\left(1_q,3_g,2_{\bar{q}}\right)\right)=2\left(\mathbf{I}_{qg,F}^{(1)}\left(\epsilon,s_{13}\right)+\mathbf{I}_{qg,F}^{(1)}\left(\epsilon,s_{23}\right)\right)A_3^0\left(1,3,2\right)\,, \tag{7.18}$$

$$\text{Poles}\left(\mathcal{A}_2^1\left(s_{123}\right)\right)=2\mathbf{I}_{q\bar{q}}^{(1)}\left(\epsilon,s_{123}\right)\,, \tag{7.19}$$

where $\mathbf{I}_{xy}^{(1)}$ are the colour-ordered singularity operators, whose expressions are reported in eqs. (B.1)–(B.6). The integral of the subtraction term $\mathrm{d}\hat{\sigma}_q^{\mathrm{S}}$ reads:

$$\begin{aligned}\int_1 \mathrm{d}\hat{\sigma}_{q(q)}^{S} =&\; N_3\,\mathrm{d}\Phi_3\left(p_1,\ldots,p_3;Q\right)\,J_3^{(3)}\left(\left\{p_1,p_2,p_3\right\};\eta p_1\right)\\ &\times\Bigg[N\left(\frac{1}{2}\mathcal{D}_3^{0,\mathrm{id}.q}\left(s_{13},z\right)+\frac{1}{2}\mathcal{D}_3^{0}\left(s_{23}\right)\right)-\frac{1}{N}\mathcal{A}_3^{0,\mathrm{id}.q}\left(s_{12},z\right)\\ &+N_F\left(\mathcal{E}_3^{0,\mathrm{id}.q}\left(s_{13},z\right)+\mathcal{E}_3^{0}\left(s_{23}\right)\right)\Bigg]A_3^0(1_q^{\mathrm{id.}},3_g,2_{\bar{q}})\,,\end{aligned} \tag{7.20}$$

$$\begin{aligned}\int_1 \mathrm{d}\hat{\sigma}_{g(q)}^{S} =&\; N_3\,\mathrm{d}\Phi_3(p_1,\ldots,p_3;Q)\,J_3^{(3)}(\{p_1,p_2,p_3\};\eta p_3)\\ &\times\mathcal{E}_3^{0,\mathrm{id}.q'}(s_{13},z)A_3^0(1_q,3_g^{\mathrm{id.}},2_{\bar{q}})\,,\end{aligned} \tag{7.21}$$

where in (7.20) we need the integral of the inclusive sub-antenna d_3^0, which is given by one-half the integral $\mathcal{D}_3^0$ of the full inclusive antenna D_3^0. The integral of the subtraction term $\mathrm{d}\hat{\sigma}_g^{\mathrm{S}}$ reads:

$$\begin{aligned}\int_1 \mathrm{d}\hat{\sigma}_{g(g)}^{S} =&\; N_3\,\mathrm{d}\Phi_3\left(p_1,\ldots,p_3;Q\right)\,J_3^{(3)}\left(\left\{p_1,p_2,p_3\right\};\eta p_3\right)\\ &\times\left\{N\left[\left(\mathcal{D}_{3,g\to g}^{0,\mathrm{id}.g}\left(s_{13},z\right)+\mathcal{D}_{3,g\to g}^{0,\mathrm{id}.g}\left(s_{23},z\right)\right)\right]-\frac{1}{N}\left[\mathcal{A}_3^0\left(s_{12}\right)\right]\right\}A_3^0\left(1_q,3_g^{\mathrm{id.}},2_{\bar{q}}\right)\,,\end{aligned} \tag{7.22}$$

$$\begin{aligned}\int_1 \mathrm{d}\hat{\sigma}_{q(g)}^{S} =&\; N_3\,\mathrm{d}\Phi_3\left(p_1,\ldots,p_3;Q\right)\,J_3^{(3)}\left(\left\{p_1,p_2,p_3\right\};\eta p_1\right)\\ &\times\left\{N\left[\mathcal{D}_{3,q\to g}^{0,\mathrm{id}.g}\left(s_{13},z\right)\right]-\frac{1}{N}\left[\mathcal{D}_{3,q\to g}^{0,\mathrm{id}.g}\left(s_{13},z\right)\right]\right\}A_3^0\left(1_q^{\mathrm{id.}},3_g,2_{\bar{q}}\right)\,.\end{aligned} \tag{7.23}$$

The integral of $\mathrm{d}\hat{\sigma}_{\bar{q}(g)}^{S}$ is given by (7.23) with $1\leftrightarrow 2$. Finally the integral of $\mathrm{d}\hat{\sigma}_{g(q')}^{S}$ is

$$\int_1 \mathrm{d}\hat{\sigma}_{g(q')}^{S}=\int_1 \mathrm{d}\hat{\sigma}_{g(q)}^{S}\,. \tag{7.24}$$

Given the pole structure of the fully integrated antenna functions [43],

$$\text{Poles}\left(\mathcal{D}_3^0\left(q^2\right)\right)=-4\mathbf{I}_{qg}^{(1)}\left(\epsilon,q^2\right)\,, \tag{7.25}$$

$$\text{Poles}\left(\mathcal{A}_3^0\left(q^2\right)\right)=-2\mathbf{I}_{q\bar{q}}^{(1)}\left(\epsilon,q^2\right)\,, \tag{7.26}$$

$$\text{Poles}\left(\mathcal{E}_3^0\left(q^2\right)\right)=-4\mathbf{I}_{qg,F}^{(1)}(\epsilon,q^2)\,, \tag{7.27}$$

and the explicit expressions of the integrated fragmentation antenna functions $\mathcal{X}_3^{0,\mathrm{id}.p}$ provided in appendix B, we see that most of the poles cancel, except the ones proportional to splitting functions, which are removed by means of the mass factorisation counterterms, such that

$$\text{Poles}\left(\mathrm{d}\hat{\sigma}_g^V + \int_1 \mathrm{d}\hat{\sigma}_g^S + \mathrm{d}\hat{\sigma}_g^{\mathrm{MF}}\right) = 0\,, \tag{7.28}$$

$$\text{Poles}\left(\mathrm{d}\hat{\sigma}_q^V + \int_1 \mathrm{d}\hat{\sigma}_q^S + \mathrm{d}\hat{\sigma}_q^{\mathrm{MF}}\right) = 0\,, \tag{7.29}$$

$$\text{Poles}\left(\int_1 \mathrm{d}\hat{\sigma}_{q'}^S + \mathrm{d}\hat{\sigma}_{q'}^{\mathrm{MF}}\right) = 0\,, \tag{7.30}$$

thus yielding an infrared-finite result. Moreover, note that there is a one-to-one correspondence between $\int \mathrm{d}\hat{\sigma}_{i(j)}$ and $\mathbf{\Gamma}^{(1)}_{j\leftarrow i}$ inside $\mathrm{d}\hat{\sigma}_j^{\mathrm{MF}}$, in the sense that the poles proportional to splitting kernels in the former are explicitly removed by the latter. In particular, the integral of IC subtraction terms such as $\mathrm{d}\hat{\sigma}^S_{g(q')}$ does not have a corresponding virtual contributions and its infrared poles are removed entirely by the mass factorisation term.

It is instructive to look explicitly at the poles of (7.28), before adding the mass factorisation term:

$$\begin{aligned}
&\text{Poles}\left(\mathrm{d}\hat{\sigma}_g^V + \int_1 \mathrm{d}\hat{\sigma}_g^S\right) \\
&= N_3 \int \mathrm{d}z\, N\Bigg\{\left[(s_{13})^{-\epsilon} + (s_{23})^{-\epsilon}\right]\left(-\frac{1}{2\epsilon}p_{gg}^{(0)}(z)\right)\mathrm{d}\hat{\sigma}_g^{\mathrm{B}}(\eta z) \\
&\qquad + (s_{13})^{-\epsilon}\left(-\frac{1}{2\epsilon}p_{gq}^{(0)}(z)\right)\mathrm{d}\hat{\sigma}_q^{\mathrm{B}}(\eta z) + (s_{23})^{-\epsilon}\left(-\frac{1}{2\epsilon}p_{gq}^{(0)}(z)\right)\mathrm{d}\hat{\sigma}_{\bar{q}}^{\mathrm{B}}(\eta z)\Bigg\} \\
&\quad - \frac{1}{N}\left\{(s_{13})^{-\epsilon}\left(-\frac{1}{2\epsilon}p_{gq}^{(0)}(z)\right)\mathrm{d}\hat{\sigma}_q^{\mathrm{B}}(\eta z) + (s_{23})^{-\epsilon}\left(-\frac{1}{2\epsilon}p_{gq}^{(0)}(z)\right)\mathrm{d}\hat{\sigma}_{\bar{q}}^{\mathrm{B}}(\eta z)\right\} \\
&\quad + N_F\left\{\left[\Re(-s_{13})^{-\epsilon} + \Re(-s_{23})^{-\epsilon}\right]\frac{1}{6\epsilon}\mathrm{d}\hat{\sigma}_g^{\mathrm{B}}(\eta z)\right\}
\end{aligned} \tag{7.31}$$

The last line contains the pole coming from $\hat{A}_3^1$, whose singularity structure (7.18) is given by twice the infrared operator $\mathbf{I}^{(1)}_{gg,F}$ (B.5). Since there is no term coming from the integral of $\mathrm{d}\hat{\sigma}_g^S$ proportional to N_F, such a pole is entirely canceled by $\Gamma^{(1)}_{gg,F}$. Note that the ϵ-poles in (7.31) appear together with different invariants raised to the $(-\epsilon)$ power i.e. differing by $\mathcal{O}(\epsilon)$, thus allowing for a cancellation of the poles, by leaving the usual logarithms of ratio of scales as leftover when $\epsilon \to 0$.

8 Conclusions

In this paper, we have described how identified final-state hadrons can be incorporated in the antenna subtraction formalism for NNLO calculations, which required the introduction of fragmentation antenna functions. These functions retain the information on a final-state parton momentum fraction, in contrast to previously considered antenna functions that were inclusive in the final state parton momenta.

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In the description of the formalism, we focused on identified hadron production processes in generic hadronic final states in e^+e^- annihilation. This restriction is largely for notational simplicity. The structure of the formalism, which amounts to the introduction of new subtraction terms for all unresolved configurations that involve the parton that subsequently fragments into the identified hadron, carries over to electron-hadron and hadron-hadron collisions, as already demonstrated for identified photons [51] at hadron colliders.

We have outlined the structure of the subtraction terms that are newly required for unresolved configurations involving an identified final-state parton. In e^+e^- annihilation, these are constructed from antenna functions with both radiator partons in the final state (final-final kinematics). We introduced suitable phase space factorisations and mappings at NLO and NNLO, which retained the dependence on the momentum fraction z of the fragmenting parton. The relevant antenna functions have been integrated over the factorised phase space by leaving z unintegrated, in order to combine with mass factorisation terms at the virtual, real-virtual and double-virtual level. Since the antenna functions are related to physical matrix elements [55–57], we have been able to check our integrated results against known expressions in the literature for single-inclusive coefficient functions in vector boson and Higgs decay.

The integrated antenna functions are inclusive over unresolved radiation, but in the context of a subtraction scheme they can be used as local subtraction terms for more *exclusive* calculations. For instance, a NNLO calculation of the hadron-in-jet fragmentation process in three-jet final states in e^+e^- annihilation, whose NLO subtraction structure has been detailed in section 7, could be envisaged. Experimental data differential in $x_E = E_h/E_{\text{jet}}$, where E_h is the energy of the hadron h and E_{jet} is the energy of the jet to which it is assigned, have been published, see e.g. [35]. In the latter paper, the experimental data are compared with NLO calculations, and they fail to describe the full set of results; a re-analysis of such e^+e^- data at NNLO accuracy would thus be warranted. Moreover, the hadron-in-jet data have been proven to provide valuable constraints on fragmentation functions [36, 37].

The fragmentation antenna functions in final-final kinematics derived here will also appear in the construction of subtraction terms for processes with identified hadrons in deep-inelastic scattering or at hadron colliders. In these cases, one (but not two) of the hard radiators can be in the initial state. The resulting fragmentation antenna functions in initial-final kinematics were already derived in parts in the context of photon fragmentation up to NNLO [51], their completion for all parton combinations will be addressed in future work.

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A Time-like mass factorisation kernels

Before factorisation of final-state mass singularities, the physical cross section is written as the convolution of a *bare* fragmentation function with the short-distance cross section still containing final-state collinear divergences: symbolically,

$$\mathrm{d}\hat{\sigma} = D_i^B \otimes \mathrm{d}\hat{\sigma}_i^B\,. \tag{A.1}$$

The bare fragmentation function is related to the physical mass-factorised fragmentation function by means of

$$D_i^B\left(z,\mu_a^2\right) = \sum_j D_j\left(z\right) \otimes \mathbf{\Gamma}_{j\leftarrow i}\left(z,\mu_a^2\right)\,, \tag{A.2}$$

where $\mathbf{\Gamma}_{j\leftarrow i}$ are the mass factorisation kernels, with a bold letter to indicate that they carry colour factors, and μ_a^2 is the fragmentation scale. The replacement $D_i^B \to D_i$ in (A.1) generates the mass factorisation terms which are added to the short-distance cross section. Symbolically, we then have:

$$D_i^B \otimes \mathrm{d}\hat{\sigma}_i^B = D_i\left(\mu_a^2\right) \otimes \mathrm{d}\hat{\sigma}_i\left(\mu_a^2\right)\,, \tag{A.3}$$

where now on the right hand side each term retains a dependence on μ_a^2, and

$$\mathrm{d}\hat{\sigma}_i\left(z,\mu_a^2\right) = \left(\mathrm{d}\hat{\sigma}_i\left(z\right) + \left(\frac{\alpha_s}{2\pi}\right)\mathrm{d}\hat{\sigma}_i^{\mathrm{MF,NLO}}\left(z,\mu_a^2\right) + \left(\frac{\alpha_s}{2\pi}\right)^2\mathrm{d}\hat{\sigma}_i^{\mathrm{MF,NNLO}}\left(z,\mu_a^2\right)\right)\,. \tag{A.4}$$

The mass factorisation terms are obtained after an expansion of (A.2), and they read

$$\mathrm{d}\hat{\sigma}_i^{\mathrm{MF,NLO}} = -\overline{C}\left(\epsilon\right)\left(\mu_a^2\right)^{-\epsilon}\sum_j \mathbf{\Gamma}^{(1)}_{i\leftarrow j} \otimes \mathrm{d}\hat{\sigma}_j^{\mathrm{LO}}\,, \tag{A.5}$$

and

$$\mathrm{d}\hat{\sigma}_i^{\mathrm{MF,NNLO}} = -\overline{C}\left(\epsilon\right)^2\left(\mu_a^2\right)^{-2\epsilon}\left[\sum_j \mathbf{\Gamma}^{(2)}_{i\leftarrow j} \otimes \mathrm{d}\hat{\sigma}_j^{\mathrm{LO}} + \sum_j \mathbf{\Gamma}^{(1)}_{i\leftarrow j} \otimes \mathrm{d}\hat{\sigma}_j^{\mathrm{NLO}}\right]\,. \tag{A.6}$$

The mass factorisation kernels are given by:

$$\mathbf{\Gamma}^{(1)}_{i\leftarrow j} = -\frac{1}{\epsilon}\,\mathbf{P}^{(0)}_{ij}\,, \tag{A.7}$$

and

$$\mathbf{\Gamma}^{(2)}_{i\leftarrow j} = -\frac{1}{2\epsilon}\mathbf{P}^{(1)}_{ij} + \frac{\beta_0}{2\epsilon^2}\,\mathbf{P}^{(0)}_{ij} + \frac{1}{2\epsilon^2}\left[\mathbf{P}^{(0)}_{ik} \otimes \mathbf{P}^{(0)}_{kj}\right]\,, \tag{A.8}$$

where $\mathbf{P}^{(0)}$ and $\mathbf{P}^{(1)}$ are the leading order [6] and next-to-leading order [13, 76, 77] time-like splitting functions, respectively, whose expression can be found in many places, see e.g. [78]. Time-like splitting functions coincide with the space-like splitting functions at leading order, but they differ at higher orders.

Due to the intrinsic colour decomposition of the antenna functions, we need to decompose the splitting kernels into the N and N_F factors, in order to define colour stripped kernels to be used in the mass factorisation term, along the lines of appendix A of [44]. The one-loop mass factorisation kernels in the time-like region are the same as the ones in the space-like region and are given by:

$$\mathbf{\Gamma}^{(1)}_{q\leftarrow q}(z) = \left(\frac{N^2-1}{N}\right)\Gamma^{(1)}_{qq}(z) = \left(\frac{N^2-1}{N}\right)\left[-\frac{1}{2\epsilon}\,p^{(0)}_{qq}(z)\right], \tag{A.9}$$

$$\mathbf{\Gamma}^{(1)}_{g\leftarrow q}(z) = \left(\frac{N^2-1}{N}\right)\Gamma^{(1)}_{gq}(z) = \left(\frac{N^2-1}{N}\right)\left[-\frac{1}{2\epsilon}\,p^{(0)}_{gq}(z)\right], \tag{A.10}$$

$$\mathbf{\Gamma}^{(1)}_{q\leftarrow g}(z) = \Gamma^{(1)}_{qg}(z) = -\frac{1}{2\epsilon}\,p^{(0)}_{qg}(z), \tag{A.11}$$

$$\mathbf{\Gamma}^{(1)}_{g\leftarrow g}(z) = N\,\Gamma^{(1)}_{gg}(z) + N_F\,\Gamma^{(1)}_{gg,F}(z) = N\left[-\frac{1}{\epsilon}\,p^{(0)}_{gg}\right] + N_F\left[-\frac{1}{\epsilon}\,p^{(0)}_{gg,F}\right], \tag{A.12}$$

where we have exploited $C_F = (N^2-1)/(2N)$ and $T_R = 1/2$. The set of $p^{(0)}_{ij}$ reads:

$$p^{(0)}_{qq}(z) = \frac{3}{2}\delta(1-z) + 2\mathcal{D}_0(1-z) - 1 - z\,, \tag{A.13}$$

$$p^{(0)}_{gq}(z) = \frac{2}{z} - 2 + z\,, \tag{A.14}$$

$$p^{(0)}_{qg}(z) = 1 - 2z + 2z^2\,, \tag{A.15}$$

$$p^{(0)}_{gg}(z) = \frac{11}{6}\delta(1-z) + 2\mathcal{D}_0(1-z) + \frac{2}{z} - 4 + 2z - 2z^2\,, \tag{A.16}$$

$$p^{(0)}_{gg,F}(z) = -\frac{1}{3}\delta(1-z)\,. \tag{A.17}$$

The two-loop mass factorisation kernels can be easily assembled according to (A.8); this is a rather straightforward procedure, so we do not report here the resulting (lengthy) explicit expressions.

B Integrated NLO fragmentation antenna functions

We report here the integrated form of the X_3^0 antenna functions, differential in the momentum fraction z, as defined in (5.2). We recall the reader that the unintegrated X_3^0 antenna functions can be found in [43]. The discussion is similar to appendix B.2 of [51]. However, note that compared to [51], we do not have a reference particle and the definition of z is different (compare (5.2) with (3.10) of [51]): this results in different integrated antenna functions.

It is convenient to introduce the NLO colour-ordered singularity operators [43], which appear in the explicit expressions of the integrated antenna functions:

$$\mathbf{I}^{(1)}_{q\bar{q}}(\epsilon, s_{q\bar{q}}) = -\frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\left[\frac{1}{\epsilon^2}+\frac{3}{2\epsilon}\right]\Re(-s_{q\bar{q}})^{-\epsilon}\,, \tag{B.1}$$

$$\mathbf{I}^{(1)}_{qg}(\epsilon, s_{qg}) = -\frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\left[\frac{1}{\epsilon^2}+\frac{5}{3\epsilon}\right]\Re(-s_{qg})^{-\epsilon}\,, \tag{B.2}$$

$$\mathbf{I}^{(1)}_{gg}(\epsilon, s_{gg}) = -\frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\left[\frac{1}{\epsilon^2}+\frac{11}{6\epsilon}\right]\Re(-s_{gg})^{-\epsilon}\,, \tag{B.3}$$

$$\mathbf{I}^{(1)}_{q\bar{q},F}(\epsilon, s_{q\bar{q}}) = 0\,, \tag{B.4}$$

$$\mathbf{I}^{(1)}_{qg,F}(\epsilon, s_{qg}) = \frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\frac{1}{6\epsilon}\Re(-s_{qg})^{-\epsilon}\,, \tag{B.5}$$

$$\mathbf{I}^{(1)}_{gg,F}(\epsilon, s_{gg}) = \frac{e^{\epsilon\gamma}}{2\Gamma(1-\epsilon)}\frac{1}{3\epsilon}\Re(-s_{gg})^{-\epsilon}\,. \tag{B.6}$$

The integrated NLO fragmentation antenna functions are reported here up to finite terms in ϵ. When they are used in the context of a NNLO calculation, e.g. in the integrated form of products of tree-level three-parton antenna functions, the knowledge of terms proportional to ϵ and ϵ^2 is also required, in order to combine with the poles proportional to $1/\epsilon$ and $1/\epsilon^2$ and result in a finite contribution. Explicit expressions for the integrated $\mathcal{X}_3^{0,\mathrm{id}.p}$ antenna functions up to $\mathcal{O}(\epsilon^2)$ are provided as supplementary material attached to this paper.

At NLO, there is one quark-quark antenna function, $A_3^0(1_q, 2_g, 3_{\bar{q}})$, symmetric under exchange of the quark pair. When the quark or anti-quark is identified, we obtain

$$\begin{aligned}\mathcal{A}_3^{0,\mathrm{id}.q}\left(q^2,z\right) = &-2\mathbf{I}^{(1)}_{q\bar{q}}\left(\epsilon,q^2\right)\delta\left(1-z\right) + \left(q^2\right)^{-\epsilon}\left[-\frac{1}{2\epsilon}p^{(0)}_{qq}(z)\right.\\ &+\delta(1-z)\left(\frac{7}{4}+\frac{\pi^2}{3}\right) - \frac{3}{4}\mathcal{D}_0(1-z)+\mathcal{D}_1(1-z)\\ &\left.+\log(z)\left(\frac{1+z^2}{1-z}\right)-\frac{1}{2}\log(1-z)\left(1+z\right)+\frac{5}{4}-\frac{3}{4}z\right]+\mathcal{O}(\epsilon)\,,\end{aligned} \tag{B.7}$$

whereas when the gluon is identified we get

$$\begin{aligned}\mathcal{A}_3^{0,\mathrm{id}.g}\left(q^2,z\right) = \left(q^2\right)^{-\epsilon}&\left[-\frac{1}{\epsilon}p^{(0)}_{gq}(z)+\log(z)\left(\frac{4}{z}+2z-4\right)\right.\\ &\left.-\log(1-z)\left(-\frac{2}{z}-z+2\right)\right]+\mathcal{O}(\epsilon)\,.\end{aligned} \tag{B.8}$$

In (B.8), there is no infrared singularity operator associated to the $q\bar{q}$ vertex (as in (B.7)), because the gluon has to be resolved in order to be identified.

There are two quark-gluon antenna functions, $D_3^0(1_q, 2_g, 3_g)$ and $E_3^0(1_q, 2_{q'}, 3_{\bar{q}'})$. The D_3^0 antenna function can be written as a sum of two sub-antenna functions [58]:

$$D_3^0(1_q,2_g,3_g) = d^0_{3,q\to g}(1_q,2_g,3_g)+d^0_{3,g\to g}(1_q,3_g,2_g)\,, \tag{B.9}$$

where the sub-antenna $d^0_{3,q\to g}(1,2,3)$ contains the collinear $1 \parallel 2$ limit, but not the collinear $1 \parallel 3$ limit nor the soft 3 limit; it is very handy in subtracting one single collinear limit — see for instance its usage in the NLO subtraction terms of section 7. Instead, the sub-antenna $d^0_{3,g\to g}(1,3,2)$ is singular in s_{13} and s_{23}, but not in s_{12}. When we identify the quark, we integrate the full antenna D^0_3, to find

$$\begin{aligned}\mathcal{D}_3^{0,\mathrm{id}.q}\left(q^2,z\right) = & -4\mathbf{I}^{(1)}_{qg}\left(\epsilon,q^2\right)\delta(1-z) + (q^2)^{-\epsilon}\Bigg[-\frac{1}{\epsilon}p^{(0)}_{gq}(z) + \delta(1-z)\left(\frac{67}{18}+\frac{2\pi^2}{3}\right)\\ & -\frac{11}{6}\mathcal{D}_0(1-z) + 2\mathcal{D}_1(1-z) + \log(z)\left(-2+\frac{4}{1-z}-2z\right)\\ & -\log(1-z)(1+z) + \frac{17}{6} + \frac{5}{6}z + \frac{1}{3}z^2\Bigg] + \mathcal{O}(\epsilon)\,. \end{aligned} \tag{B.10}$$

Instead, when we identify the gluon, we integrate the sub-antenna functions introduced in (B.9). In both cases, we identify the gluon 2. If we integrate $d^0_{3,q\to g}$ we obtain

$$\begin{aligned}\mathcal{D}_{3,q\to g}^{0,\mathrm{id}.g}\left(q^2,z\right) = & \left(q^2\right)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{gq}(z) + \log(z)\left(-2+\frac{2}{z}+z\right)\\ & -\log(1-z)\left(1-\frac{1}{z}-\frac{1}{2}z\right) - z + \frac{3}{4}z^2\Bigg] + \mathcal{O}(\epsilon)\,, \end{aligned} \tag{B.11}$$

whereas if we integrate $d^0_{3,g\to g}$ we get

$$\begin{aligned}\mathcal{D}_{3,g\to g}^{0,\mathrm{id}.g}\left(q^2,z\right) = & -2\mathbf{I}^{(1)}_{qg}\left(\epsilon,q^2\right)\delta(1-z) + \left(q^2\right)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{gg}(z) + \delta(1-z)\left(\frac{7}{4}+\frac{\pi^2}{3}\right)\\ & -\frac{3}{4}\mathcal{D}_0(1-z) + \mathcal{D}_1(1-z) + \log(z)\left(-4+\frac{2}{z}+\frac{2}{1-z}+2z-2z^2\right)\\ & -\log(1-z)\left(2-\frac{1}{z}-z+z^2\right) + \frac{3}{4} + \frac{9}{4}z\Bigg] + \mathcal{O}(\epsilon)\,. \end{aligned} \tag{B.12}$$

The pattern emerging from (B.11) and (B.12) is interesting. Eq. (B.11) contains only a single pole proportional to the splitting kernel $p^{(0)}_{gq}$, related to the $q \to qg$ branching. Eq. (B.12), instead, has a richer structure, with the presence of the infrared singularity operator $\mathbf{I}^{(1)}_{qg}$ (encoding the virtual correction to a qg vertex) and the splitting kernel $p^{(0)}_{gg}$ (encoding the outgoing gluon splitting into a pair of gluons).

The other quark-gluon antenna function, $E^0_3(1_q, 2_{q'}, 3_{\bar{q}'})$, is symmetric under the exchange of q' and $\bar{q}'$. When we identify the primary quark q, we find

$$\begin{aligned}\mathcal{E}_3^{0,\mathrm{id}.q}\left(q^2,z\right) = & -4\mathbf{I}^{(1)}_{qg,F}\left(\epsilon,q^2\right)\delta(1-z) + \left(q^2\right)^{-\epsilon}\Bigg[-\frac{5}{9}\delta(1-z)\\ & +\frac{1}{3}\mathcal{D}_0(1-z) - \frac{1}{3} - \frac{1}{3}z + \frac{1}{6}z^2\Bigg] + \mathcal{O}(\epsilon)\,; \end{aligned} \tag{B.13}$$

when we identify the secondary quark q' or $\bar{q}'$, we get

$$\begin{aligned}\mathcal{E}_3^{0,\mathrm{id}.q'}\left(q^2,z\right) = & \left(q^2\right)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{qg}(z) + \log(z)\left(1-2z+2z^2\right)\\ & -\log(1-z)\left(-\frac{1}{2}+z-z^2\right) + \frac{3}{2}z - 2z^2\Bigg] + \mathcal{O}(\epsilon)\,. \end{aligned} \tag{B.14}$$

In (B.13), we note the presence of the $\mathbf{I}^{(1)}_{qg,F}$ infrared operator, but the absence of a pole proportional to a splitting kernel, since there are no collinear limits between quarks of different flavour. Instead, when we identify a secondary quark, we do not have any infrared operator, since the secondary quark flavour is absent at the virtual level, but we have $p^{(0)}_{qg}$, encoding the splitting $g \to q'\bar{q}'$.

Finally, we have the gluon-gluon antenna function with all gluons $F^0_3(1_g, 2_g, 3_g)$, whose integral reads

$$\begin{aligned}\mathcal{F}_3^{0,\mathrm{id}.g}(q^2,z) = &-4\mathbf{I}^{(1)}_{gg}\left(\epsilon,q^2\right)\delta(1-z) + \left(q^2\right)^{-\epsilon}\Bigg[-\frac{1}{\epsilon}p^{(0)}_{gg}(z) + \delta(1-z)\left(\frac{67}{18}+\frac{2\pi^2}{3}\right)\\ &-\frac{11}{6}\mathcal{D}_0(1-z) + 2\mathcal{D}_1(1-z) + \log(z)\left(-8+\frac{4}{z}+\frac{4}{1-z}+4z-4z^2\right)\\ &-\log(1-z)\left(4-\frac{2}{z}-2z+2z^2\right)+\frac{11}{6}+\frac{11}{6}z+\frac{11}{6}z^2\Bigg] + \mathcal{O}(\epsilon)\,,\end{aligned} \tag{B.15}$$

and the gluon-gluon antenna function with a quark pair $G^0_3(1_g, 2_{q'}, 3_{\bar{q}'})$, symmetric under exchange of the quark line: when we identify the gluon, we obtain

$$\begin{aligned}\mathcal{G}_3^{0,\mathrm{id}.g}\left(q^2,z\right) = &-2\mathbf{I}^{(1)}_{gg,F}\left(\epsilon,q^2\right)\delta(1-z) + (q^2)^{-\epsilon}\Bigg[-\frac{5}{9}\delta(1-z)\\ &+\frac{1}{3}\mathcal{D}_0(1-z)-\frac{1}{3}-\frac{1}{3}z-\frac{1}{3}z^2\Bigg]+\mathcal{O}(\epsilon)\,,\end{aligned} \tag{B.16}$$

whereas when we identify a quark we get

$$\begin{aligned}\mathcal{G}_3^{0,\mathrm{id}.q}\left(q^2,z\right) = &\left(q^2\right)^{-\epsilon}\Bigg[-\frac{1}{2\epsilon}p^{(0)}_{qg}(z) + \log(z)\left(1-2z+2z^2\right)\\ &-\log(1-z)\left(-\frac{1}{2}+z-z^2\right)+z-\frac{7}{4}z^2\Bigg]+\mathcal{O}(\epsilon)\,.\end{aligned} \tag{B.17}$$

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