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Adequate bases of phase space master integrals for $gg \to h$ at NNLO and beyond

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Abstract: We study master integrals needed to compute the Higgs boson production cross section via gluon fusion in the infinite top quark mass limit, using a canonical form of differential equations for master integrals, recently identified by Henn, which makes their solution possible in a straightforward algebraic way. We apply the known criteria to derive such a suitable basis for all the phase space master integrals in afore mentioned process at next-to-next-to-leading order in QCD and demonstrate that the method is applicable to next-to-next-to-next-to-leading order as well by solving a non-planar topology. Furthermore, we discuss in great detail how to find an adequate basis using practical examples. Special emphasis is devoted to master integrals which are coupled by their differential equations.

Keywords: Higgs production, QCD, master integrals, method of differential equations

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1 Introduction

In order to study the compatibility of the assumed Higgs particle discovered by ATLAS and CMS [1, 2] with the standard model precise theoretical predictions are required. One of the basic physical observables is the total inclusive Higgs production cross section which is, as is well known, dominated by gluon fusion at the LHC. For a long time the state of the art in fixed-order perturbative calculations of the total inclusive Higgs production cross section in the gluon fusion channel has been next-to-leading-order (NLO) for electroweak corrections and next-to-next-to-leading order (NNLO) for QCD corrections (see ref. [3] for comprehensive reviews). The latter ones have firstly been calculated in the infinite top mass limit [4–6] while finite mass corrections were included in refs. [7–12].

In recent years, various next-to-next-to-next-to-leading order (N^{3}LO) QCD approximations have become available [13, 14] but the full calculation remains a challenging frontier.

Some partial results have been obtained with full dependence on the partonic center-of-mass energy (in the infinite top mass limit), including the three-loop matrix elements [15–17], the one-loop squared single-real-emission contributions [18, 19] and the convolutions of NNLO cross sections with splitting functions [20–22] which require the knowledge of the NNLO master integrals to higher orders in ϵ [23, 24]. Other results are only available as threshold expansions. They include the partonic cross section of the purely three-parton real emission [25], the two-loop soft current [26, 27], the one-loop two emission contribution [28], culminating in the hadronic Higgs production cross section at threshold [29].

In this paper we calculate the dependence of master integrals, appearing in calculations of the total inclusive Higgs production cross section via gluon fusion in the infinite top mass limit, on the kinematic variable x, which is derived by the method of differential equations [30–34] (see refs. [35, 36] for comprehensive reviews). The differential equations become, however, more and more complicated with growing loop order. At $\mathrm{N^3LO}$ level it seems rather difficult to obtain solutions of the differential equations high enough in the ϵ-expansion in a naively chosen basis of master integrals. Recently, a very elegant form of differential equations was introduced in ref. [37] which is supposed to exist at any loop order. This conjecture has been strengthened by plenty of examples at two-loop [37–42] and three-loop order [43–45] which show the applicability to various kinematic configurations, even to single-scale integrals [44]. Although there exist algorithms for constructing an adequate basis in cases of differential equations depending on ϵ polynomially [39] and for finite integrals in $D = 4$ dimensions [45] as well as a strategy for the construction from a basis with a triangular finite part of the homogeneous differential equation matrix [42], a general algorithm to find such a basis is still missing. However, a lot of methods, tricks and ideas do exist which are discussed in the references above and used in practice.

The purpose of this paper is twofold. On the one hand, we review the techniques for finding an adequate basis using NLO and NNLO master integrals for Higgs production cross section in sections 2 and 3, respectively, giving the explicit bases as well. We also present a trick using a characteristic form of higher order differential equations for the case of coupled master integrals in section 3.2, which, to our knowledge, has hitherto not been discussed in the literature. On the other hand, we show the applicability of the method to the state of the art problem of finding solutions with full x-dependence to master integrals appearing in $\mathrm{N^3LO}$ Higgs production by solving a non-planar topology in section 4. In section 5 we state our conclusions and outlook.

2 General idea and NLO warm-up

2.1 Reduction to master integrals

Suppose that we have families of Feynman integrals, also called topologies, to be evaluated where the propagator labelled by i is raised to a power a_i, usually called index. Within dimensional regularization [46] integration-by-parts (IBP) identities give linear relations among integrals with different values of indices a_i [47]. Starting from a large set of values of a_i, all integrals can be reduced to a linearly independent set of master integrals by making use of the IBP identities by means of, e.g., Laporta algorithm [48].

We treat phase space integrals contributing to the Higgs production cross section as cut integrals [49]. In the same way as loop integrals, cut integrals can be reduced to master integrals via IBP identities by means of the reverse-unitarity method [5, 25]. The only difference stems from the fact that integrals containing a cut line with a non-positive index $a_c \leq 0$ vanish. In order to identify subtopologies, families of Feynman integrals obtained by setting subsets of indices to be zero, that have no cuts or are scaleless within dimensional regularization, we use the private `Mathematica` package `TopoID`. This code also provides symmetries useful for the reduction and allows us to identify a minimal set of master integrals.

In this work, we have used an in-house implementation of Laporta algorithm, as well as the program `FIRE` [50, 51] together with its unpublished C++ version. The result is stored in a reduction table for later repeated use.

In the reduction, we use Feynman propagators in Euclidean metric, which applies also to the master integrals given in this paper.

2.2 Differential equations for master integrals

In the case of Higgs production via gluon fusion in the infinite top mass limit, each topology has only one massive Higgs line and we have forward scattering kinematics, i.e., the incoming partons' momenta p_1 and p_2 are equal to the outgoing partons' momenta $p_3 = p_1$ and $p_4 = p_2$, respectively. Therefore, aside from the trivial overall mass scale, the integrals depend only on one kinematic variable $x = m_h^2/s$ with $s = (p_1 + p_2)^2$ and the space-time dimension $D = 4 - 2\epsilon$. Without loss of generality we can set $s = 1$. The derivative of each master integral with respect to x is given, up to a constant prefactor, by raising the index of the massive line by one and the resulting integral can be reduced to a linear combination of master integrals. In this way, we arrive at a set of differential equations for N master integrals, which can be expressed as the following matrix form:

$$\partial_x \tilde{f}(x,\epsilon) = \tilde{A}(x,\epsilon)\tilde{f}(x,\epsilon), \tag{2.1}$$

where $\tilde{f}$ is a column vector of master integrals of length N and $\tilde{A}$ is an $N \times N$ matrix.

2.3 Change of basis

The choice of master integrals is not unique and one can always choose another basis of master integrals. The basis transformation can be obtained by looking up the entries in the reduction table for the *new* basis integrals f which are by construction linear combinations of the *old* basis integrals $\tilde{f}$:

$$f(x,\epsilon) = B(x,\epsilon)\tilde{f}(x,\epsilon), \tag{2.2}$$

with an $N \times N$ matrix B. Taking the derivative of eq. (2.2) with respect to x, one arrives at the differential equations for the new basis integrals:

$$\partial_x f(x,\epsilon) = A(x,\epsilon)f(x,\epsilon), \qquad \text{with } A := \left[(\partial_x B) + B\tilde{A}\right] B^{-1}. \tag{2.3}$$

This means that, providing an alternative basis f, we instantly know the form of its differential equation A by use of the reduction table to obtain B as well as $\tilde{A}$.

2.4 Master integral basis in canonical form

Following Henn's conjecture [37], a basis f of integrals exists in which all master integrals become so-called *pure functions*[1] and satisfy the differential equations

$$\partial_x f(x,\epsilon) = \epsilon \bar{A}(x) f(x,\epsilon), \tag{2.4}$$

i.e., the dependence of the matrix A on the dimensional parameter ϵ is factored out as $A = \epsilon \bar{A}$. To ensure the basis integrals are pure functions, $\bar{A}$ should have the form

$$\bar{A}(x) = \sum_k \frac{\alpha_k}{x - x_k}, \tag{2.5}$$

where x_k are constants and α_k are constant matrices. The system of differential equations (2.4) can be expanded in ϵ as

$$\partial_x f^{[n]}(x) = \bar{A}(x) f^{[n-1]}(x), \qquad \text{with} \quad f(x,\epsilon) = \sum_{n=-\infty}^{\infty} \epsilon^n f^{[n]}(x), \tag{2.6}$$

and one can solve it order by order. The expanded system (2.6) is triangular in the sense that only lower order functions $f^{[n-1]}$ appear in the right-hand side of the set of differential equations for $f^{[n]}$, hence the solution can be easily obtained in terms of iterated integrals, provided the boundary condition is fixed at some point $x = x_0$.

The matrix $\bar{A}$ respects singular points of the process, in this case we have: for $x = 0$ the Higgs line becomes massless and additional infra-red singularities may be introduced. In addition, at $x = 1$, more precisely for approach from $x < 1$, the diagrams develop a non-zero imaginary part, since the Higgs may be produced indeed. In our calculation, we observe another singular point at $x = -1$ for some NNLO integrals[2], yielding the canonical form (2.5) for the differential equations:

$$\bar{A}(x) = \frac{a}{x} + \frac{b}{1-x} + \frac{c}{1+x}, \tag{2.7}$$

where we find the matrices a, b and c to just contain rational numbers. This assures that at any order the ϵ-expansion of the solution of the differential equations are iterated integrals expressible as harmonic polylogarithms (HPLs) [53], which can be easily manipulated with `HPL` package implemented in `Mathematica` [54, 55]. The first term of the solution in the expansion is a constant, the next in general contains also HPLs of weight one, the next in addition HPLs of weight two, etc. Therefore, the result will be a linear combination of HPLs with constant prefactors. If the integration constants have suitable weight the master integrals are pure functions.

[1] The number of iterated integrations needed to define a function is called weight. If a function f consists of terms having a uniform weight and if taking a derivative of f also gives a function in which all summands have a uniform weight lowered by one, then f is called *pure* [37, 52]. This definition forbids transcendental functions in f from being multiplied by algebraic coefficients apart from numbers, thus master integrals given by pure functions usually have more compact expressions.

[2] Our results for the canonical basis integrals contain one more singular point for $x \to \infty$ in the unphysical region.

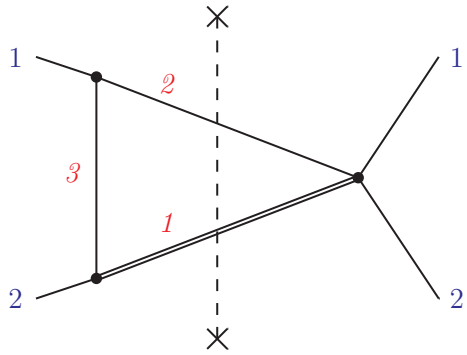


Figure 1. The NLO topology $\mathrm{TNLO}_2(a_1, a_2, a_3)$. The massive Higgs line is depicted by a double line, whereas the dashed line denotes the cut. Numbers in roman indicate the incoming and outgoing momenta p_1 and p_2, and numbers in italic label the propagators according to the corresponding indices.

2.5 Parametric representations of integrals

Although there is no algorithm to obtain an optimal basis from arbitrary basis integrals in general, there exist some guiding principles how to find candidate integrals that may give a canonical form. For example, integrals having unit leading singularities [52, 56] are expected to be uniform weight functions. Another one is investigating parametric representations of integrals, which is described as follows.

The notion that pure functions are built from iteratively integrated logarithms [37] imposes strong constraints on the candidates. Sketching the Feynman parameter representation for an integral I (see, e.g., [36])

$$\begin{aligned} I(x,\epsilon) &\sim \int \prod_j d\alpha_j \frac{[U(\{\alpha_i\})]^{e_U} \prod_i \alpha_i^{a_i-1} \delta(\sum_k \alpha_k - 1)}{[W(x,\{\alpha_i\})]^{e_W}}, \\ e_U &= a - (l+1)D/2, \\ e_W &= a - lD/2, \\ a &= \sum_i a_i, \end{aligned} \tag{2.8}$$

where l is the number of loops, U and W are polynomials in the Feynman parameters α_i and a_i are the corresponding indices. An integral of form

$$\int \prod_j d\alpha_j \frac{1}{[g(\{\alpha_i\}, x)]^k}, \qquad \text{with } k \in \mathbb{N}, \tag{2.9}$$

where g is an irreducible polynomial, is favored over those of different form as it yields more likely a pure function in x, see the discussion about d-log forms in ref. [57].

Let us illustrate this statement by considering the NLO problem. After applying symmetries of diagrams and performing partial fraction decomposition, one is left with only one topology $\mathrm{TNLO}_2(a_1, a_2, a_3)$ depicted in fig. 1. A standard Laporta algorithm finds one

master integral, typically given by $\mathrm{TNLO}_2(1,1,0)$ obeying the differential equation

$$\partial_x \mathrm{TNLO}_2(1,1,0) = -\frac{1-2\epsilon}{1-x}\mathrm{TNLO}_2(1,1,0). \tag{2.10}$$

Although the missmatch from eq. (2.4) can be cured with a suitable x-normalization (see section 3), let us try to understand it from the parametric representation eq. (2.8). We have $U = 1$ from the δ-function for all NLO integrals. Furthermore, $\mathrm{TNLO}_2(1,1,0)$ has $a = 2$ and therefore $e_W \approx 0$, where we understand the "$\approx$" symbol as the $D = 4$ approximation[3]. Therefore, we find $k \approx 0$ in eq. (2.9), accounting for the non-canonical form of eq. (2.10). The other way around, we need $a = 3$ to obtain $k = e_W \approx 1$. This can be achieved, e.g., by raising the index of the massive Higgs line by one, $\mathrm{TNLO}_2(2,1,0)$, or adding another propagator, $\mathrm{TNLO}_2(1,1,1)$. In the former case, raising the index of the Higgs line causes an additional α_1 in the numerator which cancels against an overall α_1 in W of the denominator. Writing down the differential equations, we see that the mentioned candidates indeed turn out to form canonical bases:[4]

$$\begin{aligned}\partial_x \mathrm{TNLO}_2(2,1,0) &= \frac{2\epsilon}{1-x}\mathrm{TNLO}_2(2,1,0),\\ \partial_x \mathrm{TNLO}_2(1,1,1) &= \frac{2\epsilon}{1-x}\mathrm{TNLO}_2(1,1,1).\end{aligned} \tag{2.11}$$

It is important to remember this fact in the following since these diagrams will appear as subgraphs at higher loop order. Performing the same manipulations, i.e. raising one index of a bubble or stretching it into a triangle, for the subgraphs will lead to promising candidates (see ref. [43] as well). In general, we observe that there are cases where adding additional lines or raising indices helps. Finally, it is worth mentioning that the arguments given here have made use of the diagrammatic structure of the integrals, but (apart from the α_1 cancellation mentioned above) not of the explicit structure of the W polynomial in eq. (2.8) and therefore were (almost) independent of the kinematics. Hence, it is not surprising that some of the integrals in canonical bases given in section 3 and section 4 resemble results for similar topologies with different kinematics found in the literature.

3 NNLO: examples and solutions

3.1 Known techniques

Let us discuss further known tricks for finding an adequate basis by looking at the example of the three-particle phase space diagram defined in terms of the topology TTA_3 (see fig. 2) occurring at NNLO via

$$\mathrm{TTA}_3(1,1,1,0,0,0,0) =: \mathrm{TTA}_3(1,1,1), \tag{3.1}$$

[3] For the purpose of finding candidates in a canonical basis, ϵ-dependence of powers can be ignored. See also, e.g., ref. [43].

[4] Although these two integrals obey the same differential equation their solutions are different due to different boundary conditions.

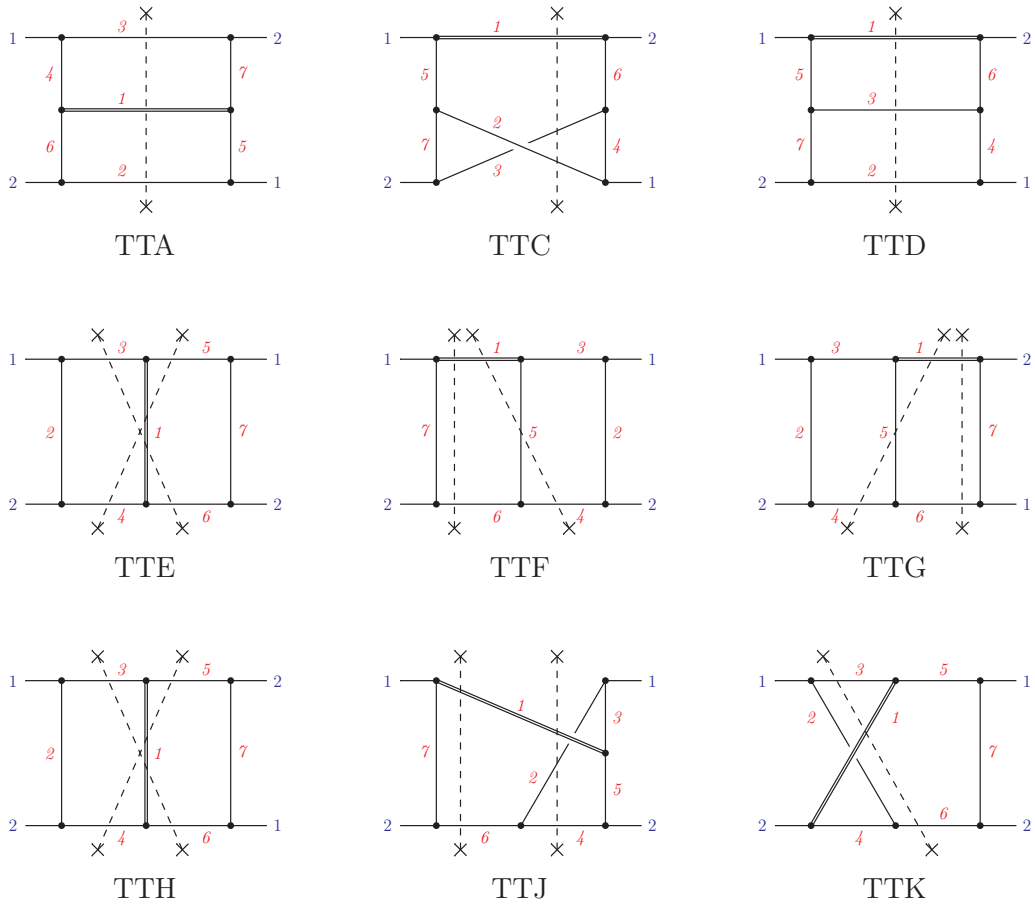


Figure 2. The NNLO topologies $\mathrm{TT}X_c(a_1, a_2, a_3, a_4, a_5, a_6, a_7)$ involving our choice for a canonical basis. The subscript $c = 2, 3$ of topologies distinguishes two-particle cuts and three-particle cuts. The massive Higgs line is depicted by a double line, whereas dashed lines denote possible cuts. Numbers in roman indicate the incoming and outgoing momenta p_1 and p_2 and numbers in italic label the propagators according to the corresponding indices. In the text we define all integrals as single-cut integrals. For TTE and TTH, two cuts give the same contribution but only one of them is taken into account in the defnition of the corresponding master integrals.

where we omit the trailing zeros in the indices for simplicity. In the reduction basis obtained from our reduction table, its differential equation is coupled to another integral $\mathrm{TTA}_3(1, 1, 1, -1, 0, 0, 0)$ having an additional scalar product in the numerator. For the purpose of finding good candidates we raise one index of the massless bubble [43]. It is well known that integrating a massless bubble with the indices b_1 and b_2 gives, up to a prefactor, a propagator with the index $b_1 + b_2 - 2 + \epsilon$. Therefore, we have

$$V_1^* = \mathrm{TTA}_3(2, 2, 1) \sim \mathrm{TNLO}_2(2, 1 + \epsilon, 0) \tag{3.2}$$

and we expect this to be a good candidate from the discussion for the NLO case in section 2. The second candidate which couples to this one can be found by constructing a subtle *linear*

combination. For that purpose, let us compare eq. (2.8) to eq. (2.9) for $k = 1$, i.e. in a first step we set $e_W \approx k = 1$. This means that we have fixed $a = 5$ and $e_U \approx -1$. For example the parametric representation of the above candidate V_1^* is of the type

$$\mathrm{TTA}_3(2,2,1) \sim \int \prod_j d\alpha_j \frac{\alpha_1\alpha_2\delta(\sum_k \alpha_k - 1)}{(\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3)\, W(x,\{\alpha_i\})}. \tag{3.3}$$

One could try $\mathrm{TTA}_3(1,2,2)$ which is of the same form, but with $\alpha_1\alpha_2$ in the numerator replaced by $\alpha_2\alpha_3$. However, the candidate does not lead to a differential equation of the desired form. Therefore, one can try to identify W in eq. (3.3) with g in eq. (2.9), which means we have to cancel the U polynomial $(\alpha_1\alpha_2 + \alpha_1\alpha_3 + \alpha_2\alpha_3)$. This is achieved by adding three integrals to

$$V_2^* = \mathrm{TTA}_3(2,2,1) + \mathrm{TTA}_3(2,1,2) + \mathrm{TTA}_3(1,2,2) = 2\mathrm{TTA}_3(2,2,1) + \mathrm{TTA}_3(1,2,2). \tag{3.4}$$

Note that the construction given above can be generalized to any loop order for this type of sunrise diagrams (see the results of section 4 for the three-loop case).

Constructing the differential equations for the candidates V_1^* and V_2^* using eq. (2.3) we find only A_{22} to be of inappropriate form

$$\lim_{\epsilon\to 0} A = \begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{1-x} \end{pmatrix}. \tag{3.5}$$

The non-vanishing *diagonal* element corresponds to the homogeneous differential equation of V_2^* in lowest order in ϵ and therefore it appears in all orders [35]. The problem is resolved by allowing for an ϵ independent $n(x)$-*normalization*, i.e. a shift $V_2^* \to n(x)V_2^*$, yielding

$$\lim_{\epsilon\to 0} A_{22} = \frac{1}{1-x} + \frac{\partial_x n(x)}{n(x)} \stackrel{!}{=} 0. \tag{3.6}$$

This determines $n(x) = 1 - x$ and we have found two elements of the canonical basis

$$\begin{aligned} V_1 &= \epsilon\mathrm{TTA}_3(2,2,1), \\ V_2 &= \epsilon(1-x)\big[2\mathrm{TTA}_3(2,2,1) + \mathrm{TTA}_3(1,2,2)\big], \end{aligned} \tag{3.7}$$

obeying the differential equation with

$$A = \epsilon \begin{pmatrix} -\frac{3}{x} & \frac{1}{x} + \frac{1}{1-x} \\ -\frac{6}{x} & \frac{2}{x} + \frac{4}{1-x} \end{pmatrix}. \tag{3.8}$$

The prefactors of ϵ have been introduced to make the integrals start at finite order.

Note that the result, we have found here, will not be changed by adding more master integrals to the considerations. In this sense, finding a canonical basis can be approached *step by step*, starting with the integrals with lowest number of lines and continuously increasing that number. Master integrals with coupled differential equations have to be added in one step to the problem, but here other strategies apply, as we show in section. 3.2.

Now we add the next master integral of the topology TTA_3 to the problem, given by $V_3^* = \mathrm{TTA}_3(1,1,1,1,0,1,0)$, where we have just taken the integral from the reduction basis as a candidate. Since it has $a = 5$ in its parametric representation (2.8), this is a good choice as motivated above. The matrix defining the differential equations becomes

$$A = \begin{pmatrix} -\frac{3\epsilon}{x} & \frac{\epsilon}{x} + \frac{\epsilon}{1-x} & 0 \\ -\frac{6\epsilon}{x} & \frac{2\epsilon}{x} + \frac{4\epsilon}{1-x} & 0 \\ -\frac{1}{\epsilon^2 x} & \frac{1}{2\epsilon^2 x} & -\frac{2\epsilon}{x} \end{pmatrix}, \tag{3.9}$$

where the upper left 2×2 block corresponds to (V_1, V_2) and forms a canonical basis already as eq. (3.8). The *off-diagonal* elements in the last row depend on ϵ differently from the desired form. These elements correspond to the inhomogeneous terms in the differential equation for V_3^*. The problem is cured by $n(\epsilon)$-*normalization*, i.e. by changing $V_3^* \to n(\epsilon)V_3^*$. In this case we find $n(\epsilon) = \epsilon^3$, such that

$$V_3 = \epsilon^3 \mathrm{TTA}_3(1,1,1,1,0,1,0) \tag{3.10}$$

completes a canonical basis of the 3×3 subproblem.

In summary, a diagonal scaling matrix

$$B^{\mathrm{s}}_{ij} = \begin{cases} s_i(x,\epsilon), & i = j, \\ 0, & i \neq j, \end{cases} \tag{3.11}$$

changes the coefficient matrix as

$$A^{\mathrm{s}}_{ij} = \frac{\partial_x s_i}{s_i}\delta_{ij} + \frac{s_i}{s_j}A_{ij}. \tag{3.12}$$

Lastly, let us remark that bases exist where ϵ factorizes from their A matrix as in eq. (2.4) but the matrix is not of the desired form given in eq. (2.7). For example, choosing

$$V_3^* = (1+\epsilon)\epsilon^2 x \mathrm{TTA}_3(1,1,1,2,0,1,0) \tag{3.13}$$

instead of V_3 the last row in eq. (3.9) changes to

$$A = \begin{pmatrix} -\frac{3\epsilon}{x} & \frac{\epsilon}{x} + \frac{\epsilon}{1-x} & 0 \\ -\frac{6\epsilon}{x} & \frac{2\epsilon}{x} + \frac{4\epsilon}{1-x} & 0 \\ -3\epsilon & \frac{\epsilon}{2} + \frac{\epsilon}{1-x} & -\frac{2\epsilon}{x} \end{pmatrix}, \tag{3.14}$$

where the off-diagonal elements in the last row induce non-logarithmic functions in the solution of V_3^* and therefore the result cannot be a pure function.

3.2 Techniques for coupled master integrals

The techniques we want to discuss next touches on the issue of master integrals coupled by their differential equations. In particular, a problem that occurs frequently is the following: when there is a system of n coupled master integrals in a reduction basis, one tries a set of n candidates for a canonical basis and sees if the resulting n differential equations are of the

canonical form or not. Even if one of the n candidates is a *good* integral that would form a canonical basis with appropriately chosen other $(n-1)$ good integrals, the corresponding differential equation may not be of the canonical form due to a choice of the other $(n-1)$ *bad* integrals, which makes it difficult to identify good integrals. Nonetheless, it would be worthwhile knowing if one of the n candidates is a canonical basis integral so one could keep good integrals and dismiss bad integrals.

In the following we want to show how to distinguish suitable candidates for canonical master integrals from unsuitable choices using the fact that the system of n coupled first order differential equations is equivalent to one nth order differential equation for one of the master integrals. The idea is that the resulting higher order differential equation is unique for each master integral in the sense that it is independent of eliminated integrals. It defines the master integral itself and furthermore takes a specific form for canonical master integrals, founding on the assumption that a set of canonical master integrals exists. Moreover, we will show that once one of canonical master integrals in a coupled system is found the assumption of the existence of a canonical basis allows us to construct a set of the other canonical master integrals coupled to it.

3.2.1 Characteristic form of higher order differential equations

Let us discuss the situation of two coupled master integrals f_1 and f_2 to explain the method in detail:

$$\begin{aligned} f_1' &= a_{11} f_1 + a_{12} f_2 + \sum_i r_{1i} g_i, \\ f_2' &= a_{21} f_1 + a_{22} f_2 + \sum_i r_{2i} g_i, \end{aligned} \tag{3.15}$$

where primes denote derivatives with respect to x and g_i in the right-hand sides are master integrals assumed to be fixed already and to form a canonical basis, obeying

$$g_i' = \sum_j \alpha_{ij} g_j. \tag{3.16}$$

All the quantities given here depend on x and ϵ. Taking one more derivative with respect to x of the first line of eq. (3.15) we find

$$f_1'' = a_{11}' f_1 + a_{11} f_1' + a_{12}' f_2 + a_{12} f_2' + \sum_i \left(r_{1i}' g_i + r_{1i} g_i' \right). \tag{3.17}$$

Eliminating f_2 and f_2' by eq. (3.15) and g_i' by eq. (3.16) we obtain a second order differential equation for f_1:

$$\begin{aligned} f_1'' &= -\left(-a_{11} - \frac{a_{12}'}{a_{12}} - a_{22} \right) f_1' + \left(a_{11}' - \frac{a_{11} a_{12}'}{a_{12}} + a_{12} a_{21} - a_{11} a_{22} \right) f_1 \\ &\quad + \sum_i \left(-\frac{a_{12}' r_{1i}}{a_{12}} - a_{22} r_{1i} + a_{12} r_{2i} + r_{1i}' + \sum_j r_{1j} \alpha_{ji} \right) g_i \\ &=: -C_1 f_1' + C_0 f_1 + \sum_i C_{0i} g_i. \end{aligned} \tag{3.18}$$

It is important to emphasize that this differential equation is independent of f_2 and uniquely defines the behaviour of f_1. The coefficients C_1, C_0 and C_{0i} are invariant under any basis transformations that change only f_2 as $f_2 \to b_{21}f_1 + b_{22}f_2 + \sum_i \beta_{2i}g_i$.

Case 1: f_1 and f_2 are canonical master integrals. Let us now reveal what characteristic form for the higher order differential equation of f_1 should appear when f_1 and f_2 are canonical master integrals as g_i are. In such a basis, a_{ij} and r_{ij} as well as α_{ij} are proportional to ϵ. Therefore, the coefficients C_1, C_0 and C_{0i} defined by eq. (3.18) can be decomposed into ϵ independent coefficients as

$$\begin{aligned} C_1 &= C_1^{(0)} + \epsilon C_1^{(1)}, \\ C_0 &= \epsilon C_0^{(1)} + \epsilon^2 C_0^{(2)}, \\ C_{0i} &= \epsilon C_{0i}^{(1)} + \epsilon^2 C_{0i}^{(2)}, \end{aligned} \tag{3.19}$$

given by

$$\begin{aligned} C_1^{(0)} &= -\frac{a'_{12}}{a_{12}}, \\ C_1^{(1)} &= \frac{1}{\epsilon}\left(-a_{11} - a_{22}\right), \\ C_0^{(1)} &= \frac{1}{\epsilon}\left(a'_{11} - \frac{a_{11}a'_{12}}{a_{12}}\right), \\ C_0^{(2)} &= \frac{1}{\epsilon^2}\left(a_{12}a_{21} - a_{11}a_{22}\right), \\ C_{0i}^{(1)} &= \frac{1}{\epsilon}\left(-\frac{a'_{12}r_{1i}}{a_{12}} + r'_{1i}\right), \\ C_{0i}^{(2)} &= \frac{1}{\epsilon^2}\left(-a_{22}r_{1i} + a_{12}r_{2i} + \sum_j r_{1j}\alpha_{ji}\right). \end{aligned} \tag{3.20}$$

Case 2: f_1 is a canonical master integral but f_2 is not. Even if f_2 is not a canonical master integral and it makes a_{ij} and r_{ij} not be of canonical form, we can utilize the uniqueness of the coefficients C_1, C_0 and C_{0i} in the higher order differential equation for f_1. They must still have decompositions in ϵ like eq. (3.19), although the identities for $C_1^{(m)}$, $C_0^{(m)}$, $C_{0i}^{(m)}$ in terms of a_{ij} and r_{ij} eq. (3.20) do not hold any longer. Furthermore, it allows us to reconstruct what coefficients a_{ij}^{p} and r_{ij}^{p} in a system of differential equations would be within a basis in which f_2 is properly chosen to be a canonical master integral f_2^{p}, under the assumption that such an f_2^{p} does exist. Since in such a proper basis C_1, C_0 and C_{0i} take the same form as **Case 1** in terms of a_{ij}^{p} and r_{ij}^{p}, we can invert eq. (3.20) to obtain a_{ij}^{p}

and $r^{\rm p}_{ij}$:

$$\begin{aligned}
a^{\rm p}_{12}{}' + C^{(0)}_1 a^{\rm p}_{12} &= 0,\\
a^{\rm p}_{11}{}' - \frac{a^{\rm p}_{12}{}'}{a^{\rm p}_{12}} a^{\rm p}_{11} &= \epsilon C^{(1)}_0,\\
a^{\rm p}_{22} &= -a^{\rm p}_{11} - \epsilon C^{(1)}_1,\\
a^{\rm p}_{21} &= \frac{a^{\rm p}_{11} a^{\rm p}_{22}}{a^{\rm p}_{12}} + \epsilon^2 \frac{C^{(2)}_0}{a^{\rm p}_{12}},\\
r^{\rm p}_{1i}{}' - \frac{a^{\rm p}_{12}{}'}{a^{\rm p}_{12}} r^{\rm p}_{1i} &= \epsilon C^{(1)}_{0i},\\
r^{\rm p}_{2i} &= \frac{a^{\rm p}_{22} r^{\rm p}_{1i}}{a^{\rm p}_{12}} - \sum_j \frac{r^{\rm p}_{1j}\alpha_{ji}}{a^{\rm p}_{12}} + \epsilon^2 \frac{C^{(2)}_{0i}}{a^{\rm p}_{12}}.
\end{aligned} \tag{3.21}$$

We can solve this system of differential equations, line by line for a_{ij} and r_{ij}, setting the integration constants of a_{12}, a_{11} and r_{1i} to constants proportional to ϵ, namely ϵc_{12}, ϵc_{11} and ϵk_{1i}, respectively.

3.2.2 Construction of canonical basis

Having all entries of $a^{\rm p}_{ij}$ and $r^{\rm p}_{ij}$ as in **Case 2** of the previous section, one can construct a canonical master integral $f^{\rm p}_2$ that satisfies the differential equations implied by $a^{\rm p}_{ij}$ and $r^{\rm p}_{ij}$. The linear basis transformation

$$B = \begin{pmatrix} \mathbb{1} & 0 & 0\\ 0 & 1 & 0\\ \beta_{2i} & b_{21} & b_{22} \end{pmatrix} \tag{3.22}$$

from the basis (g_i, f_1, f_2) obeying the differential equation with the matrix A to the canonical basis $(g_i, f_1, f^{\rm p}_2)$ with $A^{\rm p}$ satisfies eq. (2.3), or

$$B' = A^{\rm p} B - B A, \tag{3.23}$$

where the matrix A and $A^{\rm p}$ are given by

$$A = \begin{pmatrix} \alpha_{ij} & 0 & 0\\ r_{1i} & a_{11} & a_{12}\\ r_{2i} & a_{21} & a_{22} \end{pmatrix}, \qquad A^{\rm p} = \begin{pmatrix} \alpha_{ij} & 0 & 0\\ r^{\rm p}_{1i} & a^{\rm p}_{11} & a^{\rm p}_{12}\\ r^{\rm p}_{2i} & a^{\rm p}_{21} & a^{\rm p}_{22} \end{pmatrix}. \tag{3.24}$$

Each component in the row corresponding to f_1 (the next to the last line) of eq. (3.23) gives a linear equation for β_{2i}, b_{21} and b_{22}, respectively. The rows above the mentioned one give trivial equations, whereas the row below gives differential equations that serve as consistency checks. Once the basis transformation B is determined, one can obtain an explicit expression of $f^{\rm p}_2$ as a linear combination of g_i, f_1 and f_2.

Note that until the end we do not need to fix the integration constants c_{12}, c_{11} and k_{1i} introduced in **Case 2**. Since from eq. (3.21) $a^{\rm p}_{12}$ is proportional to c_{12} and $a^{\rm p}_{21}$ and $r^{\rm p}_{2i}$ are

proportional to c_{12}^{-1} whereas a_{11}^{p}, a_{22}^{p} and r_{1i}^{p} are independent of it, c_{12}^{-1} can be interpreted as a numerical normalization factor of f_2^{p}, see eqs. (3.11) and (3.12). In addition to the normalization factor c_{12}^{-1}, c_{11} and k_{1i} span a multi-dimensional space of solutions for f_2^{p} and cover the full class of canonical master integrals that are coupled partners to f_1.

So far, we have seen that if f_1 is a canonical master integral one can construct another canonical master integral f_2^{p} coupled to f_1. This leads to an algorithm to see whether f_1 can be a canonical master integral: assuming f_1 is a canonical master integral, one tries to construct f_2^{p} on the basis of the above considerations. If it fails at any step, one concludes that f_1 cannot be a canonical master integral. Once f_2^{p} is explicitly constructed, one can see whether f_1 and f_2^{p} form a canonical basis as they should, which is equivalent to find a consistent solution of B in eq. (3.23). The details are as follows:

1. Calculate the coefficients C_1, C_0 and C_{0i} in the higher order differential equation for f_1 from a_{ij} and r_{ij} by eq. (3.18).

2. Assuming f_1 is a canonical master integral, one should find that C_1, C_0 and C_{0i} have decompositions in ϵ as eq. (3.19), otherwise f_1 cannot be a canonical master integral and should be dismissed.

3. Reconstruct a_{ij}^{p} and r_{ij}^{p} from $C_1^{(m)}$, $C_0^{(m)}$ and $C_{0i}^{(m)}$ by eq. (3.21). If one requires them to be of the desired form

$$a_{ij}^{\mathrm{p}}, r_{ij}^{\mathrm{p}} \sim \epsilon \left(\frac{n_0}{x} + \frac{n_1}{1-x} + \frac{n_{-1}}{1+x} \right), \tag{3.25}$$

   where n_0, n_1 and n_{-1} are numbers, the differential equations for a_{12}^{p}, a_{11}^{p} and r_{1i}^{p} must be easily solved, and if they are difficult to solve most likely they do not have the above form[5]. If one of the reconstructed entries a_{ij}^{p} and r_{ij}^{p} are not of the form eq. (3.25), f_1 cannot be a canonical master integral.

4. Find the basis transformation (3.22) to the basis that satisfies the differential equations given by a_{ij}^{p} and r_{ij}^{p} from eq. (3.23). From this transformation one obtains f_2^{p}. If there is no solution of eq. (3.23) with eq. (3.22), f_1 cannot be a canonical master integral.

Note that in our case eq. (3.25) is imposed on the canonical form, but for the derivation of f_2^{p} we only needed the assumption that a_{ij}^{p} and r_{ij}^{p} are proportional to ϵ. Therefore this algorithm should also work for other calculations within the framework of canonical differential equations having different forms (2.5) in x.

3.2.3 Example in the three-particle phase space at NNLO

Let us apply the above algorithm to the example of the two coupled phase space integrals of $\mathrm{TTA}_3(a_1, a_2, a_3)$ we have already encountered in section 3.1. More specifically, we put

$$\begin{aligned} f_1 &= \epsilon \mathrm{TTA}_3(2,2,1), \\ f_2 &= \mathrm{TTA}_3(2,1,1). \end{aligned} \tag{3.26}$$

[5] Actually, eq. (3.25) can be taken as an ansatz for the differential equations such that all differential equations we need to solve are reduced to algebraic equations.

We have previously seen that $f_1 = V_1$ is a canonical master integral, nevertheless we will apply the algorithm to this pair of integrals and see what happens. The differential equations have no inhomogeneous terms and therefore

$$\begin{aligned} r_{1i} &= 0, \\ r_{2i} &= 0. \end{aligned} \tag{3.27}$$

Writing down the second order differential equation for f_1, we can reconstruct A^{p} from its coefficients:

$$A^{\mathrm{p}} = \epsilon \begin{pmatrix} \frac{c_{11}}{x} + \frac{c_{11}+3}{1-x} & \frac{c_{12}}{x} + \frac{c_{12}}{1-x} \\ -\frac{c_{11}(c_{11}+1)}{c_{12}x} - \frac{(c_{11}+3)(c_{11}-1)}{c_{12}(1-x)} & -\frac{c_{11}+1}{x} - \frac{c_{11}-1}{1-x} \end{pmatrix}. \tag{3.28}$$

Correspondingly, we can find f_2^{p} as

$$f_2^{\mathrm{p}} = \frac{1 - c_{11}(1-4\epsilon) - 2\epsilon(1+x)}{c_{12}(1-4\epsilon)} f_1 - \frac{2\epsilon(1-2\epsilon)(1-3\epsilon)}{c_{12}(1-4\epsilon)} f_2. \tag{3.29}$$

Once f_2^{p} is obtained, one can easily check that f_1 and f_2^{p} form a canonical basis with A^{p}.

Note that we have not fixed the integration constants c_{11} and c_{12}. As discussed before, c_{12} determines the normalization of f_2^{p}. If we choose $c_{11} = -3$ and $c_{12} = 1$, A^{p} turns into eq. (3.8) and f_2^{p} becomes V_2, which can be verified by the reduction. Other interesting solutions are given by $c_{11} = 1$, $c_{12} = 1$ or $c_{11} = -1$, $c_{12} = 2$, for which $a_{21}^{\mathrm{p}} = a_{22}^{\mathrm{p}}$ and the second row of A^{p} becomes independent of $1/(1-x)$ or $1/x$, respectively.

By contrast, if we interchange f_1 and f_2 in the above example (3.26) and put

$$\begin{aligned} f_1 &= \mathrm{TTA}_3(2,1,1), \\ f_2 &= \epsilon \mathrm{TTA}_3(2,2,1), \end{aligned} \tag{3.30}$$

the first coefficient stemming from $C_1^{(0)}$ already yields

$$a_{12}^{\mathrm{p}} = -\epsilon c_{12} + \epsilon \frac{c_{12}}{x}, \tag{3.31}$$

in disagreement with the desired form (3.25). Therefore we can conclude $f_1 = \mathrm{TTA}_3(2,1,1)$ cannot be a canonical master integral.

3.2.4 Example with a non-zero inhomogeneity

As we will see in section 3.3, there is another pair of coupled integrals V_{11} and V_{12} among the NNLO canonical master integrals. Their differential equations contain V_1 and V_2 as inhomogeneous terms. Let us apply the algorithm to a basis in which V_{11} is correctly chosen as well as V_1 and V_2 but the coupled integral is chosen differently from V_{12}. By putting

$$\begin{aligned} g_1 = V_1 &= \epsilon \mathrm{TTA}_3(2,2,1), \\ g_2 = V_2 &= \epsilon(1-x)\left[\mathrm{TTA}_3(1,2,2) + 2\mathrm{TTA}_3(2,2,1)\right], \\ f_1 = V_{11} &= \epsilon^3 \mathrm{TTF}_3(1,0,1,1,1,0,1), \\ f_2 &= \epsilon^2 \mathrm{TTF}_3(1,0,2,1,1,0,1), \end{aligned} \tag{3.32}$$

the algorithm gives $A^{\rm p}$ in the desired form:

$$A^{\rm p} = \epsilon \left(\frac{a^{\rm p}}{x} + \frac{b^{\rm p}}{1-x} \right), \tag{3.33}$$

with

$$a^{\rm p} = \begin{pmatrix} -3 & 1 & 0 & 0 \\ -6 & 2 & 0 & 0 \\ k_{11} & k_{12} & c_{11} & c_{12} \\ -\frac{c_{11}k_{11}-6k_{12}+2}{c_{12}} & -\frac{2c_{11}k_{12}+2k_{11}+10k_{12}-1}{2c_{12}} & -\frac{(c_{11}+1)(c_{11}+2)}{c_{12}} & -(c_{11}+3) \end{pmatrix}, \tag{3.34}$$

and

$$b^{\rm p} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{2(k_{11}-1)}{c_{12}} & -\frac{2k_{11}+4k_{12}-1}{2c_{12}} & \frac{2(c_{11}+2)}{c_{12}} & 2 \end{pmatrix}. \tag{3.35}$$

If we choose the integration constants as

$$c_{12} = 1, \qquad c_{11} = -1, \qquad k_{12} = \frac{1}{4}, \qquad k_{11} = -1, \tag{3.36}$$

we find agreement with the differential equation matrix given in section 3.3, and the reconstructed $f_2^{\rm p}$ turns into V_{12}.

3.2.5 Three or more coupled differential equations

In the case that there are three or more coupled master integrals, one can straightforwardly generalize the arguments in the above. Suppose that one has n coupled master integrals ($n \geq 2$) to be added into a canonical basis all at once. Starting from the differential equations of order m ($m \geq 1$)[6]

$$f^{(m)} = A^{[m-1]} f, \tag{3.37}$$

where the matrix $A^{[m]}$ is recursively defined by

$$A^{[m]} := \left(A^{[m-1]} \right)' + A^{[m-1]} A, \qquad A^{[0]} := A, \tag{3.38}$$

one can obtain the nth order differential equation for f_i by eliminating $(n-1)$ integrals f_{j_1}, f_{j_2}, …, $f_{j_{n-1}}$ from the system of n differential equations for f_i', $f_i^{(2)}$, …, $f_i^{(n)}$. The result has the following form

$$\sum_{m=1}^{n} C_m f_i^{(m)} = \sum_{k \notin \{j_1,\ldots,j_{n-1}\}} C_{0k} f_k, \tag{3.39}$$

where the summation in the right-hand side is taken for all integrals except the eliminated integrals; in other words, all canonical master integrals already fixed as well as f_i. The coefficients C_m and C_{0k} are given by

$$C_m = \frac{\Delta_{mn}}{\Delta_{nn}}, \qquad C_{0k} = \frac{\Delta_k}{\Delta_{nn}} = \sum_{m=1}^{n} C_m A_{ik}^{[m-1]}, \tag{3.40}$$

[6] To keep the formulae simple, integrals that are already properly chosen as canonical master integrals and regarded as inhomogeneous terms are now also included in the basis vector f.

where we have normalized C_n as unity, $\Delta_k = \det(M_k)$ is the determinant of the following $n \times n$ matrix:

$$M_k = \begin{pmatrix} A^{[0]}_{ij_1} & \dots & A^{[0]}_{ij_{n-1}} & A^{[0]}_{ik} \\ \vdots & & \vdots & \vdots \\ A^{[n-1]}_{ij_1} & \dots & A^{[n-1]}_{ij_{n-1}} & A^{[n-1]}_{ik} \end{pmatrix}, \tag{3.41}$$

and Δ_{mn} is the cofactor obtained by multiplying $(-1)^{m+n}$ to the determinant of M_k with omitting the mth row and the nth column (hence does not depend on k).

Assuming f_i is a canonical master integral, one can conclude that the coefficients must have the following structure in ϵ:

$$\begin{aligned} C_m &= \frac{\epsilon^{n-1} C_m^{(n-1)} + \dots + \epsilon^{n(n+1)/2-m} C_m^{(n(n+1)/2-m)}}{\epsilon^{n-1} D^{(n-1)} + \dots + \epsilon^{n(n-1)/2} D^{(n(n-1)/2)}}, \\ C_{0k} &= \frac{\epsilon^{n} C_{0k}^{(n)} + \dots + \epsilon^{n(n+1)/2} C_{0k}^{(n(n+1)/2)}}{\epsilon^{n-1} D^{(n-1)} + \dots + \epsilon^{n(n-1)/2} D^{(n(n-1)/2)}}. \end{aligned} \tag{3.42}$$

The coefficients C_m and C_{0k} are rational functions in ϵ and thus the set of differential equations for reconstructing the matrix $A^{\rm p}$, appearing in the basis in which the eliminated integrals $f_{j_1}, f_{j_2}, \dots, f_{j_{n-1}}$ are properly chosen, becomes quite tedious. However, taking only the leading terms of C_m and C_{0k} in ϵ by replacing $A^{[n]}$ with $A^{(n)}$

$$A^{[n]}_{kl} = A^{(n)}_{kl} + \mathcal{O}(\epsilon^2), \tag{3.43}$$

may alleviate the complexity of the problem[7]. The first terms of C_m, i.e., $C_m^{(n-1)}/D^{(n-1)}$ give a set of $(n-1)$ differential equations of $(n-1)$ variables $A^{\rm p}_{ij_1}, \dots, A^{\rm p}_{ij_{n-1}}$. After solving them, one substitutes the result into the first terms of C_{0k}, $C_{0k}^{(n)}/D^{(n-1)}$, which gives a differential equation for $A^{\rm p}_{ik}$. In this way, one can reconstruct the ith row of the matrix $A^{\rm p}$.

In general, higher order terms of the coefficients in ϵ expansions are needed to reconstruct the full matrix $A^{\rm p}$. From a naive counting, n orders of each coefficient have to be taken into account.

Once $A^{\rm p}$ is completely determined, one can construct the basis transformation B to this basis. The matrix B can be parametrized by filling $(n-1)$ rows corresponding to $f_{j_1}, \dots, f_{j_{n-1}}$ with variables b_{kl}. The matrix equation eq. (3.23) contains derivatives of the variables; however, one does not need to solve any differential equations. Non-trivial equations in n rows of the matrix equation can be solved as follows. Starting with ith row, whose components are all zero in the left-hand side, one has a set of linear equations, which can be solved for all variables of a row[8]. Next, one considers this row. On the left-hand side, one can use the chain rule of the derivative and replace derivatives of unsolved

[7] This does not apply to the cases where $C_m^{(n-1)}$, $D^{(n-1)}$ or $C_{0k}^{(n)}$ obtained from the components of $A^{\rm p}$ become zero. For example, with the ansatz eq. (3.25), one finds $C_m^{(n-1)}$ and $D^{(n-1)}$ vanish for $n \geq 5$, and $C_{0k}^{(n)}$ vanishes for $n \geq 4$.

[8] There exist cases where some components of $A^{\rm p}$ are zero, and some variables do not appear in a set of equations generated from a row of the matrix equation. However, the set of equations must give solutions for variables of a row at least provided the integral corresponding to the row giving the equations is coupled to the other integrals in the basis with $A^{\rm p}$.

variables with the corresponding components of the matrix equation. Then one substitutes the solution for the solved variables. The resulting equations give the next set of linear equations that can determine all variables of another row. Repeating this procedure, one can solve for all the variables by using $(n-1)$ rows, and the remaining row can serve as a consistency check.

The generalized version of the algorithm given in section 3.2.2 that checks whether f_i is a canonical master integral is formulated as follows:

1. Derive higher order differential equation for f_i, i.e. calculate the coefficients C_m and C_{0k} given in eq. (3.40).

2. Check ϵ-dependence of C_m and C_{0k}, which should be as in eq. (3.42).

3. Expand C_m and C_{0k} in ϵ. Take enough terms to be able to solve for the elements of A^{p}. The differential equations should be solvable by the ansatz eq. (3.25). In order to proceed, it is enough to find one particular solution for A^{p}.

4. Construct B and check its consistency by use of eq. (3.23).

If the checks fail at any step, one can conclude f_i cannot be a canonical master integral.

Let us conclude with a few final remarks:

- By using the ansatz eq. (3.25) in solving for the elements of A^{p}, all differential equations appearing in this algorithm can be reduced to algebraic equations.

- In practice A sometimes contains elements equal to zero. Setting the elements at the same positions in A^{p} to zero may simplify the derivation a lot, provided this additional constraints on the form of A^{p} gives a solution for A^{p} and B.

- By changing the ansatz eq. (3.25), the algorithm can be extended to other forms (2.5) in x.

3.3 Canonical master integrals for NNLO Higgs boson production

Here we present a canonical basis we found at NNLO, together with the differential equation matrix A it satisfies. All master integrals of topology T in this basis have the form

$$M_i^{(T)} = \epsilon^{d_i} n_i(x) \sum_k c_{ik} T\left(\{a\}_k\right), \tag{3.44}$$

where d_i is an integer, $n_i(x)$ is an x-dependent prefactor, c_{ik} are numerical constants and $\{a\}_k$ are distinct sets of indices. All integrals are defined as single-cut integrals. The definitions of the individual topologies are given in fig. 2. Note that the choice of a canonical basis is not unique. In many cases we have found alternative master integrals forming a canonical basis which have a more complicated $n(\epsilon)$ normalization. We present here a basis

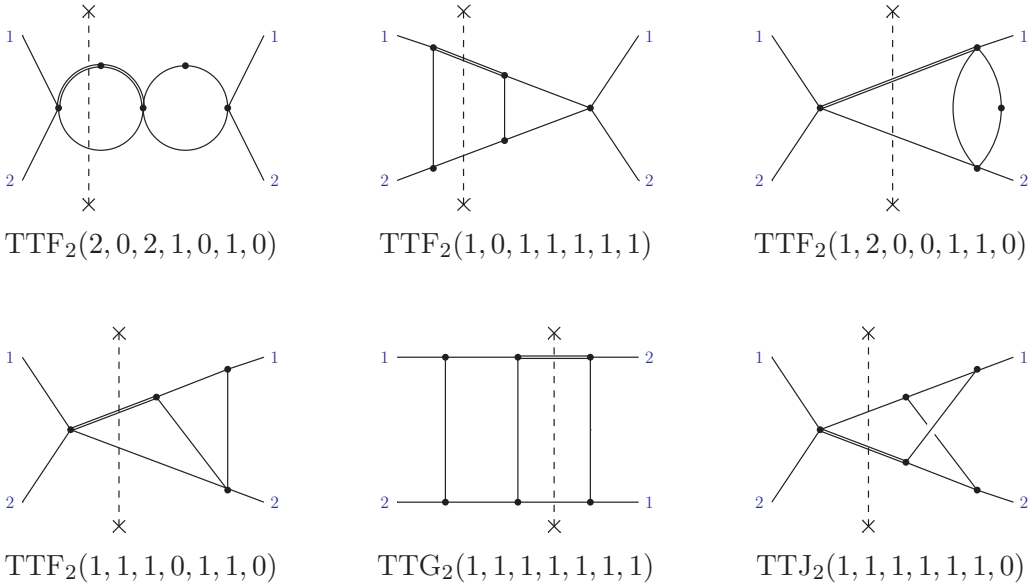


Figure 3. Two-particle cut diagrams appearing in our choice of canonical master integrals at NNLO.

of the simple monomial form in ϵ as eq. (3.44):

$$
\begin{aligned}
W_1 &= \epsilon \mathrm{TTF}_2(2,0,2,1,0,1,0), \\
W_2 &= \epsilon^3(1-x)\mathrm{TTF}_2(1,0,1,1,1,1,1), \\
W_3 &= \epsilon^2 \mathrm{TTF}_2(1,2,0,0,1,1,0), \\
W_4 &= \epsilon^3 \mathrm{TTF}_2(1,1,1,0,1,1,0), \\
W_5 &= \epsilon^3(1-x)\mathrm{TTG}_2(1,1,1,1,1,1,1), \\
W_6 &= \epsilon^3(1-x)\mathrm{TTJ}_2(1,1,1,1,1,1,0),
\end{aligned}
\tag{3.45}
$$

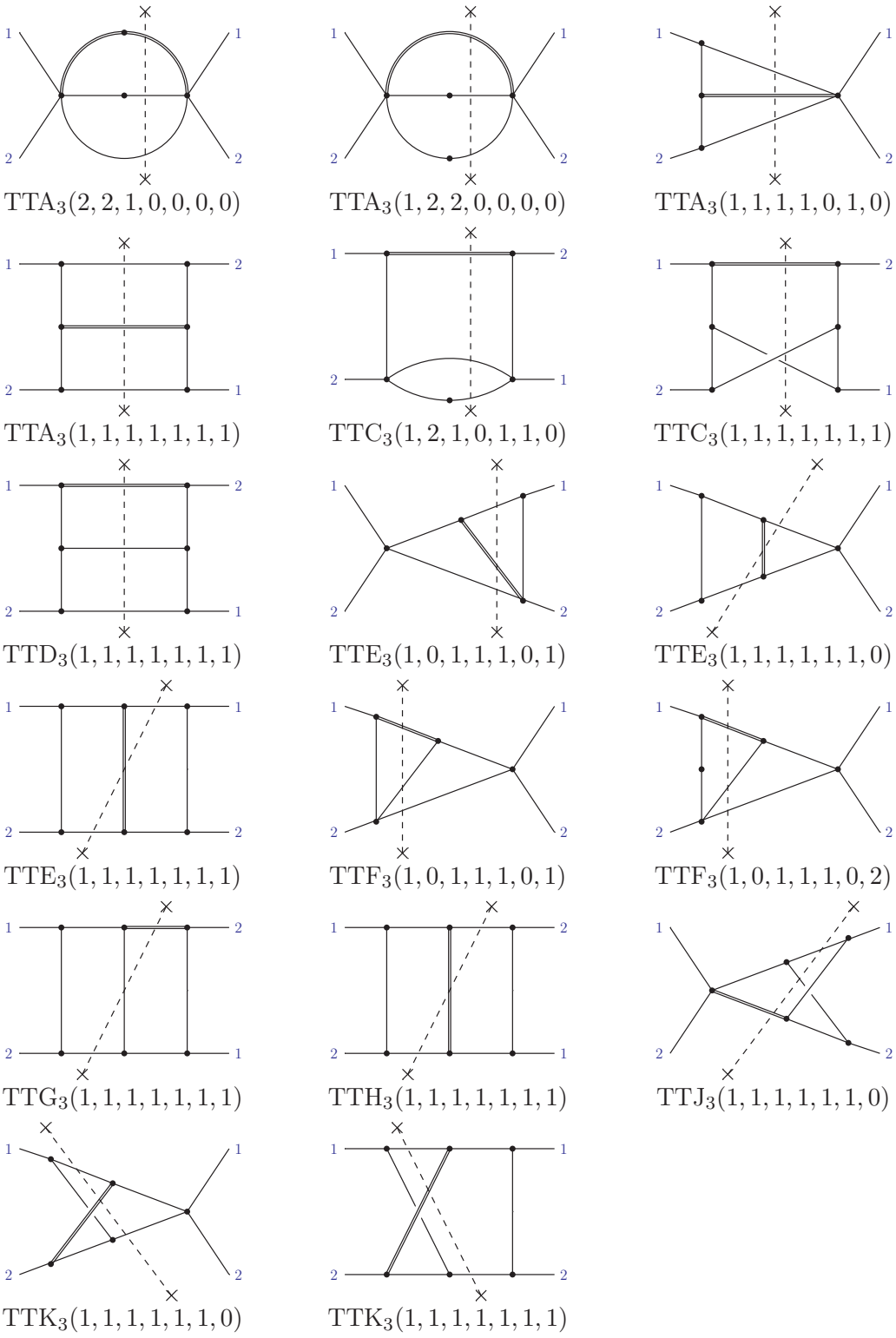


Figure 4. Three-particle cut diagrams appearing in our choice of canonical master integrals at NNLO.

are the two-particle cut master integrals, whereas

$$
\begin{aligned}
V_1 &= \epsilon \mathrm{TTA}_3(2,2,1,0,0,0,0),\\
V_2 &= \epsilon(1-x)\big[\mathrm{TTA}_3(1,2,2,0,0,0,0) + 2\mathrm{TTA}_3(2,2,1,0,0,0,0)\big],\\
V_3 &= \epsilon^3 \mathrm{TTA}_3(1,1,1,1,0,1,0),\\
V_4 &= \epsilon^3(1-x)\mathrm{TTA}_3(1,1,1,1,1,1,1),\\
V_5 &= \epsilon^2(1-x)\mathrm{TTC}_3(1,2,1,0,1,1,0),\\
V_6 &= \epsilon^3(1-x)x\mathrm{TTC}_3(1,1,1,1,1,1,1),\\
V_7 &= \epsilon^3(1-x)\mathrm{TTD}_3(1,1,1,1,1,1,1),\\
V_8 &= \epsilon^3 \mathrm{TTE}_3(1,0,1,1,1,0,1),\\
V_9 &= \epsilon^3 \mathrm{TTE}_3(1,1,1,1,1,1,0),\\
V_{10} &= \epsilon^3 x\mathrm{TTE}_3(1,1,1,1,1,1,1),\\
V_{11} &= \epsilon^3 \mathrm{TTF}_3(1,0,1,1,1,0,1),\\
V_{12} &= \epsilon^2 x\mathrm{TTF}_3(1,0,1,1,1,0,2),\\
V_{13} &= \epsilon^3(1-x)\mathrm{TTG}_3(1,1,1,1,1,1,1),\\
V_{14} &= \epsilon^3(1+x)\mathrm{TTH}_3(1,1,1,1,1,1,1),\\
V_{15} &= \epsilon^3(1-x)\mathrm{TTJ}_3(1,1,1,1,1,1,0),\\
V_{16} &= \epsilon^3(1+x)\mathrm{TTK}_3(1,1,1,1,1,1,0),\\
V_{17} &= \epsilon^3 x\big[\mathrm{TTK}_3(1,1,1,1,1,1,1) - \mathrm{TTK}_3(1,1,1,1,1,1,0)\big],
\end{aligned}
\tag{3.46}
$$

are the three-particle cut master integrals[9]. They are normalized in such a way as to start at finite order. Two- and three-particle cut diagrams appearing in this basis are shown in figs. 3 and 4, respectively.

The two-particle cut master integrals satisfy the differential equations (2.4) and (2.7) with

$$
a_2 = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0\\
1 & -1 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
1 & -1 & -2 & -2 & 0 & 0\\
2 & -2 & 2 & 2 & 0 & 0\\
0 & 0 & -4 & -4 & 0 & 0
\end{pmatrix},
\tag{3.47}
$$

$$
b_2 = \begin{pmatrix}
2 & 0 & 0 & 0 & 0 & 0\\
0 & 2 & 0 & 0 & 0 & 0\\
0 & 0 & 3 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 6 & 0 & 2 & 0\\
0 & 0 & 0 & 0 & 0 & 4
\end{pmatrix},
\tag{3.48}
$$

[9]The basis given here has the same number of integrals as the reduction basis given in ref. [23] which is known to be not minimal as there is a linear relation between the integrals U_1, U_{1a}, U_6 and U_8 given there.

$$c_2 = 0, \tag{3.49}$$

whereas for the three-particle cut master integrals we have

$$a_3 = \begin{pmatrix}
-3 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-6 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & \frac{1}{2} & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-2 & 1 & -4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{2} & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & \frac{1}{2} & -2 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-2 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-5 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & -2 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-1 & \frac{1}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\
-\frac{3}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 \\
-4 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -\frac{1}{2} & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
3 & -1 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 0 & 0 & 0 & 0 & 0 \\
1 & -\frac{1}{2} & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2
\end{pmatrix}, \tag{3.50}$$

$$b_3 = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\frac{1}{2} & 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 2 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-4 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 \\
-4 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
4 & -\frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & -2 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}, \tag{3.51}$$

$$c_3 = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-4 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & -2 & 0 & 0 & 0 & 0 & 0 & 2 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0
\end{pmatrix}. \tag{3.52}$$

As discussed previously, (V_1, V_2) and (V_{11}, V_{12}) form coupled differential equations. The other integrals form a triangular system, hence one can add a candidate integral to a subset of a canonical basis and check if it successfully gives a larger canonical basis or not, approaching a whole canonical basis step by step. Some of the integrals in the canonical basis given here are diagrammatically similar to those given in ref. [37] where four-point two-loop diagrams have been investigated as well, although with different kinematics.

We computed the given master integrals W_i and V_i up to order ϵ^6 corresponding to a maximum weight of six in the appearing HPLs, using their reduction to the reduction basis and the $x \to 1$ limit of the latter as boundary conditions. We checked that the solutions for the master integrals in the canonical basis are pure functions. Furthermore, by applying the matrix B^{-1} we transformed back to the reduction basis and found agreement with the results given in ref. [23] up to the order in ϵ given there which is high enough for the N^{3}LO calculation (see also the result in ref. [24]). We emphasize that in the canonical basis master integrals decouple order by order in ϵ and therefore only the first term in the $x \to 1$ limit for each master integral is sufficient to fix all the boundary constants.

4 N^{3}LO: example and solution

In this section we discuss the N^{3}LO topology TTS$_4$, shown in fig. 5, which we refer to as *sea snake* topology. It is non-planar, has ten lines with two additional irreducible scalar products and exhibits a four-particle cut only. Integrals belonging to this topology are reduced to eleven master integrals, which we choose to be also of the form of eq. (3.44) and

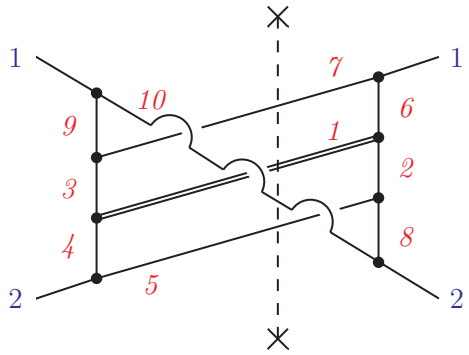


Figure 5. The sea snake topology $\mathrm{TTS}_4(a_1, a_2, a_3, a_4, a_5, a_6, a_7, a_8, a_9, a_{10}, n_{11}, n_{12})$. The notation is the same as in fig. 2. The indices n_{11} and n_{12} denote irreducible scalar products which appear in the numerator and are always less than or equal to zero.

with the last two indices for the irreducible scalar products set to be zero, namely,

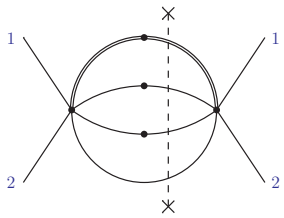
$$
\begin{aligned}
S_1 &= \epsilon^2 \mathrm{TTS}_4(2,0,0,0,2,0,2,0,0,1,0,0), \\
S_2 &= \epsilon^2 (1-x) \left[\mathrm{TTS}_4(1,0,0,0,2,0,2,0,0,2,0,0) + 3\mathrm{TTS}_4(2,0,0,0,2,0,2,0,0,1,0,0)\right], \\
S_3 &= \epsilon^3 \mathrm{TTS}_4(2,0,1,0,1,0,2,0,0,1,0,0), \\
S_4 &= \epsilon^4 \mathrm{TTS}_4(2,0,0,1,1,1,1,0,0,1,0,0), \\
S_5 &= \epsilon^4 \mathrm{TTS}_4(1,2,1,0,1,0,1,0,0,1,0,0), \\
S_6 &= \epsilon^4 \mathrm{TTS}_4(2,1,1,0,1,0,1,0,0,1,0,0), \\
S_7 &= \epsilon^3 (1-x) \mathrm{TTS}_4(1,1,1,0,2,0,2,0,0,1,0,0), \\
S_8 &= \epsilon^3 x \mathrm{TTS}_4(1,2,2,0,1,0,1,0,0,1,0,0), \\
S_9 &= \epsilon^3 x \mathrm{TTS}_4(2,1,1,0,1,0,1,0,0,2,0,0), \\
S_{10} &= \epsilon^5 \mathrm{TTS}_4(1,0,0,1,1,1,1,1,1,1,0,0), \\
S_{11} &= \epsilon^5 \mathrm{TTS}_4(1,1,1,0,1,0,1,1,1,1,0,0).
\end{aligned}
\tag{4.1}
$$

Diagrams appearing in this basis are shown in fig. 6.

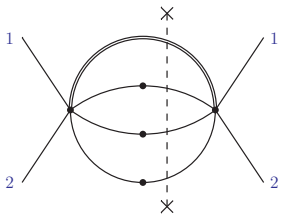
The choice of master integrals S_1 and S_2 is motivated by the discussion given in section 3 in analogy to eq. (3.7). S_3 and S_4 are not coupled and can be found by trying possible candidates. S_{10} and S_{11} stem up to ϵ-normalization from the reduction basis. This can be motivated from the sum of indices $a = 8$ leading to the favored $e_W = 1$ given in eq. (2.8), as discussed in section 2. Integrals S_5 to S_9 are coupled. It is worth mentioning that the subtopology spanned by their six propagators defines the K_4 topology discussed in ref. [44]. Although kinematics and mass-configuration are different from the present case, the basis integrals S_5 to S_9 can be established by direct diagrammatic correspondence to five of the seven coupled integrals for the off-shell K_4 case $g_6, \ldots, g_{10}$ given in ref. [44]:

$$
g_6 \mathrel{\hat{=}} S_6, \qquad g_7 \mathrel{\hat{=}} S_5, \qquad g_8 \mathrel{\hat{=}} S_7, \qquad g_9 \mathrel{\hat{=}} S_9, \qquad g_{10} \mathrel{\hat{=}} S_8,
\tag{4.2}
$$

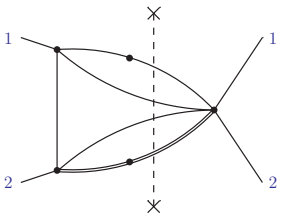
where "$\hat{=}$" states that the indices of the integrals have the same structure. For this case of five coupled master integrals, we do not use the algorithm described in section 3.2.5, because the equations to be solved become highly complicated.



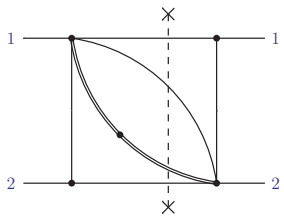
$\mathrm{TTS}_4(2,0,0,0,2,0,2,0,0,1,0,0)$



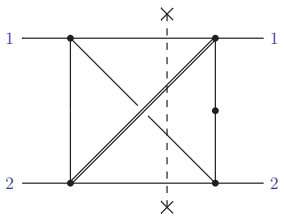
$\mathrm{TTS}_4(1,0,0,0,2,0,2,0,0,2,0,0)$



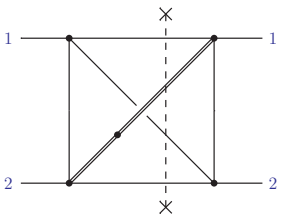
$\mathrm{TTS}_4(2,0,1,0,1,0,2,0,0,1,0,0)$



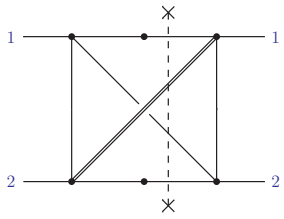
$\mathrm{TTS}_4(2,0,0,1,1,1,1,0,0,1,0,0)$



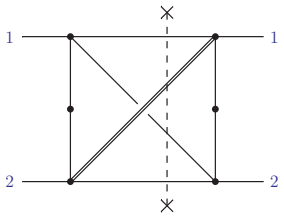
$\mathrm{TTS}_4(1,2,1,0,1,0,1,0,0,1,0,0)$



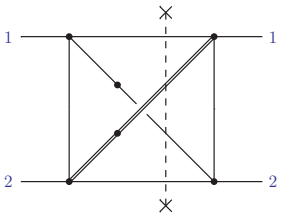
$\mathrm{TTS}_4(2,1,1,0,1,0,1,0,0,1,0,0)$



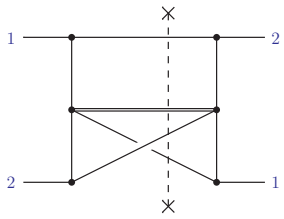
$\mathrm{TTS}_4(1,1,1,0,2,0,2,0,0,1,0,0)$



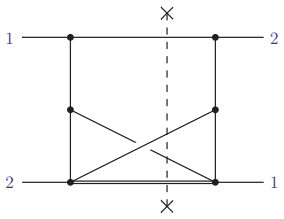
$\mathrm{TTS}_4(1,2,2,0,1,0,1,0,0,1,0,0)$



$\mathrm{TTS}_4(2,1,1,0,1,0,1,0,0,2,0,0)$



$\mathrm{TTS}_4(1,0,0,1,1,1,1,1,1,1,0,0)$



$\mathrm{TTS}_4(1,1,1,0,1,0,1,1,1,1,0,0)$

Figure 6. Diagrams appearing in our choice of canonical master integrals for the sea snake topology.

The basis given here satisfies the differential equation of eq. (2.4) with eq. (2.7):

$$a_4 = \begin{pmatrix}
-4 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-12 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{2} & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & -\frac{1}{6} & 0 & -3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\frac{1}{6} & 0 & 0 & 0 & -\frac{2}{3} & \frac{2}{3} & -\frac{1}{6} & \frac{1}{2} & \frac{1}{3} & 0 & 0 \\
\frac{5}{6} & 0 & 1 & 0 & \frac{7}{3} & -\frac{7}{3} & \frac{7}{12} & \frac{1}{4} & -\frac{1}{6} & 0 & 0 \\
\frac{11}{3} & -\frac{1}{2} & 2 & 0 & \frac{14}{3} & -\frac{14}{3} & \frac{7}{6} & \frac{5}{2} & \frac{8}{3} & 0 & 0 \\
\frac{7}{3} & -\frac{1}{2} & 2 & 0 & -\frac{2}{3} & \frac{2}{3} & -\frac{1}{6} & -\frac{7}{2} & -\frac{2}{3} & 0 & 0 \\
\frac{7}{3} & -\frac{1}{2} & 2 & 0 & -\frac{2}{3} & \frac{2}{3} & -\frac{1}{6} & -\frac{1}{2} & -\frac{11}{3} & 0 & 0 \\
0 & -\frac{1}{6} & 0 & 2 & 0 & 24 & 0 & 0 & 0 & -3 & 0 \\
-3 & 0 & -7 & 0 & -13 & -2 & -\frac{3}{2} & -\frac{5}{2} & -2 & 0 & -3
\end{pmatrix}, \tag{4.3}$$

$$b_4 = \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{11}{3} & -\frac{1}{2} & 6 & 0 & \frac{50}{3} & \frac{10}{3} & \frac{37}{6} & \frac{7}{2} & \frac{5}{3} & 0 & 0 \\
\frac{11}{3} & -\frac{1}{2} & 6 & 0 & \frac{50}{3} & \frac{10}{3} & \frac{1}{6} & \frac{7}{2} & \frac{5}{3} & 0 & 0 \\
-\frac{11}{3} & -\frac{1}{2} & -6 & 0 & -\frac{50}{3} & -\frac{10}{3} & -\frac{19}{6} & -\frac{7}{2} & -\frac{5}{3} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix} \tag{4.4}$$

and

$$c_4 = 0. \tag{4.5}$$

We computed the master integrals S_i up to order ϵ^6 corresponding to a maximum weight of six in the HPLs. As boundary conditions we computed the master integrals in the reduction basis in the $x \to 1$ limit with our `Mathematica` implementation of the soft expansion algorithm given in ref. [25], using the program `FIRE` for reduction. It is worth mentioning that all master integrals are reduced to the four-particle phase space integral only, i.e., the integral $F_1(\epsilon)$ given in ref. [25] which is known for general values of ϵ, therefore the result given here can be extended to arbitrary orders in ϵ. We checked our results transformed to the reduction basis against the soft expansion around $x = 1$, including at least three non-vanishing terms in the expansion. Furthermore, we found that all S_i are indeed pure functions. The results, up to order ϵ^5 for brevity, are given in appendix A.

5 Conclusions and outlook

In this work we recomputed all necessary double-real and real-virtual master integrals for $gg \to h$ at NNLO within the framework of canonical differential equations [37]. By solving a non-planar three-loop topology as well, we have explicitly shown the use of the method to Higgs production in gluon fusion in full x-dependence at N^{3}LO. The method can be applied to other master integrals at N^{3}LO, which will contribute to the completion of the calculation of the total inclusive Higgs production cross section with full x-dependence in the future. To accomplish this, one needs to provide boundary conditions for the differential equations. For the triple-real emission diagrams, the reduction of phase space integrals in the soft limit [25] works efficiently to obtain the soft expansions around threshold. For other diagrams containing loop integrals, techniques such as asymptotic expansions by strategy of regions [18, 58, 59], those in the α-parameter representations [36, 60] or asymptotic expansions of Mellin-Barnes integral representations [36] may be useful to obtain the soft expansions. Sophisticated treatments for phase space integrals may also do the job. In any case, the fact that the framework of canonical differential equations requires only the leading terms of expansions for boundary conditions can make the computation simple.

Furthermore, working in this new framework we were able to derive a new criterion to find a canonical master integral being part of a coupled system by use of a characteristic form for higher order differential equations, allowing also for the construction of a canonical basis for the coupled integrals. This criterion was derived in a quite general way and can also be used in coupled systems of differential equations for master integrals appearing in other processes.

Acknowledgments

We are grateful to J.M. Henn for a comprehensive introduction to his method as well as for pointing out the applicability of it to the process of Higgs production in gluon fusion at N^{3}LO. We thank J.M. Henn and M. Steinhauser for reading the manuscript and giving useful comments. Furthermore, we thank M. Steinhauser, J. Grigo and C. Anzai for valuable discussion. We also thank A.V. Smirnov for allowing us to use the unpublished C++ version of `FIRE`. The Feynman diagrams were drawn by using `JaxoDraw` [61], based on `Axodraw` [62]. This work was supported by Deutsche Forschungsgemeinschaft through Sonderforschungsbereich/Transregio 9 "Computational Particle Physics".

A Results for sea snake topology

In the appendix, we present the results of the master integrals S_i for the sea snake topology TTS_4. We have normalized the results by multiplying an ϵ-dependent prefactor, which is chosen such that the four-particle phase space integral in the limit $x \to 1$, corresponding to $F_1(\epsilon)$ defined in ref. [25], becomes

$$\lim_{x\to 1} \mathrm{TTS}_4(1,0,0,0,1,0,1,0,0,1,0,0) = \frac{\Gamma^3(1-\epsilon)}{\Gamma(6-6\epsilon)\Gamma^3(1+\epsilon)}. \tag{A.1}$$

Furthermore, we omit the common argument x of HPLs as $\mathrm{H}_{i_1,\ldots i_n} := \mathrm{H}_{i_1,\ldots i_n}(x)$.

$$\begin{aligned}
S_1 = {} & 1 + 2\epsilon\big[\,\mathrm{H}_0 + 3\,\mathrm{H}_1\,\big] + 2\epsilon^2\big[6\,\mathrm{H}_2 - \mathrm{H}_{0,0} + 3\,\mathrm{H}_{1,0} + 18\,\mathrm{H}_{1,1} - 12\zeta_2\big] - 2\epsilon^3\big[6\,\mathrm{H}_3 - 18\,\mathrm{H}_{1,2} \\
& - 6\,\mathrm{H}_{2,0} - 36\,\mathrm{H}_{2,1} - \mathrm{H}_{0,0,0} + 3\,\mathrm{H}_{1,0,0} - 18\,\mathrm{H}_{1,1,0} - 108\,\mathrm{H}_{1,1,1} + \big(6\,\mathrm{H}_0 + 54\,\mathrm{H}_1\,\big)\zeta_2 + 32\zeta_3\big] \\
& + 2\epsilon^4\big[6\,\mathrm{H}_4 - 18\,\mathrm{H}_{1,3} + 36\,\mathrm{H}_{2,2} - 6\,\mathrm{H}_{3,0} - 36\,\mathrm{H}_{3,1} + 108\,\mathrm{H}_{1,1,2} + 18\,\mathrm{H}_{1,2,0} + 108\,\mathrm{H}_{1,2,1} \\
& - 6\,\mathrm{H}_{2,0,0} + 36\,\mathrm{H}_{2,1,0} + 216\,\mathrm{H}_{2,1,1} - \mathrm{H}_{0,0,0,0} + 3\,\mathrm{H}_{1,0,0,0} - 18\,\mathrm{H}_{1,1,0,0} + 108\,\mathrm{H}_{1,1,1,0} \\
& + 648\,\mathrm{H}_{1,1,1,1} + \big(-108\,\mathrm{H}_2 + 6\,\mathrm{H}_{0,0} - 18\,\mathrm{H}_{1,0} - 324\,\mathrm{H}_{1,1}\,\big)\zeta_2 + 123\zeta_4 + \big(-10\,\mathrm{H}_0 \\
& - 138\,\mathrm{H}_1\,\big)\zeta_3\big] - 2\epsilon^5\big[6\,\mathrm{H}_5 - 18\,\mathrm{H}_{1,4} + 36\,\mathrm{H}_{2,3} + 36\,\mathrm{H}_{3,2} - 6\,\mathrm{H}_{4,0} - 36\,\mathrm{H}_{4,1} + 108\,\mathrm{H}_{1,1,3} \\
& - 108\,\mathrm{H}_{1,2,2} + 18\,\mathrm{H}_{1,3,0} + 108\,\mathrm{H}_{1,3,1} - 216\,\mathrm{H}_{2,1,2} - 36\,\mathrm{H}_{2,2,0} - 216\,\mathrm{H}_{2,2,1} - 6\,\mathrm{H}_{3,0,0} \\
& + 36\,\mathrm{H}_{3,1,0} + 216\,\mathrm{H}_{3,1,1} - 648\,\mathrm{H}_{1,1,1,2} - 108\,\mathrm{H}_{1,1,2,0} - 648\,\mathrm{H}_{1,1,2,1} + 18\,\mathrm{H}_{1,2,0,0} \\
& - 108\,\mathrm{H}_{1,2,1,0} - 648\,\mathrm{H}_{1,2,1,1} - 6\,\mathrm{H}_{2,0,0,0} + 36\,\mathrm{H}_{2,1,0,0} - 216\,\mathrm{H}_{2,1,1,0} - 1296\,\mathrm{H}_{2,1,1,1} \\
& - \mathrm{H}_{0,0,0,0,0} + 3\,\mathrm{H}_{1,0,0,0,0} - 18\,\mathrm{H}_{1,1,0,0,0} + 108\,\mathrm{H}_{1,1,1,0,0} - 648\,\mathrm{H}_{1,1,1,1,0} - 3888\,\mathrm{H}_{1,1,1,1,1} \\
& + \big(-21\,\mathrm{H}_0 - 513\,\mathrm{H}_1\,\big)\zeta_4 + \zeta_2\big(-108\,\mathrm{H}_3 + 324\,\mathrm{H}_{1,2} + 36\,\mathrm{H}_{2,0} + 648\,\mathrm{H}_{2,1} + 6\,\mathrm{H}_{0,0,0} \\
& - 18\,\mathrm{H}_{1,0,0} + 108\,\mathrm{H}_{1,1,0} + 1944\,\mathrm{H}_{1,1,1} - 444\zeta_3\big) + \big(276\,\mathrm{H}_2 - 10\,\mathrm{H}_{0,0} + 30\,\mathrm{H}_{1,0}
\end{aligned}$$

$$+ 828\,\mathrm{H}_{1,1}\big)\zeta_3 + 324\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \tag{A.2}$$

$$S_2 = 6 + 6\epsilon\big[\,\mathrm{H}_0 + 6\,\mathrm{H}_1\,\big] + 6\epsilon^2\big[6\,\mathrm{H}_2 - \mathrm{H}_{0,0} + 6\,\mathrm{H}_{1,0} + 36\,\mathrm{H}_{1,1} - 18\zeta_2\big] - 6\epsilon^3\big[6\,\mathrm{H}_3 - 36\,\mathrm{H}_{1,2}$$
$$- 6\,\mathrm{H}_{2,0} - 36\,\mathrm{H}_{2,1} - \mathrm{H}_{0,0,0} + 6\,\mathrm{H}_{1,0,0} - 36\,\mathrm{H}_{1,1,0} - 216\,\mathrm{H}_{1,1,1} + \big(6\,\mathrm{H}_0 + 108\,\mathrm{H}_1\big)\zeta_2$$
$$+ 46\zeta_3\big] + 6\epsilon^4\big[6\,\mathrm{H}_4 - 36\,\mathrm{H}_{1,3} + 36\,\mathrm{H}_{2,2} - 6\,\mathrm{H}_{3,0} - 36\,\mathrm{H}_{3,1} + 216\,\mathrm{H}_{1,1,2} + 36\,\mathrm{H}_{1,2,0}$$
$$+ 216\,\mathrm{H}_{1,2,1} - 6\,\mathrm{H}_{2,0,0} + 36\,\mathrm{H}_{2,1,0} + 216\,\mathrm{H}_{2,1,1} - \mathrm{H}_{0,0,0,0} + 6\,\mathrm{H}_{1,0,0,0} - 36\,\mathrm{H}_{1,1,0,0}$$
$$+ 216\,\mathrm{H}_{1,1,1,0} + 1296\,\mathrm{H}_{1,1,1,1} + \big(-108\,\mathrm{H}_2 + 6\,\mathrm{H}_{0,0} - 36\,\mathrm{H}_{1,0} - 648\,\mathrm{H}_{1,1}\big)\zeta_2 + 171\zeta_4$$
$$+ \big(-10\,\mathrm{H}_0 - 276\,\mathrm{H}_1\big)\zeta_3\big] - 6\epsilon^5\big[6\,\mathrm{H}_5 - 36\,\mathrm{H}_{1,4} + 36\,\mathrm{H}_{2,3} + 36\,\mathrm{H}_{3,2} - 6\,\mathrm{H}_{4,0} - 36\,\mathrm{H}_{4,1}$$
$$+ 216\,\mathrm{H}_{1,1,3} - 216\,\mathrm{H}_{1,2,2} + 36\,\mathrm{H}_{1,3,0} + 216\,\mathrm{H}_{1,3,1} - 216\,\mathrm{H}_{2,1,2} - 36\,\mathrm{H}_{2,2,0} - 216\,\mathrm{H}_{2,2,1}$$
$$- 6\,\mathrm{H}_{3,0,0} + 36\,\mathrm{H}_{3,1,0} + 216\,\mathrm{H}_{3,1,1} - 1296\,\mathrm{H}_{1,1,1,2} - 216\,\mathrm{H}_{1,1,2,0} - 1296\,\mathrm{H}_{1,1,2,1}$$
$$+ 36\,\mathrm{H}_{1,2,0,0} - 216\,\mathrm{H}_{1,2,1,0} - 1296\,\mathrm{H}_{1,2,1,1} - 6\,\mathrm{H}_{2,0,0,0} + 36\,\mathrm{H}_{2,1,0,0} - 216\,\mathrm{H}_{2,1,1,0}$$
$$- 1296\,\mathrm{H}_{2,1,1,1} - \mathrm{H}_{0,0,0,0,0} + 6\,\mathrm{H}_{1,0,0,0,0} - 36\,\mathrm{H}_{1,1,0,0,0} + 216\,\mathrm{H}_{1,1,1,0,0} - 1296\,\mathrm{H}_{1,1,1,1,0}$$
$$- 7776\,\mathrm{H}_{1,1,1,1,1} + \big(-21\,\mathrm{H}_0 - 1026\,\mathrm{H}_1\big)\zeta_4 + \zeta_2\big(-108\,\mathrm{H}_3 + 648\,\mathrm{H}_{1,2} + 36\,\mathrm{H}_{2,0} + 648\,\mathrm{H}_{2,1}$$
$$+ 6\,\mathrm{H}_{0,0,0} - 36\,\mathrm{H}_{1,0,0} + 216\,\mathrm{H}_{1,1,0} + 3888\,\mathrm{H}_{1,1,1} - 612\zeta_3\big) + \big(276\,\mathrm{H}_2 - 10\,\mathrm{H}_{0,0} + 60\,\mathrm{H}_{1,0}$$
$$+ 1656\,\mathrm{H}_{1,1}\big)\zeta_3 + 450\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \tag{A.3}$$

$$S_3 = -\frac{\epsilon}{2}\,\mathrm{H}_0 - 3\epsilon^2\big[\,\mathrm{H}_2 - \zeta_2\big] + \epsilon^3\big[-3\,\mathrm{H}_{2,0} - 18\,\mathrm{H}_{2,1} + \mathrm{H}_{0,0,0} + 6\,\mathrm{H}_0\,\zeta_2 + 12\zeta_3\big]$$
$$+ \epsilon^4\big[6\,\mathrm{H}_4 - 18\,\mathrm{H}_{2,2} + 3\,\mathrm{H}_{2,0,0} - 18\,\mathrm{H}_{2,1,0} - 108\,\mathrm{H}_{2,1,1} - 3\,\mathrm{H}_{0,0,0,0} + \big(54\,\mathrm{H}_2 - 6\,\mathrm{H}_{0,0}\big)\zeta_2$$
$$- 51\zeta_4 + 8\,\mathrm{H}_0\,\zeta_3\big] + \epsilon^5\big[-18\,\mathrm{H}_5 + 18\,\mathrm{H}_{2,3} + 6\,\mathrm{H}_{4,0} + 36\,\mathrm{H}_{4,1} - 108\,\mathrm{H}_{2,1,2} - 18\,\mathrm{H}_{2,2,0}$$
$$- 108\,\mathrm{H}_{2,2,1} - 3\,\mathrm{H}_{2,0,0,0} + 18\,\mathrm{H}_{2,1,0,0} - 108\,\mathrm{H}_{2,1,1,0} - 648\,\mathrm{H}_{2,1,1,1} + 7\,\mathrm{H}_{0,0,0,0,0} - 21\,\mathrm{H}_0\,\zeta_4$$
$$+ \zeta_2\big(18\,\mathrm{H}_{2,0} + 324\,\mathrm{H}_{2,1} + 6\,\mathrm{H}_{0,0,0} - 192\zeta_3\big) + \big(138\,\mathrm{H}_2 - 6\,\mathrm{H}_{0,0}\big)\zeta_3 + 138\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \tag{A.4}$$

$$S_4 = \epsilon^2\,\mathrm{H}_{0,0} + 2\epsilon^3\big[3\,\mathrm{H}_3 - 2\,\mathrm{H}_{0,0,0} - 3\,\mathrm{H}_0\,\zeta_2 - 3\zeta_3\big] + \epsilon^4\big[-24\,\mathrm{H}_4 + 6\,\mathrm{H}_{3,0} + 36\,\mathrm{H}_{3,1}$$
$$+ 13\,\mathrm{H}_{0,0,0,0} + 12\,\mathrm{H}_{0,0}\,\zeta_2 + 33\zeta_4\big] + 2\epsilon^5\big[39\,\mathrm{H}_5 + 18\,\mathrm{H}_{3,2} - 12\,\mathrm{H}_{4,0} - 72\,\mathrm{H}_{4,1} - 3\,\mathrm{H}_{3,0,0}$$
$$+ 18\,\mathrm{H}_{3,1,0} + 108\,\mathrm{H}_{3,1,1} - 20\,\mathrm{H}_{0,0,0,0,0} - 12\,\mathrm{H}_0\,\zeta_4 - 5\,\mathrm{H}_{0,0}\,\zeta_3 + \zeta_2\big(-54\,\mathrm{H}_3 - 15\,\mathrm{H}_{0,0,0}$$
$$+ 36\zeta_3\big) - 33\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \tag{A.5}$$

$$S_5 = \frac{\epsilon^3}{2}\big[\,\mathrm{H}_{2,0} + \mathrm{H}_{0,0,0} + \mathrm{H}_0\,\zeta_2 + 2\zeta_3\big] + \epsilon^4\big[3\,\mathrm{H}_4 + 3\,\mathrm{H}_{2,2} - 2\,\mathrm{H}_{3,0} - \mathrm{H}_{2,0,0} + \mathrm{H}_{2,1,0}$$
$$- 4\,\mathrm{H}_{0,0,0,0} + \big(-2\,\mathrm{H}_2 - 5\,\mathrm{H}_{0,0}\big)\zeta_2 - 2\zeta_4 - \mathrm{H}_0\,\zeta_3\big] + \frac{\epsilon^5}{8}\big[-192\,\mathrm{H}_5 - 48\,\mathrm{H}_{2,3} - 96\,\mathrm{H}_{3,2}$$
$$+ 84\,\mathrm{H}_{4,0} + 144\,\mathrm{H}_{4,1} + 48\,\mathrm{H}_{2,1,2} + 4\,\mathrm{H}_{2,2,0} + 144\,\mathrm{H}_{2,2,1} + 32\,\mathrm{H}_{3,0,0} - 32\,\mathrm{H}_{3,1,0}$$
$$- 20\,\mathrm{H}_{2,0,0,0} - 48\,\mathrm{H}_{2,1,0,0} + 172\,\mathrm{H}_{0,0,0,0,0} + 323\,\mathrm{H}_0\,\zeta_4 + \zeta_2\big(64\,\mathrm{H}_3 - 20\,\mathrm{H}_{2,0} - 48\,\mathrm{H}_{2,1}$$
$$+ 204\,\mathrm{H}_{0,0,0} - 56\zeta_3\big) + \big(56\,\mathrm{H}_2 + 24\,\mathrm{H}_{0,0}\big)\zeta_3 + 184\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \tag{A.6}$$

$$S_6 = \frac{\epsilon^4}{4}\big[4\,\mathrm{H}_{3,0} + 8\,\mathrm{H}_{2,0,0} + 4\,\mathrm{H}_{2,1,0} + 8\,\mathrm{H}_{0,0,0,0} + \big(4\,\mathrm{H}_2 + 4\,\mathrm{H}_{0,0}\big)\zeta_2 - 17\zeta_4 - 4\,\mathrm{H}_0\,\zeta_3\big]$$
$$+ \frac{\epsilon^5}{2}\big[24\,\mathrm{H}_5 + 24\,\mathrm{H}_{2,3} + 12\,\mathrm{H}_{3,2} - 12\,\mathrm{H}_{4,0} + 12\,\mathrm{H}_{2,1,2} + 6\,\mathrm{H}_{2,2,0} - 16\,\mathrm{H}_{3,0,0} - 2\,\mathrm{H}_{3,1,0}$$
$$+ 20\,\mathrm{H}_{2,1,0,0} + 16\,\mathrm{H}_{2,1,1,0} - 36\,\mathrm{H}_{0,0,0,0,0} - 29\,\mathrm{H}_0\,\zeta_4 + \big(-24\,\mathrm{H}_2 - 6\,\mathrm{H}_{0,0}\big)\zeta_3 + \zeta_2\big(-14\,\mathrm{H}_3$$
$$- 18\,\mathrm{H}_{2,0} + 4\,\mathrm{H}_{2,1} - 36\,\mathrm{H}_{0,0,0} + 10\zeta_3\big) - 27\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \tag{A.7}$$

$$
\begin{aligned}
S_7 = &-\frac{3}{2} + \frac{\epsilon}{4}\big[-7\,\mathrm{H}_0 - 36\,\mathrm{H}_1 \big] + \frac{\epsilon^2}{2}\big[-21\,\mathrm{H}_2 + 4\,\mathrm{H}_{0,0} - 19\,\mathrm{H}_{1,0} - 108\,\mathrm{H}_{1,1} + 56\zeta_2 \big] \\
&+ \frac{\epsilon^3}{4}\big[48\,\mathrm{H}_3 - 228\,\mathrm{H}_{1,2} - 37\,\mathrm{H}_{2,0} - 252\,\mathrm{H}_{2,1} - \mathrm{H}_{0,0,0} + 48\,\mathrm{H}_{1,0,0} - 216\,\mathrm{H}_{1,1,0} - 1296\,\mathrm{H}_{1,1,1} \\
&+ \big(41\,\mathrm{H}_0 + 660\,\mathrm{H}_1 \big)\zeta_2 + 262\zeta_3 \big] + \frac{\epsilon^4}{8}\big[-12\,\mathrm{H}_4 + 576\,\mathrm{H}_{1,3} - 444\,\mathrm{H}_{2,2} + 72\,\mathrm{H}_{3,0} \\
&+ 576\,\mathrm{H}_{3,1} - 2592\,\mathrm{H}_{1,1,2} - 412\,\mathrm{H}_{1,2,0} - 2736\,\mathrm{H}_{1,2,1} + 80\,\mathrm{H}_{2,0,0} - 476\,\mathrm{H}_{2,1,0} - 3024\,\mathrm{H}_{2,1,1} \\
&- 68\,\mathrm{H}_{0,0,0,0} - 52\,\mathrm{H}_{1,0,0,0} + 560\,\mathrm{H}_{1,1,0,0} - 2528\,\mathrm{H}_{1,1,1,0} - 15552\,\mathrm{H}_{1,1,1,1} + \big(1480\,\mathrm{H}_2 \\
&- 204\,\mathrm{H}_{0,0} + 380\,\mathrm{H}_{1,0} + 7840\,\mathrm{H}_{1,1} \big)\zeta_2 - 2547\zeta_4 + \big(68\,\mathrm{H}_0 + 3160\,\mathrm{H}_1 \big)\zeta_3 \big] + \frac{\epsilon^5}{16}\big[-816\,\mathrm{H}_5 \\
&- 624\,\mathrm{H}_{1,4} + 960\,\mathrm{H}_{2,3} + 864\,\mathrm{H}_{3,2} + 84\,\mathrm{H}_{4,0} - 144\,\mathrm{H}_{4,1} + 6720\,\mathrm{H}_{1,1,3} - 4944\,\mathrm{H}_{1,2,2} \\
&+ 944\,\mathrm{H}_{1,3,0} + 6912\,\mathrm{H}_{1,3,1} - 5712\,\mathrm{H}_{2,1,2} - 940\,\mathrm{H}_{2,2,0} - 5328\,\mathrm{H}_{2,2,1} - 192\,\mathrm{H}_{3,0,0} \\
&+ 1008\,\mathrm{H}_{3,1,0} + 6912\,\mathrm{H}_{3,1,1} - 30336\,\mathrm{H}_{1,1,1,2} - 4800\,\mathrm{H}_{1,1,2,0} - 31104\,\mathrm{H}_{1,1,2,1} + 864\,\mathrm{H}_{1,2,0,0} \\
&- 5232\,\mathrm{H}_{1,2,1,0} - 32832\,\mathrm{H}_{1,2,1,1} - 268\,\mathrm{H}_{2,0,0,0} + 928\,\mathrm{H}_{2,1,0,0} - 5920\,\mathrm{H}_{2,1,1,0} - 36288\,\mathrm{H}_{2,1,1,1} \\
&+ 596\,\mathrm{H}_{0,0,0,0,0} - 464\,\mathrm{H}_{1,0,0,0,0} - 864\,\mathrm{H}_{1,1,0,0,0} + 6464\,\mathrm{H}_{1,1,1,0,0} - 30080\,\mathrm{H}_{1,1,1,1,0} \\
&- 186624\,\mathrm{H}_{1,1,1,1,1} + \big(1343\,\mathrm{H}_0 - 27600\,\mathrm{H}_1 \big)\zeta_4 + \zeta_2\big(-3312\,\mathrm{H}_3 + 16128\,\mathrm{H}_{1,2} + 764\,\mathrm{H}_{2,0} \\
&+ 17936\,\mathrm{H}_{2,1} + 972\,\mathrm{H}_{0,0,0} - 1888\,\mathrm{H}_{1,0,0} + 4032\,\mathrm{H}_{1,1,0} + 93568\,\mathrm{H}_{1,1,1} - 13352\zeta_3 \big) \\
&+ \big(7816\,\mathrm{H}_2 - 200\,\mathrm{H}_{0,0} + 720\,\mathrm{H}_{1,0} + 38208\,\mathrm{H}_{1,1} \big)\zeta_3 + 8976\zeta_5 \big] + \mathcal{O}\big(\epsilon^6\big), \qquad \text{(A.8)} \\
S_8 = &-\frac{\epsilon}{4}\,\mathrm{H}_0 + \frac{\epsilon^2}{2}\big[-3\,\mathrm{H}_2 + 3\,\mathrm{H}_{0,0} + 2\,\mathrm{H}_{1,0} + 5\zeta_2 \big] + \frac{\epsilon^3}{4}\big[36\,\mathrm{H}_3 + 24\,\mathrm{H}_{1,2} - 19\,\mathrm{H}_{2,0} \\
&- 36\,\mathrm{H}_{2,1} - 27\,\mathrm{H}_{0,0,0} + 12\,\mathrm{H}_{1,1,0} + \big(-37\,\mathrm{H}_0 - 12\,\mathrm{H}_1 \big)\zeta_2 - 2\zeta_3 \big] + \frac{\epsilon^4}{4}\big[-162\,\mathrm{H}_4 \\
&- 114\,\mathrm{H}_{2,2} + 78\,\mathrm{H}_{3,0} + 216\,\mathrm{H}_{3,1} + 72\,\mathrm{H}_{1,1,2} + 16\,\mathrm{H}_{1,2,0} + 144\,\mathrm{H}_{1,2,1} + 8\,\mathrm{H}_{2,0,0} - 74\,\mathrm{H}_{2,1,0} \\
&- 216\,\mathrm{H}_{2,1,1} + 108\,\mathrm{H}_{0,0,0,0} - 20\,\mathrm{H}_{1,0,0,0} - 8\,\mathrm{H}_{1,1,0,0} + 32\,\mathrm{H}_{1,1,1,0} + \big(148\,\mathrm{H}_2 + 132\,\mathrm{H}_{0,0} \\
&- 56\,\mathrm{H}_{1,0} - 40\,\mathrm{H}_{1,1} \big)\zeta_2 + 215\zeta_4 + \big(10\,\mathrm{H}_0 + 8\,\mathrm{H}_1 \big)\zeta_3 \big] + \frac{\epsilon^5}{16}\big[2592\,\mathrm{H}_5 - 480\,\mathrm{H}_{1,4} \\
&+ 192\,\mathrm{H}_{2,3} + 1872\,\mathrm{H}_{3,2} - 1188\,\mathrm{H}_{4,0} - 3888\,\mathrm{H}_{4,1} - 192\,\mathrm{H}_{1,1,3} + 384\,\mathrm{H}_{1,2,2} + 80\,\mathrm{H}_{1,3,0} \\
&- 1776\,\mathrm{H}_{2,1,2} - 340\,\mathrm{H}_{2,2,0} - 2736\,\mathrm{H}_{2,2,1} - 192\,\mathrm{H}_{3,0,0} + 1344\,\mathrm{H}_{3,1,0} + 5184\,\mathrm{H}_{3,1,1} \\
&+ 768\,\mathrm{H}_{1,1,1,2} + 144\,\mathrm{H}_{1,1,2,0} + 1728\,\mathrm{H}_{1,1,2,1} - 96\,\mathrm{H}_{1,2,0,0} + 480\,\mathrm{H}_{1,2,1,0} + 3456\,\mathrm{H}_{1,2,1,1} \\
&+ 236\,\mathrm{H}_{2,0,0,0} + 288\,\mathrm{H}_{2,1,0,0} - 1248\,\mathrm{H}_{2,1,1,0} - 5184\,\mathrm{H}_{2,1,1,1} - 1620\,\mathrm{H}_{0,0,0,0,0} + 352\,\mathrm{H}_{1,0,0,0,0} \\
&- 240\,\mathrm{H}_{1,1,0,0,0} - 256\,\mathrm{H}_{1,1,1,0,0} + 256\,\mathrm{H}_{1,1,1,1,0} + \big(-2935\,\mathrm{H}_0 + 2964\,\mathrm{H}_1 \big)\zeta_4 + \zeta_2\big(-3120\,\mathrm{H}_3 \\
&- 1632\,\mathrm{H}_{1,2} + 836\,\mathrm{H}_{2,0} + 3120\,\mathrm{H}_{2,1} - 1836\,\mathrm{H}_{0,0,0} + 560\,\mathrm{H}_{1,0,0} - 528\,\mathrm{H}_{1,1,0} - 512\,\mathrm{H}_{1,1,1} \\
&- 264\zeta_3 \big) + \big(952\,\mathrm{H}_2 - 168\,\mathrm{H}_{0,0} - 96\,\mathrm{H}_{1,0} + 288\,\mathrm{H}_{1,1} \big)\zeta_3 - 176\zeta_5 \big] + \mathcal{O}\big(\epsilon^6\big), \qquad \text{(A.9)} \\
S_9 = &-\frac{1}{4} + \frac{\epsilon}{2}\big[\mathrm{H}_0 - 3\,\mathrm{H}_1 \big] + \frac{\epsilon^2}{4}\big[12\,\mathrm{H}_2 - 3\,\mathrm{H}_{0,0} - 7\,\mathrm{H}_{1,0} - 36\,\mathrm{H}_{1,1} - \zeta_2 \big] + \frac{\epsilon^3}{2}\big[-9\,\mathrm{H}_3 \\
&- 21\,\mathrm{H}_{1,2} + 7\,\mathrm{H}_{2,0} + 36\,\mathrm{H}_{2,1} - 21\,\mathrm{H}_{1,1,0} - 108\,\mathrm{H}_{1,1,1} + \big(-2\,\mathrm{H}_0 + 54\,\mathrm{H}_1 \big)\zeta_2 + \zeta_3 \big] \\
&+ \frac{\epsilon^4}{16}\big[336\,\mathrm{H}_{2,2} - 84\,\mathrm{H}_{3,0} - 432\,\mathrm{H}_{3,1} - 1008\,\mathrm{H}_{1,1,2} - 196\,\mathrm{H}_{1,2,0} - 1008\,\mathrm{H}_{1,2,1} + 32\,\mathrm{H}_{2,0,0} \\
&+ 352\,\mathrm{H}_{2,1,0} + 1728\,\mathrm{H}_{2,1,1} + 108\,\mathrm{H}_{0,0,0,0} - 4\,\mathrm{H}_{1,0,0,0} + 32\,\mathrm{H}_{1,1,0,0} - 992\,\mathrm{H}_{1,1,1,0}
\end{aligned}
$$

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\begin{aligned}
&- 5184\,\mathrm{H}_{1,1,1,1} + \big(- 848\,\mathrm{H}_2 + 132\,\mathrm{H}_{0,0} + 308\,\mathrm{H}_{1,0} + 2608\,\mathrm{H}_{1,1} \big)\zeta_2 + 141\zeta_4 + \big(- 8\,\mathrm{H}_0 \\
&+ 1240\,\mathrm{H}_1 \big)\zeta_3 \big] + \frac{\epsilon^5}{8}\big[324\,\mathrm{H}_5 - 12\,\mathrm{H}_{1,4} + 96\,\mathrm{H}_{2,3} - 252\,\mathrm{H}_{3,2} + 96\,\mathrm{H}_{1,1,3} - 588\,\mathrm{H}_{1,2,2} \\
&+ 32\,\mathrm{H}_{1,3,0} + 1056\,\mathrm{H}_{2,1,2} + 220\,\mathrm{H}_{2,2,0} + 1008\,\mathrm{H}_{2,2,1} - 96\,\mathrm{H}_{3,0,0} - 300\,\mathrm{H}_{3,1,0} - 1296\,\mathrm{H}_{3,1,1} \\
&- 2976\,\mathrm{H}_{1,1,1,2} - 564\,\mathrm{H}_{1,1,2,0} - 3024\,\mathrm{H}_{1,1,2,1} + 96\,\mathrm{H}_{1,2,0,0} - 540\,\mathrm{H}_{1,2,1,0} - 3024\,\mathrm{H}_{1,2,1,1} \\
&+ 4\,\mathrm{H}_{2,0,0,0} + 48\,\mathrm{H}_{2,1,0,0} + 1056\,\mathrm{H}_{2,1,1,0} + 5184\,\mathrm{H}_{2,1,1,1} - 324\,\mathrm{H}_{0,0,0,0,0} + 76\,\mathrm{H}_{1,0,0,0,0} \\
&- 12\,\mathrm{H}_{1,1,0,0,0} + 176\,\mathrm{H}_{1,1,1,0,0} - 2912\,\mathrm{H}_{1,1,1,1,0} - 15552\,\mathrm{H}_{1,1,1,1,1} + \big(- 389\,\mathrm{H}_0 \\
&- 2049\,\mathrm{H}_1 \big)\zeta_4 + \big(- 1336\,\mathrm{H}_2 - 12\,\mathrm{H}_{0,0} + 324\,\mathrm{H}_{1,0} + 3624\,\mathrm{H}_{1,1} \big)\zeta_3 + \zeta_2\big(600\,\mathrm{H}_3 \\
&+ 1560\,\mathrm{H}_{1,2} - 380\,\mathrm{H}_{2,0} - 2592\,\mathrm{H}_{2,1} - 324\,\mathrm{H}_{0,0,0} + 44\,\mathrm{H}_{1,0,0} + 852\,\mathrm{H}_{1,1,0} + 7840\,\mathrm{H}_{1,1,1} \\
&+ 4\zeta_3\big) - 88\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \qquad \text{(A.10)}
\end{aligned}
$$

$$
\begin{aligned}
S_{10} = &- \epsilon\,\mathrm{H}_0 - 2\epsilon^2\big[3\,\mathrm{H}_2 - \mathrm{H}_{0,0} - 3\zeta_2\big] + 3\epsilon^3\big[4\,\mathrm{H}_3 - 2\,\mathrm{H}_{2,0} - 12\,\mathrm{H}_{2,1} - \mathrm{H}_{0,0,0} + 4\zeta_3\big] \\
&- 2\epsilon^4\big[9\,\mathrm{H}_4 + 18\,\mathrm{H}_{2,2} - 6\,\mathrm{H}_{3,0} - 36\,\mathrm{H}_{3,1} - 3\,\mathrm{H}_{2,0,0} + 18\,\mathrm{H}_{2,1,0} + 108\,\mathrm{H}_{2,1,1} + \big(- 54\,\mathrm{H}_2 \\
&+ 3\,\mathrm{H}_{0,0} \big)\zeta_2 + 27\zeta_4 + \mathrm{H}_0\,\zeta_3\big] + \epsilon^5\big[36\,\mathrm{H}_{2,3} + 72\,\mathrm{H}_{3,2} - 18\,\mathrm{H}_{4,0} - 108\,\mathrm{H}_{4,1} - 216\,\mathrm{H}_{2,1,2} \\
&- 36\,\mathrm{H}_{2,2,0} - 216\,\mathrm{H}_{2,2,1} - 12\,\mathrm{H}_{3,0,0} + 72\,\mathrm{H}_{3,1,0} + 432\,\mathrm{H}_{3,1,1} - 6\,\mathrm{H}_{2,0,0,0} + 36\,\mathrm{H}_{2,1,0,0} \\
&- 216\,\mathrm{H}_{2,1,1,0} - 1296\,\mathrm{H}_{2,1,1,1} + 27\,\mathrm{H}_{0,0,0,0,0} + 57\,\mathrm{H}_0\,\zeta_4 + \zeta_2\big(- 216\,\mathrm{H}_3 + 36\,\mathrm{H}_{2,0} \\
&+ 648\,\mathrm{H}_{2,1} + 36\,\mathrm{H}_{0,0,0} - 132\zeta_3\big) + \big(276\,\mathrm{H}_2 + 16\,\mathrm{H}_{0,0} \big)\zeta_3 + 120\zeta_5\big] + \mathcal{O}\big(\epsilon^6\big), \qquad \text{(A.11)}
\end{aligned}
$$

$$
\begin{aligned}
S_{11} = &- \frac{\epsilon}{4}\,\mathrm{H}_0 + \frac{\epsilon^2}{2}\big[- 3\,\mathrm{H}_2 + \mathrm{H}_{0,0} + 3\zeta_2\big] + \frac{\epsilon^3}{4}\big[12\,\mathrm{H}_3 - 11\,\mathrm{H}_{2,0} - 36\,\mathrm{H}_{2,1} - 3\,\mathrm{H}_{0,0,0} \\
&- 5\,\mathrm{H}_0\,\zeta_2 + 2\zeta_3\big] + \frac{\epsilon^4}{2}\big[- 9\,\mathrm{H}_4 - 33\,\mathrm{H}_{2,2} + 11\,\mathrm{H}_{3,0} + 36\,\mathrm{H}_{3,1} - 27\,\mathrm{H}_{2,1,0} - 108\,\mathrm{H}_{2,1,1} \\
&+ \big(60\,\mathrm{H}_2 + 2\,\mathrm{H}_{0,0} \big)\zeta_2 - 18\zeta_4 - 9\,\mathrm{H}_0\,\zeta_3\big] + \frac{\epsilon^5}{16}\big[528\,\mathrm{H}_{3,2} - 132\,\mathrm{H}_{4,0} - 432\,\mathrm{H}_{4,1} \\
&- 1296\,\mathrm{H}_{2,1,2} - 260\,\mathrm{H}_{2,2,0} - 1584\,\mathrm{H}_{2,2,1} + 432\,\mathrm{H}_{3,1,0} + 1728\,\mathrm{H}_{3,1,1} + 76\,\mathrm{H}_{2,0,0,0} \\
&+ 64\,\mathrm{H}_{2,1,0,0} - 1120\,\mathrm{H}_{2,1,1,0} - 5184\,\mathrm{H}_{2,1,1,1} + 108\,\mathrm{H}_{0,0,0,0,0} + 97\,\mathrm{H}_0\,\zeta_4 + \big(1208\,\mathrm{H}_2 \\
&+ 232\,\mathrm{H}_{0,0} \big)\zeta_3 + \zeta_2\big(- 960\,\mathrm{H}_3 + 532\,\mathrm{H}_{2,0} + 2768\,\mathrm{H}_{2,1} + 84\,\mathrm{H}_{0,0,0} + 456\zeta_3\big) - 200\zeta_5\big] \\
&+ \mathcal{O}\big(\epsilon^6\big). \qquad \text{(A.12)}
\end{aligned}
$$

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