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# Beam functions for $N$-jettiness at N$^3$LO in perturbative QCD

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Abstract: We present a calculation of all matching coefficients for $N$-jettiness beam functions at next-to-next-to-next-to-leading order (N$^3$LO) in perturbative quantum chromodynamics (QCD). Our computation is performed starting from the respective collinear splitting kernels, which we integrate using the axial gauge. We use reverse unitarity to map the relevant phase-space integrals to loop integrals, which allows us to employ multi-loop techniques including integration-by-parts identities and differential equations. We find a canonical basis and use an algorithm to establish non-trivial partial fraction relations among the resulting master integrals, which allows us to reduce their number substantially. By use of regularity conditions, we express all necessary boundary constants in terms of an independent set, which we compute by direct integration of the corresponding integrals in the soft limit. In this way, we provide an entirely independent calculation of the matching coefficients which were previously computed in Ref. [1].

## Contents

## 1 Introduction

The high energy and luminosity of the Large Hadron Collider, as well as the excellent performance of the ATLAS and CMS detectors allow one to conduct high-precision studies of a large number of processes with the goal to stress-test the Standard Model and to search for possible deviations from its predictions. Perturbative QCD enables an accurate description of hadron collisions through a systematically improvable computation of partonic cross sections and kinematic distributions, and plays a central role in this endeavour.

However, making theoretical predictions for partonic QCD processes is complicated. One reason for that are the infra-red and collinear divergences which have to be carefully extracted and cancelled between elastic and inelastic contributions to the final result in any fixed-order perturbative computation. While such divergences naturally appear as poles in the dimensional regularisation parameter $\epsilon$ when elastic contributions to a given process are computed, the situation is more complex for inelastic ones, where additional partons appear in the final state. In such cases, the singularities arise when these partons become either soft or collinear to other partons, but they only turn into poles in $\epsilon$ once an integration over the energies and angles of these additional partons is performed. Since such integrations are not suitable for computations that aim at describing arbitrary infra-red safe distributions of final state particles, special methods have to be designed to allow the extraction of soft and collinear singularities without the integration over the kinematic variables of the resolved partons.

Two distinct methods to do this have been proposed and developed since the early days of perturbative computations; one is called subtraction and the other one is called slicing. The idea of the subtraction method is to subtract and add back an approximate expression of the product of the relevant matrix elements squared and the multi-particle phase space. The difference between the exact and approximate expressions should be integrable in four dimensions. The integral of the subtraction term over the unresolved phase space of final state particles should be performed in $d = 4 - 2\epsilon$ dimensions either numerically or analytically. Several subtraction methods for generic hadron collider processes have been worked out at next-to-leading order (NLO) [2, 3] and at next-to-next-to-leading order (NNLO) in perturbative QCD [4–9] but their extension to next-next-to-next-to-leading order ($\mathrm{N^3LO}$) in QCD is not available.

The slicing method seeks to split the phase space of final state particles into the (most) singular and non-singular (or less singular) parts. The most singular contributions typically arise when all particles in the final state, beyond those present in the Born process, become soft or collinear. The less singular parts correspond to processes which contain resolved partons in addition to the Born ones; such processes can be dealt with by computing lower-order perturbative corrections to higher-multiplicity processes. Hence, if one is interested in computing $\mathrm{N^3LO}$ QCD corrections to the partonic process $pp \to X$ using the slicing method, one needs to know NNLO QCD corrections to the process $pp \to X + \mathrm{jet}$ and $\mathrm{N^3LO}$ QCD contribution to $pp \to X$ which comes from the fully-unresolved region of phase space.

The exact definition of resolved and unresolved phase-space regions requires the introduction of a slicing variable. The choice of the slicing variable can be arbitrary but recently two such variables have been used for several NNLO and N$^3$LO QCD computations. For processes where colour-singlet (e.g., $H$, $Z$, $W$, $ZZ$, $WW$ etc.) or heavy colour-charged (e.g., $t\bar{t}$ etc.) particles are produced in hadron collisions at the Born level, one can use their total transverse momentum $q_\perp$ [10] to distinguish elastic and inelastic contributions. Another option is to use the $N$-jettiness variable [11, 12], first introduced in the context of Soft Collinear Effective Theory (SCET) [13–17], to distinguish processes with a different number of jets. The advantage of using $N$-jettiness for slicing stems from the fact that it can be employed for processes with jets at leading order, whereas dealing with such processes remains a challenge for $q_\perp$-slicing.

The construction of a slicing scheme that uses the $N$-jettiness variable benefits from the existence of a factorisation theorem that describes the behaviour of relevant cross sections at small values of the $N$-jettiness variable. To present this theorem, we consider the case of colour-singlet production in proton-proton collision. Since the Born process in this case contains no final-state jets, the generic $N$-jettiness variable becomes zero-jettiness. It is defined as

$$\mathcal{T}_0 = \sum_{j=1}^{N} \min_{i\in\{1,2\}} \left[ \frac{2p_i \cdot k_j}{Q_i} \right] . \tag{1.1}$$

In Eq. (1.1) the sum runs over all final state QCD partons. For each final state parton $j$, the smallest scalar product of its momentum $k_j$ and the momenta of the incoming partons $p_{1,2}$ contributes to the value of $\mathcal{T}_0$. The $Q_i$ are the so-called hardness variables; they can be chosen in different ways and are of no relevance for the computations described in this paper.

Schematically, the cross section of the process $pp \to V + X$, where $V$ is a colour-singlet system, at small values of zero-jettiness can be written as [11, 12, 18]

$$\lim_{\mathcal{T}_0\to 0} \mathrm{d}\sigma^{\mathrm{N^3LO}}_{pp\to V+X} \approx B \otimes B \otimes S_0 \otimes H \otimes \mathrm{d}\sigma^{\mathrm{LO}}_{pp\to V} . \tag{1.2}$$

In Eq. (1.2), the summation over different partonic species is implied and $\otimes$ stands for the convolutions. Furthermore, $H$ is a process-specific hard function which, essentially, accounts for loop corrections to the Born process, $S_0$ is the zero-jettiness soft function and $B$ is the beam function that accounts for the effects of the collinear QCD radiation off the incoming partons.

We note that in contrast to the soft and hard functions, the beam function in Eq. (1.2) is universal in that it does not depend on the process and on the number of jets in the final state. Eq. (1.2) suggests that, in order to calculate the cross section for small values of $\mathcal{T}_0$ through, say, N$^3$LO in perturbative QCD, one has to compute the beam function, the soft function and the hard function to third perturbative order and then combine them to obtain the unresolved contribution to $pp \to V + X$ cross section.

We note that, in principle, beam functions are non-perturbative objects. However, at leading power in $\Lambda_{\mathrm{QCD}}/\mathcal{T}$, their non-perturbative parts are related to parton distribution functions (PDFs) $f_j$ through the following formula

$$B_i = \sum_{\text{partons } j} \mathcal{I}_{ij} \otimes f_j \,, \quad \text{where} \quad i,j \in \{g, u, \bar{u}, d, \bar{d}, \dots\} \,. \tag{1.3}$$

The quantities $\mathcal{I}_{ij}$ are the so-called matching coefficients; they can be computed in perturbative QCD and used to describe fixed-order cross sections at small values of $N$-jettiness.

The calculation of the matching coefficients $\mathcal{I}_{ij}$ has a long history. The NLO and NNLO results for the matching coefficients were obtained in Refs. [19–21]. The N$^3$LO QCD computations were initiated in Refs. [22, 23] and first physics results for $\mathcal{I}_{qq}$ in the generalised large-$N_c$ approximation were presented in Ref. [24]. In Ref. [1] the matching coefficients for all partonic channels were computed through N$^3$LO in perturbative QCD using the method described in Ref. [25].

The goal of this paper is to complete the calculation described in Ref. [24]. We do this by going beyond the generalised large-$N_c$ approximation and by computing beam-function matching coefficients for all partonic channels. As explained in the next section, we perform this calculation by utilising the connection between partonic beam functions and integrals of the collinear splitting kernels pointed out in Ref. [26] (see also Ref. [27] for a recent discussion). We note that this method of computing the matching coefficients is very different from the method used in Refs. [1, 25]. Thus, our calculation provides a fully independent check of the results reported in Ref. [1] and demonstrates the practical utility of working in a ghost-free physical gauge.

The rest of the paper is organised as follows. In Section 2, we discuss the calculation of the matching coefficients. We begin with the description of the computational setup. Then, we discuss the derivation of the differential equations for master integrals and their solutions, the computation of the boundary conditions and the assembly of the partonic beam functions. In Section 3, we describe the renormalisation of the beam function and the extraction of the matching coefficients. We present the results of the computation in Section 4 and conclude in Section 5. Additional discussion of particular aspects of the calculation can be found in the appendices.

## 2 Calculation

Beam functions were originally defined in SCET as matrix elements of particular operators calculated with respect to external hadronic states [11, 18]. The matching relation in Eq. (1.3) arises from an operator product expansion (OPE) in the limit $\Lambda_{\text{QCD}}/\mathcal{T} \ll 1$. Since the OPE is independent of the external states, the matching coefficients $\mathcal{I}_{ij}$ remain the same if we replace the hadronic external states by the partonic ones. The matching relation between partonic beam functions $B_{ij}$ and partonic PDFs $f_{ij}$ reads

$$B_{ij} = \sum_{k \in \{g,u,\bar{u},d,\bar{d},\dots\}} \mathcal{I}_{ik} \otimes f_{kj} \,. \tag{2.1}$$

In comparison to hadronic quantities, the partonic ones carry an additional index $j$ which specifies the flavour of the external parton. Thus, one possibility to compute the matching coefficients is to directly calculate the matrix elements of SCET operators on both sides of the matching relation with external partonic states.

However, it is more practical to forgo the SCET-based definition and to calculate the matching coefficients directly by integrating collinear splitting functions over momenta of the collinear partons subject to certain phase-space constraints [26]. The advantage of this procedure is that it allows one to work with familiar objects such as Feynman diagrams and scattering amplitudes instead of matrix elements of complicated SCET operators.

Let us sketch the computation of the matching coefficient $\mathcal{I}_{ij}$. According to Eqs. (1.2) and (1.3), the matching coefficient is related to the behaviour of the cross section at small values of zero-jettiness. Zero-jettiness becomes small if final state partons are soft or collinear to incoming partons. By forcing the final state partons to be in the collinear limit to one of the incoming ones, we effectively project the differential cross section onto beam functions. As explained above, replacing the external hadronic states by partonic states introduces partonic beam functions. The partonic beam function describes a process where a parton $j$ in the initial state emits collinear partons, loses some of its original momentum, goes slightly off-shell, changes its identity to a parton $i$ and continues into the hard process. The final state kinematics of this collinear-splitting process is subject to a constraint on the zero-jettiness variable. According to Eq. (2.1), the matching coefficients are then obtained by removing contributions, that have to be associated with partonic PDFs, from the partonic beam functions. In the rest of this section, we describe how to calculate the fully unrenormalised, bare partonic beam functions $B_{ij}^{\rm bare}$ from phase-space integrals over splitting functions. We will explain how to use these results to derive the matching coefficients in Section 3.

In total, there are five independent flavour combinations to consider for $i$ and $j$ and, therefore, also five different matching coefficients, $(ij) \in \{q_i q_j, qg, gq, gg, q_i \bar{q}_j\}$. In addition, depending on the order of QCD perturbation theory, there are contributions with different numbers of final-state partons. To compute the N$^3$LO contribution to the matching coefficient, we need to consider final states with up to three additional partons, depending on how many virtual loops appear in a particular amplitude. We will refer to these different processes as triple-real (RRR), double-real virtual (RRV) and real double-virtual (RVV) contributions.

For the sake of concreteness, we consider a triple-real contribution to a partonic beam function. To compute it, we study the partonic process

$$j(p) + \bar{f}(\bar{p}) \to V + f_1(k_1) + f_2(k_2) + f_3(k_3) \tag{2.2}$$

for a colour-singlet state $V$, and investigate its squared matrix element in the collinear limit $k_1||k_2||k_3||p$. We illustrate our notations in Figure 1. It is well-known [28] that in this limit the squared matrix element factorises into a product of the splitting function that describes a transition of a parton $j$ to a parton $i$ along with three collinear partons $f_{1,2,3}$, and the hard matrix element of the process $i + \bar{f}(\bar{p}) \to V$. We write

$$\lim_{k_1||k_2||k_3||p} |\mathcal{M}(j(p), \bar{f}(\bar{p}); f_1, f_2, f_3)|^2 \sim \frac{P_{ij}(p, \bar{p}, \{k_1, k_2, k_3\})}{s_{123}^2} |\mathcal{M}(i(zp), \bar{f}(\bar{p}))|^2 \,, \tag{2.3}$$

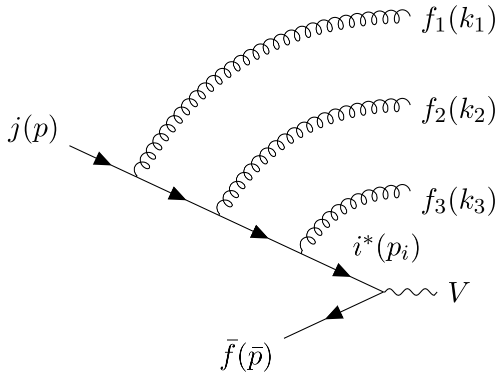


**Figure 1**. Sketch of a triple-real contribution to the process $j(p) + \bar{f}(\bar{p}) \to V + f_1(k_1) + f_2(k_2) + f_3(k_3)$, for $j = q$, $\bar{f} = \bar{q}$ and $f_{1,2,3} = g$, to illustrate the notation for the momenta and flavours.

where $s_{123} = (p - k_1 - k_2 - k_3)^2$ is the off-shell propagator of the parton $i$ which enters the hard process and $P_{ij}$ is the corresponding splitting function. In principle, the factorisation formula shown in Eq. (2.3) is not exact because of spin correlations but since, eventually, we integrate over momenta of collinear partons, the spin correlations average out.

To define the variable $z$ in Eq. (2.3), we use the Sudakov decomposition of the momentum $p_i = p - k_1 - k_2 - k_3$ and write

$$p_i = zp + y\bar{p} + k_\perp \,, \tag{2.4}$$

where $p \cdot k_\perp = \bar{p} \cdot k_\perp = 0$. Thanks to momentum conservation, we find

$$k_{123} = k_1 + k_2 + k_3 = (1 - z)p - y\bar{p} - k_\perp \,. \tag{2.5}$$

Multiplying this equation with $\bar{p}$ and using $\bar{p}^2 = 0$, we obtain

$$1 - z = \frac{\bar{p} \cdot k_{123}}{\bar{p} \cdot p} \,. \tag{2.6}$$

In the collinear limit where $k_{1,2,3} || p$, the zero-jettiness defined in Eq. (1.1) simplifies and becomes[1]

$$\mathcal{T}_0 \approx \frac{2p \cdot k_{123}}{Q_p} \,. \tag{2.7}$$

To compute the matching coefficient at fixed zero-jettiness, we introduce a new variable, the so-called transverse virtuality $t$, defined as

$$t = 2zp \cdot k_{123} \,. \tag{2.8}$$

Once the matching coefficients at fixed $t$ are available, it is straightforward to change variables from $t$ to $\mathcal{T}_0$ using Eq. (2.7), if needed.

[1]We note that this formula applies to an arbitrary $N$-jettiness variable $\mathcal{T}$, not only to the zero-jettiness, in the limit where unresolved final state partons are collinear to the incoming parton with momentum $p$.

To compute the partonic beam functions, we need to integrate over energies and angles of the emitted partons, keeping $z$ and $t$ fixed. To account for these constraints, we follow the common practice and introduce two delta functions into the phase-space integral, writing the triple-real contribution to the partonic beam function as follows

$$B_{ij}^{\rm bare} \sim \int {\rm d}\Phi_B^{(3,0)} \, \frac{P_{ij}(k_1,k_2,k_3)}{s_{123}^2} \,. \tag{2.9}$$

In Eq. (2.9) ${\rm d}\Phi_B^{(3,0)}$ is defined as

$${\rm d}\Phi_B^{(3,0)} = \prod_{m=1}^{3} [{\rm d}k_m] \delta\left(2p\cdot k_{123} - \frac{t}{z}\right) \delta\left(\frac{2\bar{p}\cdot k_{123}}{s} - (1-z)\right) , \tag{2.10}$$

with $s = 2p\cdot\bar{p}$ and

$$[{\rm d}k_m] = \frac{{\rm d}^d k_m}{(2\pi)^{d-1}} \delta^+(k_m^2), \tag{2.11}$$

is the phase-space element for the parton $f_m$ with the momentum $k_m$. We note that contributions of lower-multiplicity final states can also be computed using Eq. (2.9) except that the corresponding splitting functions should include loop contributions, and the number of final-state partons should be reduced accordingly.

Since NLO and NNLO QCD splitting functions are known [28–30], one can integrate them directly to compute the partonic beam functions. In principle, many ingredients required for an $\rm N^3LO$ QCD computation are also known [31–36] but the results at this order are so complex that using them for our purposes does not appear to be beneficial. We thus decided to compute the collinear projections of the relevant matrix elements and their contributions to the various $\rm N^3LO$ QCD splitting functions on our own, to have full control over their possible simplifications.

To do that, we follow Ref. [28] where it is explained how to extract the splitting functions by applying collinear projections to parton scattering amplitudes. To perform the calculation in a process-independent way, we need to use the *axial gauge* for real and virtual gluons since, if such a gauge is used, collinear singularities only appear in diagrams where virtual and real gluons are emitted and absorbed by the *same* external parton $j$. Hence, when computing the sum over polarisations for a gluon with the momentum $k$, we use the following formula

$$\sum_\lambda \epsilon_\lambda{}^\mu(k)\epsilon_\lambda^{*\,\nu}(k) = -g^{\mu\nu} + \frac{k^\mu\bar{p}^\nu + k^\nu\bar{p}^\mu}{k\cdot\bar{p}} \,, \tag{2.12}$$

where have chosen $\bar{p}$ as the auxiliary light-like vector required to define the axial gauge. We note that this formula also defines the numerator of the gluon propagator which we use to compute the virtual corrections and also, since we use the axial gauge, no ghost particles need to be included.

The next step in constructing the splitting functions consists in choosing the "hard process" in a smart way. As explained in Ref. [28], one has to distinguish between cases

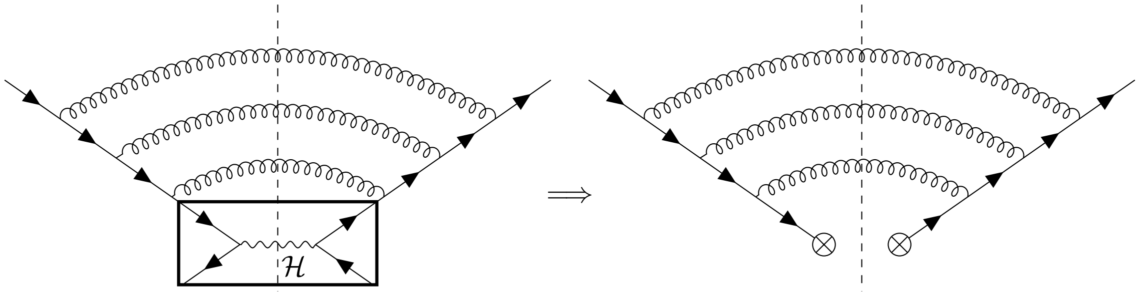


**Figure 2**. Sketch of a squared diagram from the RRR contribution of $q\bar{q} \to V + ggg$ (left-hand side) and the same contribution to the partonic beam function where the hard process ($\mathcal{H}$) has been replaced by a projector denoted by the crossed dots (right-hand side). The dashed vertical line represents the final state cut. The Feynman rules used for the projector are explained in the main text.

where a quark or a gluon enters the hard scattering. In the quark case, $i = q$, we obtain the splitting functions by simply replacing the hard scattering kernel defined in Figure 2 with $\hat{\bar{p}}/(4\,p_i \cdot \bar{p}) = \hat{\bar{p}}/(4z\,p \cdot \bar{p})$ where $\hat{\bar{p}} = \bar{p}^\mu \gamma_\mu$. Hence, the matrix element becomes

$$\mathrm{Tr}\left[\ldots \hat{p}_i\,\mathcal{H}\,\hat{p}_i \ldots\right] \to \frac{\mathrm{Tr}\left[\ldots \hat{p}_i\,\hat{\bar{p}}\,\hat{p}_i \ldots\right]}{4z\,p \cdot \bar{p}}\,, \tag{2.13}$$

where ellipses stand for other contributions stemming from the Feynman diagrams that describe the $j \to i^* + f_1 + f_2 + f_3$ transition. The trace originates from the summation over polarisation states of initial or final state quarks. Thanks to the universal nature of the splitting functions and to the properties of the collinear limit, this procedure projects the relevant amplitudes onto singular contributions which arise when the emitted partons become collinear to the incoming ones [28]. Finally, we note that in order to compute partonic beam functions which describe processes where gluons enter the hard process, i.e. $B_{gq}$ and $B_{gg}$, we simply use $-g^{\mu\nu}/(d-2)$ as a proxy for the hard matrix element.

This procedure allows us to compute the contributions to the splitting functions from individual Feynman diagrams which describe a process where partons are emitted by an incoming parton $j$ with momentum $p$, and an off-shell parton $i$ with momentum $zp$ enters the hard process. Once these contributions to the splitting functions are computed, they need to be integrated over the unresolved phase space of all final state partons while keeping the transverse virtuality $t$ and the $z$-parameter fixed, c.f. Eqs. (2.9,2.10). We perform this integration by employing the method of reverse unitarity [37]. The main idea behind this method is to map all delta functions that appear in a given integrand, for example the on-shell conditions for final state partons $\delta(k^2)$ or the kinematic constraints such as $\delta(2p \cdot k_{123} - t/z)$, onto propagator-like structures using the identity

$$\delta(X) = \frac{1}{2\pi\mathrm{i}}\left[\frac{1}{X - \mathrm{i}0} - \frac{1}{X + \mathrm{i}0}\right]. \tag{2.14}$$

This mapping is beneficial because it turns constrained phase-space integrals into "loop-like" integrals, enabling the use of standard multi-loop technologies, such as the integration-by-parts method (IBPs) [38, 39] and differential equations technique [40–43], to compute them.

The rest of the calculation proceeds in a relatively standard way. We use QGRAF [44] to generate diagrams that describe the various partonic processes, e.g., $j(p) \to i^*(p_i) + f_1(k_1) + f_2(k_2) + f_3(k_3)$. We note that since the parton $i$ is off-shell, we have to account for self-energy corrections on this leg. We use FORM [45–48] to deal with the Dirac and Lorentz algebra and COLOR.H [49] for the colour algebra. For each partonic process and final state multiplicity we define suitable integral families which close under IBPs. We use REDUZE2 [50] and KIRA [51–54] to solve the system of IBP identities and express all integrals in terms of a (relatively) small number of master integrals.

Since the Laporta algorithm requires the propagators of each integral family to be linearly independent, we have to apply a partial fraction decomposition to integrals where linearly dependent propagators appear. In our calculation, linear dependencies between propagators arise because of the phase-space delta functions and the axial-gauge propagators. For example, the delta functions in the RRV contributions imply the following constraint

$$2(k_1 + k_2) \cdot \bar{p} = s(1 - z)\,, \tag{2.15}$$

and it gives rise to partial fraction identities such as

$$\frac{\delta(2k_{12} \cdot \bar{p}/s - (1 - z))}{(k_1 \cdot \bar{p})(k_2 \cdot \bar{p})} = \frac{2\,\delta(2k_{12} \cdot \bar{p}/s - (1 - z))}{s(1 - z)} \left[\frac{1}{k_1 \cdot \bar{p}} + \frac{1}{k_2 \cdot \bar{p}}\right]. \tag{2.16}$$

Moreover, the propagator of a gluon with momentum $k$ in the axial gauge features a term proportional to $(k \cdot \bar{p})^{-1}$. As every integral has to contain the cut propagator corresponding to $\delta(2k_{1\ldots n_R} \cdot \bar{p}/s - (1 - z))$, where $k_{1\ldots n_R} = \sum\limits_{i=1}^{n_R} k_i$ is the total momentum of final state partons, and since at N$^3$LO there are at most three linearly independent scalar products $k_i \cdot \bar{p}$, $i = 1, 2, 3$, diagrams with sufficiently many gluon propagators will contain linearly dependent propagators. We remove such linear dependencies by systematically applying partial fraction relations using polynomial reduction over Gröbner bases. The algorithm that we use has been described in Refs. [55, 56] (see also Refs. [57–59] for related work). We discuss an example of the application of this algorithm in Appendix A.

The above discussion applies to the mapping of integrals that appear in the transition amplitudes onto the integral families. However, it turns out to be important to identify linearly-dependent master integrals which belong to *different* families. This step reduces the number of integrals that need to be computed and it contributes towards significant simplifications of systems of differential equations that the master integrals satisfy. An example of such a relation between three RRR master integrals is

$$\overbrace{\int \frac{\mathrm{d}\Phi_B^{(3,0)}}{(k_1 - p)^2 (k_{13} - p)^2 (k_3 \cdot \bar{p})(k_{13} \cdot \bar{p})}}^{=I^{\mathrm{T29}}_{3391}}$$

$$= \underbrace{\int \frac{\mathrm{d}\Phi_B^{(3,0)}}{(k_1-p)^2(k_{12}-p)^2(k_1\cdot\bar{p})(k_2\cdot\bar{p})}}_{=I^{\mathrm{T1}}_{3263}} - \underbrace{\int \frac{\mathrm{d}\Phi_B^{(3,0)}}{(k_1-p)^2(k_{13}-p)^2(k_1\cdot\bar{p})(k_{13}\cdot\bar{p})}}_{=I^{\mathrm{T28}}_{3291}}, \tag{2.17}$$

where $I_s^f$ denotes an integral from family $f$ and sector $s$ and $\mathrm{d}\Phi_B^{(3,0)}$ is the phase-space measure, c.f. Eq. (2.10). This relation becomes obvious after relabeling $k_2 \leftrightarrow k_3$ in the first integral on the right hand side of Eq. (2.17); it arises because the propagators $1/(k_1\cdot\bar{p})$, $1/(k_3\cdot\bar{p})$ and $1/(k_{13}\cdot\bar{p})$ are linearly dependent.

To construct partial fraction relations between master integrals we generate a list of seed integrals from *all sectors* of *all* integral families. We then calculate a Gröbner basis for the overcomplete set of all propagators obtained by joining all integral families. After polynomial reduction of the seed integrals with respect to this Gröbner basis, we map the integrals to integral families and apply IBP reduction to all integrals. This yields a large system of linear equations which involve integrals that are identified as master integrals by the Laporta algorithm. Finally, we solve the system taking into account the Laporta ordering of the integrals. The non-trivial solutions of this system give us linear relations between master integrals. By applying these relations, we observe a significant reduction in the number of master integrals that are required to express the transition amplitude.

Nevertheless, the question whether *all* linear relations are found in this way remains open. As we explained earlier, this is an important question because eliminating linear dependencies is crucial for achieving the simplest possible form of the differential equations for the master integrals. Unfortunately, some of these linear dependencies only become apparent after relabeling and shifting real and virtual momenta. Since the Gröbner basis is calculated for one particular choice of the integration momenta, it is conceivable that some partial dependencies are not captured by the procedure described above. Extending it in a way that avoids loopholes related to choices of integration momenta and symmetry transformations of the integrals is an interesting question worthy of further investigation.

We note here that, as a matter of fact, we do find further relations between master integrals but only a posteriori, by looking for linear combinations of master integrals that fulfil purely *homogeneous* differential equations, see Section 2.1. More details are given in Ref. [22].

To simplify the computation of master integrals, we remark that their dependence on the variables $t$ and $s$ is homogeneous; this allows us to treat the integrals as functions of the single variable $z$. To see this, we note that, for example, a triple-real integral can be schematically written as follows

$$I(s,t,z) = \int \prod_{m=1}^{3} [\mathrm{d}k_m]\delta\left(2p\cdot k_{123} - \frac{t}{z}\right)\delta\left(\frac{2\bar{p}\cdot k_{123}}{s} - (1-z)\right) F(p,\bar{p},\{k_i\}), \tag{2.18}$$

where $F$ is given by a product of propagators constructed from inverse powers of

$$(p-l_A)^2 \quad \text{and} \quad \bar{p}\cdot l_A, \qquad \text{where } l_A \in \{k_1,k_2,k_3,k_{12},k_{13},k_{23},k_{123}\}, \tag{2.19}$$

and

$$l_A^2\,, \qquad\qquad \text{with } l_A \in \{k_{12}, k_{13}, k_{23}, k_{123}\}\,. \tag{2.20}$$

It is now easy to see that Eq. (2.18) simplifies if we introduce new (tilded) momenta according to

$$k_i = \sqrt{\frac{t}{z}}\tilde{k}_i\,, \qquad\qquad p = \sqrt{\frac{t}{z}}\,\tilde{p}\,, \qquad\qquad \bar{p} = s\sqrt{\frac{z}{t}}\tilde{\bar{p}}\,. \tag{2.21}$$

Using the tilded momenta in Eq. (2.18), we obtain

$$\begin{aligned} I(s,t,z) &= s^{n_s}\left(\frac{t}{z}\right)^{n_t-3\epsilon}\int \mathrm{d}\tilde{\Phi}_B F(\tilde{p},\tilde{\bar{p}},\{\tilde{k}_i\}) \\ &= s^{n_s}\left(\frac{t}{z}\right)^{n_t-3\epsilon} I(1,1,z)\,, \end{aligned} \tag{2.22}$$

where $\mathrm{d}\tilde{\Phi}_B$ can be obtained from Eq. (2.10) by substituting $t \to 1$, $s \to 1$, $p \to \tilde{p}$ and $\bar{p} \to \tilde{\bar{p}}$ there. Also, $n_{s,t}$ are integral-dependent integers and the last step in Eq. (2.22) follows from the fact that $\tilde{p} \cdot \tilde{\bar{p}} = 1/2$. By a slight abuse of notation, we will occasionally use $p$ and $\bar{p}$ instead of $\tilde{p}$ and $\tilde{\bar{p}}$; it should be clear from the context which normalisation is used in a particular part of the calculation. Note that an analogous discussion also holds for RRV integrals.

To derive the differential equations for the master integrals with respect to the variable $z$, we follow the standard procedure. We differentiate the integrands with respect to $z$ and use IBP identities and partial fraction relations to express the derivatives through the master integrals. For solving the differential equations, we need to supply the boundary conditions; to do that, we compute the required master integrals in the $z \to 1$ limit where all emitted partons become soft. In the next sections we first describe how we choose the basis of master integrals to simplify the solution of the differential equations and then elaborate on the details of the computation of the relevant boundary conditions.

### 2.1 Differential equations for master integrals

We use differential equations [40–43] to compute the master integrals. As the integrals depend non-trivially on a single variable $z$, we have to deal with the following system of differential equations

$$\partial_z \vec{I}(z,\epsilon) = \mathbf{A}(z,\epsilon)\vec{I}(z,\epsilon)\,. \tag{2.23}$$

In Eq. (2.23) $\vec{I}(z,\epsilon)$ is the vector of master integrals and $\mathbf{A}(z,\epsilon)$ is a matrix of (rational) functions of $z$ and of the dimensional regularisation parameter $\epsilon$.

It is well known that different choices of master integrals can significantly impact the form of the matrix $\mathbf{A}(z,\epsilon)$ and the complexity of the system of differential equations. When it exists, a canonical basis of master integrals [60] is a particularly convenient choice.

For integrals in a canonical basis the differential equations assume the especially simple form

$$\partial_z \vec{I}_c(z,\epsilon) = \epsilon \mathbf{A}_c(z) \vec{I}_c(z,\epsilon)\,, \quad \text{where} \quad \mathbf{A}_c(z) = \sum_i f_i(z) \mathbf{A}_{c,i}\,. \tag{2.24}$$

A further crucial property of a canonical basis is that the matrix $\mathbf{A}_c(z)$ must be in the so-called dlog form. This means that in Eq. (2.24) $f_i(z) = \mathrm{d}\log g_i(z)/\mathrm{d}z$ for some algebraic functions $g_i(z)$, and the entries of the $z$-independent matrices $\mathbf{A}_{c,i}$ are just numbers.

Since the $\epsilon$-dependence of the right-hand side in Eq. (2.24) is completely factorised, the solutions of the homogeneous equation at each order in $\epsilon$ are just constants, and one can construct an iterative solution of this equation in a straightforward manner. Inserting a Laurent-series ansatz in $\epsilon$ for the integrals $\vec{I}_c(z,\epsilon) = \sum\limits_{k=0} \epsilon^k \vec{I}_c^{(k)}(z)$, we obtain the solutions

$$\vec{I}_c^{(k)}(z) = \vec{B}^{(k)} + \sum_i \mathbf{A}_{c,i} \int^z \mathrm{d}z'\, f_i(z') \vec{I}_c^{(k-1)}(z')\,. \tag{2.25}$$

Here, $\vec{B}^{(k)}$ are the vectors of integration constants which need to be determined by computing the integrals for a particular value of $z$. The $z$-dependence of the solution is calculated through iterated integration over $z$. The kernels of such iterated integrals are specified by the logarithmic differential forms in $\mathbf{A}_c(z)$. A famous result [61] in the theory of iterated integrals guarantees that, as long as the logarithmic forms are independent, the resulting iterated integrals will also be linearly independent of each other. Besides the simplicity of the differential equations, another benefit of having a canonical basis is that the cancellation of spurious poles in $\epsilon$ in the amplitude is made explicit so that we do not have to compute the master integrals to higher orders in $\epsilon$ than strictly necessary.

Finding a canonical basis for master integrals is a non-trivial task. Starting from a generic choice of master integrals, one performs a basis transformation

$$\vec{I}_c(z,\epsilon) = \mathbf{T}(z,\epsilon) \vec{I}(z,\epsilon)\,. \tag{2.26}$$

The differential equation for $\vec{I}_c(z,\epsilon)$ becomes

$$\partial_z \vec{I}_c(z,\epsilon) = \tilde{\mathbf{A}}(z,\epsilon) \vec{I}_c(z,\epsilon)\,, \tag{2.27}$$

where

$$\tilde{\mathbf{A}}(z,\epsilon) = \mathbf{T}(z,\epsilon)\mathbf{A}(z,\epsilon)\mathbf{T}^{-1}(z,\epsilon) + (\partial_z \mathbf{T}(z,\epsilon))\mathbf{T}^{-1}(z,\epsilon)\,. \tag{2.28}$$

If one is able to find a matrix $\mathbf{T}(z,\epsilon)$ such that $\tilde{\mathbf{A}}(z,\epsilon) = \epsilon \mathbf{A}_c(z)$, one arrives at a canonical basis.

Various semi-automated methods have been developed to find the transformation to a canonical basis. Iterative approaches to constructing the matrix $\mathbf{T}$ starting from a general matrix $\mathbf{A}(z,\epsilon)$, have been discussed in Refs. [57, 62–68]. An alternative procedure based on constructing candidates for the canonical basis through the analysis of the so-called leading singularities was suggested in Refs. [60, 69, 70]. Other approaches to finding canonical bases were discussed in Refs. [71–74].

While the advantage of having canonical bases is clear and significant progress in developing algorithms to determine them has been achieved, their application to non-trivial problems, such as the calculation of the N$^3$LO QCD contributions to beam functions, remains a difficult task. In fact, upon inspecting the differential equations for our problem, we observe that their solutions involve rational functions of $z$ and three different square roots

$$\sqrt{z}\sqrt{4-z}\,, \qquad \sqrt{z}\sqrt{4+z}\,, \qquad \text{and} \qquad \sqrt{4+z^2}\,. \tag{2.29}$$

The presence of algebraic functions renders the application of the majority of automated algorithms for finding a canonical basis either impossible or highly non-trivial. Hence, we have decided to adopt a pragmatic approach to finding the canonical basis for our system of differential equations. It is based on the following steps:

1. As a starting point, we choose a basis of integrals whose differential equations do not contain denominators which mix the kinematic variable $z$ with the dimensional regularisation parameter $\epsilon$. Such denominators unnecessarily complicate the calculation and can be avoided by choosing the master integrals appropriately (see Refs. [75–77] for related discussions). Here, we encountered such denominators only for a handful of integrals so that we searched for appropriate replacements on a case-by-case basis. It was sufficient to replace integrals for which this occurs either by other integrals from the same sector[2] or, in a small number of cases, by integrals from a supersector which does not contain any master integrals.[3]

2. To make use of the automated packages for the determination of a canonical basis, it was beneficial to rationalise square roots. We note that according to Eq. (2.29) all square roots involve second-degree polynomials in the variable $z$. Hence, each of them can be easily rationalised by a particular variable transformation. On the other hand, we could not find a transformation that rationalises all three square roots at the same time.

   To take full advantage of the possibility to rationalise individual roots, we split up the differential equations for the master integrals into subsystems which close and contain at most one square root. It turns out that this can be achieved for the majority of the relevant integrals. For the sake of completeness, we present the variable transformations which rationalise three square roots in Eq. (2.29)

$$\sqrt{z}\sqrt{4-z}: \qquad\qquad z \to z = \frac{(1+x)^2}{x}\,, \tag{2.30}$$

[2]As usual, the term *sector* denotes the set of propagators that is present in the denominator of an integral. We call a sector $S'$ a *subsector* of another sector $S$ if the set of denominators of $S'$ is a subset of those present in $S$ and a *supersector* if the set of denominators in $S'$ is a superset of those present in $S$.

[3]A heuristic for choosing candidates for the replacement integrals was whether or not the reductions of the candidate integrals to the original master integrals contain the offending factors in the denominator.

$$\sqrt{z}\sqrt{4+z}: \qquad z \to z = \frac{(1-y)^2}{y}\,, \tag{2.31}$$

$$\sqrt{4+z^2}: \qquad z \to z = \frac{w^2-1}{w}\,. \tag{2.32}$$

The last transformation is a generalisation of the Landau transformation introduced in the first two.

While the process of rationalisation can make previously simple linear letters more complicated, once the equations are rationalised, we can use FUCHSIA [65] and CANONICA [57, 66] to algorithmically construct a canonical basis.

3. For a relatively small number of equations where multiple square roots appear simultaneously, we constructed a canonical basis without rationalising the square roots. To achieve this, we employed a heuristic strategy based on the analysis of some of the leading singularities of the corresponding integrals, combined with the procedure described in Ref. [62] that allows the simplification of possible remaining non-canonical entries in the differential equations. We performed the analysis of the leading singularities for both triple-real and double-real virtual integrals using the Baikov representation [78, 79]. For completeness, we present an example of such a construction in Appendix B.

4. Once canonical systems of differential equations are constructed, we switch back to the original variable $z$ even if the canonical basis was calculated using $x, y$ or $w$ variables. This allows us to integrate all master integrals in a uniform way, as we explain below.

Once the equations are written in canonical form, we can easily solve them in terms of iterated integrals. As already hinted to above, a general result from the theory of iterated integrals ensures that, as long as the dlog forms that we integrate over are independent, also the corresponding iterated integrals are linearly independent of each other. We stress for clarity that this is only true once all products of different iterated integrals evaluated at the same argument have been removed using the standard shuffle product relations, which hold for any (properly regulated) iterated integral. This implies that our integration procedure is literally as simple as in the well-known case of multiple polylogarithms [80–83], being entirely reduced to the iterative addition of a new "index" to the iterated integrals for each differential form. We define iterated integrals as follows

$$L_{a,\vec{b}}(x) = \int_0^x f_a(t)\, L_{\vec{b}}(t)\,\mathrm{d}t\,, \qquad L_a(x) = \int_0^x f_a(t)\,\mathrm{d}t\,, \qquad L_{\underbrace{0,\,\ldots,\,0}_{n}}(x) = \frac{1}{n!}\log^n x\,, \tag{2.33}$$

where the functions $f_a(t)$ are differentials of logarithms, as discussed right after Eq. (2.24). Note that this definition makes sense since, in our problem there is only one function $f(t)$ that diverges at zero, c.f. Eq. (2.34) below.

Of course, as already mentioned earlier, to completely determine the integrals from their system of differential equations, we need to know their values at a certain point in order to fix all the relevant boundary conditions. For all the integrals considered, it is convenient to choose their soft ($z \to 1$) limit as a reference point. To simplify the evaluation of the iterated integrals close to the soft limit, we rewrite the differential equations using the auxiliary variable $\bar{z} = 1 - z$. In fact, when using $\bar{z}$ we find that we need to consider iterated integrals defined over the following alphabet

$$f_i(\bar{z}) \in \left\{ \frac{1}{\bar{z}-1}, \frac{1}{\bar{z}}, \frac{1}{\bar{z}+1}, \frac{1}{\bar{z}-2}, \frac{1}{\bar{z}-3}, \frac{1}{\bar{z}+3}, \frac{1}{\bar{z}-5}, \frac{2\bar{z}-3}{\bar{z}^2-3\bar{z}+3}, \frac{2\bar{z}-2}{\bar{z}^2-2\bar{z}+5}, \right. \\ \left. \frac{1}{\sqrt{1-\bar{z}}\sqrt{5-\bar{z}}}, \frac{1}{\sqrt{1-\bar{z}}\sqrt{3+\bar{z}}}, \frac{1}{\sqrt{\bar{z}^2-2\bar{z}+5}}, \frac{1}{(\bar{z}-1)\sqrt{\bar{z}^2-2\bar{z}+5}} \right\}. \tag{2.34}$$

We note here that iterated integrals of rational functions and square roots of polynomials up to degree two have been studied extensively in the literature [84–89].

Since we defined the iterated integrals by integrating from 0 to $\bar{z}$, c.f. Eq. (2.33), their $\bar{z} \to 0$ limits either vanish or behave as $\log^n(\bar{z})$ for some $n \in \mathbb{N}$. Moreover, the fact that the only letter in Eq. (2.34) that diverges in the soft $\bar{z} \to 0$ limit is $1/\bar{z}$, guarantees that all logarithmic $\log^n(\bar{z})$ singularities can be systematically extracted by un-shuffling all the occurrences of this letter, similar to what is done for standard multiple polylogarithms.

In this way, we obtain the canonical master integrals as expansions in $\epsilon$ through $\mathcal{O}(\epsilon^5)$, i.e. including $I_c^{(5)}(\bar{z})$, as functions of $\bar{z}$. We note that, although the rational letters with quadratic denominators can be further factorised at the expense of introducing complex numbers, we keep the quadratic forms to achieve a more compact representation. To manipulate iterated integrals we make extensive use of the packages HarmonicSums [81, 86, 90–98], HPL [99, 100] and PolyLogTools [101], as well as GiNaC [82, 102] for the numerical evaluation of multiple polylogarithms.

Since the soft ($\bar{z} \to 0$) singularities of the beam functions are regularised dimensionally, we have to solve the differential equations for the master integrals in this limit in closed form in $\epsilon$, but as generalised power series expansions in $\bar{z}$. Due to spurious poles in $1/\bar{z}$ in the amplitudes, in some cases we need the expansions through $\bar{z}^2$ terms. Since we work with a canonical basis, obtaining a solution in the limit $\bar{z} \to 0$ is particularly simple. The leading behaviour of the canonical integrals in this limit can be obtained by solving

$$\partial_{\bar{z}} \vec{I}_c^{(0)}(\bar{z}, \epsilon) = \epsilon \frac{\mathbf{A}_{c,0}}{\bar{z}} \vec{I}_c^{(0)}(\bar{z}, \epsilon), \tag{2.35}$$

where $\mathbf{A}_{c,0}$ is the coefficient matrix of the letter $f_0(\bar{z}) = 1/\bar{z}$. The solution of Eq. (2.35) is expressed through the matrix exponential

$$\vec{I}_c^{(0)} = \mathbf{\Phi}(\bar{z}, \epsilon) \vec{B}_{\text{soft}}(\epsilon), \qquad \text{where } \mathbf{\Phi} = \exp\left(\epsilon \log(\bar{z}) \mathbf{A}_{c,0}\right) = \bar{z}^{\epsilon \mathbf{A}_{c,0}}. \tag{2.36}$$

The matrix $\mathbf{\Phi}(\bar{z}, \epsilon)$ contains the fundamental system of the solutions to Eq. (2.35). The subleading terms are then obtained by expanding the coefficient matrix $\mathbf{A}_c(\bar{z})$ around $\bar{z} = 0$ as $\mathbf{A}_c(\bar{z}) = \sum_{n=0}^{\infty} \bar{z}^{n-1} \mathbf{A}_c^{(n)}$ and then solving the differential equations

$$\partial_z \vec{I}_c^{(n)}(\bar{z}, \epsilon) = \epsilon \sum_{k=0}^{n} \bar{z}^{k-1} \mathbf{A}_c^{(k)} \vec{I}_c^{(n-k)}(\bar{z}, \epsilon)$$

$$= \epsilon \left[ \underbrace{\sum_{k=1}^{n} \bar{z}^{k-1} \mathbf{A}_c^{(k)} \vec{I}_c^{(n-k)}(\bar{z},\epsilon)}_{\equiv \vec{R}^{(n)}(\bar{z},\epsilon)} + \frac{\mathbf{A}_{c,0}}{\bar{z}} \vec{I}_c^{(n)}(\bar{z},\epsilon) \right]. \tag{2.37}$$

It is obvious that, for $n = 0$, Eq. (2.37) simplifies to Eq. (2.35).

We note that we require solutions $\vec{I}_c^{(n)}(\bar{z},\epsilon)$ of Eq. (2.37) that behave asymptotically as $\bar{z}^n$ in the limit $\bar{z} \to 0$. This implies that for $n > 0$ we only need to consider the inhomogeneous solutions of the above equation. We obtain them using the method of variation of constants. We note that the fundamental system of the homogeneous equation that is needed to construct the inhomogeneous solution is always $\mathbf{\Phi}(\bar{z},\epsilon)$ defined in Eq. (2.36). We find

$$I_c^{(n)}(\bar{z},\epsilon) = \mathbf{\Phi}(\bar{z},\epsilon) \int_0^{\bar{z}} \mathrm{d}\bar{z}' \, \mathbf{\Phi}^{-1}(\bar{z}',\epsilon) \vec{R}^{(n)}(\bar{z}',\epsilon) \,, \tag{2.38}$$

where $\vec{R}^{(n)}(\bar{z},\epsilon)$ is defined in Eq. (2.37). Having computed the boundary constants, we find that the soft limit of the master integrals can be written as

$$\vec{I}_{c,\text{soft}}(\bar{z},\epsilon) = \sum_{n=0}^{\infty} \left[ \vec{B}_{\text{soft},3,n}(\epsilon) \bar{z}^{n-3\epsilon} + \vec{B}_{\text{soft},2,n}(\epsilon) \bar{z}^{n-2\epsilon} \right] . \tag{2.39}$$

In the triple-real case we observe that $\vec{B}_{\text{soft},2,n}(\epsilon) = \vec{0}$ for all $n$. Finally, we merge the solutions in the soft limit with those expanded order by order in $\epsilon$ via

$$\vec{I}_c(\bar{z},\epsilon) = \left[ \sum_i \epsilon^k \vec{I}_c^{(k)}(\bar{z}) - \vec{I}_{c,\text{soft}}(\bar{z},\epsilon) \right]_{\epsilon-\text{exp}} + \vec{I}_{c,\text{soft}}(\bar{z},\epsilon) \,. \tag{2.40}$$

This way, the soft singularity stays dimensionally regulated, which is important for computing convolution integrals over $z$.

### 2.2 Boundary constants

The calculation of the boundary conditions is one of the most demanding parts of this computation and we have used different methods to derive them. We have discussed the computation of some of these constants in Refs. [22, 23] which the interested reader should consult. Here we address the problem from a slightly different perspective.

We start with the discussion of the triple-real integrals which appear in the calculation. We will show that their soft, $z \to 1$, limits can be related to integrals which appear in the calculation of the Higgs cross section in the threshold limit. A generic triple-real integral $I$ can be written as

$$I = \int \prod_{i=1}^{3} [\mathrm{d}k_i] \, \delta\left(2p \cdot k_{123} - \frac{t}{z}\right) \delta\left(\frac{2\bar{p} \cdot k_{123}}{s} - (1-z)\right) F(p,\bar{p},\{k_i\}) \,, \tag{2.41}$$

where the function $F(p,\bar{p},\{k_i\})$ describes the collection of propagators that are displayed in Eqs. (2.19) and (2.20).

The boundary constant $C$ for the integral $I$ is defined as follows

$$\lim_{z\to 1} I = C s^{n_1} t^{n_2-3\epsilon}(1-z)^{n_3-3\epsilon}\,\{1+\mathcal{O}(1-z)\}\,, \tag{2.42}$$

where $n_{1,..,3}$ are integers that depend on the exact definition of the integral $I$. As explained in Ref. [22], the constant $C$ can be computed by replacing all propagators that appear in Eq. (2.41) with their eikonal counterparts. For example,

$$\frac{1}{(p-k_{123})^2} \to \frac{1}{-2p\cdot k_{123}}\,, \qquad \frac{1}{(p-k_{12})^2} \to \frac{1}{-2p\cdot k_{12}}\,, \qquad \text{etc.} \tag{2.43}$$

Once these simplifications are performed, the integral becomes a homogeneous function of $(1-z)$ in addition to being a homogeneous function of $s$ and $t/z$. Hence, we can write

$$\begin{aligned} I_{\rm eik} &= \int \prod_{i=1}^{3} [\mathrm{d}k_i]\,\delta\left(2p\cdot k_{123} - \frac{t}{z}\right)\delta\left(\frac{2\bar{p}\cdot k_{123}}{s} - (1-z)\right) F(p,\bar{p},\{k_i\})|_{\rm eik} \\ &= C\, s^{n_1}\left(\frac{t}{z}\right)^{n_2-3\epsilon}(1-z)^{n_3-3\epsilon}\,. \end{aligned} \tag{2.44}$$

We emphasise that the constant $C$ in Eq. (2.44) is the same as in Eq. (2.42) and that the dependence of $I_{\rm eik}$ on $z$, as displayed in the second line of Eq. (2.44), is exact.

We now explain how to make use of this fact to simplify the computation of the integration constant. To this end, we take $t = sz^2$ in Eq. (2.44) and integrate that equation over $z$. We find

$$\begin{aligned} \bar{I} = \int_0^1 \mathrm{d}z\, I_{\rm eik} &= \int \prod_{i=1}^{3} [\mathrm{d}k_i]\,\delta\left(2P\cdot k_{123} - s\right) F(p,\bar{p},\{k_i\})|_{\rm eik} \\ &= C\, s^{n_1+n_2-3\epsilon}\frac{\Gamma(n_2+1-3\epsilon)\Gamma(n_3+1-3\epsilon)}{\Gamma(n_2+n_3+2-6\epsilon)}\,, \end{aligned} \tag{2.45}$$

where $P = p+\bar{p}$.

Eq. (2.45) is useful because the integral there can be related to the triple-real soft integrals calculated for the Higgs boson production in gluon fusion in Refs. [103–106]. Hence, many of the boundary constants required for the calculation of the N$^3$LO $N$-jettiness beam functions can be compared with the boundary constants computed in Ref. [103–106]. Moreover, we can use the integration-by-parts identities for triple-real soft Higgs integrals to relate the various boundary constants required in our case.

In fact, we have checked that our computation of the boundary constants for triple-real integrals covers all of the ten integrals described in Ref. [103] as well as the 13 inclusive RRR integrals calculated recently in Ref. [106]. We checked that our results agree with those references up to the $\epsilon$-order required for our calculation. We note that whereas Refs. [103, 106] heavily relied on using the Mellin-Barnes representation to compute the triple-real soft integrals, in Ref. [22] we calculated most of them by a direct integration over Sudakov parameters. Hence, in addition to serving its original purpose, our computation of the boundary constants provides an independent confirmation of the triple-real soft integrals for Higgs boson production calculated in Ref. [103].

The absolute majority of the RRV boundary constants can be computed by a direct integration over Feynman and Sudakov parameters following the discussion in Ref. [23]. We used a convenient Feynman parameter representation of the one-loop integrals and calculated the relevant[4] $(1-z)$-branches by making suitable approximations. Most of the required boundary conditions are discussed in Ref. [23]; however, we discovered that a few additional boundary constants are needed.

All but one of these additional constants can be computed following the discussion in Ref. [23]. The RRV integral for which this approach fails reads

$$
\begin{aligned}
I = &\int \prod_{i=1}^{2} [\mathrm{d}k_i]\, \delta\left(2p\cdot k_{12} - \frac{t}{z}\right) \delta\left(\frac{2\bar{p}\cdot k_{12}}{s} - (1-z)\right) \frac{1}{(k_1-p)^2}\frac{1}{k_2\cdot\bar{p}} \\
&\times \int \frac{\mathrm{d}^d k_3}{(2\pi)^d} \frac{1}{k_3^2 k_{13}^2 k_{123}^2\,(k_{123}-p)^2\,(k_3\cdot\bar{p})}\,,
\end{aligned}
\tag{2.46}
$$

where $k_{13} = k_1 + k_3$ and $k_{123} = k_1 + k_2 + k_3$. Similar to the triple-real case, this integral is a homogeneous function of $t/z$ and $s$. Hence, in what follows we will set $t/z \to 1$, $s \to 1$ and $p\cdot\bar{p} \to 1/2$ when discussing the RRV integral in Eq. (2.46).

To determine the boundary constant, we need to know the coefficient of the $(1-z)^{-2-3\epsilon}$ branch of this integral, i.e.

$$
\lim_{z\to 1} I \approx C(1-z)^{-2-3\epsilon} + \ldots \tag{2.47}
$$

One can show that, in the $z \to 1$ limit, this branch can be calculated from a simplified integral that is obtained by using the soft approximation for *both* real and virtual-loop momenta (the *soft region* in the terminology of the method of expansion by regions [107]). This amounts to the replacement $1/(k_{123}-p)^2 \to 1/(-2p\cdot k_{123})$ in Eq. (2.46). Denoting the approximate integral by $I_s$, and making use of the fact that it is a homogeneous function of $(1-z)$ we can write

$$
I_s = C(1-z)^{-2-3\epsilon}\,. \tag{2.48}
$$

To proceed further, we write the soft approximation for the integral shown in Eq. (2.46) in the following way

$$
I_s = \int \mathrm{d}^d q\, \delta\left(2p\cdot q - 1\right) \delta\left(2\bar{p}\cdot q - (1-z)\right)\, F_s(p\cdot q, \bar{p}\cdot q, q^2)\,, \tag{2.49}
$$

where

$$
\begin{aligned}
F_s(p\cdot q, \bar{p}\cdot q, q^2) = &\int \prod_{i=1}^{2} [\mathrm{d}k_i]\, \delta^{(d)}\left(q - k_1 - k_2\right) \frac{1}{(-2k_1\cdot p)}\frac{1}{k_2\cdot\bar{p}} \\
&\times \int \frac{\mathrm{d}^d k_3}{(2\pi)^d} \frac{1}{k_3^2 k_{13}^2 k_{123}^2\,(-2p\cdot k_{123})\,(\bar{p}\cdot k_3)}\,.
\end{aligned}
\tag{2.50}
$$

[4] We have found empirically that only the branches $(1-z)^{m_1-2\epsilon}$ and $(1-z)^{m_2-3\epsilon}$ with $m_1, m_2 \in \mathbb{Z}$ appear in RRV integrals. If the homogeneous part of the differential equation for a RRV integral allows a different branch, its coefficient can be immediately set to zero.

To integrate over $q$ in Eq. (2.49), we introduce the Sudakov decomposition

$$q_\mu = \alpha_q \, p_\mu + \beta_q \, \bar{p}_\mu + q_{\perp,\mu} \,, \tag{2.51}$$

and write

$$\mathrm{d}^d q = \frac{1}{2} \mathrm{d}\alpha_q \, \mathrm{d}\beta_q \, \mathrm{d}^{d-2} q_\perp = \frac{1}{4} \, \mathrm{d}q^2 \, \mathrm{d}\alpha_q \, \mathrm{d}\beta_q \, \mathrm{d}\Omega^{(d-2)} \, (\alpha_q \beta_q - q^2)^{-\epsilon} \,, \tag{2.52}$$

where in the last step we traded the integration over $q_\perp^2$ for the integration over $q^2$. Using the fact that the function $F_s$ in Eq. (2.49) is independent of the directions of the vector $q_\perp$, we integrate over directions of the vector $q_\perp$ and the variables $\alpha_q$ and $\beta_q$, and obtain

$$I_s = \frac{\Omega^{(d-2)}}{4} \int_0^{1-z} \mathrm{d}q^2 \, \left( (1-z) - q^2 \right)^{-\epsilon} \, F_s(p \cdot q, \bar{p} \cdot q, q^2) \big|_{p \cdot q = 1/2, \, \bar{p} \cdot q = (1-z)/2} \,. \tag{2.53}$$

We now discuss how this integral can be computed. We note that, in spite of its appearance, the function $F_s$ in Eq. (2.50) is a non-trivial function of a *single variable* $x = q^2/(4(p \cdot q)\,(\bar{p} \cdot q))$; the remaining dependences on the other two variables, say $p \cdot q$ and $\bar{p} \cdot q$, follow from dimensional analysis and are homogeneous. Hence, we can write

$$F_s(p \cdot q, \bar{p} \cdot q, q^2) = (2p \cdot q)^{\omega_1} (2\bar{p} \cdot q)^{\omega_2} \, \tilde{F}_s \left( \frac{q^2}{4(p \cdot q)\,(\bar{p} \cdot q)} \right) \,, \tag{2.54}$$

where $\omega_{1,2}$ are two, potentially $\epsilon$-dependent, constants.

Using this representation in Eq. (2.53) and observing that the factor $(2\bar{p} \cdot q)^{\omega_2}$ provides the only source of the $(1-z)$-dependence in the function $F_s$, we find

$$I_s = \frac{\Omega^{(d-2)}}{4} (1-z)^{-2-3\epsilon} \int_0^1 \mathrm{d}x \, (1-x)^{-\epsilon} \, \tilde{F}_s(x) \,. \tag{2.55}$$

Hence, to compute the boundary constant $C$ we need to determine the function $\tilde{F}_s(x)$ and integrate it over $x$ from zero to one with the weight shown in Eq. (2.55).

It is quite challenging to compute the function $\tilde{F}_s(x)$ by directly integrating Eq. (2.50). A more elegant way to do this is to use the definition of the function $\tilde{F}_s$ to construct a differential equation that this function satisfies; we do this by using integration-by-parts identities. Of course, closing the system of differential equations requires the introduction of many more integrals in addition to the one in Eq. (2.50), but these integrals are simpler. We find that 22 integrals, including $\tilde{F}_s$, are needed to close the system of differential equations with respect to the variable $x$.

To solve these differential equations we require boundary constants; we determine them by considering the $x \to 1$ limit. Physically, this limit corresponds to vanishing transverse momentum $q_\perp$. We will now discuss a few examples of integrals that need to be calculated to determine the boundary conditions.

The simplest integral reads

$$I_1 = \int [\mathrm{d}k_1][\mathrm{d}k_2] (2\pi)^{d-1} \delta^{(d)}(q - k_1 - k_2) \int \frac{\mathrm{d}^d k_3}{(2\pi)^d} \frac{1}{k_3^2 (k_3 + q)^2} \,. \tag{2.56}$$

In contrast to other cases considered below, this integral can be computed exactly. We begin by integrating over the loop momentum $k_3$ and find

$$\int \frac{\mathrm{d}^d k_3}{(2\pi)^d} \frac{1}{k_3^2 (k_3+q)^2} = \frac{\mathrm{i}}{(4\pi)^{d/2}} \frac{\Gamma^2(1-\epsilon)\Gamma(\epsilon)}{\Gamma(2-2\epsilon)} \left(-q^2\right)^{-\epsilon} . \tag{2.57}$$

The remaining integrations over $k_{1,2}$ are also elementary. Performing them, we obtain

$$I_1 = \frac{\mathrm{i}\Gamma^2(1+\epsilon)}{(4\pi)^d} \mathrm{e}^{\mathrm{i}\pi\epsilon} \frac{\Gamma^3(1-\epsilon)}{\epsilon\,\Gamma^2(2-2\epsilon)\Gamma(1+\epsilon)}\, x^{-2\epsilon} \left(4(p\cdot q)\,(\bar{p}\cdot q)\right)^{-2\epsilon} . \tag{2.58}$$

A slightly more complicated integral reads

$$I_2 = \int [\mathrm{d}k_1][\mathrm{d}k_2](2\pi)^{d-1}\delta^{(d)}(q-k_1-k_2) \int \frac{\mathrm{d}^d k_3}{(2\pi)^d} \frac{1}{k_{13}^2\,(\bar{p}\cdot k_3)\,(p\cdot k_{123})} . \tag{2.59}$$

To compute it, we calculate the loop integral and find

$$\int \frac{\mathrm{d}^d k_3}{(2\pi)^d} \frac{1}{k_{13}^2\,(\bar{p}\cdot k_3)\,(p\cdot k_{123})} = -\frac{\mathrm{i}}{(4\pi)^{d/2}} \frac{4\,\mathrm{e}^{\mathrm{i}\pi\epsilon}\,\Gamma^2(1+\epsilon)\Gamma(1-\epsilon)}{\epsilon^2} \left(2p\cdot k_2\right)^{-\epsilon} \left(2k_1\cdot\bar{p}\right)^{-\epsilon} . \tag{2.60}$$

To integrate over $k_{1,2}$, we consider the rest frame of the vector $q$ and determine the energies of the two partons with momenta $k_{1,2}$ by removing the delta function $\delta^{(d)}(q-k_1-k_2)$. We obtain

$$I_2 = -\frac{\mathrm{i}\Gamma^2(1+\epsilon)}{(4\pi)^d} \mathrm{e}^{\mathrm{i}\pi\epsilon} \frac{4\Gamma^2(1-\epsilon)}{\epsilon^2\Gamma(2-2\epsilon)} \left((q\cdot p)\,(q\cdot\bar{p})\right)^{2\epsilon} (4x)^{-\epsilon} I_\Omega\,, \tag{2.61}$$

where

$$I_\Omega = \frac{1}{\Omega^{(d-1)}} \int \frac{\mathrm{d}\Omega_{\vec{n}}^{(d-1)}}{(1+\vec{a}\cdot\vec{n})^\epsilon (1-\vec{b}\cdot\vec{n})^\epsilon} . \tag{2.62}$$

In Eq. (2.62), $\vec{n}$, $\vec{a}$ and $\vec{b}$ are $(d-1)$-dimensional[5] unit vectors which describe the directions of vectors $k_1$, $p$ and $\bar{p}$ in the rest frame of the vector $q$. Furthermore, when writing Eq. (2.62), we have used the fact that in this frame $\vec{k}_1$ and $\vec{k}_2$ are back-to-back.

It follows from Eq. (2.61) that, in order to determine the boundary condition for the integral $I_2$, we need to analyse the behaviour of $I_\Omega$ in the $x \to 1$ limit. This can be done by noticing that, since $\vec{a}^2 = \vec{b}^2 = 1$, $I_\Omega$ is a function of the scalar product $\vec{a}\cdot\vec{b}$. To relate this scalar product to the variable $x$, we compute the scalar product $p\cdot\bar{p}$ in the rest frame of $q$. We find

$$1 - \vec{a}\cdot\vec{b} = \frac{p\cdot\bar{p}}{p^0\bar{p}^0} = \frac{(p\cdot\bar{p})q^2}{(p\cdot q)(\bar{p}\cdot q)} = 2x\,. \tag{2.63}$$

[5] As indicated by the arrow.

Hence, we conclude that the limit $x \to 1$ corresponds to vectors $\vec{a}$ and $\vec{b}$ being back-to-back. Therefore, computation of the boundary conditions for the integral $I_2$ requires extracting relevant branches from $I_\Omega$ in the limit $\vec{a} \to -\vec{b}$.

The relevant branches can be analysed by introducing a Feynman parameter to combine the two denominators which appear in the integrand in Eq. (2.62). We write

$$\frac{1}{(1+\vec{a}\cdot\vec{n})^\epsilon(1-\vec{b}\cdot\vec{n})^\epsilon} = \frac{\Gamma(2\epsilon)}{\Gamma^2(\epsilon)} \int_0^1 \mathrm{d}y \, \frac{y^{\epsilon-1}(1-y)^{\epsilon-1}}{(1-\vec{\eta}\cdot\vec{n})^{2\epsilon}} \,, \tag{2.64}$$

where $\vec{\eta} = \vec{b}(1-y) - \vec{a}y$. We use this representation in Eq. (2.62) and integrate over the directions of $\vec{n}$ choosing the $z$-axis along the vector $\vec{\eta}$. We find

$$I_\Omega = \frac{\Gamma(2\epsilon)}{\Gamma^2(\epsilon)} \int_0^1 \mathrm{d}y \, \frac{y^{\epsilon-1}(1-y)^{\epsilon-1}}{(1+\eta)^{2\epsilon}} \; {}_2F_1\left(2\epsilon, 1-\epsilon, 2-2\epsilon, \frac{2\eta}{1+\eta}\right) , \tag{2.65}$$

where $\eta = |\vec{\eta}| = \sqrt{1-2y(1-y)(1+\vec{a}\cdot\vec{b})} = \sqrt{1-4(1-x)y(1-y)}$. Hence, $\eta = 1$ at $x = 1$.

Although Eq. (2.65) has no explicit $x \to 1$ or $\eta \to 1$ branches, implicit branches are hidden in the hypergeometric function. To expose them and to extract the relevant $x \to 1$ branches, it is sufficient to rewrite the hypergeometric function in Eq. (2.65) as follows

$$\begin{aligned} {}_2F_1\left(2\epsilon, 1-\epsilon, 2-2\epsilon, \frac{2\eta}{1+\eta}\right) &= \frac{\Gamma(1-3\epsilon)\Gamma(2-2\epsilon)}{\Gamma(2-4\epsilon)\Gamma(1-\epsilon)} {}_2F_1\left(2\epsilon, 1-\epsilon, 3\epsilon, \frac{1-\eta}{1+\eta}\right) \\ &+ \left(\frac{1-\eta}{1+\eta}\right)^{1-3\epsilon} \frac{\Gamma(2-2\epsilon)\Gamma(-1+3\epsilon)}{\Gamma(1-\epsilon)\Gamma(2\epsilon)} {}_2F_1\left(2-4\epsilon, 1-\epsilon, 2-3\epsilon, \frac{1-\eta}{1+\eta}\right) . \end{aligned} \tag{2.66}$$

Both hypergeometric functions in Eq. (2.66) can be expanded in Taylor series around $\eta = 1$ which corresponds to $x = 1$. Furthermore, the two terms in Eq. (2.66) provide two distinct branches that arise in the $x \to 1$ limit, i.e. $\mathcal{O}((1-x)^0)$ and $\mathcal{O}((1-x)^{1-3\epsilon})$.

It follows from the system of differential equations, that coefficients of *both* of these branches can be used to fix some of the boundary constants. Hence, we require the two coefficients $C_{1,2}$ defined through the following equation

$$\lim_{x\to 1} I_2 \sim C_1 + C_2(1-x)^{1-3\epsilon} + \ldots \,, \tag{2.67}$$

These two constants can be readily computed using Eqs. (2.65) and (2.66). Indeed, to compute $C_1$ we can simply set $x = 1$ in these equations. Since we work at fixed $\epsilon$, $(1-x)^{1-3\epsilon} = 0$ at $x = 1$ and we obtain

$$I_\Omega|_{x=1} = \frac{2^{-2\epsilon}\Gamma(1-3\epsilon)\Gamma(2-2\epsilon)}{\Gamma(2-4\epsilon)\Gamma(1-\epsilon)} \,, \tag{2.68}$$

from where $C_1$ is easily determined.

For $C_2$, we need to consider the second term in Eq. (2.66). To extract the $(1-x)^{1-3\epsilon}$ branch, we write

$$\left(\frac{1-\eta}{1+\eta}\right)^{1-3\epsilon} = \left(\frac{1-\eta^2}{(1+\eta)^2}\right)^{1-3\epsilon} \approx (1-x)^{1-3\epsilon} \, (y(1-y))^{1-3\epsilon} \,. \tag{2.69}$$

Hence, by taking the second term in Eq. (2.66), setting the hypergeometric function that appears there to one, and using the simplifications indicated in Eq. (2.69), we obtain

$$
\begin{aligned}
I_\Omega|_{\mathcal{O}((1-x)^{1-3\epsilon})} &= \frac{2^{-2\epsilon}\Gamma(2\epsilon)}{\Gamma^2(\epsilon)} \frac{\Gamma(2-2\epsilon)\Gamma(-1+3\epsilon)}{\Gamma(1-\epsilon)\Gamma(2\epsilon)} (1-x)^{1-3\epsilon} \int_0^1 \mathrm{d}y\, y^{-2\epsilon}\,(1-y)^{-2\epsilon} \\
&= \frac{2^{-2\epsilon}\Gamma(2-2\epsilon)\Gamma(-1+3\epsilon)}{\Gamma(1-\epsilon)\Gamma^2(\epsilon)} \frac{\Gamma^2(1-2\epsilon)}{\Gamma(2-4\epsilon)} (1-x)^{1-3\epsilon}\,,
\end{aligned}
\tag{2.70}
$$

The required boundary conditions are then obtained by combining Eqs. (2.68) and (2.70) with Eq. (2.61).

Finally, we note that a similar analysis of boundary conditions can be performed for all integrals needed for the computation of the original integral $\tilde{F}_s$ shown in Eq. (2.50). However, since $\tilde{F}_s$ *itself* needs to be determined from the system of differential equations, it could have required a calculation of its own boundary constant. Luckily, this is not the case. Indeed, the analysis of the homogeneous part of the differential equations for $\tilde{F}_s$ shows that

$$
\tilde{F}_s = C_s \frac{x^{-1-\epsilon}}{1-x} + \ldots\,, \tag{2.71}
$$

where the ellipses stand for the integral of the inhomogeneous contributions to the differential equation for $\tilde{F}_s$. The striking feature of the homogeneous contribution is that it predicts an $\epsilon$-unregulated singularity in the $x \to 1$ limit and one can use an integral representation for $\tilde{F}_s$ to show that such a singularity does not occur. In fact, in the $x \to 1$ limit, $\tilde{F}_s$ is described by two branches $(1-x)^{-1-3\epsilon}$ and $(1-x)^{-1-\epsilon}$ whose coefficients can be computed but are not needed to construct the solution of the differential equation for $\tilde{F}_s$.

The result for $\tilde{F}_s(x)$ is written in terms of harmonic polylogarithms. To compute the required boundary condition for the original integral $I$, we need to substitute $\tilde{F}_s(x)$ into Eq. (2.55) and integrate over $x$. In principle, this procedure is straightforward but it is made complicated by the fact that, after expansion in $\epsilon$, $\tilde{F}_s(x)$ develops non-integrable singularities at $x = 0$. Hence, before the integration can be completed, one has to re-sum singular $x \to 0$ terms in the expression for $\tilde{F}_s(x)$. We achieve this using the $x \neq 0$ solution as well as the differential equation which predicts the structure of branches of $\tilde{F}_s(x)$ at small values of $x$.

After integrating over $x$, we obtain the following result for the soft limit of the integral

$$
\begin{aligned}
I_s = \mathrm{i}\left(\frac{\mathrm{e}^{\epsilon\gamma_E}}{(4\pi)^\epsilon}4\pi^2\right)^{-3} (1-z)^{-2-3\epsilon}\Bigg[&-\frac{25}{64\epsilon^4} - \frac{23}{32\epsilon^3} + \frac{\frac{11}{4}+\frac{533\pi^2}{768}}{\epsilon^2} \\
&+ \frac{1}{\epsilon}\left(-\frac{85}{8}+\frac{139\pi^2}{128}+\frac{853\zeta_3}{64}\right) + \left(\frac{331}{8} - 4\pi^2 + \frac{361\zeta_3}{32} + \frac{997\pi^4}{30720}\right) \\
&+ \epsilon\left(-\frac{1297}{8}+\frac{479\pi^2}{32}-\frac{157\zeta_3}{4}-\frac{7157\pi^4}{15360}-\frac{15025\pi^2\zeta_3}{768}+\frac{13015\zeta_5}{64}\right) \\
&+ \epsilon^2\left(\frac{5107}{8}-\frac{1817\pi^2}{32}+\frac{1115\zeta_3}{8}+\frac{3401\pi^4}{1920}+\frac{5739\zeta_5}{160}-\frac{2069\pi^2\zeta_3}{128}\right.
\end{aligned}
\tag{2.72}
$$

$$+\frac{416141\pi^6}{1548288}-\frac{14289\zeta_3^2}{128}\Bigg)+\mathcal{O}\left(\epsilon^3\right)\Bigg]\,.$$

According to the above discussion, this result provides the required boundary condition for the integral $I$ defined in Eq. (2.46).

Overall, the RRV master integrals require explicit calculation for eight boundary constants in addition to those discussed in Ref. [23]. The method for relating boundary constants of RRR integrals to integrals for Higgs production in gluon fusion at threshold, discussed at the beginning of this section, can also be applied to the soft region of RRV integrals. This allows us to map these integrals onto those for Higgs production computed in Ref. [108]. We have not systematically employed this connection to calculate the RRV boundary constants, but we did use it to cross-check our results for some of the boundary constants, including the one for $I_s$ in Eq. (2.72) which can be mapped on to the most complicated integral $\mathcal{M}_{13}^S$ from Ref. [108]. More recently, results up to weight 8 for the soft RRV integrals have been published in Ref. [106].

Once the boundary constants are computed and incorporated into the solutions of the differential equations following the steps outlined in the previous section, we obtain the final results for the master integrals that are used to compute the bare beam function. We discuss how this is done in the next section. Before proceeding with this discussion, we note that the results for master integrals can be checked numerically as described in Refs. [22, 23]. We performed this check for many master integrals to ensure their correctness.

### 2.3 Assembly of the bare beam functions

Having discussed the computation of the amplitudes and the integrals required for the calculation of the beam function, we explain how the different contributions are put together. The expansion of the fully unrenormalised, bare partonic beam functions in the strong coupling constant reads

$$B_{ij}^{\rm bare}(t,z)=\sum_{k=0}^{\infty}\left(\frac{\alpha_s^{(0)}}{4\pi}\right)^k B_{ij}^{{\rm bare},(k)}(t,z)\,. \tag{2.73}$$

In Eq. (2.73) $\alpha_s^{(0)}$ denotes the unrenormalised strong coupling constant and the expansion coefficients through N$^3$LO read

$$B_{ij}^{{\rm bare},(0)}(t,z)=\delta_{ij}\delta(t)\delta(1-z)\,, \tag{2.74}$$

$$B_{ij}^{{\rm bare},(1)}(t,z)=\int {\rm d}\Phi_B^{(1,0)}\,|\mathcal{A}_{ij}^{\rm R}|^2\,, \tag{2.75}$$

$$B_{ij}^{{\rm bare},(2)}(t,z)=\int {\rm d}\Phi_B^{(2,0)}\sum_f|\mathcal{A}_{ij,f}^{\rm RR}|^2+\int {\rm d}\Phi_B^{(1,1)}\,2\,{\rm Re}\left[\mathcal{A}_{ij}^{\rm RV}(\mathcal{A}_{ij}^{\rm R})^*\right]\,, \tag{2.76}$$

$$\begin{aligned}B_{ij}^{{\rm bare},(3)}(t,z)=&\int {\rm d}\Phi_B^{(3,0)}\sum_f|\mathcal{A}_{ij,f}^{\rm RRR}|^2+\int {\rm d}\Phi_B^{(2,1)}\sum_f 2\,{\rm Re}\left[\mathcal{A}_{ij,f}^{\rm RRV}(\mathcal{A}_{ij,f}^{\rm RR})^*\right]\\&+\int {\rm d}\Phi_B^{(1,2)}\,2\,{\rm Re}\left[\mathcal{A}_{ij}^{\rm RVV}(\mathcal{A}_{ij}^{\rm R})^*\right]+\int {\rm d}\Phi_B^{(1,2)}\,|\mathcal{A}_{ij}^{\rm RV}|^2\,.\end{aligned} \tag{2.77}$$

The sums over $f$ run over different partonic final states. For example, the term $\sum_f |\mathcal{A}^{\mathrm{RRR}}_{q_iq_j,f}|^2$ includes the processes $q_j \to q_i^* + ggg$ and $q_j \to q_i^* + g\bar{q}_k q_k$. The squared amplitudes for the splitting functions can be generated from diagrams for the partonic process $j \to i^* + f$ as explained in the beginning of this section. Finally, the integration measure is defined as

$$\mathrm{d}\Phi_B^{(n_R,n_V)} = \prod_{i=1}^{n_R}[\mathrm{d}k_i]\prod_{j=1}^{n_V}\frac{\mathrm{d}^d l_j}{(2\pi)^d}\delta\left(2p\cdot k_{1\ldots n_R} - \frac{t}{z}\right)\delta\left(\frac{2\bar{p}\cdot k_{1\ldots n_R}}{s} - (1-z)\right), \tag{2.78}$$

where $k_{1\ldots n_R} = \sum_{i=1}^{n_R} k_i$, $n_R$ is the number of final state partons and $n_V$ is the number of virtual loops that appear in the particular contribution.

While we calculate the RRR and RRV contributions in the way we described in the previous sections, we use a different approach to compute the RVV contribution. As we previously described in Ref. [24], we can bypass a two-loop calculation in a physical gauge by making use of the fact that the splitting functions are gauge invariant and that for the single-collinear limit at two-loop order they have been calculated from limits of $2 \to 2$ scattering matrix elements in Refs. [29, 30, 109]. We use the expressions for the two-loop single-collinear splitting functions $P_{a^*\to a_1 a_2}(z)$ from Ref. [109] together with the soft current from Ref. [110] and cross them to the case of initial state splitting $a_1 \to a^* a_2$ via

$$P_{a_1\to a^* a_2}(z) = (-1)^{2s_a+2s_{a_1}}\frac{n_a}{n_{a_1}}\, z\, P_{a^*\to a_1 a_2}\left(\frac{1}{z}\right). \tag{2.79}$$

In Eq. (2.79) $a^*$, $a_1$ and $a_2$ are the flavours of the partons involved in the splitting and $s_a$ and $s_{a_1}$ are the respective spin quantum numbers. The factors $n_a$ and $n_{a_1}$ are the corresponding spin and colour averaging factors, i.e. $n_q = 2N_c$ and $n_g = (d-2)(N_c^2-1)$. Finally, we integrate them over the constrained single-emission phase space

$$\begin{aligned}\int \mathrm{d}\Phi_B^{(1,2)} 2\,\mathrm{Re}\left[\mathcal{A}^{\mathrm{RVV}}_{ij}(\mathcal{A}^{\mathrm{R}}_{ij})^*\right] = &\int [\mathrm{d}^d k]\,\delta\left(2k\cdot p - \frac{t}{z}\right)\delta\left(\frac{2k\cdot\bar{p}}{s} - (1-z)\right)\\ &\times (64\pi^2)\frac{2}{\tilde{s}_{12}}\left(-\frac{\tilde{s}_{12}}{\mu^2}\right)^{-2\epsilon}\frac{2\,\mathrm{Re}[P^{(2)}_{j\to i^* f}(z)]}{z},\end{aligned} \tag{2.80}$$

where $\tilde{s}_{12} = (p-k)^2 = -t/z$. The phase-space integration is trivial because of the delta functions.

For the RV$^2$ contribution, which contains the square of one-loop amplitudes, we generate the relevant amplitudes while keeping track of which propagators belong to $\mathcal{A}^{\mathrm{RV}}_{ij}$ and which to $(\mathcal{A}^{\mathrm{RV}}_{ij})^*$. It turns out that we can re-use the master integrals calculated in Ref. [111] provided that we do not use symmetries of integrals which mix propagators with their complex conjugate counterparts.

For the RRR and RRV contributions we generate the amplitudes for the splitting functions using the setup described above. The number of combinations of relevant diagrams, as well as the number of scalar integrals before IBP reduction, and the number of master integrals before and after applying partial fraction relations are collected in Table 1. Once

**Table 1**. We show, for individual partonic processes, the number of combinations of relevant diagrams, the number of scalar integrals before IBP reduction, as well as the number of master integrals before and after eliminating partial fraction (PF) relations between master integrals.

| Contrib. | Process | Diagram comb. | Scalar int. | MIs before PF | MIs after PF |
|---|---|---|---|---|---|
| RRR | $q \to q^* + ggg$ | $16 \times 16 = 256$ | 126255 | 139 | 91 |
| | $q \to q^* + gq\bar{q}$ | $10 \times 10 = 100$ | 33700 | 241 | 200 |
| | $\bar{q} \to q^* + g\bar{q}\bar{q}$ | $10 \times 10 = 100$ | 3649 | 207 | 175 |
| | $g \to q^* + \bar{q}gg$ | $16 \times 16 = 256$ | 212882 | 329 | 214 |
| | $g \to q^* + \bar{q}q\bar{q}$ | $10 \times 10 = 100$ | 25707 | 136 | 123 |
| | $q \to g^* + qgg$ | $16 \times 16 = 256$ | 146630 | 335 | 222 |
| | $q \to g^* + qq\bar{q}$ | $10 \times 10 = 100$ | 18151 | 73 | 65 |
| | $g \to g^* + ggg$ | $25 \times 25 = 625$ | 394415 | 399 | 219 |
| | $g \to g^* + gq\bar{q}$ | $16 \times 16 = 256$ | 49468 | 169 | 153 |
| | overall | | 404086 | 431 | 278 |
| RRV | $q \to q^* + gg$ | $30 \times 3 = 90$ | 97801 | 271 | 115 |
| | $q \to q^* + q\bar{q}$ | $18 \times 2 = 36$ | 24029 | 178 | 119 |
| | $\bar{q} \to q^* + \bar{q}\bar{q}$ | $18 \times 2 = 36$ | 5056 | 184 | 110 |
| | $g \to q^* + \bar{q}g$ | $30 \times 3 = 90$ | 131856 | 367 | 166 |
| | $q \to g^* + qg$ | $33 \times 3 = 99$ | 112301 | 363 | 152 |
| | $g \to g^* + gg$ | $68 \times 4 = 272$ | 282894 | 365 | 149 |
| | $g \to g^* + q\bar{q}$ | $33 \times 3 = 99$ | 23796 | 72 | 63 |
| | overall | | 290843 | 420 | 195 |

the master integrals are known, we first rewrite the fully unrenormalised, bare partonic beam function in terms of canonical master integrals

$$B_{ij}^{\text{bare}} = \sum_n c_n I_n = \sum_{n,m} c_n (T^{-1})_{nm} I_{c,m}\,, \tag{2.81}$$

which makes cancellations of spurious poles in $\epsilon$ explicit. Next, we insert the solutions for the canonical master integrals in terms of iterated integrals of the variable $\bar{z}$. As we explained earlier, the $\bar{z} \to 0$ as well as the $t \to 0$ singularities are regulated dimensionally. To construct their expansions in $\epsilon$, we have to use the distributional identities

$$\bar{z}^{-1+b\epsilon} = \frac{\delta(\bar{z})}{b\epsilon} + \sum_{k=0}^{\infty} \frac{b^k \epsilon^k}{k!} \mathcal{D}_k(\bar{z})\,, \tag{2.82}$$

$$\frac{1}{\mu^2}\left(\frac{t}{\mu^2}\right)^{-1+b\epsilon} = \frac{\delta(t)}{b\epsilon} + \sum_{k=0}^{\infty} \frac{b^k \epsilon^k}{k!} \mathcal{L}_k\left(\frac{t}{\mu^2}\right)\,, \tag{2.83}$$

where we use the notation

$$\mathcal{D}_k(\bar{z}) = \left[\frac{\log^k(\bar{z})}{\bar{z}}\right]_+\,, \qquad \mathcal{L}_k\left(\frac{t}{\mu^2}\right) = \frac{1}{\mu^2}\left[\frac{\log^k(t/\mu^2)}{t/\mu^2}\right]_+\,. \tag{2.84}$$

In Eq. (2.84) $[\dots]_+$ denotes standard plus-distributions which regulate limits when their arguments become infinite.[6]

The highest possible pole of the amplitude is $\epsilon^{-6}$ so that, in principle, the canonical master integrals have to be known up to weight six, i.e. including $\vec{I}_c^{(6)}(z)$. However, if we express the amplitude in terms of canonical master integrals, the highest pole that appears there is $\epsilon^{-4}$. The additional poles can only arise from the terms proportional to delta functions in Eqs. (2.82) and (2.83). Therefore, the weight six terms $\vec{I}_c^{(6)}(z)$ of the canonical master integrals are only needed for $\bar{z} = 0$, i.e. for terms proportional to $\delta(\bar{z})$. As such, they can be obtained from the soft limit of the amplitudes and master integrals.

## 3 Matching coefficients

Having computed the fully unrenormalised, bare partonic beam functions, we discuss the extraction of the matching coefficients. As explained in Ref. [11], this is done by absorbing certain collinear $1/\epsilon$-poles of the partonic beam functions into the corresponding parton distribution functions and by removing the remaining $1/\epsilon$-poles through an appropriate renormalisation. A detailed discussion of this procedure was provided in our earlier paper [24], but we repeat it here for completeness. A schematic overview of the required steps is shown in Figure 3.

As the first step, we replace the bare QCD coupling constant with the renormalised one. We use

$$\alpha_s^{(0)} = R(\mu^2) Z_{\alpha_s} \alpha_s(\mu^2)\,, \tag{3.1}$$

where $R(\mu^2) = \left(\mu^2 e^{\gamma_E}/(4\pi)\right)^\epsilon$ and

$$Z_{\alpha_s} = 1 - \frac{\alpha_s}{4\pi}\frac{\beta_0}{\epsilon} + \left(\frac{\alpha_s}{4\pi}\right)^2 \left(\frac{\beta_0^2}{\epsilon^2} - \frac{\beta_1}{2\epsilon}\right) + \mathcal{O}(\alpha_s^3)\,. \tag{3.2}$$

Once this is done, we obtain the bare partonic beam functions $\bar{B}_{ij}^{\text{bare}}$ from the original *fully unrenormalised* bare partonic beam functions $B_{ij}^{\text{bare}}$.

Expanding $\bar{B}_{ij}^{\text{bare}}$ in the renormalised strong coupling yields

$$\bar{B}_{ij}^{\text{bare}} = \sum_{k=0}^{\infty} \left(\frac{\alpha_s}{4\pi}\right)^k \bar{B}_{ij}^{\text{bare},(k)}\,, \tag{3.3}$$

where the expansion coefficients read

$$\bar{B}_{ij}^{\text{bare},(0)} = B_{ij}^{\text{bare},(0)}\,, \tag{3.4}$$

$$\bar{B}_{ij}^{\text{bare},(1)} = \left[R(\mu^2) B_{ij}^{\text{bare},(1)}\right]\,, \tag{3.5}$$

[6]The exact definitions are

$$\int_0^1 \mathrm{d}\bar{z}\, \mathcal{D}_k(\bar{z}) f(\bar{z}) = \int_0^1 \frac{\mathrm{d}\bar{z}}{\bar{z}} \log^k \bar{z}\, \left(f(\bar{z}) - f(0)\right)\,, \quad \int_0^\infty \mathrm{d}t\, \mathcal{L}_k\left(\frac{t}{\mu^2}\right) f(t) = \int_0^\infty \frac{\mathrm{d}t}{t} \log^k\left(\frac{t}{\mu^2}\right) \left(f(t) - f(0)\right)\,.$$

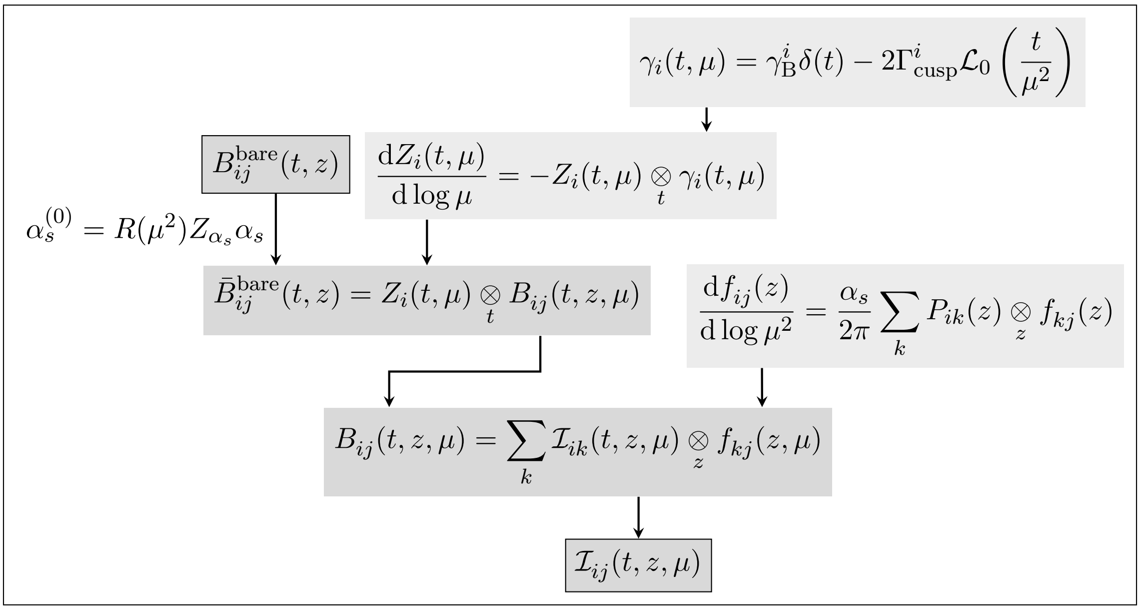


**Figure 3**. Steps required for the extraction of the matching coefficients $\mathcal{I}_{ij}(t,z,\mu)$ from the fully unrenormalised, bare partonic beam functions $B_{ij}^{\rm bare}(t,z,\mu)$, whose calculation is described in the previous section. For a detailed description of the steps see the main text.

$$\bar{B}_{ij}^{\rm bare,(2)} = \left[R(\mu^2)^2 B_{ij}^{\rm bare,(2)}\right] - \frac{\beta_0}{\epsilon}\left[R(\mu^2) B_{ij}^{\rm bare,(1)}\right], \tag{3.6}$$

$$\begin{aligned}\bar{B}_{ij}^{\rm bare,(3)} &= \left[R(\mu^2)^3 B_{ij}^{\rm bare,(3)}\right] - \frac{2\beta_0}{\epsilon}\left[R(\mu^2)^2 B_{ij}^{\rm bare,(2)}\right] \\ &\quad + \left(\frac{\beta_0^2}{\epsilon^2} - \frac{\beta_1}{2\epsilon}\right)\left[R(\mu^2) B_{ij}^{\rm bare,(1)}\right]. \end{aligned}\tag{3.7}$$

The bare partonic beam function is related to the partonic beam function by a renormalisation [11]

$$\bar{B}_{ij}^{\rm bare}(t,z) = Z_i(t,\mu) \underset{t}{\otimes} B_{ij}(t,z,\mu)\,. \tag{3.8}$$

In the above equation the convolution with respect to $t$ is defined through the following equation

$$f_1(t) \underset{t}{\otimes} f_2(t) = \int_0^\infty {\rm d}t_1\,{\rm d}t_2\, f(t_1) f(t_2)\,\delta(t - t_1 - t_2)\,. \tag{3.9}$$

We write expansions for the partonic beam function and the renormalisation constant in $\alpha_s$

$$B_{ij}(t,z,\mu) = \sum_{k=0}^\infty \left(\frac{\alpha_s}{4\pi}\right)^k B_{ij}^{(k)}(t,z,\mu)\,, \tag{3.10}$$

$$Z_i(t,\mu) = \sum_{k=0}^\infty \left(\frac{\alpha_s}{4\pi}\right)^n Z_i^{(k)}(t,\mu)\,, \tag{3.11}$$

make use of the fact that the leading-order coefficients are given by

$$\bar{B}_{ij}^{\text{bare},(0)}(t,z) = B_{ij}^{(0)}(t,z,\mu) = \delta_{ij}\delta(t)\delta(1-z)\,, \qquad Z_i^{(0)}(t,\mu) = \delta(t)\,, \tag{3.12}$$

insert those expansions into Eq. (3.8) and obtain the expansion coefficients of the beam function in terms of those of the bare beam function,

$$B_{ij}^{(1)}(t,z,\mu) = \bar{B}_{ij}^{\text{bare},(1)}(t,z) - \delta_{ij}\delta(1-z)Z_i^{(1)}(t,\mu)\,, \tag{3.13}$$

$$B_{ij}^{(2)}(t,z,\mu) = \bar{B}_{ij}^{\text{bare},(2)}(t,z) - \delta_{ij}\delta(1-z)Z_i^{(2)}(t,\mu) - B_{ij}^{(1)}(t,z,\mu) \underset{t}{\otimes} Z_i^{(1)}(t,\mu)\,, \tag{3.14}$$

$$\begin{aligned} B_{ij}^{(3)}(t,z,\mu) = \bar{B}_{ij}^{\text{bare},(3)}(t,z) &- \delta_{ij}\delta(1-z)Z_i^{(3)}(t,\mu) - B_{ij}^{(2)}(t,z,\mu) \underset{t}{\otimes} Z_i^{(1)}(t,\mu) \\ &- B_{ij}^{(1)}(t,z,\mu) \underset{t}{\otimes} Z_i^{(2)}(t,\mu)\,. \end{aligned} \tag{3.15}$$

To compute the matching coefficients $\mathcal{I}_{ij}$, we use the matching relation for the partonic beam function

$$B_{ij}(t,z,\mu) = \sum_{k\in\{g,u,\bar{u},d,\bar{d},\dots\}} \mathcal{I}_{ik}(t,z,\mu) \underset{z}{\otimes} f_{kj}(z,\mu)\,. \tag{3.16}$$

In Eq. (3.16), $\underset{z}{\otimes}$ stands for the Mellin convolution with respect to the variable $z$. It is defined as follows

$$f_1(z) \underset{z}{\otimes} f_2(z) = \int_0^1 \mathrm{d}z_1 \mathrm{d}z_2\, f_1(z_1) f_2(z_2) \delta(z - z_1 z_2)\,. \tag{3.17}$$

We again expand all quantities in the strong coupling

$$\mathcal{I}_{ij}(t,z,\mu) = \sum_n \left(\frac{\alpha_s}{4\pi}\right)^n \mathcal{I}_{ij}^{(n)}(t,z,\mu)\,, \qquad f_{ij}(z,\mu) = \sum_n \left(\frac{\alpha_s}{2\pi}\right)^n f_{ij}^{(n)}(z)\,, \tag{3.18}$$

use the leading-order coefficients

$$\mathcal{I}_{ij}^{(0)} = \delta_{ij}\delta(t)\delta(1-z)\,, \qquad f_{ij}^{(0)} = \delta_{ij}\delta(1-z)\,, \tag{3.19}$$

insert these expansions in Eq. (3.16), and obtain

$$\mathcal{I}_{ij}^{(1)}(t,z,\mu) = B_{ij}^{(1)}(t,z,\mu) - 2\delta(t) f_{ij}^{(1)}(z)\,, \tag{3.20}$$

$$\mathcal{I}_{ij}^{(2)}(t,z,\mu) = B_{ij}^{(2)}(t,z,\mu) - 4\delta(t) f_{ij}^{(2)}(z) - 2\sum_k \mathcal{I}_{ik}^{(1)}(t,z,\mu) \underset{z}{\otimes} f_{kj}^{(1)}(z)\,, \tag{3.21}$$

$$\begin{aligned} \mathcal{I}_{ij}^{(3)}(t,z,\mu) = B_{ij}^{(3)}(t,z,\mu) &- 8\delta(t) f_{ij}^{(3)}(z) - 4\sum_k \mathcal{I}_{ik}^{(1)}(t,z,\mu) \underset{z}{\otimes} f_{kj}^{(2)}(z) \\ &- 2\sum_k \mathcal{I}_{ik}^{(2)}(t,z,\mu) \underset{z}{\otimes} f_{kj}^{(1)}(z)\,. \end{aligned} \tag{3.22}$$

Finally, we combine Eqs. (3.13,3.14,3.15) with Eqs. (3.20,3.21,3.22), and obtain the expressions for the matching coefficients in terms of the bare beam function

$$\mathcal{I}_{ij}^{(1)}(t,z,\mu) = \bar{B}_{ij}^{\text{bare},(1)}(t,z) - \delta_{ij}\delta(1-z)\, Z_i^{(1)}(t,\mu) - 2\,\delta(t)\, f_{ij}^{(1)}(z)\,, \tag{3.23}$$

$$\begin{aligned}\mathcal{I}_{ij}^{(2)}(t,z,\mu) &= \bar{B}_{ij}^{\text{bare},(2)}(t,z) - \delta_{ij}\delta(1-z)\,Z_i^{(2)}(t,\mu) - 2Z_i^{(1)}(t,\mu)\,f_{ij}^{(1)}(z)\\ &\quad - 4\,\delta(t)\,f_{ij}^{(2)}(z) - Z_i^{(1)}(t,\mu)\underset{t}{\otimes}\mathcal{I}_{ij}^{(1)}(t,z,\mu)\\ &\quad - 2\sum_k \mathcal{I}_{ik}^{(1)}(t,z,\mu)\underset{z}{\otimes} f_{kj}^{(1)}(z)\,,\end{aligned} \tag{3.24}$$

$$\begin{aligned}\mathcal{I}_{ij}^{(3)}(t,z,\mu) &= \bar{B}_{ij}^{\text{bare},(3)}(t,z) - \delta_{ij}\delta(1-z)\,Z_i^{(3)}(t,\mu) - 2Z_i^{(2)}(t,\mu)\,f_{ij}^{(1)}(z)\\ &\quad - 4Z_i^{(1)}(t,\mu)\,f_{ij}^{(2)}(z) - Z_i^{(2)}(t,\mu)\underset{t}{\otimes}\mathcal{I}_{ij}^{(1)}(t,z,\mu) - 8\,\delta(t)\,f_{ij}^{(3)}(z)\\ &\quad - 2\sum_k Z_i^{(1)}(t,\mu)\underset{t}{\otimes}\mathcal{I}_{ik}^{(1)}(t,z,\mu)\underset{z}{\otimes} f_{kj}^{(1)}(z)\\ &\quad - Z_i^{(1)}(t,\mu)\underset{t}{\otimes}\mathcal{I}_{ij}^{(2)}(t,z,\mu) - 4\sum_k \mathcal{I}_{ik}^{(1)}(t,z,\mu)\underset{z}{\otimes} f_{kj}^{(2)}(z)\\ &\quad - 2\sum_k \mathcal{I}_{ik}^{(2)}(t,z,\mu)\underset{z}{\otimes} f_{kj}^{(1)}(z).\end{aligned} \tag{3.25}$$

As Eqs. (3.23,3.24,3.25) demonstrate, we have to compute convolutions of the renormalisation constants and divergent partonic distribution functions with lower-order matching coefficients. For this reason, both NLO and NNLO partonic beam functions are required to higher orders in the expansion in the dimensional regularisation parameter $\epsilon$. The corresponding computations for all relevant partonic beam functions were performed in Ref. [111] and we use the results of that reference in the current calculation.

It remains to explain how to compute the expansion coefficients of the renormalisation constants and of partonic distribution functions. We begin with the renormalisation constants $Z_i$. It is known [11] that these constants satisfy the renormalisation group equation

$$\mu\frac{\mathrm{d}Z_i}{\mathrm{d}\mu} = -Z_i(t,\mu)\underset{t}{\otimes}\gamma_i(t,\mu)\,, \tag{3.26}$$

where the anomalous dimensions read

$$\gamma_i(t,\mu) = \gamma_{\text{B}}^i\delta(t) - 2\Gamma_{\text{cusp}}^i\,\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\,. \tag{3.27}$$

The anomalous dimensions $\Gamma_{\text{cusp}}$ and $\gamma_{\text{B}}^i$ are known through $\mathcal{O}(\alpha_s^4)$ [18, 106, 112–129]. In Eq. (3.27), $\mathcal{L}_0(t/\mu^2)$ is a plus-distribution defined in Eq. (2.84). We integrate Eq. (3.27) to determine the renormalisation constants $Z_{q,g}$. The analytic expressions for these constants through $\mathcal{O}(\alpha_s^3)$ are provided in Appendix C and in an ancillary file.

The perturbative expansion of the partonic distribution functions is obtained by solving the Altarelli-Parisi equation

$$\mu^2\frac{\mathrm{d}f_{ij}(z,\mu^2)}{\mathrm{d}\mu^2} = \frac{\alpha_s(\mu^2)}{2\pi}\sum_k P_{ik}(z)\underset{z}{\otimes} f_{kj}(z,\mu^2)\,, \tag{3.28}$$

order by order in $\alpha_s$ and using the boundary conditions in Eq. (3.19). Since the parton distribution functions in Eq. (3.16) are defined in the $\overline{\text{MS}}$ scheme, the perturbative parton distribution functions should only contain poles in $\epsilon$. Explicit results for the functions

$f_{kj}^{(n)}(z)$, with $n = 1, 2, 3$, in terms of Altarelli-Parisi splitting functions are given in Ref. [24]; we present them in Appendix C for completeness.

We note in passing that the cancellation of infra-red poles that occurs once the renormalisation procedure described in this section is performed, provides a direct cross-check on the three-loop Altarelli-Parisi splitting functions computed in Refs. [113, 114, 130–134].

## 4 Results

We used the procedure described in Sections 2 and 3 to compute the N$^3$LO matching coefficients $\mathcal{I}_{ij}^{(3)}(t, z, \mu)$ for all partonic combinations $(ij) \in \{q_i q_j, qg, gq, gg, q_i\bar{q}_j\}$.

We observe a significant simplification of the alphabet of the iterated integrals that appear in the final result for the matching coefficients compared to the alphabet for the individual master integrals given in Eq. (2.34). Already when inserting the master integrals into the RRR and RRV squared amplitudes some letters cancel completely. In particular, the square root $\sqrt{z}\sqrt{4+z} = \sqrt{1-\bar{z}}\sqrt{5-\bar{z}}$ only appears in integrals entering the RRR contribution and cancels at the level of squared amplitudes. Moreover, upon combining the RRR and RRV contributions, the two letters with the square root $\sqrt{4+z^2} = \sqrt{\bar{z}^2 - 2\bar{z} + 5}$ drop out. The iterated integrals in the final results for the matching coefficients depend only on the following letters

$$f_i(\bar{z}) \in \left\{ \frac{1}{\bar{z}-1}, \frac{1}{\bar{z}}, \frac{1}{\bar{z}+1}, \frac{1}{\bar{z}-2}, \frac{1}{\sqrt{1-\bar{z}}\sqrt{3+\bar{z}}} \right\}. \tag{4.1}$$

The remaining square root corresponds to $\sqrt{z}\sqrt{4-z}$ when written in terms of the variable $\bar{z}$. We note that in total only twelve different iterated integrals that depend on square roots appear in the results and that they only occur in four distinct combinations. We illustrate this below.

It is instructive to discuss the general structure of the matching coefficients. For all partonic channels the $n$-th order matching coefficient can be written as

$$\mathcal{I}_{ij}^{(n)} = \sum_{k=0}^{2n-1} \mathcal{L}_k\left(\frac{t}{\mu^2}\right) F_{ij,+}^{(n,k)}(z) + \delta(t) F_{ij,\delta}^{(n)}(z)\,. \tag{4.2}$$

The function $F_{ij,\delta}^{(n)}$ can be further decomposed as

$$F_{ij,\delta}^{(n)} = C_{ij,-1}^{(n)}\delta(1-z) + \sum_{k=0}^{2n-1} C_{ij,k}^{(n)}\mathcal{D}_k(z) + F_{ij,\delta,h}^{(n)}(z)\,. \tag{4.3}$$

The above decomposition is important because it isolates all the contributions to N$^3$LO matching coefficients which can be predicted without explicit computation. Indeed, the functions $F_{ij,+}^{(n,k)}(z)$ can be obtained from the renormalisation group equation for the beam function [11]. Similarly, the coefficients $C_{ij,k}^{(n)}$ for $k = -1, \ldots, 5$, can be derived by analysing soft contributions to the beam function [135]. The genuinely new result that cannot be obtained without a dedicated calculation is the hard contribution $F_{ij,\delta,h}^{(n)}(z)$. Clearly, the above predictions for certain contributions to the matching coefficients are important since they allow us to check our calculation in a non-trivial way. Finally, we note that our results for the matching coefficients agree with the results published in Ref. [1].

Unfortunately, the results for the matching coefficients are quite sizeable. Because of that, we refrain from displaying them in the paper and, instead, provide them in electronically readable form in an ancillary file. However, to illustrate their structure, we will describe a particular contribution to the matching coefficient $\mathcal{I}_{q_iq_j}$.

In addition to being a function of the energy fraction $z$, the hard contribution $F^{(3)}_{q_iq_j,\delta,h}$ is also a function of the number of colours $N_c$ and the number of fermion species $n_f$. Explicitly, this dependence reads[7]

$$\begin{aligned}F^{(3)}_{q_iq_j,\delta,h}(z) = \delta_{ij}\Bigg[& n_f^2\left(N_c F_{n_f^2 N_c} + \frac{F_{n_f^2 N_c^{-1}}}{N_c}\right) + n_f\left(N_c^2 F_{n_f N_c^2} + F_{n_f} + \frac{F_{n_f N_c^{-2}}}{N_c^2}\right)\\ &+ N_c^3 F_{N_c^3} + N_c F_{N_c} + \frac{F_{N_c^{-1}}}{N_c} + \frac{F_{N_c^{-3}}}{N_c^3}\Bigg] + n_f\left(N_c F_{n_f N_c} + \frac{F_{n_f N_c^{-1}}}{N_c}\right)\\ &+ N_c^2 F_{N_c^2} + F_1 + \frac{F_{N_c^{-2}}}{N_c^2}\,. \end{aligned} \tag{4.4}$$

In writing this decomposition we have used $T_F = \frac{1}{2}$. The coefficients $F_{N_c^3}$, $F_{n_f N_c^2}$ and $F_{n_f^2 N_c}$ were published in Ref. [24]. To illustrate the structure of the new results, we show the coefficient $F_{N_c^{-3}}$, which only contributes for equal flavours, $i = j$, below.

The function $F_{N_c^{-3}}$ features iterated integrals with square-root-valued letters as well as square roots in the coefficients of the iterated integrals. We use the notation

$$L_{a,\vec{b}}(\bar{z}) = \int_0^{\bar{z}} \mathrm{d}t\, f_a(t) L_{\vec{b}}(t)\,, \qquad L_a(\bar{z}) = \int_0^{\bar{z}} \mathrm{d}t\, f_a(t)\,, \qquad L_{\underbrace{0,\ldots,0}_{n}}(\bar{z}) = \frac{1}{n!}\log^n(\bar{z}) \tag{4.5}$$

for the iterated integrals and the letters

$$\begin{aligned} f_{-1}(\bar{z}) &= \frac{1}{\bar{z}+1}\,, & f_0(\bar{z}) &= \frac{1}{\bar{z}}\,, & f_1(\bar{z}) &= \frac{1}{\bar{z}-1}\,,\\ f_2(\bar{z}) &= \frac{1}{\bar{z}-2}\,, & f_r(\bar{z}) &= \frac{1}{\sqrt{1-\bar{z}}\sqrt{3+\bar{z}}}\,. \end{aligned} \tag{4.6}$$

Following the standard practice, we suppress the argument $\bar{z}$ of the iterated integrals for brevity. We note that the iterated integrals that depend on square roots only occur in four distinct combinations throughout all matching coefficients. They are given by

$$R_1 = L_{r,0,1} + \frac{2}{3}L_{r,1,1} - \frac{\pi^2}{6}L_r\,, \tag{4.7}$$

$$R_2 = L_{r,r,0,1} + \frac{2}{3}L_{r,r,1,1} - \frac{\pi^2}{6}L_{r,r}\,, \tag{4.8}$$

[7] For better readability, we suppress flavour- and order-related indices and the argument $z$ on the right-hand side in Eq. (4.4).

$$R_3 = L_{0,r,r,0,1} + \frac{2}{3}L_{0,r,r,1,1} - \frac{\pi^2}{6}L_{0,r,r}\,, \tag{4.9}$$

$$R_4 = L_{1,r,r,0,1} + \frac{2}{3}L_{1,r,r,1,1} - \frac{\pi^2}{6}L_{1,r,r}\,. \tag{4.10}$$

With these abbreviations the coefficient $F_{N_c^{-3}}$ reads

$$\begin{aligned}
F_{N_c^{-3}} = &\frac{1}{12}\big(-2116\bar{z}+15\big) + \frac{1}{12}\big(1344\bar{z}+31\big)L_0 + \frac{1}{48}\big(-947\bar{z}-2390\big)L_1 \\
&+ \frac{1}{3}\big(5\bar{z}-12\big)L_{0,0} + \frac{1}{6}\big(143\bar{z}-68\big)L_{0,1} + \frac{1}{6}\big(-253\bar{z}+569\big)L_{1,0} \\
&+ \frac{1}{24}\big(16\bar{z}^2-1147\bar{z}+482\big)L_{1,1} + 3\big(9\bar{z}+1\big)L_{0,0,0} + \frac{1}{6}\big(-113\bar{z}+34\big)L_{0,0,1} \\
&+ \frac{1}{2}\big(-61\bar{z}-26\big)L_{0,1,0} + \frac{1}{6}\big(95\bar{z}-6\big)L_{0,1,1} - \frac{19}{6}\big(19\bar{z}-14\big)L_{1,0,0} \\
&+ \frac{1}{2}\big(60\bar{z}-31\big)L_{1,0,1} + \frac{1}{12}\big(1307\bar{z}-936\big)L_{1,1,0} + \frac{1}{6}\big(118\bar{z}-197\big)L_{1,1,1} \\
&- \frac{2}{3}\big(24\bar{z}-17\big)L_{1,2,1} + 12\bar{z}L_{0,0,0,0} + \frac{1}{3}\big(-41\bar{z}+2\big)L_{0,0,0,1} \\
&+ \frac{1}{3}\big(-57\bar{z}+26\big)L_{0,0,1,0} + \frac{4}{3}\big(10\bar{z}+3\big)L_{0,0,1,1} - \frac{2}{3}\big(11\bar{z}+2\big)L_{0,1,0,0} \\
&+ \frac{1}{3}\big(47\bar{z}-2\big)L_{0,1,0,1} + \frac{2}{3}\big(3\bar{z}-10\big)L_{0,1,1,0} - \frac{4}{3}\big(41\bar{z}-6\big)L_{0,1,1,1} \\
&+ \frac{4}{3}\big(7\bar{z}-2\big)L_{0,1,2,1} - 3\big(13\bar{z}-14\big)L_{1,0,0,0} + \frac{1}{6}\big(143\bar{z}-150\big)L_{1,0,0,1} \\
&+ \frac{1}{2}\big(99\bar{z}-130\big)L_{1,0,1,0} + \frac{1}{2}\big(-83\bar{z}+108\big)L_{1,0,1,1} + \frac{1}{6}\big(409\bar{z}-442\big)L_{1,1,0,0} \\
&+ \frac{1}{3}\big(-101\bar{z}+113\big)L_{1,1,0,1} + \frac{1}{6}\big(-463\bar{z}+568\big)L_{1,1,1,0} - \frac{1}{2}\big(\bar{z}+9\big)L_{1,1,1,1} \\
&+ 4\big(13\bar{z}-14\big)L_{1,1,2,1} - 4\big(5\bar{z}-4\big)L_{1,2,1,0} + \frac{4}{3}\big(42\bar{z}-37\big)L_{1,2,1,1} \\
&- \frac{4}{3}\big(53\bar{z}-54\big)L_{1,2,2,1} + \big(1+\bar{z}\big)\Bigg(\frac{1}{3}\big(2\bar{z}-11\big)L_{2,1} - \frac{8}{3}L_{2,1,0} + \frac{94}{3}L_{2,1,1} \\
&- \frac{44}{3}L_{2,2,1} + 16L_{2,1,0,1} + \frac{28}{3}L_{2,1,1,0} - 24L_{2,1,1,1} + 40L_{2,1,2,1} - \frac{56}{3}L_{2,2,1,0} \\
&+ 32L_{2,2,1,1} - \frac{152}{3}L_{2,2,2,1} + 60L_{0,0,0,0,0} - 12L_{1,0,0,0,0} + 16L_{1,0,0,0,1} \\
&+ 14L_{1,0,0,1,0} - \frac{55}{3}L_{1,0,0,1,1} + 12L_{1,0,1,0,0} - \frac{50}{3}L_{1,0,1,0,1} - 27L_{1,0,1,1,0} \\
&+ 29L_{1,0,1,1,1} + 24L_{1,1,0,0,0} - 28L_{1,1,0,0,1} - \frac{64}{3}L_{1,1,0,1,0} + \frac{70}{3}L_{1,1,0,1,1} \\
&- \frac{73}{3}L_{1,1,1,0,0} + \frac{58}{3}L_{1,1,1,0,1} + \frac{97}{6}L_{1,1,1,1,0} + \frac{5}{2}L_{1,1,1,1,1} + \frac{28}{3}L_{1,1,1,2,1} \\
&- 4L_{1,1,2,1,0} + \frac{20}{3}L_{1,1,2,1,1} - 4L_{1,1,2,2,1} + \bigg(-\frac{22}{9}L_{2,1} - 9L_{0,0,0} + \frac{11}{6}L_{1,0,0} \\
&- \frac{35}{18}L_{1,0,1} - \frac{29}{9}L_{1,1,0} + \frac{31}{12}L_{1,1,1}\bigg)\pi^2 + \bigg(40L_{0,0} - 8L_{1,0} + 11L_{1,1}\bigg)\zeta_3
\end{aligned}$$

$$
\begin{aligned}
&+\left(\frac{25}{72}L_0-\frac{13}{180}L_1\right)\pi^4-6\pi^2\zeta_3+24\zeta_5\Bigg)+\frac{\bar{z}^2-2\bar{z}+2}{\bar{z}}\Bigg(\frac{83}{48}L_1+L_{0,1}\\
&-\frac{1}{3}L_{1,0}-\frac{29}{24}L_{1,1}-4L_{0,0,1}-\frac{11}{3}L_{0,1,0}+14L_{0,1,1}-\frac{13}{3}L_{1,0,0}+15L_{1,0,1}\\
&-\frac{9}{4}L_{1,1,0}+\frac{11}{3}L_{1,1,1}+\frac{5}{3}L_{1,2,1}+3L_{0,0,1,0}-\frac{9}{2}L_{0,0,1,1}+6L_{0,1,0,0}\\
&-8L_{0,1,0,1}-\frac{41}{2}L_{0,1,1,0}+\frac{63}{2}L_{0,1,1,1}+9L_{1,0,0,0}-\frac{27}{2}L_{1,0,0,1}-\frac{23}{2}L_{1,0,1,0}\\
&+23L_{1,0,1,1}-\frac{23}{2}L_{1,1,0,0}+18L_{1,1,0,1}+\frac{7}{2}L_{1,1,1,0}+4L_{1,2,1,1}+84L_{0,0,0,0,1}\\
&+72L_{0,0,0,1,0}-114L_{0,0,0,1,1}+66L_{0,0,1,0,0}-80L_{0,0,1,0,1}-68L_{0,0,1,1,0}\\
&+\frac{296}{3}L_{0,0,1,1,1}+\frac{32}{3}L_{0,0,1,2,1}+66L_{0,1,0,0,0}-\frac{236}{3}L_{0,1,0,0,1}-68L_{0,1,0,1,0}\\
&+\frac{226}{3}L_{0,1,0,1,1}-\frac{248}{3}L_{0,1,1,0,0}+\frac{164}{3}L_{0,1,1,0,1}+74L_{0,1,1,1,0}+14L_{0,1,1,1,1}\\
&-\frac{128}{3}L_{0,1,1,2,1}+24L_{0,1,2,1,0}-\frac{140}{3}L_{0,1,2,1,1}+\frac{112}{3}L_{0,1,2,2,1}+4L_{1,0,-1,0,1}\\
&+72L_{1,0,0,0,0}-82L_{1,0,0,0,1}-\frac{206}{3}L_{1,0,0,1,0}+\frac{220}{3}L_{1,0,0,1,1}-\frac{208}{3}L_{1,0,1,0,0}\\
&+\frac{212}{3}L_{1,0,1,0,1}+\frac{182}{3}L_{1,0,1,1,0}-50L_{1,0,1,1,1}-\frac{32}{3}L_{1,0,1,2,1}-74L_{1,1,0,0,0}\\
&+68L_{1,1,0,0,1}+\frac{152}{3}L_{1,1,0,1,0}-\frac{58}{3}L_{1,1,0,1,1}+\frac{170}{3}L_{1,1,1,0,0}-44L_{1,1,1,0,1}\\
&-4L_{1,1,1,1,0}-4L_{1,1,1,1,1}-\frac{40}{3}L_{1,1,1,2,1}-\frac{16}{3}L_{1,1,2,1,0}-10L_{1,1,2,1,1}\\
&+28L_{1,1,2,2,1}+16L_{1,2,1,0,1}+\frac{28}{3}L_{1,2,1,1,0}-24L_{1,2,1,1,1}+40L_{1,2,1,2,1}\\
&-\frac{56}{3}L_{1,2,2,1,0}+32L_{1,2,2,1,1}-\frac{152}{3}L_{1,2,2,2,1}+\Bigg(\frac{35}{36}L_1-\frac{5}{6}L_{0,1}-\frac{17}{12}L_{1,0}\\
&+\frac{21}{8}L_{1,1}-\frac{28}{3}L_{0,0,1}-\frac{82}{9}L_{0,1,0}+\frac{21}{2}L_{0,1,1}-\frac{1}{3}L_{1,0,-1}-\frac{59}{6}L_{1,0,0}\\
&+\frac{64}{9}L_{1,0,1}+\frac{73}{9}L_{1,1,0}-\frac{14}{3}L_{1,1,1}-\frac{22}{9}L_{1,2,1}\Bigg)\pi^2+\Bigg(13L_1+34L_{0,1}\\
&+42L_{1,0}-\frac{76}{3}L_{1,1}\Bigg)\zeta_3+\frac{371}{1080}L_1\pi^4\Bigg)+\Bigg(\frac{1}{18}\big(-\bar{z}^2-22\bar{z}+26\big)\\
&+\frac{1}{36}\big(-108\bar{z}+11\big)L_0+\frac{1}{18}\big(55\bar{z}-47\big)L_1-\frac{16}{9}\bar{z}L_{0,0}+\frac{1}{9}\big(18\bar{z}-1\big)L_{0,1}\\
&+\frac{1}{12}\big(55\bar{z}-52\big)L_{1,0}+\frac{1}{72}\big(-553\bar{z}+586\big)L_{1,1}\Bigg)\pi^2+\Bigg(\frac{1}{6}\big(235\bar{z}-18\big)\\
&-\frac{2}{3}\big(29\bar{z}-64\big)L_1\Bigg)\zeta_3+\frac{1}{1080}\big(187\bar{z}+92\big)\pi^4-\frac{3\sqrt{1-\bar{z}}\big(5\bar{z}+14\big)}{\sqrt{3+\bar{z}}}R_1\\
&-15\bar{z}R_2+6\big(\bar{z}-2\big)R_4+\frac{\bar{z}^2-2\bar{z}+2}{\bar{z}}\left(18R_3-6R_4\right)\,. \qquad (4.11)
\end{aligned}
$$

We note that the expressions that contain square roots either as coefficients or as letters of the iterated integrals are confined to the *last four terms* of the above formula and are very compact. The structure of the results for other colour factors and also for the other matching coefficients is quite similar to what is shown in Eq. (4.11).

It is obvious that, for practical computations, it is important to be able to evaluate the matching coefficients numerically. From this perspective, the result shown above is not optimal as the numerical evaluation of iterated integrals with square-root-valued letters is complicated. It is possible to get around this problem by providing the expansion of the matching coefficient in powers of $z$ and/or $\bar{z}$ as was done in Ref. [1].

Here, we note that it is also possible to obtain an expression for the matching coefficient which is suitable for numerical evaluation, by rationalising the only square-root-valued letter that appears in the final result. Indeed, since the matching coefficients only depend on a single square root, we express those iterated integrals which actually depend on this square root in terms of Goncharov polylograrithms (GPLs) using the rationalising variable transformation from Eq. (2.30). These GPLs are then evaluated at the argument

$$x = \frac{\sqrt{z} + \mathrm{i}\sqrt{4-z}}{\sqrt{z} - \mathrm{i}\sqrt{4-z}}\,. \tag{4.12}$$

The remaining iterated integrals only depend on linear letters and therefore also fall into the class of GPLs, but they are still evaluated at the argument $\bar{z}$. Also the algebraic coefficients in front of the integrals are expressed in terms of $\bar{z}$. The use of these mixed arguments in the iterated integrals allows for a relatively compact representation of the matching coefficients which is straightforward to evaluate numerically. The corresponding expressions for the matching coefficients are also included in an ancillary file.

## 5 Conclusions

In this paper, we have described the computation of the matching coefficients for $N$-jettiness beam functions through third order in perturbative QCD. This computation extends our previous results reported in Ref. [24], where only the generalised leading-colour contribution to the $q \to q$ matching coefficient was presented.

Although beam functions were originally defined in soft-collinear effective theory, we benefited from the observation made in Ref. [26] that matching coefficients can be computed by integrating collinear splitting functions over the $N$-jettiness phase space simplified in the collinear limits. This observation together with the known fact that collinear splitting functions can be calculated in a process-independent way if physical gauges are used, opened up a way to compute the matching coefficients as described in this paper.

To simplify the actual computation, we made use of reverse unitarity which allowed us to map the various real emission integrals onto loop-like integrals. We then employed the (by now) standard machinery for computing loop integrals, such as integration by parts, differential equations, canonical bases etc. to make the computation manageable. It is worth noting that, although we were able to construct a canonical basis for all the master integrals involved in the computation, this could not be always done with publicly-available programs because multiple square roots appeared in an alphabet associated with the differential equations. Because of this, we had to resort to a manual construction of candidate integrals for the canonical basis by studying their leading singularities in the Baikov representation.

Another non-trivial aspect of the calculation involves the computation of the boundary conditions for the master integrals. We calculated the required boundary conditions by studying the soft $z \to 1$ limit of the master integrals. Interestingly, it turns out that many boundary constants that we require for this computation are related to the boundary constants which appear in the calculation of the N$^3$LO QCD corrections to Higgs boson production cross section obtained in Refs. [103]. This relation allows us to compare the boundary constants that we computed in this and earlier papers [22, 23] with the results of Refs. [103], offering a welcome cross-check at the intermediate stages of the calculation.

We computed the matching coefficients for the $q_i q_j$, $qg$, $gq$, $gg$ and $q_i \bar{q}_j$ partonic channels. The results are written as linear combinations of plus-distributions and regular functions given by linear combinations of iterated integrals with mostly rational $z$-dependent coefficients. As we pointed out in Section 2, the differential equations for individual master integrals involve various square roots of second degree $z$-polynomials. It is interesting that many of these square roots disappear from the final answer, when all the master integrals are combined. In fact, *all* such square roots should disappear in the divergent parts of the partonic beam functions since these divergences are removed, e.g., by collinear counter-terms that involve Altarelli-Parisi splitting functions. These functions were first calculated through N$^3$LO in Refs. [113, 114] and are known to contain no square roots of $z$-polynomials.

The matching coefficients computed in this paper have been already calculated in Ref. [1]. Our calculation agrees with these results and provides a completely independent check of the matching coefficients reported in that reference. It goes without saying that for computations of such a complexity, an independent confirmation is always welcome.

The application of the $N$-jettiness slicing scheme to collider processes requires calculation of beam functions, jet functions and soft functions. The beam functions are universal in that they do not depend on the number of jets in the final state; the same applies to jet functions and, by now, both are known through N$^3$LO in perturbative QCD.[8] The soft functions, on the other hand, are not known at that perturbative order even for the simplest zero-jettiness case, in spite of the interesting progress in recent years [138–140]. Hence, to fully unlock the potential of the $N$-jettiness slicing scheme for N$^3$LO QCD computations, further progress with computing $N$-jettiness soft-functions at N$^3$LO is needed.

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[8]The N$^3$LO QCD contributions to jet functions were computed in Refs. [136, 137]

**Table 2**. Integral family definitions for the example on partial fraction relations.

| $f$ | T1 | T28 | T29 | T30 |
|---|---|---|---|---|
| $D_1^f$ | $k_1^2$ | | | |
| $D_2^f$ | $k_2^2$ | | | |
| $D_3^f$ | $k_3^2$ | | | |
| $D_4^f$ | $2k_{123} \cdot p - \frac{t}{z}$ | | | |
| $D_5^f$ | $\frac{2k_{123} \cdot \bar{p}}{s} - (1-z)$ | | | |
| $D_6^f$ | $(k_1 - p)^2$ | $(k_1 - p)^2$ | $(k_1 - p)^2$ | $k_{12}^2$ |
| $D_7^f$ | $(k_2 - p)^2$ | $(k_2 - p)^2$ | $(k_2 - p)^2$ | $(k_1 - p)^2$ |
| $D_8^f$ | $(k_{12} - p)^2$ | $(k_{12} - p)^2$ | $(k_{12} - p)^2$ | $(k_{12} - p)^2$ |
| $D_9^f$ | $(k_{13} - p)^2$ | $(k_{13} - p)^2$ | $(k_{13} - p)^2$ | $(k_{13} - p)^2$ |
| $D_{10}^f$ | $(k_{123} - p)^2$ | $(k_{123} - p)^2$ | $(k_{123} - p)^2$ | $(k_{123} - p)^2$ |
| $D_{11}^f$ | $k_1 \cdot \bar{p}$ | $k_1 \cdot \bar{p}$ | $k_{13} \cdot \bar{p}$ | $k_1 \cdot \bar{p}$ |
| $D_{12}^f$ | $k_2 \cdot \bar{p}$ | $k_{13} \cdot \bar{p}$ | $k_3 \cdot \bar{p}$ | $k_{12} \cdot \bar{p}$ |

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## A Example of deriving partial fraction relations

In this appendix, we discuss an example to illustrate the algorithm that was used to find partial fraction relations between different integrals. This algorithm was first proposed in Ref. [55]; a clear and concise description was provided in Ref. [56]. More details about the relevant mathematical concepts can be found in standard textbooks on the subject (see, for example, Ref. [142]).

We consider the following problem. Suppose that there exists a number of integral families constructed in some way starting from relevant Feynman diagrams. An example is given in Table 2 where four families are displayed. The integrals described by these families read

$$I^f_{a_1\ldots a_{12}} = \frac{1}{(2\pi)^{3d}} \int \frac{\mathrm{d}^d k_1\, \mathrm{d}^d k_2\, \mathrm{d}^d k_3}{[D^f_1]^{a_1}_c \ldots [D^f_5]^{a_5}_c (D^f_6)^{a_6} \ldots (D^f_{12})^{a_{12}}}\,, \tag{A.1}$$

where $[\ldots]_c$ denotes a cut propagator which implements a delta-function constraint via reverse unitarity. We would like to find if all integrals that belong to these four families are independent, and to derive linear relations between them if they are not.

Since each family contains enough inverse propagators to describe all independent scalar products between $p$, $\bar{p}$ and $k_{1,2,3}$, there exist linear relations between inverse propagators of different families shown in Table 2, and it is these linear relations that, potentially, lead to useful partial fraction relations. To find these relations, the first step is to combine all inverse propagators that belong to different families into an overcomplete set. For the sake of simplicity, we consider the topology T1 and add $D^{\mathrm{T30}}_{12}$ to its inverse propagators, so that a toy version of the overcomplete set reads

$$\left\{D^{\mathrm{T1}}_1, \ldots, D^{\mathrm{T1}}_{12}, D^{\mathrm{T30}}_{12}\right\}\,. \tag{A.2}$$

Since there are twelve independent scalar products and thirteen inverse propagators, there is one linear relation between elements of the list in Eq. (A.2); it reads

$$0 = D^{\mathrm{T1}}_{11} + D^{\mathrm{T11}}_{12} - D^{\mathrm{T30}}_{12}\,. \tag{A.3}$$

To find a partial fraction relation, we divide Eq. (A.3) by the product of the three propagators and obtain

$$0 = \frac{1}{D^{\mathrm{T1}}_{12} D^{\mathrm{T30}}_{12}} + \frac{1}{D^{\mathrm{T1}}_{11} D^{\mathrm{T30}}_{12}} - \frac{1}{D^{\mathrm{T1}}_{11} D^{\mathrm{T1}}_{12}}\,. \tag{A.4}$$

Our goal is to treat both linear relations for the numerators and partial fraction relations for the denominators on the same footing and systematically apply them to integrands of Feynman integrals. To unify the description of numerator and denominator relations, we describe the integrands not as rational functions of the $D^f_i$, but as polynomials in $D^f_i$ and $\tilde{D}^f_i = 1/D^f_i$. We treat the $D^f_i$ and $\tilde{D}^f_i$ as a priori independent variables which are then subject to the relations $D^f_i \tilde{D}^f_i - 1 = 0$, that describe cancelling numerators against denominators. Moreover, in the example at hand the variables are also subject to the linear relation in Eq. (A.3) and the partial fraction relation in Eq. (A.4) which becomes

$$0 = \tilde{D}^{\mathrm{T1}}_{12} \tilde{D}^{\mathrm{T30}}_{12} + \tilde{D}^{\mathrm{T1}}_{11} \tilde{D}^{\mathrm{T30}}_{12} - \tilde{D}^{\mathrm{T1}}_{11} \tilde{D}^{\mathrm{T1}}_{12}\,. \tag{A.5}$$

In this language, the relations between the variables $D^f_i$ and $\tilde{D}^f_i$ are encoded by polynomials that we equate to zero and applying one of these relations can be thought of as extracting one of the polynomials, setting it to zero and keeping the remainder. A trivial example would be a cancellation of some factors in a numerator and a denominator using

$$D^{\mathrm{T1}}_7 \tilde{D}^{\mathrm{T1}}_7 \tilde{D}^{\mathrm{T1}}_8 \tilde{D}^{\mathrm{T1}}_9 = \underbrace{\left(D^{\mathrm{T1}}_7 \tilde{D}^{\mathrm{T1}}_7 - 1\right)}_{=0} \tilde{D}^{\mathrm{T1}}_8 \tilde{D}^{\mathrm{T1}}_9 + \tilde{D}^{\mathrm{T1}}_8 \tilde{D}^{\mathrm{T1}}_9 = \tilde{D}^{\mathrm{T1}}_8 \tilde{D}^{\mathrm{T1}}_9\,. \tag{A.6}$$

Similarly, extracting $D_{11}^{\mathrm{T1}}+D_{12}^{\mathrm{T11}}-D_{12}^{\mathrm{T30}}$ corresponds to eliminating a linear relation between numerators in Eq. (A.3), and extracting $\tilde{D}_{12}^{\mathrm{T1}}\tilde{D}_{12}^{\mathrm{T30}}+\tilde{D}_{11}^{\mathrm{T1}}\tilde{D}_{12}^{\mathrm{T30}}-\tilde{D}_{11}^{\mathrm{T1}}\tilde{D}_{12}^{\mathrm{T1}}$ corresponds to eliminating a partial fraction relation in Eq. (A.4).

To phrase this more generally, given an integrand of a Feynman integral $\mathcal{I}_D$ written as a polynomial in the variables $D_i^f$ and $\tilde{D}_i^f$ and a set of polynomials $\{p_i\}$ that encode relations between the variables, we would like to systematically construct a decomposition

$$\mathcal{I}_D = \sum_i c_{D,i}\, p_i + r_D\,, \tag{A.7}$$

where the coefficients $c_{D,i}$ and the remainder $r_D$ are also polynomials in $D_i^f$ and $\tilde{D}_i^f$. The remainder $r_D$ is equivalent to $\mathcal{I}_D$ because if we consider the case where all relations encoded by the polynomials $p_i$ hold, i.e. where all the $p_i$'s vanish simultaneously, then Eq. (A.7) becomes

$$\mathcal{I}_D\big|_{\{p_i=0\}} = r_D\,. \tag{A.8}$$

Moreover, the remainder should be unique so that if we decompose two or more integrands in this way and find that their remainders are linearly independent over functions of the kinematic variables, the integrands have to be independent. Thus, such a procedure allows us to remove all linear and partial fraction relations between integrands.

In order to make this approach systematic, we have to specify which monomials are preferred over others. For example, in Eq. (A.6) we preferred terms with a lower total degree, i.e. we preferred the term 1 over $D_7^{\mathrm{T1}}\tilde{D}_7^{\mathrm{T1}}$. Intuitively, this ensures that numerators are cancelled against denominators whenever possible. For the linear and partial fraction relations in Eqs. (A.3) and (A.5) all terms have same total degree, so we must use other additional criteria to specify preferred terms. In general, this is done by specifying a *monomial ordering*, which defines an ordering of the exponents of the variables.[9]

The problem we just described is a classic problem in the field of algebraic geometry and corresponds to *finding a canonical representative modulo polynomial ideal*. The set of all linear combinations $\langle\{p_i\}\rangle = \sum_i c_{D,i}\, p_i$, where the $c_{D,i}$ are polynomials in the $D_i^f$ and $\tilde{D}_i^f$, is called the *polynomial ideal* spanned by the polynomials $p_i$. Decomposing a polynomial $\mathcal{I}_D$ into an element of the ideal $\langle\{p_i\}\rangle$ and a remainder $r$ can be achieved using a procedure called *polynomial reduction*. In general, this decomposition is not unique for an arbitrary set of polynomials $\{p_i\}$. However, what is important for us is the set of simultaneous zeros of the polynomials $\{p_i\}$. Therefore, we can choose different sets of polynomials $\{\tilde{p}_i\}$ which have the same set of simultaneous zeros and generate the same polynomial ideal. For each given set of polynomials there exists a particular choice of polynomials, called a *Gröbner basis*, for which the remainder $r_D$ becomes unique. Here, we will not go into detail of how to construct a Gröbner basis and only note that the construction of Gröbner bases

[9] We follow the suggestion from Refs. [55, 56] and use a monomial ordering where we first compare the total degree of two monomials for the variables $\{\tilde{D}_1^f,\ldots,\tilde{D}_{12}^f,D_1^f,\ldots,D_{12}^f\}$. If that is the same, we successively compare the total degrees considering fewer variables, i.e. $\{\tilde{D}_2^f,\ldots,\tilde{D}_{12}^f,D_1^f,\ldots,D_{12}^f\}$, then $\{\tilde{D}_3^f,\ldots,\tilde{D}_{12}^f,D_1^f,\ldots,D_{12}^f\}$, etc.

is implemented in many computer algebra systems. We have used the implementations in Mathematica and Singular [143] for our calculation.

To apply this method to find relations between integrands of Feynman integrals, the idea is to start from the polynomials that encode cancellations between numerators $D_i^f$ and denominators $\tilde{D}_i^f$, i.e. $D_i^f \tilde{D}_i^f - 1$, as well as the linear relations between the numerators. The partial fraction relations between denominators automatically arise as a consequence of the numerator relations.[10] For the toy overcomplete set from Eq. (A.2) we start with

$$L_D = \{D_1^{\rm T1}\tilde{D}_1^{\rm T1} - 1,\ \ldots,\ D_{12}^{\rm T1}\tilde{D}_{12}^{\rm T1} - 1,\ D_{12}^{\rm T30}\tilde{D}_{12}^{\rm T30} - 1,\ D_{11}^{\rm T1} + D_{12}^{\rm T1} - D_{12}^{\rm T30}\}\,. \tag{A.9}$$

We now compute the Gröbner basis for this set and find

$$\begin{aligned} L_D^G = \Big\{ & D_1^{\rm T1}\tilde{D}_1^{\rm T1} - 1,\ \ldots,\ D_{12}^{\rm T1}\tilde{D}_{12}^{\rm T1} - 1,\ (D_{12}^{\rm T1} + D_{11}^{\rm T1})\tilde{D}_{12}^{\rm T30} - 1, \\ & D_{12}^{\rm T30} - D_{12}^{\rm T1} - D_{11}^{\rm T1},\ \tilde{D}_{12}^{\rm T1}\tilde{D}_{12}^{\rm T30} + \tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T30} - \tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T1} \Big\}\,. \end{aligned} \tag{A.10}$$

Compared to Eq. (A.9), the next-to-last polynomial in Eq. (A.9) war reexpressed and the last polynomial in Eq. (A.10) was added. Finally, this Gröbner basis can be used to compute the remainders of the integrands of Feynman integrals via polynomial reduction.

We illustrate this procedure by considering an integral from the topology T1 defined by the integrand

$$I^{\rm T1}_{11111;1010011} = \tilde{D}_1^{\rm T1}\ldots\tilde{D}_5^{\rm T1}\tilde{D}_6^{\rm T1}\tilde{D}_8^{\rm T1}\tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T1}\,. \tag{A.11}$$

Decomposing $I^{\rm T1}_{11111;1010011}$ with respect to the Gröbner basis $L_D^G$ in Eq. (A.10) yields

$$\begin{aligned} I^{\rm T1}_{11111;1010011} = & \left[\tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T1} - \tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T30} - \tilde{D}_{12}^{\rm T1}\tilde{D}_{12}^{\rm T30}\right]\tilde{D}_1^{\rm T1}\ldots\tilde{D}_5^{\rm T1}\tilde{D}_6^{\rm T1}\tilde{D}_8^{\rm T1} \\ & + \tilde{D}_1^{\rm T1}\ldots\tilde{D}_5^{\rm T1}\tilde{D}_6^{\rm T1}\tilde{D}_8^{\rm T1}\tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T30} + \tilde{D}_1^{\rm T1}\ldots\tilde{D}_5^{\rm T1}\tilde{D}_6^{\rm T1}\tilde{D}_8^{\rm T1}\tilde{D}_{12}^{\rm T1}\tilde{D}_{12}^{\rm T30}\,. \end{aligned} \tag{A.12}$$

The first term on the right hand side of Eq. (A.12) is proportional to the last element of the Gröbner basis and therefore vanishes; the last two terms represent the remainder. Hence, we obtain

$$I^{\rm T1}_{11111;1010011} = \tilde{D}_1^{\rm T1}\ldots\tilde{D}_5^{\rm T1}\tilde{D}_6^{\rm T1}\tilde{D}_8^{\rm T1}\tilde{D}_{11}^{\rm T1}\tilde{D}_{12}^{\rm T30} + \tilde{D}_1^{\rm T1}\ldots\tilde{D}_5^{\rm T1}\tilde{D}_6^{\rm T1}\tilde{D}_8^{\rm T1}\tilde{D}_{12}^{\rm T1}\tilde{D}_{12}^{\rm T30}\,. \tag{A.13}$$

Upon inspecting the two integrals on the right hand side of Eq. (A.13), we find that we can map them to the integral families shown in Table 2 provided that we redefine the loop momenta $k_2 \leftrightarrow k_3$. We obtain

$$I^{\rm T1}_{11111;1010011} = I^{\rm T28}_{11111;1001011} + I^{\rm T29}_{11111;1001011}\,. \tag{A.14}$$

This is the partial fraction relation that was displayed in Eq. (2.17). We note that, although we added the linearly-dependent propagator from a family T30 to the twelve propagators of the family T1, the linear relation that we found involves integrals from the families T1, T28, T29. As a final comment we note that, in general, it may still be necessary to reduce integrals found in the last step to master integrals using the IBP relations.

[10] As pointed out in Refs. [58, 59] it is also possible to directly use the independent scalar products as the variables for the numerators. In that case one does not even have to specify the linear relations between numerators since they will automatically be found though the construction of the Gröbner basis.

## B Leading-singularity analysis: an example

In this appendix, we give an explicit example of finding a candidate for a canonical integral based on the analysis of the leading singularities in the Baikov representation [78, 79]. For this example, we consider a family of RRV integrals defined by the inverse propagators[11]

$$\begin{aligned}
&D_1 = k_1^2\,, && D_2 = k_2^2\,, && D_3 = 2k_{12}\cdot p - \frac{t}{z}\,, && D_4 = \frac{2k_{12}\cdot p}{s} - \bar{z}\,,\\
&D_5 = k_3^2\,, && D_6 = k_{12}^2\,, && D_7 = k_{13}^2\,, && D_8 = k_{123}^2\,,\\
&D_9 = (k_1-p)^2\,, && D_{10} = (k_{123}-p)^2\,, && D_{11} = k_2\cdot\bar{p}\,, && D_{12} = k_3\cdot\bar{p}\,.
\end{aligned} \tag{B.1}$$

We focus on the following integral

$$I^{\rm A3}_{1111;10111111} = \frac{1}{(2\pi)^{3d}}\int \frac{{\rm d}^d k_1\,{\rm d}^d k_2\,{\rm d}^d k_3}{[D_1]_c[D_2]_2[D_3]_c[D_4]_c D_5 D_7 D_8 D_9 D_{10} D_{11} D_{12}}\,. \tag{B.2}$$

In Eq. (B.2) $[\ldots]_c$ denotes a cut propagator introduced via reverse unitarity. Note that the propagator $D_6$ is absent in the integrand in Eq. (B.2). We assume that $s = 2p\cdot\bar{p} = 1$ and $t = 1$ since, as we explained in the main text of the paper, the dependence of all integrals on $s$ and $t$ is uniform and can be easily restored. The differential equation in $z$, that $I^{\rm A3}_{1111;10111111}$ satisfies, is not in canonical form. Hence, our goal is to find a new master integral which is directly related to $I^{\rm A3}_{1111;10111111}$ and is canonical.

To proceed, we start by employing the Baikov representation [78, 79] to render the integrand into a convenient form where the propagators $D_i$ take the role of the integration variables. Up to an irrelevant overall prefactor, we therefore write

$$I^{\rm A3}_{1111;10111111} \sim \underset{D_1,D_2,D_3,D_4}{\rm Cut}\int \frac{{\rm d}D_1\ldots{\rm d}D_{12}}{D_1\ldots D_5\,D_7\ldots D_{12}} P(D_1,\ldots,D_{12})^{(d-6)/2}\,. \tag{B.3}$$

In Eq. (B.3) $P(D_1,\ldots,D_{12}) = G(k_1,k_2,k_3,p,\bar{p})|_{p_i\cdot p_j=\sum_k c_k D_k}$ is the so-called Baikov polynomial, i.e. the Gram determinant of the momenta $k_{1,2,3}$ and external momenta $p$ and $\bar{p}$ where all scalar products have been expressed in terms of inverse propagators. The advantage of the Baikov representation for the problem at hand is that it allows us to derive a convenient starting point for the analysis of the cut integrals. Indeed, cutting propagators corresponds to taking residues at $D_i = 0$, $i = 1,2,3,4$, in Eq. (B.3) which, in turn, amounts to simply evaluating the Baikov polynomial at the point $D_1 = D_2 = D_3 = D_4 = 0$.

For the cut integral in Eq. (B.3), the Baikov polynomial reads

$$\begin{aligned}
&P(0,0,0,0,D_5,\ldots,D_{12})\\
&\quad = \frac{1}{16z^2}\big(D_5\bar{z}^2 - D_6\bar{z}^2 - D_7\bar{z}^2 + D_8\bar{z}^2 - D_{5,6}z\bar{z} + D_6^2 z\bar{z} + D_{5,7}z\bar{z} - D_7^2 z\bar{z}\\
&\qquad - D_{5,8}z\bar{z} - D_{6,8}z^2\bar{z} + D_{7,8}(2-z)z\bar{z} - D_8^2 z\bar{z}^2 + 2D_{5,9}z\bar{z}^2 - D_{6,9}z\bar{z}^2 - D_{7,9}z\bar{z}^2\\
&\qquad + D_{8,9}z\bar{z}^2 - D_{6,10}z\bar{z}^2 - D_{7,10}z\bar{z}^2 + D_{8,10}z\bar{z}^2 - 2D_{5,11}\bar{z} + 2D_{6,11}\bar{z} + 2D_{7,11}\bar{z}\\
&\qquad - 4D_{8,11}\bar{z} + 2D_{5,12}\bar{z} - 2D_{6,12}\bar{z} - 2D_{7,12}\bar{z} - D_{5,6,7}z^2 + D_6^2 D_7 z^2 + D_6 D_7^2 z^2
\end{aligned}$$

[11] The first four propagators correspond to delta-function constraints re-written as propagators using reverse unitarity.

$$
\begin{aligned}
&+ D_{5,6,8}z^2 - D_6^2 D_8 z^2\bar{z} - D_{6,7,8}(2-z)z^2 + D_6 D_8^2 z^2\bar{z} - D_{5,6,9}z^2\bar{z} + D_6^2 D_9 z^2\bar{z} \\
&+ D_{5,7,9}z^2\bar{z} + D_{6,7,9}z^2\bar{z} - D_{5,8,9}z^2\bar{z} - D_{6,8,9}z^2(z+1)\bar{z} - D_{7,8,9}z^3\bar{z} + D_8^2 D_9 z^3\bar{z} \\
&+ D_5 D_9^2 z^2\bar{z}^2 + D_6^2 D_{10} z^2\bar{z} + D_{6,7,10}z^2\bar{z} - D_{6,8,10}z^2\bar{z} - D_{6,9,10}z^2\bar{z}^2 - D_{7,9,10}z^2\bar{z}^2 \\
&+ D_{8,9,10}z^2\bar{z}^2 - 2D_5^2 D_{11} z + 4D_{5,6,11}z - 2D_6^2 D_{11} z + 2D_{5,7,11}z - 2D_{6,7,11}z \\
&+ 2D_{5,8,11}z^2 + 2D_{6,8,11}z - 2D_{7,8,11}(2-z)z + 4D_8^2 D_{11} z\bar{z} - 2D_{5,9,11}z\bar{z} \\
&+ 2D_{6,9,11}z\bar{z} - 2D_{8,9,11}z\bar{z} + 2D_{5,10,11}z\bar{z} + 2D_{7,10,11}z\bar{z} - 4D_{8,10,11}z\bar{z} - 2D_{5,6,12}z \\
&+ 2D_6^2 D_{12} z + 2D_{6,7,12}z + D_8 D_{11}^2 4 + 2D_{6,8,12}z\bar{z} + 4D_{5,9,12}z\bar{z} - 2D_{7,9,12}z\bar{z} \\
&- 2D_{8,9,12}z\bar{z} - 2D_{6,10,12}z\bar{z} + D_{5,11,12} - 4 + D_{6,11,12}4 + D_{7,11,12}4 - 2D_{5,6,8,11}z^2 \\
&+ 2D_6^2 D_{8,11} z^2 + 4D_{6,7,8,11}z^2 - 2D_8^2 D_{6,11}(2-z)z^2 - 2D_5^2 D_{9,11} z^2 + 4D_{5,6,9,11}z^2 \\
&- 2D_6^2 D_{9,11} z^2 + 2D_{5,8,9,11}z^2(z+1) + 2D_{6,8,9,11}z^2(z+1) - 2D_8^2 D_{9,11} z^3 \\
&+ 2D_{5,6,10,11}z^2 - 2D_6^2 D_{10,11} z^2 - 4D_{6,7,10,11}z^2 + 2D_{6,8,10,11}(3-2z)z^2 \\
&+ 2D_{5,9,10,11}z^2\bar{z} + 2D_{6,9,10,11}z^2\bar{z} - 2D_{8,9,10,11}z^2\bar{z} - 2D_{10}^2 D_{6,11} z^2\bar{z} + 4D_{11}^2 D_{5,8} z \\
&- 4D_{11}^2 D_{6,8} z - 2D_6^2 D_{8,12} z^2 - 4D_{8,11}^2 z - 2D_{5,6,9,12}z^2 + 2D_6^2 D_{9,12} z^2 + 4D_{6,7,9,12}z^2 \\
&- 2D_{6,8,9,12}z^3 - 4D_{11}^2 D_{5,10} z + 2D_9^2 D_{5,12} z^2\bar{z} + 4D_{11}^2 D_{6,10} z + 2D_9^2 D_{6,12} z^2\bar{z} \\
&+ 2D_6^2 D_{10,12} z^2 + 4D_{11}^2 D_{8,10} z - 2D_9^2 D_{8,12} z^2\bar{z} - 2D_{6,9,10,12}z^2\bar{z} - 4D_{6,8,11,12}z \\
&- 4D_{5,9,11,12}z + 4D_{6,9,11,12}z + 4D_{8,9,11,12}z + 4D_{6,10,11,12}z + 4D_{12}^2 D_{6,9} z \\
&+ 4D_6 D_{8,11}^2 z^2 - 8D_{11}^2 D_{6,8,10} z^2 + 4D_6 D_{10,11}^2 z^2 - 8D_{6,8,9,11,12}z^2 + 8D_{6,9,10,11,12}z^2 \\
&+ 4D_6 D_{9,12}^2 z^2\big)\,,
\end{aligned}
\tag{B.4}
$$

where we have used the abbreviations $D_{a,b,c,\ldots} = D_a D_b D_c \ldots$.

Calculation of the leading singularities requires us to compute (iterated) residues in all integration variables at all possible locations of the poles, eventually including those induced by the Baikov polynomial $P(D_1,\ldots,D_{12})$. Conjecturally [70], this analysis allows us to determine candidates for canonical integrals by searching for linear combinations of integrals

1. which are ultra-violet (UV) finite;
2. which do not have any double poles in any of the integration variables;
3. whose leading singularities, i.e. the maximally iterated residues at all single poles, are constant in the sense that they do not depend on the kinematic variable $z$.

To find candidate integrals, we work in $d = 4$ dimensions. As we already mentioned, the integral in Eq. (B.2) is not canonical and has to be modified appropriately. Hence, we make a general ansatz for the numerator and write

$$
I_{\text{can}} \sim \underset{D1,D2,D3,D4}{\text{Cut}} \int \frac{\mathrm{d}D_1 \ldots \mathrm{d}D_{12}}{D_1 \ldots D_5\, D_7 \ldots D_{12}} \frac{N_{\text{can}}(D_1,\ldots,D_{12})}{P(D_1,\ldots,D_{12})^2}\,, \tag{B.5}
$$

$$
N_{\text{can}}(D_1,\ldots,D_{12}) = a_0 + \sum_{k=5}^{12} a_k D_k + \sum_{k=5}^{12}\sum_{l=5}^{k} a_{k,l} D_k D_l\,, \tag{B.6}
$$

where the degree of $N_{\text{can}}(D_1,\ldots,D_{12})$ is bounded by the requirement of UV finiteness.[12] This formula implies that the candidate integral is a linear combination of $I^{\text{A3}}_{1111;10111111}$ and simpler integrals that belong to the same integral family. Our goal is to find the coefficients $a_0$, $a_k$ and $a_{k,l}$ that make $I_{\text{can}}$ satisfy the three requirements listed above.

We note that the analysis of the leading singularities of the full integral, which necessarily involves studying the pole structure of the Baikov polynomial $P(D_1,\ldots,D_{12})$, is quite demanding. To simplify it, we organise the analysis iteratively, starting with the computation of simplest residues, and then moving to more complex ones. Experience shows that we do not need to carry this analysis to the very end and that after several iterations a clear candidate for a canonical integral emerges. Below we illustrate how this is done in practice.

A glance at Eq. (B.5) reveals that the simplest residue to compute (the maximal cut) is the one at $D_i = 0$, with $i = 1,\ldots,5,7,\ldots,12$. Computing this residue, we find

$$\underset{D_1,\ldots,\widehat{D_6},\ldots,D_{12}}{\text{Cut}}[I_{\text{can}}] \sim \frac{16z^2}{1-z}\int \mathrm{d}D_6\,\frac{a_0 + a_6 D_6 + a_{6,6}D_6^2}{D_6(zD_6-(1-z))}\,, \tag{B.7}$$

where $\widehat{D_6}$ means that no residue in $D_6$ has been calculated. The denominator of the integrand in Eq. (B.7) comes from the Baikov polynomial which simplifies once all the other propagators are set to zero.

For the maximal-cut computation we need to analyse residues in $D_6$ in Eq. (B.7). We note that absence of double poles at infinity immediately implies $a_{6,6} = 0$. It is then clear that there are two simple poles in Eq. (B.7), one at $D_6 = 0$ and another one at $D_6 = (1-z)/z$. Computing the two residues we obtain

$$\underset{D_1,\ldots,D_6,\ldots,D_{12}}{\text{Cut}}[I_{\text{can}}] \sim \left\{-\frac{16z^2}{(1-z)^2}a_0\,,\quad \frac{16z^2}{(1-z)^2}\left(a_0+\frac{1-z}{z}a_6\right)\right\}. \tag{B.8}$$

These residues are called the "leading singularities". According to the third requirement mentioned above, a candidate for a canonical master integral should have constant (i.e. $z$-independent) leading singularities. We accomplish this by choosing

$$a_0 = \frac{(1-z)^2}{16z^2}\,,\quad a_6 = 0\,. \tag{B.9}$$

Computing the maximal cut allows us to determine some, but not all coefficients in the general ansatz shown in Eq. (B.6). To fix more coefficients, we need to inspect the next-to-maximal cuts. This means that, instead of computing the residues at $D_i = 0$ for all $i = 5,7,8,\ldots,12$, we do this for all but one of them. It is clear that the number of next-to-maximal cuts that need to be considered is seven in this case.

As an example, we consider the next-to-maximal cut where we do not take the residue at $D_7 = 0$. The corresponding integrand reads

$$\underset{D_1,\ldots,\widehat{D_6},\widehat{D_7},\ldots,D_{12}}{\text{Cut}} I_{\text{can}} \sim 16z^2\int \mathrm{d}D_6\,\mathrm{d}D_7\frac{\frac{(1-z)^2}{16z^2}+a_7D_7+a_{7,6}D_6D_7+a_{7,7}D_7^2}{D_7(D_6+D_7)((1-z)+zD_7)(zD_6-(1-z))}\,. \tag{B.10}$$

[12] This requirement can be relaxed in some cases allowing for logarithmic UV divergences.

To avoid poles at $D_7 \to \infty$, we set $a_{7,7} = 0$. Computing the remaining poles in $D_7$, we find that this induces double poles in $D_6$ at $D_6 = (1-z)/z$ unless we choose

$$a_{7,6} = 0\,, \quad a_7 = \frac{1-z}{16z}\,. \tag{B.11}$$

Calculating all the remaining residues in $D_6$ and $D_7$ in Eq. (B.10), we find that with this choice of constants the leading singularities are $\{-1, 1\}$.

As another example, we consider the next-to-maximal cut where the $D_8 = 0$ residue is not taken. We then find

$$\underset{D_1,\ldots,\widehat{D_6},D_7,\widehat{D_8},\ldots,D_{12}}{\text{Cut}} I_{\text{can}} \sim \frac{16z^2}{1-z} \int \mathrm{d}D_6\, \mathrm{d}D_8 \frac{\frac{(1-z)^2}{16z^2} + a_8 D_8 + a_{8,6} D_6 D_8 + a_{8,8} D_8^2}{D_8(D_6 - D_8)(1 - zD_8)(zD_6 - (1-z))}\,, \tag{B.12}$$

We can again set $a_{8,8} = 0$ to avoid poles at infinity. Computing residues at $D_8$, we find that the result does not have double poles in the variable $D_6$. However, since our goal is to find candidates for canonical integrals, we can choose the simplest option whenever possible. Thus, we choose $a_{8,6} = 0$ and find the following leading singularities

$$\left\{\pm 1, \pm\left(\frac{1}{z} + \frac{16a_8}{1-z}\right), \pm\left(1 - \frac{1}{z} + \frac{16a_8}{1-z}\right)\right\}. \tag{B.13}$$

They become $z$-independent if we choose

$$a_8 = -\frac{(1-z)^2}{16z}\,. \tag{B.14}$$

We perform the analysis of all next-to-maximal and next-to-next-to-maximal cuts and find that with the choice of the following numerator polynomial

$$N_{\text{can}}(D_1, \ldots, D_{12}) = \frac{1-z}{16z}\left(\frac{1-z}{z} + D_7 - (1-z)D_8 + \frac{2}{z}D_{12} + 2D_{10}D_{11}\right)\,, \tag{B.15}$$

all requirements mentioned above are satisfied.

The presence of the integration variables $D_i$ in the numerator of the integrand removes the corresponding propagators in the original integral. Therefore, the candidate for a canonical integral to replace $I^{\text{A3}}_{1111;10111111}$ reads

$$\begin{aligned} I_{\text{can}} = \frac{1-z}{16z}\bigg(&\frac{1-z}{z} I^{\text{A3}}_{1111;10111111} + I^{\text{A3}}_{1111;10011111} - (1-z) I^{\text{A3}}_{1111;10101111} \\ &+ \frac{2}{z} I^{\text{A3}}_{1111;10111110} + 2 I^{\text{A3}}_{1111;10111001}\bigg)\,. \end{aligned} \tag{B.16}$$

We can easily check whether or not this candidate integral is indeed canonical since we know the differential equations for all integrals that appear in Eq. (B.16). Although in this particular case $I_{\text{can}}$ turns out to be canonical, in general this does not happen since we terminated the cut analysis once the next-to-next-to-maximal cut was computed.

Nevertheless, even if the candidate integral turns out to be not fully canonical after the next-to-leading cut analysis, knowing a good candidate is extremely helpful. Indeed, we note that once the differential equations for the integrals that $I_{\text{can}}$ couples to have been brought to a canonical form, also the differential equation that $I_{\text{can}}$ satisfies becomes partially canonical. Since the integral we started from has eleven propagators and we analysed the leading singularities up to the next-to-next-to-maximal cuts, all blocks in the differential equation corresponding to sectors with at least nine propagators are canonical. To deal with the rest, we resorted to methods described in Ref. [62] where a bottom-up construction of the canonical basis is described. As a final remark we note that an analysis of leading singularities combined with the methods of Ref. [62] allowed us to find canonical bases for all integrals that appear in the computation of the beam function at N$^3$LO in perturbative QCD.

## C Building blocks for the beam-function renormalisation

In this appendix, we collect formulas that are needed for the extraction of the matching coefficients from the bare partonic beam functions.

First, we describe how to construct the $\overline{\text{MS}}$ parton distribution functions in perturbation theory. The starting point is the Altarelli-Parisi equation, Eq. (3.28), and the perturbative expansion of the splitting functions

$$P_{ij}(z) = \sum_{n=0}^{\infty} \left(\frac{\alpha_s}{2\pi}\right)^n P_{ij}^{(n)}(z)\,. \tag{C.1}$$

To construct the parton distribution functions $f_{ij}$, we integrate the Altarelli-Parisi equation with the boundary condition $f_{ij}^{(0)}(z) = \delta(1-z)$. We employ the evolution equation for the strong coupling constant

$$\mu^2 \frac{\mathrm{d}}{\mathrm{d}\mu^2} \alpha_s(\mu^2) = \beta(\alpha_s) - \epsilon\, \alpha_s(\mu^2)\,, \tag{C.2}$$

where

$$\beta(\alpha_s) = -\frac{\alpha_s^2}{4\pi}\beta_0 - \frac{\alpha_s^3}{(4\pi)^2}\beta_1 + \mathcal{O}(\alpha_s^4)\,, \tag{C.3}$$

and

$$\beta_0 = \frac{11}{3}C_A - \frac{4}{3}T_F N_f\,, \qquad \beta_1 = \frac{34}{3}C_A^2 - \left(\frac{20}{3}C_A + 4C_F\right) T_F N_f\,, \tag{C.4}$$

are the well-known expansion coefficients of the beta function. We write the result for the partonic PDFs as

$$f_{ij}^{(1)} = -\frac{1}{\epsilon} P_{ij}^{(0)}\,, \tag{C.5}$$

$$f_{ij}^{(2)} = \frac{1}{2\epsilon^2} \sum_k P_{ik}^{(0)} \underset{z}{\otimes} P_{kj}^{(0)} + \frac{\beta_0}{4\epsilon^2} P_{ij}^{(0)} - \frac{1}{2\epsilon} P_{ij}^{(1)}\,, \tag{C.6}$$

$$
\begin{aligned}
f_{ij}^{(3)} = & -\frac{1}{6\epsilon^3}\sum_{k,\ell} P_{ik}^{(0)} \underset{z}{\otimes} P_{k\ell}^{(0)} \underset{z}{\otimes} P_{\ell j}^{(0)} - \frac{\beta_0}{4\epsilon^3}\sum_{k} P_{ik}^{(0)} \underset{z}{\otimes} P_{kj}^{(0)} - \frac{\beta_0^2}{12\epsilon^3} P_{ij}^{(0)} \\
& + \frac{1}{3\epsilon^2}\sum_{k} P_{ik}^{(1)} \underset{z}{\otimes} P_{kj}^{(0)} + \frac{\beta_0}{6\epsilon^2} P_{ij}^{(1)} + \frac{1}{6\epsilon^2}\sum_{k} P_{ik}^{(0)} \underset{z}{\otimes} P_{kj}^{(1)} \\
& + \frac{\beta_1}{12\epsilon^2} P_{ij}^{(0)} - \frac{1}{3\epsilon} P_{ij}^{(2)} ,
\end{aligned}
\tag{C.7}
$$

where the dependence of $f_{ij}$'s and $P_{ij}$'s on $z$ has been suppressed.

The expansion coefficients of the renormalisation constants for the quark case ($i = q$) read

$$
Z_q^{(1)} = C_F\left[-\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\frac{4}{\epsilon} + \delta(t)\left[\frac{4}{\epsilon^2} + \frac{3}{\epsilon}\right]\right] , \tag{C.8}
$$

$$
\begin{aligned}
Z_q^{(2)} = & C_A C_F\Bigg[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\left[\frac{22}{3\epsilon^2} + \frac{1}{\epsilon}\left(-\frac{134}{9} + \frac{2}{3}\pi^2\right)\right] + \delta(t)\Bigg[-\frac{11}{\epsilon^3} \\
& + \frac{1}{\epsilon^2}\left(\frac{35}{18} - \frac{1}{3}\pi^2\right) + \frac{1}{\epsilon}\left(\frac{1769}{108} + \frac{11}{18}\pi^2 - 20\zeta_3\right)\Bigg]\Bigg] + C_F^2\Bigg[\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\frac{16}{\epsilon^2} \\
& + \mathcal{L}_0\left(\frac{t}{\mu^2}\right)\left[-\frac{16}{\epsilon^3} - \frac{12}{\epsilon^2}\right] + \delta(t)\Bigg[\frac{8}{\epsilon^4} + \frac{12}{\epsilon^3} + \frac{1}{\epsilon^2}\left(\frac{9}{2} - \frac{4}{3}\pi^2\right) + \frac{1}{\epsilon}\Bigg(\frac{3}{4} - \pi^2 \\
& + 12\zeta_3\Bigg)\Bigg]\Bigg] + C_F N_F T_F\Bigg[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\left[-\frac{1}{\epsilon^2}\frac{8}{3} + \frac{1}{\epsilon}\frac{40}{9}\right] + \delta(t)\Bigg[\frac{4}{\epsilon^3} - \frac{2}{9\epsilon^2} \\
& + \frac{1}{\epsilon}\left(-\frac{121}{27} - \frac{2}{9}\pi^2\right)\Bigg]\Bigg] ,
\end{aligned}
\tag{C.9}
$$

and

$$
\begin{aligned}
Z_q^{(3)} = & C_A^2 C_F\Bigg[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Bigg[-\frac{484}{27\epsilon^3} + \frac{1}{\epsilon^2}\left(\frac{4172}{81} - \frac{44}{27}\pi^2\right) + \frac{1}{\epsilon}\Bigg(-\frac{490}{9} + \frac{536}{81}\pi^2 \\
& - \frac{88}{9}\zeta_3 - \frac{44}{135}\pi^4\Bigg)\Bigg] + \delta(t)\Bigg[\frac{2662}{81\epsilon^4} + \frac{1}{\epsilon^3}\left(-\frac{8999}{243} + \frac{110}{81}\pi^2\right) \\
& + \frac{1}{\epsilon^2}\left(-\frac{16147}{486} - \frac{899}{243}\pi^2 + \frac{1408}{27}\zeta_3 + \frac{44}{405}\pi^4\right) + \frac{1}{\epsilon}\Bigg(\frac{412907}{8748} + \frac{419}{729}\pi^2 \\
& - \frac{5500}{27}\zeta_3 + \frac{19}{30}\pi^4 + \frac{88}{27}\pi^2\zeta_3 + \frac{232}{3}\zeta_5\Bigg)\Bigg]\Bigg] \\
& + C_A C_F^2\Bigg[\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\left[-\frac{1}{\epsilon^3}\frac{176}{3} + \frac{1}{\epsilon^2}\left(\frac{1072}{9} - \frac{16}{3}\pi^2\right)\right] \\
& + \mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Bigg[\frac{220}{3\epsilon^4} + \frac{1}{\epsilon^3}\left(-\frac{136}{3} + 4\pi^2\right) - \frac{1}{\epsilon^2}\Bigg(\frac{2975}{27} + \frac{4}{9}\pi^2 \\
& - 80\zeta_3\Bigg)\Bigg] + \delta(t)\Bigg[-\frac{44}{\epsilon^5} - \frac{1}{\epsilon^4}\left(\frac{227}{9} + \frac{4}{3}\pi^2\right) + \frac{1}{\epsilon^3}\Bigg(\frac{3853}{54} + \frac{19}{3}\pi^2 \\
& - 80\zeta_3\Bigg) + \frac{1}{\epsilon^2}\left(\frac{1703}{36} - \frac{305}{54}\pi^2 - \frac{268}{3}\zeta_3 + \frac{4}{9}\pi^4\right) + \frac{1}{\epsilon}\Bigg(\frac{151}{12} - \frac{205}{27}\pi^2
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{844}{9}\zeta_3-\frac{247}{405}\pi^4+\frac{8}{9}\pi^2\zeta_3+40\zeta_5\Big)\Big]\Big]+C_F^3\Big[-\mathcal{L}_2\left(\frac{t}{\mu^2}\right)\frac{32}{\epsilon^3}\\
&+\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\left[\frac{64}{\epsilon^4}+\frac{48}{\epsilon^3}\right]+\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Big[-\frac{32}{\epsilon^5}-\frac{48}{\epsilon^4}-\frac{1}{\epsilon^3}\Big(18-\frac{16}{3}\pi^2\Big)\\
&-\frac{1}{\epsilon^2}\Big(3-4\pi^2+48\zeta_3\Big)\Big]+\delta(t)\Big[\frac{32}{3\epsilon^6}+\frac{24}{\epsilon^5}+\frac{1}{\epsilon^4}\Big(18-\frac{16}{3}\pi^2\Big)\\
&+\frac{1}{\epsilon^3}\Big(\frac{15}{2}-8\pi^2+\frac{80}{3}\zeta_3\Big)+\frac{1}{\epsilon^2}\Big(\frac{9}{4}-3\pi^2+36\zeta_3\Big)+\frac{1}{\epsilon}\Big(\frac{29}{6}+\pi^2\\
&+\frac{68}{3}\zeta_3+\frac{8}{15}\pi^4-\frac{16}{9}\pi^2\zeta_3-80\zeta_5\Big)\Big]\Big]\\
&+C_AC_FT_FN_F\Big[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Big[\frac{352}{27\epsilon^3}-\frac{1}{\epsilon^2}\Big(\frac{2672}{81}-\frac{16}{27}\pi^2\Big)+\frac{1}{\epsilon}\Big(\frac{1672}{81}\\
&-\frac{160}{81}\pi^2+\frac{224}{9}\zeta_3\Big)\Big]+\delta(t)\Big[-\frac{1}{\epsilon^4}\frac{1936}{81}+\frac{1}{\epsilon^3}\Big(\frac{5384}{243}-\frac{40}{81}\pi^2\Big)\\
&+\frac{1}{\epsilon^2}\Big(\frac{6148}{243}+\frac{424}{243}\pi^2-\frac{704}{27}\zeta_3\Big)+\frac{1}{\epsilon}\Big(\frac{5476}{2187}-\frac{1180}{729}\pi^2+\frac{2656}{81}\zeta_3\\
&-\frac{46}{135}\pi^4\Big)\Big]\Big]+C_F^2T_FN_F\Big[\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\Big[\frac{64}{3\epsilon^3}-\frac{1}{\epsilon^2}\frac{320}{9}\Big]\\
&+\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Big[-\frac{80}{3\epsilon^4}+\frac{32}{3\epsilon^3}+\frac{1}{\epsilon^2}\Big(\frac{700}{27}+\frac{8}{9}\pi^2\Big)+\frac{1}{\epsilon}\Big(\frac{220}{9}-\frac{64}{3}\zeta_3\Big)\Big]\\
&+\delta(t)\Big[\frac{16}{\epsilon^5}+\frac{100}{9\epsilon^4}-\frac{1}{\epsilon^3}\Big(\frac{310}{27}+\frac{8}{3}\pi^2\Big)-\frac{1}{\epsilon^2}\Big(\frac{457}{27}-\frac{38}{27}\pi^2-\frac{160}{9}\zeta_3\Big)\\
&-\frac{1}{\epsilon}\Big(\frac{4664}{81}-\frac{32}{27}\pi^2+\frac{208}{27}\zeta_3-\frac{164}{405}\pi^4\Big)\Big]\Big]\\
&+C_FT_F^2N_F^2\Big[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Big[-\frac{64}{27\epsilon^3}+\frac{320}{81\epsilon^2}+\frac{64}{81\epsilon}\Big]+\delta(t)\Big[\frac{352}{81\epsilon^4}\\
&-\frac{368}{243\epsilon^3}-\frac{1}{\epsilon^2}\Big(\frac{344}{81}+\frac{16}{81}\pi^2\Big)-\frac{1}{\epsilon}\Big(\frac{13828}{2187}-\frac{80}{243}\pi^2-\frac{256}{81}\zeta_3\Big)\Big]\Big]. \qquad \text{(C.10)}
\end{aligned}
$$

For gluons ($i=g$) we find

$$
Z_g^{(1)}=C_A\Big[-\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\frac{4}{\epsilon}+\delta(t)\Big[\frac{4}{\epsilon^2}+\frac{11}{3\epsilon}\Big]\Big]-N_FT_F\delta(t)\frac{4}{3\epsilon}\,, \qquad \text{(C.11)}
$$

$$
\begin{aligned}
Z_g^{(2)}=C_A^2\Big[&\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\frac{16}{\epsilon^2}+\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Big[-\frac{16}{\epsilon^3}-\frac{22}{3\epsilon^2}+\frac{1}{\epsilon}\Big(-\frac{134}{9}+\frac{2}{3}\pi^2\Big)\Big]\\
&+\delta(t)\Big[\frac{8}{\epsilon^4}+\frac{11}{3\epsilon^3}+\frac{1}{\epsilon^2}\Big(\frac{67}{9}-\frac{5}{3}\pi^2\Big)+\frac{1}{\epsilon}\Big(\frac{548}{27}-\frac{11}{18}\pi^2-8\zeta_3\Big)\Big]\Big]\\
&+C_AN_FT_F\Big[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Big[\frac{8}{3\epsilon^2}+\frac{40}{9\epsilon}\Big]+\delta(t)\Big[-\frac{4}{3\epsilon^3}-\frac{20}{9\epsilon^2}
\end{aligned}
$$

$$
+\frac{1}{\epsilon}\left(-\frac{184}{27}+\frac{2}{9}\pi^2\right)\Bigg]\Bigg]-C_F N_F T_F \delta(t)\frac{2}{\epsilon}\,, \tag{C.12}
$$

and

$$
\begin{aligned}
Z_g^{(3)} = C_A^3\Bigg[&-\mathcal{L}_2\left(\frac{t}{\mu^2}\right)\frac{32}{\epsilon^3}+\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\left[\frac{64}{\epsilon^4}+\frac{1}{\epsilon^2}\left(\frac{1072}{9}-\frac{16}{3}\pi^2\right)\right]\\
&+\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Bigg[-\frac{32}{\epsilon^5}+\frac{44}{3\epsilon^4}-\frac{1}{\epsilon^3}\left(\frac{2170}{27}-\frac{28}{3}\pi^2\right)-\frac{1}{\epsilon^2}\Bigg(\frac{6826}{81}\\
&-\frac{88}{27}\pi^2-32\zeta_3\Bigg)+\frac{1}{\epsilon}\left(-\frac{490}{9}+\frac{536}{81}\pi^2-\frac{88}{9}\zeta_3-\frac{44}{135}\pi^4\right)\Bigg]\\
&+\delta(t)\Bigg[\frac{32}{3\epsilon^6}-\frac{44}{3\epsilon^5}+\frac{1}{\epsilon^4}\left(\frac{1807}{81}-\frac{20}{3}\pi^2\right)+\frac{1}{\epsilon^3}\Bigg(\frac{14095}{243}-\frac{187}{81}\pi^2\\
&-\frac{160}{3}\zeta_3\Bigg)+\frac{1}{\epsilon^2}\left(\frac{7072}{243}-\frac{6259}{486}\pi^2-\frac{176}{27}\zeta_3+\frac{224}{405}\pi^4\right)\\
&+\frac{1}{\epsilon}\left(\frac{331153}{4374}-\frac{6217}{729}\pi^2-\frac{260}{3}\zeta_3+\frac{583}{810}\pi^4+\frac{64}{27}\pi^2\zeta_3+\frac{112}{3}\zeta_5\right)\Bigg]\Bigg]\\
&+C_A^2 T_F N_F\Bigg[-\mathcal{L}_1\left(\frac{t}{\mu^2}\right)\frac{320}{9\epsilon^2}+\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\Bigg[-\frac{16}{3\epsilon^4}+\frac{544}{27\epsilon^3}\\
&+\frac{1}{\epsilon^2}\left(\frac{2464}{81}-\frac{32}{27}\pi^2\right)+\frac{1}{\epsilon}\left(\frac{1672}{81}-\frac{160}{81}\pi^2+\frac{224}{9}\zeta_3\right)\Bigg]\\
&+\delta(t)\Bigg[\frac{16}{3\epsilon^5}-\frac{280}{81\epsilon^4}+\frac{1}{\epsilon^3}\left(-\frac{3256}{243}+\frac{68}{81}\pi^2\right)-\frac{1}{\epsilon^2}\Bigg(\frac{2684}{243}\\
&-\frac{1012}{243}\pi^2+\frac{128}{27}\zeta_3\Bigg)+\frac{1}{\epsilon}\left(-\frac{42557}{2187}+\frac{2612}{729}\pi^2+\frac{16}{81}\zeta_3-\frac{154}{405}\pi^4\right)\Bigg]\Bigg]\\
&+C_A C_F T_F N_F\Bigg[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\left[\frac{8}{3\epsilon^2}+\frac{1}{\epsilon}\left(\frac{220}{9}-\frac{64}{3}\zeta_3\right)\right]+\delta(t)\Bigg[-\frac{1}{\epsilon^3}\frac{8}{9}\\
&+\frac{1}{\epsilon^2}\left(-\frac{154}{27}+\frac{64}{9}\zeta_3\right)+\frac{1}{\epsilon}\left(-\frac{4145}{81}+\frac{4}{9}\pi^2+\frac{608}{27}\zeta_3+\frac{16}{135}\pi^4\right)\Bigg]\Bigg]\\
&+C_F^2 T_F N_F\delta(t)\frac{1}{\epsilon}\frac{2}{3}+C_A T_F^2 N_F^2\Bigg[\mathcal{L}_0\left(\frac{t}{\mu^2}\right)\left[\frac{32}{27\epsilon^3}-\frac{160}{81\epsilon^2}+\frac{64}{81\epsilon}\right]\\
&+\delta(t)\Bigg[-\frac{80}{81\epsilon^4}-\frac{80}{243\epsilon^3}-\frac{1}{\epsilon^2}\left(\frac{16}{81}+\frac{8}{81}\pi^2\right)-\frac{1}{\epsilon}\Bigg(\frac{3622}{2187}+\frac{80}{243}\pi^2\\
&-\frac{448}{81}\zeta_3\Bigg)\Bigg]\Bigg]+C_F N_F^2 T_F^2\delta(t)\left[-\frac{8}{9\epsilon^2}+\frac{44}{27\epsilon}\right].
\end{aligned} \tag{C.13}
$$

The NLO and NNLO coefficients agree with Ref. [26].

## References


[1] M. A. Ebert, B. Mistlberger, and G. Vita, "$N$-jettiness beam functions at N$^3$LO," *JHEP* **09** (2020) 143, arXiv:2006.03056 [hep-ph].

[2] S. Catani and M. H. Seymour, "A General algorithm for calculating jet cross-sections in NLO QCD," *Nucl. Phys. B* **485** (1997) 291–419, arXiv:hep-ph/9605323. [Erratum: Nucl. Phys. B **510** (1998) 503].

[3] S. Frixione, Z. Kunszt, and A. Signer, "Three jet cross-sections to next-to-leading order," *Nucl. Phys. B* **467** (1996) 399–442, arXiv:hep-ph/9512328.

[4] G. Somogyi, Z. Trocsanyi, and V. Del Duca, "Matching of singly- and doubly-unresolved limits of tree-level QCD squared matrix elements," *JHEP* **06** (2005) 024, arXiv:hep-ph/0502226.

[5] A. Gehrmann-De Ridder, T. Gehrmann, and E. W. N. Glover, "Antenna subtraction at NNLO," *JHEP* **09** (2005) 056, arXiv:hep-ph/0505111.

[6] M. Czakon, "A novel subtraction scheme for double-real radiation at NNLO," *Phys. Lett. B* **693** (2010) 259–268, arXiv:1005.0274 [hep-ph].

[7] F. Caola, K. Melnikov, and R. Röntsch, "Nested soft-collinear subtractions in NNLO QCD computations," *Eur. Phys. J. C* **77** no. 4, (2017) 248, arXiv:1702.01352 [hep-ph].

[8] F. Herzog, "Geometric IR subtraction for final state real radiation," *JHEP* **08** (2018) 006, arXiv:1804.07949 [hep-ph].

[9] L. Magnea, E. Maina, G. Pelliccioli, C. Signorile-Signorile, P. Torrielli, and S. Uccirati, "Local analytic sector subtraction at NNLO," *JHEP* **12** (2018) 107, arXiv:1806.09570 [hep-ph]. [Erratum: JHEP **06** (2019) 013].

[10] S. Catani and M. Grazzini, "An NNLO subtraction formalism in hadron collisions and its application to Higgs boson production at the LHC," *Phys. Rev. Lett.* **98** (2007) 222002, arXiv:hep-ph/0703012.

[11] I. W. Stewart, F. J. Tackmann, and W. J. Waalewijn, "Factorization at the LHC: From PDFs to Initial State Jets," *Phys. Rev. D* **81** (2010) 094035, arXiv:0910.0467 [hep-ph].

[12] I. W. Stewart, F. J. Tackmann, and W. J. Waalewijn, "N-Jettiness: An Inclusive Event Shape to Veto Jets," *Phys. Rev. Lett.* **105** (2010) 092002, arXiv:1004.2489 [hep-ph].

[13] C. W. Bauer and I. W. Stewart, "Invariant operators in collinear effective theory," *Phys. Lett. B* **516** (2001) 134–142, arXiv:hep-ph/0107001.

[14] C. W. Bauer, D. Pirjol, and I. W. Stewart, "Soft collinear factorization in effective field theory," *Phys. Rev. D* **65** (2002) 054022, arXiv:hep-ph/0109045.

[15] C. W. Bauer, S. Fleming, D. Pirjol, I. Z. Rothstein, and I. W. Stewart, "Hard scattering factorization from effective field theory," *Phys. Rev. D* **66** (2002) 014017, arXiv:hep-ph/0202088.

[16] M. Beneke, A. P. Chapovsky, M. Diehl, and T. Feldmann, "Soft collinear effective theory and heavy to light currents beyond leading power," *Nucl. Phys. B* **643** (2002) 431–476, arXiv:hep-ph/0206152.

[17] M. Beneke and T. Feldmann, "Multipole expanded soft collinear effective theory with non-abelian gauge symmetry," *Phys. Lett. B* **553** (2003) 267–276, arXiv:hep-ph/0211358.

[18] I. W. Stewart, F. J. Tackmann, and W. J. Waalewijn, "The Quark Beam Function at NNLL," *JHEP* **09** (2010) 005, arXiv:1002.2213 [hep-ph].

[19] J. Gaunt, M. Stahlhofen, and F. J. Tackmann, "The Gluon Beam Function at Two Loops," *JHEP* **08** (2014) 020, arXiv:1405.1044 [hep-ph].

[20] J. R. Gaunt, M. Stahlhofen, and F. J. Tackmann, "The Quark Beam Function at Two Loops," *JHEP* **04** (2014) 113, arXiv:1401.5478 [hep-ph].

[21] R. Boughezal, F. Petriello, U. Schubert, and H. Xing, "Spin-dependent quark beam function at NNLO," *Phys. Rev. D* **96** no. 3, (2017) 034001, arXiv:1704.05457 [hep-ph].

[22] K. Melnikov, R. Rietkerk, L. Tancredi, and C. Wever, "Triple-real contribution to the quark beam function in QCD at next-to-next-to-next-to-leading order," *JHEP* **06** (2019) 033, arXiv:1904.02433 [hep-ph].

[23] K. Melnikov, R. Rietkerk, L. Tancredi, and C. Wever, "Double-real contribution to the quark beam function at N$^3$LO QCD," *JHEP* **02** (2019) 159, arXiv:1809.06300 [hep-ph].

[24] A. Behring, K. Melnikov, R. Rietkerk, L. Tancredi, and C. Wever, "Quark beam function at next-to-next-to-next-to-leading order in perturbative QCD in the generalized large-$N_c$ approximation," *Phys. Rev. D* **100** no. 11, (2019) 114034, arXiv:1910.10059 [hep-ph].

[25] M. A. Ebert, B. Mistlberger, and G. Vita, "Collinear expansion for color singlet cross sections," *JHEP* **09** (2020) 181, arXiv:2006.03055 [hep-ph].

[26] M. Ritzmann and W. J. Waalewijn, "Fragmentation in Jets at NNLO," *Phys. Rev. D* **90** no. 5, (2014) 054029, arXiv:1407.3272 [hep-ph].

[27] S. Catani and P. K. Dhani, "Collinear functions for QCD resummations," arXiv:2208.05840 [hep-ph].

[28] S. Catani and M. Grazzini, "Infrared factorization of tree level QCD amplitudes at the next-to-next-to-leading order and beyond," *Nucl. Phys. B* **570** (2000) 287–325, arXiv:hep-ph/9908523.

[29] Z. Bern, L. J. Dixon, and D. A. Kosower, "Two-loop $g \to gg$ splitting amplitudes in QCD," *JHEP* **08** (2004) 012, arXiv:hep-ph/0404293.

[30] S. D. Badger and E. W. N. Glover, "Two loop splitting functions in QCD," *JHEP* **07** (2004) 040, arXiv:hep-ph/0405236.

[31] V. Del Duca, C. Duhr, R. Haindl, A. Lazopoulos, and M. Michel, "Tree-level splitting amplitudes for a quark into four collinear partons," *JHEP* **02** (2020) 189, arXiv:1912.06425 [hep-ph].

[32] V. Del Duca, C. Duhr, R. Haindl, A. Lazopoulos, and M. Michel, "Tree-level splitting amplitudes for a gluon into four collinear partons," *JHEP* **10** (2020) 093, arXiv:2007.05345 [hep-ph].

[33] S. Catani, D. de Florian, and G. Rodrigo, "The Triple collinear limit of one loop QCD amplitudes," *Phys. Lett. B* **586** (2004) 323–331, arXiv:hep-ph/0312067.

[34] S. Badger, F. Buciuni, and T. Peraro, "One-loop triple collinear splitting amplitudes in QCD," *JHEP* **09** (2015) 188, arXiv:1507.05070 [hep-ph].

[35] G. F. R. Sborlini, D. de Florian, and G. Rodrigo, "Triple collinear splitting functions at NLO for scattering processes with photons," *JHEP* **10** (2014) 161, arXiv:1408.4821 [hep-ph].

[36] M. Czakon and S. Sapeta, "Complete collection of one-loop triple-collinear splitting operators for dimensionally-regulated QCD," *JHEP* **07** (2022) 052, arXiv:2204.11801 [hep-ph].

[37] C. Anastasiou and K. Melnikov, “Higgs boson production at hadron colliders in NNLO QCD,” *Nucl. Phys. B* **646** (2002) 220–256, arXiv:hep-ph/0207004.

[38] F. V. Tkachov, “A Theorem on Analytical Calculability of Four Loop Renormalization Group Functions,” *Phys. Lett. B* **100** (1981) 65–68.

[39] K. G. Chetyrkin and F. V. Tkachov, “Integration by Parts: The Algorithm to Calculate beta Functions in 4 Loops,” *Nucl. Phys. B* **192** (1981) 159–204.

[40] A. V. Kotikov, “Differential equations method: New technique for massive Feynman diagrams calculation,” *Phys. Lett. B* **254** (1991) 158–164.

[41] Z. Bern, L. J. Dixon, and D. A. Kosower, “Dimensionally regulated pentagon integrals,” *Nucl. Phys. B* **412** (1994) 751–816, arXiv:hep-ph/9306240.

[42] E. Remiddi, “Differential equations for Feynman graph amplitudes,” *Nuovo Cim. A* **110** (1997) 1435–1452, arXiv:hep-th/9711188.

[43] T. Gehrmann and E. Remiddi, “Differential equations for two loop four point functions,” *Nucl. Phys. B* **580** (2000) 485–518, arXiv:hep-ph/9912329.

[44] P. Nogueira, “Automatic Feynman graph generation,” *J. Comput. Phys.* **105** (1993) 279–289.

[45] J. Vermaseren, “New features of FORM,” arXiv:math-ph/0010025.

[46] J. Kuipers, T. Ueda, J. Vermaseren, and J. Vollinga, “FORM version 4.0” *Comput. Phys. Commun.* **184** (2013) 1453–1467, arXiv:1203.6543 [cs.SC].

[47] J. Kuipers, T. Ueda, and J. Vermaseren, “Code Optimization in FORM,” *Comput. Phys. Commun.* **189** (2015) 1–19, arXiv:1310.7007 [cs.SC].

[48] B. Ruijl, T. Ueda, and J. Vermaseren, “FORM version 4.2” arXiv:1707.06453 [hep-ph].

[49] T. van Ritbergen, A. Schellekens, and J. Vermaseren, “Group theory factors for Feynman diagrams,” *Int. J. Mod. Phys. A* **14** (1999) 41–96, arXiv:hep-ph/9802376.

[50] A. von Manteuffel and C. Studerus, “Reduze 2 - Distributed Feynman Integral Reduction,” arXiv:1201.4330 [hep-ph].

[51] P. Maierhöfer, J. Usovitsch, and P. Uwer, “Kira—A Feynman integral reduction program,” *Comput. Phys. Commun.* **230** (2018) 99–112, arXiv:1705.05610 [hep-ph].

[52] P. Maierhöfer and J. Usovitsch, “Kira 1.2 Release Notes,” arXiv:1812.01491 [hep-ph].

[53] P. Maierhöfer and J. Usovitsch, “Recent developments in Kira,” *CERN Yellow Reports: Monographs* **3** (2020) 201–204.

[54] J. Klappert, F. Lange, P. Maierhöfer, and J. Usovitsch, “Integral reduction with Kira 2.0 and finite field methods,” *Comput. Phys. Commun.* **266** (2021) 108024, arXiv:2008.06494 [hep-ph].

[55] A. Pak, “The Toolbox of modern multi-loop calculations: novel analytic and semi-analytic techniques,” *J. Phys. Conf. Ser.* **368** (2012) 012049, arXiv:1111.0868 [hep-ph].

[56] J. S. Hoff, *Methods for multiloop calculations and Higgs boson production at the LHC*. PhD thesis, KIT, Karlsruhe, 2015.

[57] C. Meyer, “Algorithmic transformation of multi-loop master integrals to a canonical basis with CANONICA,” *Comput. Phys. Commun.* **222** (2018) 295–312, arXiv:1705.06252 [hep-ph].

[58] S. Abreu, J. Dormans, F. Febres Cordero, H. Ita, B. Page, and V. Sotnikov, "Analytic Form of the Planar Two-Loop Five-Parton Scattering Amplitudes in QCD," *JHEP* **05** (2019) 084, arXiv:1904.00945 [hep-ph].

[59] M. Heller and A. von Manteuffel, "MultivariateApart: Generalized partial fractions," *Comput. Phys. Commun.* **271** (2022) 108174, arXiv:2101.08283 [cs.SC].

[60] J. M. Henn, "Multiloop integrals in dimensional regularization made simple," *Phys. Rev. Lett.* **110** (2013) 251601, arXiv:1304.1806 [hep-th].

[61] K.-T. Chen, "Iterated path integrals," *Bull. Am. Math. Soc.* **83** (1977) 831–879.

[62] T. Gehrmann, A. von Manteuffel, L. Tancredi, and E. Weihs, "The two-loop master integrals for $q\bar{q} \to VV$," *JHEP* **06** (2014) 032, arXiv:1404.4853 [hep-ph].

[63] R. N. Lee, "Reducing differential equations for multiloop master integrals," *JHEP* **04** (2015) 108, arXiv:1411.0911 [hep-ph].

[64] M. Argeri, S. Di Vita, P. Mastrolia, E. Mirabella, J. Schlenk, U. Schubert, and L. Tancredi, "Magnus and Dyson Series for Master Integrals," *JHEP* **03** (2014) 082, arXiv:1401.2979 [hep-ph].

[65] O. Gituliar and V. Magerya, "Fuchsia: a tool for reducing differential equations for Feynman master integrals to epsilon form," *Comput. Phys. Commun.* **219** (2017) 329–338, arXiv:1701.04269 [hep-ph].

[66] C. Meyer, "Transforming differential equations of multi-loop Feynman integrals into canonical form," *JHEP* **04** (2017) 006, arXiv:1611.01087 [hep-ph].

[67] M. Prausa, "epsilon: A tool to find a canonical basis of master integrals," *Comput. Phys. Commun.* **219** (2017) 361–376, arXiv:1701.00725 [hep-ph].

[68] R. N. Lee, "Libra: A package for transformation of differential systems for multiloop integrals," *Comput. Phys. Commun.* **267** (2021) 108058, arXiv:2012.00279 [hep-ph].

[69] N. Arkani-Hamed, J. L. Bourjaily, F. Cachazo, and J. Trnka, "Local Integrals for Planar Scattering Amplitudes," *JHEP* **06** (2012) 125, arXiv:1012.6032 [hep-th].

[70] J. Henn, B. Mistlberger, V. A. Smirnov, and P. Wasser, "Constructing d-log integrands and computing master integrals for three-loop four-particle scattering," *JHEP* **04** (2020) 167, arXiv:2002.09492 [hep-ph].

[71] M. Höschele, J. Hoff, and T. Ueda, "Adequate bases of phase space master integrals for gg → h at NNLO and beyond," *JHEP* **09** (2014) 116, arXiv:1407.4049 [hep-ph].

[72] C. Dlapa, J. Henn, and K. Yan, "Deriving canonical differential equations for Feynman integrals from a single uniform weight integral," *JHEP* **05** (2020) 025, arXiv:2002.02340 [hep-ph].

[73] J. Chen, X. Jiang, X. Xu, and L. L. Yang, "Constructing canonical Feynman integrals with intersection theory," *Phys. Lett. B* **814** (2021) 136085, arXiv:2008.03045 [hep-th].

[74] J. Chen, X. Jiang, C. Ma, X. Xu, and L. L. Yang, "Baikov representations, intersection theory, and canonical Feynman integrals," *JHEP* **07** (2022) 066, arXiv:2202.08127 [hep-th].

[75] K. Melnikov, L. Tancredi, and C. Wever, "Two-loop $gg \to Hg$ amplitude mediated by a nearly massless quark," *JHEP* **11** (2016) 104, arXiv:1610.03747 [hep-ph].

[76] J. Usovitsch, "Factorization of denominators in integration-by-parts reductions," arXiv:2002.08173 [hep-ph].

[77] A. V. Smirnov and V. A. Smirnov, "How to choose master integrals," *Nucl. Phys. B* **960** (2020) 115213, arXiv:2002.08042 [hep-ph].

[78] P. A. Baikov, "Explicit solutions of the three loop vacuum integral recurrence relations," *Phys. Lett. B* **385** (1996) 404–410, arXiv:hep-ph/9603267.

[79] P. A. Baikov, "Explicit solutions of the multiloop integral recurrence relations and its application," *Nucl. Instrum. Meth. A* **389** (1997) 347–349, arXiv:hep-ph/9611449.

[80] A. B. Goncharov, "Multiple polylogarithms, cyclotomy and modular complexes," *Math. Res. Lett.* **5** (1998) 497–516, arXiv:1105.2076 [math.AG].

[81] E. Remiddi and J. A. M. Vermaseren, "Harmonic polylogarithms," *Int. J. Mod. Phys.* **A15** (2000) 725–754, arXiv:hep-ph/9905237 [hep-ph].

[82] J. Vollinga and S. Weinzierl, "Numerical evaluation of multiple polylogarithms," *Comput. Phys. Commun.* **167** (2005) 177, arXiv:hep-ph/0410259.

[83] T. Gehrmann and E. Remiddi, "Two loop master integrals for $\gamma^* \to 3$ jets: The Planar topologies," *Nucl. Phys. B* **601** (2001) 248–286, arXiv:hep-ph/0008287.

[84] U. Aglietti and R. Bonciani, "Master integrals with 2 and 3 massive propagators for the 2 loop electroweak form-factor - planar case," *Nucl. Phys. B* **698** (2004) 277–318, arXiv:hep-ph/0401193.

[85] S. Weinzierl, "Expansion around half integer values, binomial sums and inverse binomial sums," *J. Math. Phys.* **45** (2004) 2656–2673, arXiv:hep-ph/0402131.

[86] J. Ablinger, J. Blümlein, and C. Schneider, "Harmonic Sums and Polylogarithms Generated by Cyclotomic Polynomials," *J. Math. Phys.* **52** (2011) 102301, arXiv:1105.6063 [math-ph].

[87] R. Bonciani, G. Degrassi, and A. Vicini, "On the Generalized Harmonic Polylogarithms of One Complex Variable," *Comput. Phys. Commun.* **182** (2011) 1253–1264, arXiv:1007.1891 [hep-ph].

[88] J. Ablinger, J. Blümlein, C. G. Raab, and C. Schneider, "Iterated Binomial Sums and their Associated Iterated Integrals," *J. Math. Phys.* **55** (2014) 112301, arXiv:1407.1822 [hep-th].

[89] J. Ablinger, J. Blümlein, and C. Schneider, "Iterated integrals over letters induced by quadratic forms," *Phys. Rev. D* **103** no. 9, (2021) 096025, arXiv:2103.08330 [hep-th].

[90] J. Ablinger, *A Computer Algebra Toolbox for Harmonic Sums Related to Particle Physics*. Diploma thesis, J. Kepler University Linz, 2009. arXiv:1011.1176 [math-ph].

[91] J. Ablinger, *Computer Algebra Algorithms for Special Functions in Particle Physics*. PhD thesis, J. Kepler University Linz, 2012. arXiv:1305.0687 [math-ph].

[92] J. A. M. Vermaseren, "Harmonic sums, Mellin transforms and integrals," *Int. J. Mod. Phys.* **A14** (1999) 2037–2076, arXiv:hep-ph/9806280 [hep-ph].

[93] J. Blümlein, "Structural Relations of Harmonic Sums and Mellin Transforms up to Weight $w = 5$," *Comput. Phys. Commun.* **180** (2009) 2218–2249, arXiv:0901.3106 [hep-ph].

[94] J. Ablinger, J. Blümlein, and C. Schneider, "Analytic and Algorithmic Aspects of Generalized Harmonic Sums and Polylogarithms," *J. Math. Phys.* **54** (2013) 082301, arXiv:1302.0378 [math-ph].

[95] J. Ablinger, "The package HarmonicSums: Computer Algebra and Analytic aspects of Nested Sums," *PoS* **LL2014** (2014) 019, arXiv:1407.6180 [cs.SC].

[96] J. Ablinger, "Inverse Mellin Transform of Holonomic Sequences," *PoS* **LL2016** (2016) 067, arXiv:1606.02845 [cs.SC].

[97] J. Ablinger, "Computing the Inverse Mellin Transform of Holonomic Sequences using Kovacic's Algorithm," *PoS* **RADCOR2017** (2017) 069, arXiv:1801.01039 [cs.SC].

[98] J. Ablinger, "Discovering and Proving Infinite Pochhammer Sum Identities," *Experimental Mathematics* **31** no. 1, (2019) 309–323, arXiv:1902.11001 [math.CO].

[99] D. Maitre, "HPL, a mathematica implementation of the harmonic polylogarithms," *Comput. Phys. Commun.* **174** (2006) 222–240, arXiv:hep-ph/0507152.

[100] D. Maitre, "Extension of HPL to complex arguments," *Comput. Phys. Commun.* **183** (2012) 846, arXiv:hep-ph/0703052.

[101] C. Duhr and F. Dulat, "PolyLogTools — polylogs for the masses," *JHEP* **08** (2019) 135, arXiv:1904.07279 [hep-th].

[102] C. W. Bauer, A. Frink, and R. Kreckel, "Introduction to the GiNaC framework for symbolic computation within the C++ programming language," *J. Symb. Comput.* **33** (2000) 1, arXiv:cs/0004015 [cs-sc].

[103] C. Anastasiou, C. Duhr, F. Dulat, and B. Mistlberger, "Soft triple-real radiation for Higgs production at N3LO," *JHEP* **07** (2013) 003, arXiv:1302.4379 [hep-ph].

[104] Y. Li, A. von Manteuffel, R. M. Schabinger, and H. X. Zhu, "$N^3$LO Higgs boson and Drell-Yan production at threshold: The one-loop two-emission contribution," *Phys. Rev. D* **90** no. 5, (2014) 053006, arXiv:1404.5839 [hep-ph].

[105] H. X. Zhu, "On the calculation of soft phase space integral," *JHEP* **02** (2015) 155, arXiv:1501.00236 [hep-ph].

[106] C. Duhr, B. Mistlberger, and G. Vita, "Soft Integrals and Soft Anomalous Dimensions at $N^3$LO and Beyond," arXiv:2205.04493 [hep-ph].

[107] M. Beneke and V. A. Smirnov, "Asymptotic expansion of Feynman integrals near threshold," *Nucl. Phys. B* **522** (1998) 321–344, arXiv:hep-ph/9711391.

[108] C. Anastasiou, C. Duhr, F. Dulat, E. Furlan, F. Herzog, and B. Mistlberger, "Soft expansion of double-real-virtual corrections to Higgs production at $N^3$LO," *JHEP* **08** (2015) 051, arXiv:1505.04110 [hep-ph].

[109] C. Duhr, T. Gehrmann, and M. Jaquier, "Two-loop splitting amplitudes and the single-real contribution to inclusive Higgs production at $N^3$LO," *JHEP* **02** (2015) 077, arXiv:1411.3587 [hep-ph].

[110] C. Duhr and T. Gehrmann, "The two-loop soft current in dimensional regularization," *Phys. Lett. B* **727** (2013) 452–455, arXiv:1309.4393 [hep-ph].

[111] D. Baranowski, "NNLO zero-jettiness beam and soft functions to higher orders in the dimensional-regularization parameter $\epsilon$," *Eur. Phys. J. C* **80** no. 6, (2020) 523, arXiv:2004.03285 [hep-ph].

[112] G. P. Korchemsky and A. V. Radyushkin, "Renormalization of the Wilson Loops Beyond the Leading Order," *Nucl. Phys. B* **283** (1987) 342–364.

[113] S. Moch, J. A. M. Vermaseren, and A. Vogt, "The Three loop splitting functions in QCD: The Nonsinglet case," *Nucl. Phys. B* **688** (2004) 101–134, arXiv:hep-ph/0403192.

[114] A. Vogt, S. Moch, and J. A. M. Vermaseren, "The Three-loop splitting functions in QCD: The Singlet case," *Nucl. Phys. B* **691** (2004) 129–181, arXiv:hep-ph/0404111.

[115] A. Grozin, J. M. Henn, G. P. Korchemsky, and P. Marquard, "Three Loop Cusp Anomalous Dimension in QCD," *Phys. Rev. Lett.* **114** no. 6, (2015) 062006, arXiv:1409.0023 [hep-ph].

[116] A. Grozin, J. M. Henn, G. P. Korchemsky, and P. Marquard, "The three-loop cusp anomalous dimension in QCD and its supersymmetric extensions," *JHEP* **01** (2016) 140, arXiv:1510.07803 [hep-ph].

[117] J. M. Henn, A. V. Smirnov, V. A. Smirnov, and M. Steinhauser, "A planar four-loop form factor and cusp anomalous dimension in QCD," *JHEP* **05** (2016) 066, arXiv:1604.03126 [hep-ph].

[118] J. Henn, A. V. Smirnov, V. A. Smirnov, M. Steinhauser, and R. N. Lee, "Four-loop photon quark form factor and cusp anomalous dimension in the large-$N_c$ limit of QCD," *JHEP* **03** (2017) 139, arXiv:1612.04389 [hep-ph].

[119] J. Davies, A. Vogt, B. Ruijl, T. Ueda, and J. A. M. Vermaseren, "Large-$n_f$ contributions to the four-loop splitting functions in QCD," *Nucl. Phys. B* **915** (2017) 335–362, arXiv:1610.07477 [hep-ph].

[120] R. N. Lee, A. V. Smirnov, V. A. Smirnov, and M. Steinhauser, "The $n_f^2$ contributions to fermionic four-loop form factors," *Phys. Rev. D* **96** no. 1, (2017) 014008, arXiv:1705.06862 [hep-ph].

[121] S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, "Four-Loop Non-Singlet Splitting Functions in the Planar Limit and Beyond," *JHEP* **10** (2017) 041, arXiv:1707.08315 [hep-ph].

[122] A. Grozin, "Four-loop cusp anomalous dimension in QED," *JHEP* **06** (2018) 073, arXiv:1805.05050 [hep-ph]. [Addendum: JHEP **01** (2019) 134].

[123] S. Moch, B. Ruijl, T. Ueda, J. A. M. Vermaseren, and A. Vogt, "On quartic colour factors in splitting functions and the gluon cusp anomalous dimension," *Phys. Lett. B* **782** (2018) 627–632, arXiv:1805.09638 [hep-ph].

[124] R. N. Lee, A. V. Smirnov, V. A. Smirnov, and M. Steinhauser, "Four-loop quark form factor with quartic fundamental colour factor," *JHEP* **02** (2019) 172, arXiv:1901.02898 [hep-ph].

[125] J. M. Henn, T. Peraro, M. Stahlhofen, and P. Wasser, "Matter dependence of the four-loop cusp anomalous dimension," *Phys. Rev. Lett.* **122** no. 20, (2019) 201602, arXiv:1901.03693 [hep-ph].

[126] A. von Manteuffel and R. M. Schabinger, "Quark and gluon form factors in four loop QCD: The $N_f^2$ and $N_{q\gamma}N_f$ contributions," *Phys. Rev. D* **99** no. 9, (2019) 094014, arXiv:1902.08208 [hep-ph].

[127] R. Brüser, A. Grozin, J. M. Henn, and M. Stahlhofen, "Matter dependence of the four-loop

QCD cusp anomalous dimension: from small angles to all angles," *JHEP* **05** (2019) 186, arXiv:1902.05076 [hep-ph].

[128] J. M. Henn, G. P. Korchemsky, and B. Mistlberger, "The full four-loop cusp anomalous dimension in $\mathcal{N} = 4$ super Yang-Mills and QCD," *JHEP* **04** (2020) 018, arXiv:1911.10174 [hep-th].

[129] A. von Manteuffel, E. Panzer, and R. M. Schabinger, "Cusp and collinear anomalous dimensions in four-loop QCD from form factors," *Phys. Rev. Lett.* **124** no. 16, (2020) 162001, arXiv:2002.04617 [hep-ph].

[130] J. Ablinger, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider, and F. Wißbrock, "The Transition Matrix Element $A_{gq}(N)$ of the Variable Flavor Number Scheme at $O(\alpha_s^3)$," *Nucl. Phys.* **B882** (2014) 263–288, arXiv:1402.0359 [hep-ph].

[131] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. Hasselhuhn, A. von Manteuffel, M. Round, C. Schneider, and F. Wißbrock, "The 3-Loop Non-Singlet Heavy Flavor Contributions and Anomalous Dimensions for the Structure Function $F_2(x, Q^2)$ and Transversity," *Nucl. Phys. B* **886** (2014) 733–823, arXiv:1406.4654 [hep-ph].

[132] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, and C. Schneider, "The 3-loop pure singlet heavy flavor contributions to the structure function $F_2(x, Q^2)$ and the anomalous dimension," *Nucl. Phys. B* **890** (2014) 48–151, arXiv:1409.1135 [hep-ph].

[133] J. Ablinger, A. Behring, J. Blümlein, A. De Freitas, A. von Manteuffel, and C. Schneider, "The three-loop splitting functions $P_{qg}^{(2)}$ and $P_{gg}^{(2,N_F)}$," *Nucl. Phys. B* **922** (2017) 1–40, arXiv:1705.01508 [hep-ph].

[134] J. Blümlein, P. Marquard, C. Schneider, and K. Schönwald, "The three-loop unpolarized and polarized non-singlet anomalous dimensions from off shell operator matrix elements," *Nucl. Phys. B* **971** (2021) 115542, arXiv:2107.06267 [hep-ph].

[135] G. Billis, M. A. Ebert, J. K. L. Michel, and F. J. Tackmann, "A toolbox for $q_T$ and 0-jettiness subtractions at N$^3$LO," *Eur. Phys. J. Plus* **136** no. 2, (2021) 214, arXiv:1909.00811 [hep-ph].

[136] R. Brüser, Z. L. Liu, and M. Stahlhofen, "Three-Loop Quark Jet Function," *Phys. Rev. Lett.* **121** no. 7, (2018) 072003, arXiv:1804.09722 [hep-ph].

[137] P. Banerjee, P. K. Dhani, and V. Ravindran, "Gluon jet function at three loops in QCD," *Phys. Rev. D* **98** no. 9, (2018) 094016, arXiv:1805.02637 [hep-ph].

[138] D. Baranowski, M. Delto, K. Melnikov, and C.-Y. Wang, "Same-hemisphere three-gluon-emission contribution to the zero-jettiness soft function at N3LO QCD," *Phys. Rev. D* **106** no. 1, (2022) 014004, arXiv:2204.09459 [hep-ph].

[139] D. Baranowski, M. Delto, K. Melnikov, and C.-Y. Wang, "On phase-space integrals with Heaviside functions," *JHEP* **02** (2022) 081, arXiv:2111.13594 [hep-ph].

[140] W. Chen, F. Feng, Y. Jia, and X. Liu, "Double-Real-Virtual and Double-Virtual-Real Corrections to the Three-Loop Thrust Soft Function," arXiv:2206.12323 [hep-ph].

[141] J. Ellis, "TikZ-Feynman: Feynman diagrams with TikZ," *Comput. Phys. Commun.* **210** (2017) 103–123, arXiv:1601.05437 [hep-ph].

[142] D. A. Cox, J. Little, and D. O'Shea, *Ideals, Varieties, and Algorithms*. Springer, Cham, 2018.

[143] W. Decker, G.-M. Greuel, G. Pfister, and H. Schönemann, "SINGULAR 4.2.1 — A computer algebra system for polynomial computations," 2021. http://www.singular.uni-kl.de.