



NATIONAL TECHNICAL UNIVERSITY OF ATHENS  
SCHOOL OF APPLIED MATHEMATICS AND PHYSICAL SCIENCES

# MULTILOOP FEYNMAN INTEGRALS FOR PRECISION CALCULATIONS IN QUANTUM CHROMODYNAMICS

DOCTORAL THESIS

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BSc in Physics, NKUA

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ATHENS, March 2022



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# Περίληψη

Στην παρούσα διατριβή παρουσιάζουμε τον αναλυτικό υπολογισμό ολοκληρωμάτων Feynman πολλαπλών βρόχων, τα οποία συνεισφέρουν σε διάφορες  $2 \rightarrow 2$  και  $2 \rightarrow 3$  σωματιδιακές σχεδιάσεις στα πλαίσια της Κβαντικής Χρωμοδυναμικής.

Στο πρώτο μέρος παρουσιάζουμε μια επισκόπηση των μεθόδων που χρησιμοποιούνται επί του παρόντος για τον αναλυτικό υπολογισμό ολοκληρωμάτων βρόχων καθώς και την επεξεργασία των ειδικών συναρτήσεων που εμφανίζονται στις λύσεις τους. Χρησιμοποιώντας Ολοκλήρωση-Κατά-Παράγοντες, μπορούμε να εκφράσουμε τα ολοκληρώματα Feynman πολλαπλών βρόχων σε μια πεπερασμένη βάση ολοκληρωμάτων, τα οποία αποκαλούνται ολοκληρώματα βάσης. Στη συνέχεια διαμορφώνουμε ένα πλαίσιο για τον αναλυτικό υπολογισμό των ολοκληρωμάτων βάσης, το οποίο συνδυάζει την μέθοδο των Απλοποιημένων Διαφορικών Εξισώσεων με τη χρήση συγκεκριμένων ολοκληρωμάτων βάσης τα οποία ικανοποιούν κανονικές διαφορικές εξισώσεις. Για τον υπολογισμό των συνοριακών τιμών χρησιμοποιούμε την μέθοδο της επέκτασης-κατά-περιοχές.

Στο δεύτερο μέρος παρουσιάζουμε αποτελέσματα για συγκεκριμένα ολοκληρώματα βάσης ενός, δύο και τριών βρόχων. Αρχικά μελετούμε επίπεδα ολοκληρώματα βάσης τριών βρόχων που σχετίζονται με σχεδιάσεις  $2 \rightarrow 2$  όπου ένα εξωτερικό σωματίδιο φέρει μάζα. Τα αποτελέσματα αυτά συνεισφέρουν σε διορθώσεις τρίτης τάξης στα πλάτη σκέδασης για την διάσπαση ενός διανυσματικού μποζονίου σε τρία αδρονικά *jet* ή στην παραγωγή ενός μποζονίου Higgs με την διάσπαση  $gg \rightarrow H + jet$ . Στη συνέχεια παρουσιάζουμε αποτελέσματα σε επίπεδο ενός και δύο βρόχων για τη σκέδαση πέντε σωματιδίων όπου ένα εξωτερικό σωματίδιο φέρει μάζα. Τα αποτελέσματα αυτά συνεισφέρουν στον υπολογισμό διορθώσεων δεύτερης τάξης για διαδικασίες όπως η παραγωγή  $W + 2 jets$  στον LHC. Τέλος, μελετούμε διαφορα ολοκληρώματα ενός βρόχου για σκέδαση πέντε σωματιδίων, τα οποία περιλαμβάνουν άμαζους διαδότες και έως τρία έμαζα εξωτερικά σωματίδια, καθώς και έναν έμαζο διαδότη και έως δύο έμαζα εξωτερικά σωματίδια.

# Abstract

In this thesis we present analytic results for the calculation of multiloop Feynman integrals contributing to virtual corrections of various  $2 \rightarrow 2$  and  $2 \rightarrow 3$  scattering processes in Quantum Chromodynamics.

The first part consists of an overview of the current methods and tools for the analytic computation of loop integrals and the manipulation of the special functions that appear in their results. Using Integration-By-Parts identities, one can reduce all multiloop Feynman integrals to a so-called finite basis of master integrals. We construct a computational framework for the analytic calculation of these master integrals, based on the Simplified Differential Equations approach, in conjunction with the ideas of working with a specific basis of master integrals that satisfies so-called canonical differential equations. The method of expansion-by-regions is employed for the determination of the necessary boundary terms.

In the second part we present results for specific one-, two- and three-loop master integrals. We first consider planar three-loop master integrals relevant to  $2 \rightarrow 2$  scattering with one external leg off-shell. These results contribute to the scattering amplitudes for a vector boson decaying to 3-jets or  $gg \rightarrow H + jet$  in gluon fusion at Next-to-Next-to-Next-to-Leading-Order (N<sup>3</sup>LO). Furthermore we present one- and two-loop results for five-point scattering with one off-shell leg that are relevant to NNLO corrections to scattering processes such as  $W + 2$  jets production at the LHC. Finally we study several one-loop five-point master integrals involving massless propagators and up to three off-shell legs and one massive propagator with up to two off-shell legs.

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# Prolegomenon

*What is the world made of?* This question has puzzled the mind of humans since the days of ancient Greek philosophers. As centuries went on, the answer to this question was refined several times, as our species reached a deeper understanding of Nature.

Our current knowledge of Nature at its most fundamental level is encoded in the mathematical structure of the Standard Model (SM) of Particle Physics. One part of this theory comprises our best understanding of electromagnetic interactions at the quantum level, described by Quantum Electrodynamics (QED), which can be unified with the description of the weak interactions into the electroweak theory. The second part of the SM provides a theoretical description for the strong interactions, given by Quantum Chromodynamics (QCD). The theories of electroweak interactions and QCD are formulated in the mathematical language of Quantum Field Theory (QFT), a framework which has allowed us to produce the most precise description of a physical phenomenon, the magnetic moment of the electron [1]–[3].

The discovery of the Higgs boson at the LHC [4], [5] solidified the mathematical consistency of the SM of Particle Physics as our best fundamental description of Nature. And yet there are still open questions that make us think that the SM is not the final answer to the initial question about the nature of the world. The discovery of neutrino masses, the postulation by astronomers and cosmologists of the existence of a new kind of matter, called *Dark Matter* in lieu of a more accurate name that specifies its constituents, are only some of the many indications that there might be physics beyond the SM.

However, experimental data coming from powerful colliders, such as the LHC, have so far shed no light in these open questions. In the absence of any clear signals for physics beyond the SM, a detailed study of the properties of the Higgs boson, along with a scrutinization of key SM processes have spearheaded the endeavour to advance our understanding of Particle Physics [6].

From a theory perspective, precision studies in collider physics means using current methods and tools, as well as developing new ones, in order to provide predictions for the outcome of particle collisions that take place in high energy accelerator experiments. This thesis is devoted to a very specific part of this endeavour, more specifically to the study and computation of the mathematical objects that we will later identify as *Feynman integrals*.

More specifically, in the first part of this thesis we will give an overview of the theoretical methods, tools and ideas that allow us to produce precise theoretical predictions for scattering processes studied at the LHC. In the second part we will present results stemming from original research concerning the so-called virtual corrections at Next-to-Next-to Leading Order (NNLO) and N3LO for various  $2 \rightarrow 2$  and  $2 \rightarrow 3$  processes.

Although the level of mathematical sophistication of our answer to the question about the structure of our physical world has increased over the years, physics is not mathematics. The ultimate goal of a physicist is to explain the world<sup>1</sup> and all calculations presented in this thesis are made with a mind to contribute to this noble endeavour.

---

<sup>1</sup>*To Explain the World, the Discovery of Modern Science* (2015), Steven Weinberg, Harper/HarperCollins Publishers.



# Part I

## Theoretical overview

# Chapter 1

## Precision calculations in Quantum Chromodynamics (QCD)

### 1.1 Elements of Quantum Field Theory

Over the course of the twentieth century, collider physics emerged as a powerful approach for the discovery of particles that exist in nature and the study of their properties and interactions. Particle colliders provide a controlled environment for the study of fundamental interactions, since they begin with initial states of fixed momenta and end up with final states with fixed momenta as well. The measurement of the mapping from initial state momenta to final state momenta is then compared to predictions coming from theoretical models formulated within the framework of Quantum Field Theory (QFT)<sup>1</sup>.

QFT is the result of combining Quantum Mechanics with Special Relativity. Each QFT is usually characterised by a Lagrangian density  $\mathcal{L}$ , which is a polynomial of the fundamental quantum fields  $\phi_i(x)$  and their derivatives. One of the main reasons for using Lagrangian densities, is that they are manifestly Lorentz invariant. The dynamics of a QFT is determined by the principle of least action, with the action being the integral of the Lagrangian density over the four-dimensional space-time

$$S = \int d^4x \mathcal{L}[\phi_i(x)]. \quad (1.1)$$

In Quantum Mechanics, the experimental measurable quantities that one can predict are differential probabilities, given by the modulus squared of inner products of states in a Hilbert space. Since QFT is by construction based on Quantum Mechanics, the experimental quantities we can predict are of the form

$$|\langle f | \mathcal{S} | i \rangle|^2. \quad (1.2)$$

The inner product  $\langle f | \mathcal{S} | i \rangle$  is known as the Scattering or S-matrix and contains all the information about how the initial and final states evolve with time. S-matrix elements are the main objects of interest in collider physics and QFT provides us with the necessary tools to compute them.

In the absence of any interactions, i.e. when considering a free theory, the S-matrix is simply the identity matrix  $\mathbb{1}$ . When interactions are present we have

$$\mathcal{S} = \mathbb{1} + i\mathcal{T} \quad (1.3)$$

with  $\mathcal{T}$  known as the *transfer matrix*, encoding all deviations from the free theory. The transfer matrix is defined as

$$\langle f | \mathcal{T} | i \rangle = (2\pi)^4 \delta^4(\Sigma p) \langle f | \mathcal{M} | i \rangle \quad (1.4)$$

---

<sup>1</sup>There is a plethora of QFT textbooks. We refer the interested reader to [7]–[10].

where  $\langle f | \mathcal{M} | i \rangle$  is what we usually mean by *matrix elements*, and  $\Sigma p = \Sigma p_i^\mu - \Sigma p_f^\mu$ . At the end of the day one finds that the S-matrix elements are related to the total cross-section of the scattering process as

$$\sigma \propto \int d\Pi_{LIPS} |\mathcal{M}_{fi}|^2 \quad (1.5)$$

where  $d\Pi_{LIPS}$  is the *Lorentz-invariant phase space* and  $|\mathcal{M}_{fi}|^2 = |\langle f | \mathcal{M} | i \rangle|^2$ .  $\mathcal{M}_{fi}$  is also referred to as *scattering amplitude*.

The complexity of the scattering amplitudes is such that their exact analytic calculation is an insurmountable task for most theories. The only viable approach is through perturbation theory, where the scattering amplitudes are written as an expansion in Feynman diagrams. Given the Lagrangian density of a theory, one can obtain in a systematic way a set of mathematical rules, known as Feynman rules, which *translate* each diagram into a mathematical formula. As one considers scattering processes of higher multiplicity, i.e. involving the interaction of many particles, and/or higher orders in the perturbative expansion, the corresponding Feynman diagrams become significantly more involved.

In what follows we will focus on a specific QFT, the one that describes the strong interactions. Its name is Quantum Chromodynamics (QCD).

## 1.2 The QCD Lagrangian and Feynman rules

The fundamental principle of QCD is that hadronic matter is made of quarks<sup>2</sup>. Two of the most known hadrons are the proton and neutron. The dynamics of the strong interaction that is responsible for binding the protons and neutrons that form the nucleus of atoms is encoded in the mathematical structure of the QCD Lagrangian density. The strong force is mediated through the interaction of quarks and gluons, the latter being the bosonic force carriers of the strong force. Quarks are spin-1/2 particles and through experiments we know that they exist in at least six different kinds, the so-called flavours, namely: up ( $u$ ), down ( $d$ ), strange ( $s$ ), charm ( $c$ ), bottom ( $b$ ) and top ( $t$ ).

The QCD Lagrangian density can be written as a sum of three terms

$$\mathcal{L}_{QCD} = \mathcal{L}_{classic} + \mathcal{L}_{gauge-fix} + \mathcal{L}_{ghost}. \quad (1.6)$$

The first term encodes the dynamics of quarks and reads

$$\mathcal{L}_{classic} = \sum_f \bar{\psi}_{f,i} (i\not{D}_{ij} - m_f \delta_{ij}) \psi_{f,j} - \frac{1}{4} F_{\mu\nu}^a F^{\mu\nu,a} \quad (1.7)$$

where  $f$  is the flavour index,  $i, j$  are the colour indices in the fundamental representation and  $a, b$  are the ones in the adjoint representation. The quark fields are represented as  $\psi_{f,i}$  and the covariant derivative is given by

$$D_{ij}^\mu = \partial_{ij}^\mu \delta_{ij} - ig_s A_a^{ij} t_{ij}^a. \quad (1.8)$$

The gluons are represented as  $A_a^{ij}$  and the matrices  $t_{ij}^a$  are the generators of the fundamental representation of  $SU(N)$ , with  $N = 3$  the number of colours. The generators  $t_{ij}^a$  fulfil the algebra

$$[t^a, t^b] = i f^{abc} t^c \quad (1.9)$$

---

<sup>2</sup>Here we provide a schematic overview of QCD. We refer the interested reader to [11], [12] for a thorough discussion of QCD in the context of collider physics.

where  $f^{abc}$  are the structure constants. The coupling strength of quarks to gluons is represented by the coupling constant  $g_s$ . The final term in (1.7) contains the gluonic field tensor

$$F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g_s f_{abc} A_\mu^b A_\nu^c. \quad (1.10)$$

The last two terms in (1.6) are required in order to be able to perform perturbation theory. The gauge fixing term reads

$$\mathcal{L}_{gauge-fix} = \frac{1}{2\xi} (\partial_\mu A_a^\mu)^2 \quad (1.11)$$

and is needed in order to define the propagator for the gluon field. The parameter  $\xi$  is arbitrary and is needed to specify the gauge in a covariant way. The so-called Feynman gauge  $\xi = 1$  is a typical choice and the one that we will use in this thesis. Physical results are of course independent of the specific value of  $\xi$ . In a non-Abelian theory such as QCD this gauge-fixing term must be supplemented by a ghost Lagrangian density which is given by

$$\mathcal{L}_{ghost} = (\partial_\mu \chi_a^*) (\partial^\mu \delta_{ab} - g_s f_{abc} A_c^\mu) \chi_b. \quad (1.12)$$

The ghost fields  $\chi_a$  are scalar fields which obey fermionic anticommutation relations. The ghost fields cancel unphysical degrees of freedom which would otherwise propagate in covariant gauges.

Eqs. (1.7), (1.11), (1.12) are sufficient to derive the Feynman rules of QCD. In the following we will use straight lines for quarks, curly lines for gluons and dashed lines for ghosts. Taking all momenta to be incoming for the vertices and using the Feynman slash-notation, i.e.  $\not{p} = p^\mu \gamma_\mu$ , with  $\gamma_\mu$  being the Dirac gamma matrices satisfying the anticommutation relations  $\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}$ , we have

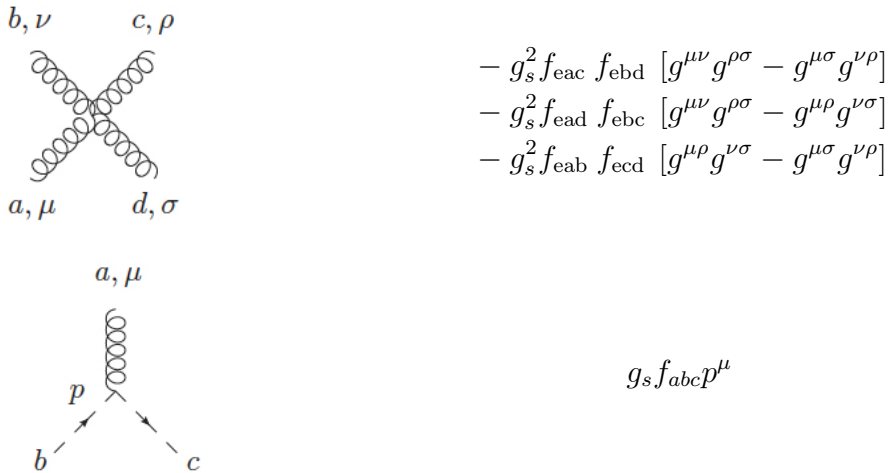
$$\begin{array}{c} i \qquad \qquad j \\ \longrightarrow \end{array} \qquad i\delta_{ij}/(\not{p} - m + i\epsilon)$$

$$\begin{array}{c} a, \mu \qquad \qquad b, \nu \\ \text{-----} \\ \text{-----} \end{array} \qquad \delta_{ab} \left[ -g_{\mu\nu} + (1 - \xi) \frac{p_\mu p_\nu}{p^2 + i\epsilon} \right] i / (p^2 + i\epsilon)$$

$$\begin{array}{c} a \qquad \qquad b \\ \text{-----} \end{array} \qquad i\delta_{ab}/(p^2 + i\epsilon)$$

$$\begin{array}{c} a, \mu \\ \text{-----} \\ \swarrow \quad \searrow \\ i \qquad \qquad j \end{array} \qquad -ig_s t_{ij}^a \gamma^\mu$$

$$\begin{array}{c} b, \nu \\ \text{-----} \\ p_2 \\ \swarrow \quad \searrow \\ p_1 \qquad \qquad p_3 \\ \text{-----} \quad \text{-----} \\ a, \mu \qquad \qquad c, \rho \end{array} \qquad -g_s f_{abc} [(p_1 - p_2)^\rho g^{\mu\nu} + (p_2 - p_3)^\mu g^{\nu\rho} + (p_3 - p_1)^\nu g^{\rho\mu}]$$



In addition to these rules, one needs to introduce symmetry factors to avoid overcounting diagrams, as well as properly treat loop diagrams using the following rules:

1. Each internal loop momentum  $k$  must be integrated over, with the integral measure being  $\int d^d k / (2\pi)^d$ , where  $d$  is the number of space-time dimensions.
2. Every fermionic loop comes with a factor of  $(-1)$ .

As can be seen, every vertex comes with its own power of the quark-gluon coupling  $g_s$ . This allows for each Feynman diagram constructed using these rules to be classified in terms of the total number of powers of the coupling constant. As this number increases, diagrams containing one or more closed loops can be drawn, which can be *translated* to the so-called *Feynman integrals*, which are the main object of interest in this thesis. A problematic feature of these integrals is that they often exhibit UV and IR divergences in  $d = 4$  space-time dimensions. The proper way to regulate these divergences is through *dimensional regularisation* [13]–[15], working in  $d = 4 - 2\epsilon$  space-time dimensions, where poles in the dimensional regulator  $\epsilon$  represent these UV and IR divergences.

### 1.3 Perturbative QCD

As we mentioned earlier, in most QFT's the only viable method of calculating S-matrix elements is through perturbation theory. Having the Feynman rules as a starting point, one can translate diagrammatic expansion in the perturbative series into specific mathematical objects. This approach yields a power tool for the production of precise phenomenological predictions, if the coupling constant of the theory under consideration is small enough at the energy level that is being studied.

In the case of QCD, the property of *asymptotic freedom* [16]–[20] states that the strong coupling constant

$$a_s = \frac{g_s^2}{4\pi} \quad (1.13)$$

where  $g_s$  is the quark-gluon coupling, decreases with the increase of energy. This means that quarks interact weakly at high energies, which allows us to use perturbative methods in QCD for the study of hadrons at high energy colliders, such as the LHC.

Comparing QCD perturbative calculations with experimental data is a non-trivial task, however the *factorisation theorem* [21] permits us to separate it into two stages:

- The *hard scattering*, described by perturbative QCD.

- The *hadronisation*, which requires different methods that go beyond the scope of this thesis.

At the level of the cross-section for the collision of two initial hadrons  $h_1$ ,  $h_2$  resulting in the production of some final state  $X$ , we have

$$d\sigma_{h_1 h_2 \rightarrow X} = \sum_{a,b=q,\bar{q},g} \int_{x_{1,\min}}^1 dx_1 \int_{x_{2,\min}}^1 dx_2 \mathcal{F}_{a/h_1}(x_1, \mu^2) \mathcal{F}_{b/h_2}(x_2, \mu^2) \hat{\sigma}_{ab \rightarrow X}(\mu^2) \quad (1.14)$$

where  $\mathcal{F}_{a/h_1}(x_1, \mu^2)$  and  $\mathcal{F}_{b/h_2}(x_2, \mu^2)$  are the Parton Distribution Functions,  $\hat{\sigma}_{ab \rightarrow X}$  is the hard scattering cross-section, and  $\mu^2$  is the factorization scale. The total cross-section for the production of the final state  $X$  in perturbative QCD,  $\hat{\sigma}(X) = \hat{\sigma}_{h_1 h_2 \rightarrow X}$  can be expanded in powers of  $a_s$ . Normalising to the number of powers of  $a_s$  of the born cross-section, we can write

$$\hat{\sigma}(X) = \hat{\sigma}(X)_{LO} + \left(\frac{a_s}{2\pi}\right) \hat{\sigma}(X)_{NLO} + \left(\frac{a_s}{2\pi}\right)^2 \hat{\sigma}(X)_{NNLO} + \left(\frac{a_s}{2\pi}\right)^3 \hat{\sigma}(X)_{NNNLO} + \dots \quad (1.15)$$

where *LO* stands for *Leading order*, *NLO* stands for *Next-to-Leading order*, *NNLO* stands for *Next-to-Next-to-Leading order*, etc.

Calculation of corrections up to *NLO* have reached a high level of maturity and have been automated in public tools [22], [23]. Since most of the calculations presented in this thesis concern *NNLO* corrections we will briefly discuss the various contributions that they receive. More specifically we have:

1. *Virtual corrections*, which include 2-loop Feynman diagrams.
2. *Mixed real-virtual corrections*, which include 1-loop Feynman diagrams with an extra particle which can become unresolved.
3. *Double-real corrections*, which include tree-level Feynman diagrams with two extra particles which can become unresolved.

Each of these contributions is individually divergent, with the divergences cancelling in the sum (after renormalization for the UV and IR divergences) leaving behind a finite result for the cross-section.

# Chapter 2

## Master integrals

The material presented in this chapter is based on reviews such as [6], [24], [25].

### 2.1 Integral families

The modern approach of thinking about the calculation of Feynman integrals (FI) which are required in the computation of a scattering amplitude, is through the notion of an *integral family*.

If we consider a scattering process involving  $N$  external particles in  $d$  space-time dimensions, then, assuming momentum conservation, only  $E = \min(N - 1, d)$  external particles will be linearly independent. We can associate to this process the following integral with  $L$  loops in  $d$  dimensions with propagator powers  $\nu_j$

$$G(\nu_1, \dots, \nu_n) = \int \prod_{l=1}^L \frac{d^d k_l}{i\pi^{d/2}} \prod_{j=1}^n \frac{1}{D_j^{\nu_j}(\{k\}, \{p\}, m_j^2)} \quad (2.1)$$

where the propagators  $D_j(\{k\}, \{p\}, m_j^2)$  depend on the loop momenta  $k_l$ , the linearly independent momenta  $\{p_1, \dots, p_E\}$  and, when present, on the propagator masses  $m_j^2$ . We work on the framework of dimensional regularisation with  $d = 4 - 2\epsilon$ , to regulate both ultraviolet and infrared divergences. This implies that the singularities in four dimensions manifest in the form of  $1/\epsilon$ -terms to some power.

For various values of propagator powers  $\nu_j$ , we see that (2.1) defines a set of integrals. We define as an *integral family* the set of integrals  $G(\nu_1, \dots, \nu_n)$  which contains all integrals with propagator configurations such that any scalar product of a loop momentum with another loop momentum or with an external momentum can be expressed as a linear combination of inverse propagators contained in the same family. A scalar integral of an integral family with no loop-momentum dependence in the numerator corresponds to  $\nu_j \geq 0$  for all  $j$ . In general, the integrals of an integral family are linearly dependent and form a vector space. Therefore one can find a basis of integrals in terms of which all integrals of the integral family can be expressed. This process is known as a *reduction to master integrals*. Finding a convenient basis of master integrals is of great importance for their efficient calculation.

For an  $N$ -point integral family with  $L$  loops, the number  $n$  of genuinely different scalar products of the type  $k_i \cdot k_j$  and  $k_i \cdot p_j$  is given by

$$n = \frac{L(L+1)}{2} + L \cdot E \quad (2.2)$$

The first term comes from contracting the loop momenta with themselves, and the second one comes from contracting the loop momenta with the external momenta. A useful way of

organising the integrals of a family is through the use of integral sectors. A sector is defined as a set of  $t$  propagators of an integral family. The number of different  $t$ -propagator sectors is  $\binom{n}{t}$  and therefore in principle  $\sum_{t=0}^n \binom{n}{t} = 2^n$  sectors are contained in an integral family, however many of them will be zero or related by symmetries.

To every  $t$ -propagator sector with propagator denominators  $D_{j_1}, \dots, D_{j_t}$  we can define a set of integrals with different propagator powers by

$$I(t, r, s) = \int \prod_{l=1}^L \frac{d^d k_l}{i\pi^{d/2}} \frac{D_{j_{t+1}}^{s_1} \dots D_{j_n}^{s_{n-t}}}{D_{j_1}^{r_1} \dots D_{j_t}^{r_t}} \quad (2.3)$$

with integer exponents  $r_i \geq 1$  and  $s_i \geq 0$ . This allows us to characterise an integral of the family by then numbers  $t, r, s$  and the indices  $\{v_1, \dots, v_n\} = \{r_1, \dots, r_t, -s_1, \dots, -s_{n-t}\}$ , where  $r = \sum_{i=1}^t r_i$  and  $s = \sum_{i=1}^{n-t} s_i$ . Positive  $v_i$  denote powers of *regular* propagators, i.e. propagators in the denominator, negative  $v_i$  denote powers of inverse propagators, i.e. they form non-trivial numerators, and  $v_i = 0$  means the absence of a propagator. The numbers  $t, r, s$  can be calculated from the vector  $\vec{v}$ , so they are redundant once  $\vec{v}$  is given.

For a  $t$ -propagator sector of an  $n$ -propagator integral family, the number of integrals that can be built for certain values of  $r$  and  $s$  is given by

$$N(n, t, r, s) = \binom{r-1}{t-1} \binom{s+n-t-1}{n-t-1} \quad (2.4)$$

The two binomial factors count all possible ways to arrange the exponents of the propagators in the denominator and numerator respectively. The integral with  $r = t$  and  $s = 0$  of some sector is called the *corner* integral of this sector.

From (2.2) we can see that all topologies with a number of propagators  $n_p > n$  are reducible, i.e. scalar products in the numerator can be expressed through linear combinations of propagators of the same integral. For  $L = 1$  one can show that the only irreducible numerators are of the type  $k_i \cdot n$ , where  $n_j$  denotes directions transverse to the hyperplane spanned by the physical external momenta. These terms however vanish after integration over the loop momenta (in integer dimensions). Starting from two loops, genuine irreducible numerators can occur, the so-called *irreducible scalar products* or isp's.

## 2.2 Integration-by-parts identities

It can be shown that for dimensionally regulated FI, the integral over a total derivative is zero [26]. If  $I$  is the integrand of an integral of the form (2.1), taking derivatives as follows

$$\prod_{l=1}^L d^d k_l \frac{\partial}{\partial k_i^\mu} [u^\mu I(\vec{v})] = 0 \quad (2.5)$$

leads to identities between different integrals, the so-called *integration-by-parts* (IBP) identities. The term  $u^\mu$  can be a loop- or external momentum which can be chosen conveniently, for example such that propagators with powers  $v_i > 1$  (known as *propagators with dots*) do not occur. If there are  $L$  loop momenta and  $E$  independent external momenta, one can therefore build  $L(L + E)$  equations from one integral.

The system of IBP identities is in general over-constrained, such that most of the integrals can be expressed as linear combinations of a small subset of integrals, the so-called master integrals (MI). Another set of identities that also provide relations among integrals are the Lorentz-invariance identities of the form

$$\sum_{i=1}^E \left( p_i^\nu \frac{\partial}{\partial p_{i\mu}} - p_i^\mu \frac{\partial}{\partial p_{i\nu}} \right) G(\vec{v}) = 0. \quad (2.6)$$



Thees relations are redundant, but can help convergence in solving the linear system.

The choice of MI is not unique. A convenient choice of the basis can make a huge difference in the calculation of integrals of a certain complexity. Further it is important to take symmetries into account as well as shifts of the loop momenta that do not change the kinematic variables.

In complicated cases, an order relation among the integrals has to be introduced to be able to solve the system for a set of MI. For example, an integral  $T_1$  is considered to be smaller than an integral  $T_2$ , if  $T_1$  can be obtained from  $T_2$  by omitting some of the propagators. Within the same topology, the integrals can be ordered according to the powers of their propagators.

The first systematic approach of IBP reduction has been formulated by Laporta [27] and is known as *Laporta's algorithm*. Several packages exist that automate *Laporta's algorithm*, such as FIRE [28], KIRA [29], AZURITE [30], REDUZE [31], just to mention some of the currently most used publicly available tools, as well as several private codes.

## 2.3 Parametric representations

There are several representations of Feynman integrals. Other than the one in momentum space (2.1), the most widely used are the *Feynman parameter representation* and the *Baikov representation*. The main advantage of these parametric representations over the one in momentum space is that the integrations involve only scalar objects in Minkowski space.

### 2.3.1 Feynman parameter representation

Starting from (2.1) one can use Schwinger's trick

$$\frac{1}{D_j^{\nu_j}} = \frac{1}{\Gamma(\nu_j)} \int_0^\infty d\alpha_j \alpha_j^{\nu_j-1} e^{-\alpha D_j} \quad (2.7)$$

for  $D_j > 0$ ,  $\text{Re}(\nu_j) > 0$ , to prove that

$$\prod_{j=1}^n \frac{1}{D_j^{\nu_j}} = \Gamma(\nu) \prod_{j=1}^n \left[ \int_0^\infty dx_j \frac{x_j^{\nu_j-1}}{\Gamma(\nu_j)} \right] \delta\left(1 - \sum_{j=1}^n x_j\right) \frac{1}{\left(\sum_{j=1}^n x_j D_j\right)^\nu} \quad (2.8)$$

with  $\nu = \sum_{j=1}^n \nu_j$  and  $x_i$  are the so-called *Feynman parameters*. Furthermore  $\sum_{j=1}^n x_j D_j$  is a quadratic form in the loop momenta  $k_l$ ,

$$\sum_{j=1}^n x_j D_j = \sum_{j,l=1}^L k_j \cdot k_l M_{jl} - 2 \sum_{j=1}^L k_j \cdot Q_j + J + i\delta \quad (2.9)$$

where  $k_j \cdot k_l$  denotes the scalar product of two  $d$ -dimensional Lorentz vectors. We can perform a shift in the loop momenta  $k_j = l_j + M_{ij}^{-1} Q_l$  and after defining

$$\mathcal{U} = \det(M) \quad , \quad \mathcal{F} = \det(M) \left[ \sum_{i,j=1}^L Q_i M_{ij}^{-1} Q_j - J - i\delta \right] \quad (2.10)$$

we can arrive at

$$G(\nu_1, \dots, \nu_n) = \Gamma\left(\nu - \frac{Ld}{2}\right) \prod_{j=1}^n \left[ \int_0^\infty dx_j \frac{x_j^{\nu_j-1}}{\Gamma(\nu_j)} \right] \delta\left(1 - \sum_{j=1}^n x_j\right) \frac{\mathcal{U}^{\nu-(L+1)d/2}}{\mathcal{F}^{\nu-Ld/2}}. \quad (2.11)$$

The polynomials  $\mathcal{U}$ ,  $\mathcal{F}$  are known as *first and second Symanzik polynomials* and also admit a graph-theoretic interpretation. The Cheng - Wu theorem [32] states that the same formula (2.11) holds even when the delta function

$$\delta\left(1 - \sum_{j=1}^n x_j\right) \quad (2.12)$$

includes only a subset of  $x_j \in \{1, \dots, n\}$ .

### 2.3.2 Baikov representation

The essence of the Baikov representation of Feynman integrals is that we change the integration variables from the loop momenta to the propagators.

Every inverse Feynman propagator  $D_a$  in (2.1) can be written as follows

$$D_a = P_a^2 - M_a^2, \quad a = 1, \dots, n \quad (2.13)$$

with  $P_a$  being a linear combination of loop and external momenta and  $M_a$  the internal masses.

Defining  $q_i = k_i$ ,  $i = 1, \dots, L$  as the loop momenta,  $q_{L+i} = p_i$ ,  $i = 1, \dots, E$  as the independent external momenta and  $M = L + E$ ,  $s_{ij} = q_i \cdot q_j$ <sup>1</sup>, allows us to write the propagators  $D_a$  in the form

$$\begin{aligned} D_a &= \sum_{i=1}^L \sum_{j=i}^M A_a^{ij} s_{ij} + f_a \\ &= \sum_{i=1}^L \sum_{j=i}^L A_a^{ij} k_i \cdot k_j + \sum_{i=1}^L \sum_{j=L+1}^M A_a^{ij} k_i \cdot p_{j-L} + f_a \end{aligned} \quad (2.14)$$

where  $f_a$  is a function depending on external kinematics and internal masses,  $A_a^{ij}$  is a matrix loosely associated with the topology of the graph with elements taken from the set  $\{-2, -1, 0, 1, 2\}$  and  $a = 1, \dots, n$ . We may view  $A_a^{ij}$  as an  $n \times n$  matrix [33]. This allows us to solve (2.14) for  $s_{ij}$

$$s_{ij} = \sum_{a=1}^n A_{ij}^a (D_a - f_a) \quad (2.15)$$

with  $A_{ij}^a = (A_a^{ij})^{-1}$ .

Now that we have set the stage, we will try at first to change the integration variables of (2.1) from the loop momenta  $k_i^\mu$  to the scalar products  $s_{ij}$ . In order to do so, we start from  $k_1^\mu$  and write it in the form

$$k_1^\mu = k_{1\parallel}^\mu + k_{1\perp}^\mu \quad (2.16)$$

where  $k_{1\parallel}^\mu$  is the projection of  $k_1^\mu$  on the hyper-plane spanned by the  $(M - 1)$  momenta  $\{k_2^\mu, \dots, k_L^\mu, p_1, \dots, p_E\}$ , and  $k_{1\perp}^\mu$  is the transverse component to the above mentioned hyper-plane. We apply this procedure to all loop momenta. For  $k_2^\mu$  for example we write

$$k_2^\mu = k_{2\parallel}^\mu + k_{2\perp}^\mu \quad (2.17)$$

with  $k_{2\parallel}^\mu$ , as in the case of  $k_{1\parallel}^\mu$ , being the projection of  $k_2^\mu$  on the hyper-plane spanned by  $\{k_3^\mu, \dots, k_L^\mu, p_1, \dots, p_E\}$  ( $M - 2$  components). This procedure allows us to write the integration measure as follows,

$$d^d k_1 \dots d^d k_L = d^{M-1} k_{1\parallel} d^{d-M+1} k_{1\perp} \dots d^{M-L} k_{L\parallel} d^{d-M+L} k_{L\perp} \quad (2.18)$$

---

<sup>1</sup>This definition of  $s_{ij}$  differs from the rest of the thesis. In later chapters we will use the notation  $s_{ij} = (p_i + p_j)^2$ , with  $p_i$  being the external momenta.

As a first step, we will make the following change of variables starting from  $k_1^\mu$ ,

$$d^{M-1}k_{1\parallel} \rightarrow ds_{12} ds_{13} \dots ds_{1M} \quad (2.19)$$

Under such a change of integration variables, the measure of integration transforms as follows,

$$d^{M-1}k_{1\parallel} = \det \left( \frac{\partial k_{1\parallel}^\mu}{\partial s_{1j}} \right) ds_{12} ds_{13} \dots ds_{1M} \quad (2.20)$$

To proceed we make the following definitions

$$\zeta_j = k_l \cdot q_j, \quad l = 1, 2, \dots, \quad j = l + 1, \dots, M \text{ and since } k_l^\mu = k_{l\parallel}^\mu + k_{l\perp}^\mu \quad (2.21)$$

$$k_l \cdot q_j = k_{l\parallel} \cdot q_j + k_{l\perp} \cdot q_j = k_{l\parallel} \cdot q_j = \zeta_j \quad (2.22)$$

From  $\zeta_j = k_l \cdot q_j$  we have for  $k_1^\mu$

$$\zeta_j = k_1 \cdot q_j = s_{1j} = k_{1\parallel} \cdot q_j \quad (2.23)$$

We may also write  $k_{l\parallel}^\mu = a_i q_i^\mu$  so we have

$$k_{l\parallel} \cdot q_j = a_i q_i \cdot q_j = a_i s_{ij} = \zeta_j \quad (2.24)$$

therefore

$$a_i = \zeta_j s_{ij}^{-1} \quad (2.25)$$

Finally we can write  $k_{1\parallel}^\mu$  as

$$k_{1\parallel}^\mu = \sum_i a_i q_i^\mu = \sum_{i,j} \zeta_j s_{ij}^{-1} q_i^\mu = s_{1j} s_{ij}^{-1} q_i^\mu, \quad i, j = 2, \dots, M \quad (2.26)$$

Following these manipulations, the Jacobian can take the form

$$\det \left( \frac{\partial k_{1\parallel}^\mu}{\partial s_{1j}} \right) = \det (s_{ij}^{-1} q_i^\mu) = \det(s_{ij})^{-1} \det (q_i^\mu) \quad (2.27)$$

To continue notice that by definition, the Gram determinant is  $|\mathbb{G}(q_1, \dots, q_n)| = \det(q_i \cdot q_j)$ , therefore for  $i, j = 2, \dots, M$

$$\det(s_{ij}) = \det(q_i \cdot q_j) = |\mathbb{G}(q_2, \dots, q_M)| \quad (2.28)$$

and we can also have

$$\left[ \det (q_i^\mu) \right]^2 = \det (q_i^\mu) \det (q_{i\mu}) = \det (q_i^\mu q_{i\mu}) = |\mathbb{G}| \quad (2.29)$$

which leads to

$$\det (q_i^\mu) = |\mathbb{G}(q_2, \dots, q_M)|^{1/2} \quad (2.30)$$

Using (2.30), the Jacobian (2.27) can take the form

$$\det \left( \frac{\partial k_{1\parallel}^\mu}{\partial s_{1j}} \right) = \frac{1}{\sqrt{|\mathbb{G}(q_2, \dots, q_M)|}} \quad (2.31)$$

Applying the above procedure to the rest of the  $k_{i\parallel}$  yields

$$d^{M-1}k_{1\parallel} = \frac{ds_{12}, ds_{13}, \dots, ds_{1M}}{|\mathbb{G}(k_2, \dots, k_L, p_1, \dots, p_E)|^{1/2}}$$

$$d^{M-2}k_{2\parallel} = \frac{ds_{23}, ds_{24}, \dots, ds_{2M}}{|\mathbb{G}(k_3, \dots, k_L, p_1, \dots, p_E)|^{1/2}} \quad (2.32)$$

⋮

$$d^{M-L}k_{L\parallel} = \frac{ds_{LL+1}, \dots, ds_{LM}}{|\mathbb{G}(p_1, \dots, p_E)|^{1/2}} \quad (2.33)$$

For  $k_{i\perp}$  we change into spherical coordinates and integrate over the angular part

$$d^n k_{i\perp} = \frac{1}{2} \Omega_n k_{i\perp}^{n-2} dk_{i\perp}^2, \quad \Omega_n = \frac{2\pi^{n/2}}{\Gamma\left(\frac{n}{2}\right)} \quad (2.34)$$

which allows us to write  $s_{ii}$  as follows

$$s_{ii} = k_i^2 = k_{i\parallel}^2 + k_{i\perp}^2 \rightarrow dk_{i\perp}^2 = ds_{ii} \quad (2.35)$$

This holds because  $k_{i\parallel}^\mu = s_{lj} s_{ij}^{-1} q_i^\mu$  and therefore

$$\begin{aligned} k_{i\parallel}^2 &= s_{lj} s_{ij}^{-1} q_i^\mu s_{lm} s_{nm}^{-1} q_{n,\mu} \\ &= s_{lj} s_{ij}^{-1} s_{lm} s_{nm}^{-1} s_{in} = s_{lj} s_{ij}^{-1} s_{lm} s_{nm}^{-1} \delta_{im} \\ &= s_{lj} s_{ij}^{-1} s_{li} \end{aligned} \quad (2.36)$$

Then we can write  $k_{1\perp}$  as follows

$$k_{1\perp} = \sqrt{s_{11} - k_{1\parallel}^2} = \sqrt{s_{11} - s_{1i} s_{ij}^{-1} s_{1j}}, \quad i, j = 2, \dots, M \quad (2.37)$$

Using the definition for the determinant of block matrices, we can write for the ratio of the following Gram determinants

$$\begin{aligned} \frac{|\mathbb{G}(k_1, \dots, k_L, p_1, \dots, p_E)|}{|\mathbb{G}(k_2, \dots, k_L, p_1, \dots, p_E)|} &= \frac{\det \begin{pmatrix} s_{11} & s_{1j} \\ s_{1j} & s_{ij} \end{pmatrix}}{\det(s_{ij})} \\ &= \frac{\det(s_{ij}) \det(s_{11} - s_{1i} s_{ij}^{-1} s_{1j})}{\det(s_{ij})} \\ &= s_{11} - s_{1i} s_{ij}^{-1} s_{1j} \end{aligned} \quad (2.38)$$

For the last step we used the fact that the determinant of a number is equal to the number itself. Putting everything together leads to

$$k_{1\perp} = \sqrt{\frac{|\mathbb{G}(k_1, \dots, k_L, p_1, \dots, p_E)|}{|\mathbb{G}(k_2, \dots, k_L, p_1, \dots, p_E)|}} \quad (2.39)$$

This allows us to write the integral measure  $d^n k_{1\perp}$  as follows

$$d^{d-M+1} k_{1\perp} = \frac{1}{2} \Omega_{d-M+1} \left( \frac{|\mathbb{G}(k_1, \dots, k_L, p_1, \dots, p_E)|}{|\mathbb{G}(k_2, \dots, k_L, p_1, \dots, p_E)|} \right)^{\frac{(d-M+1)}{2}} ds_{11} \quad (2.40)$$

Applying the above procedure to the rest of  $k_{i\perp}$  and replacing the resulting  $d^n k_{i\perp}$  and  $d^n k_{i\parallel}$  all Gram determinants except  $|\mathbb{G}(k_1, \dots, k_L, p_1, \dots, p_E)|$  and  $|\mathbb{G}(p_1, \dots, p_E)|$  cancel, yielding

$$G(\nu_1, \dots, \nu_n) = \frac{\pi^{-\frac{L(L-1)}{4} - \frac{LE}{2}}}{\prod_{i=1}^L \Gamma\left(\frac{d-M+i}{2}\right)} \left[ |\mathbb{G}(p_1, \dots, p_E)| \right]^{\frac{-d+E+1}{2}}$$

$$\times \int \prod_{i=1}^L \prod_{j=1}^M ds_{ij} \frac{\left[ |\mathbb{G}(k_1, \dots, k_L, p_1, \dots, p_E)| \right]^{\frac{d-M-1}{2}}}{D_1^{\nu_1} \dots D_n^{\nu_n}} \quad (2.41)$$

Now change integration variables from  $s_{ij}$  to  $x_a = D_a$  (baikov variables). Because of (2.15), the Jacobian of this transformation will be  $\det(A_{ij}^a)$ , which leads to the Baikov representation of Feynman Integrals:

$$G(\nu_1, \dots, \nu_n) = C_n^L \left[ |\mathbb{G}(p_1, \dots, p_E)| \right]^{\frac{-d+E+1}{2}} \times \int \frac{dx_1 \dots dx_n}{x_1^{a_1} \dots x_n^{\nu_n}} \left[ \mathcal{P}_n^L(x_1 - f_1, \dots, x_n - f_n) \right]^{\frac{d-M-1}{2}} \quad (2.42)$$

with

$$C_n^L = \frac{\pi^{-\frac{L(L-1)}{4} - \frac{LE}{2}} \det(A_{ij}^a)}{\prod_{i=1}^L \Gamma\left(\frac{d-M+i}{2}\right)} \quad (2.43)$$

and

$$\mathcal{P}_n^L(x_1 - f_1, \dots, x_n - f_n) = |\mathbb{G}(k_1, \dots, k_L, p_1, \dots, p_E)| \quad (2.44)$$

is the Baikov polynomial. Notice that in the rhs of (2.44) we impose (2.15) and we take  $s_{ij} = s_{ji}$ . The integration region is defined so that

$$\mathcal{P}_n^L(x_1 - f_1, \dots, x_n - f_n) \geq 0 \quad (2.45)$$

which practically means that the Baikov polynomial vanishes at the boundaries.

# Chapter 3

## Analytical calculation of master integrals

In principle one can use the parametric representation of a MI and proceed to perform all the necessary integrations analytically. However, as the number of loops and kinematic scales of the MI increases, so does their mathematical complexity. In the last decade the established method to obtain analytical results for MI is the method of *Differential Equations* (DE) [34]–[37]. In this chapter we will give an introduction to this method, focusing on a variant called *Simplified Differential Equations approach* (SDE) [38]. We will also build a computational framework that will allow us to obtain in a systematic way analytical results for the integral families that will be considered in the second part of this thesis. Dedicated reviews on the method of differential equations can be found in [39], [40].

### 3.1 Differential equations for master integrals

The basic idea of the method of DE is to have a basis of MI, obtained after IBP reduction of a given family of FI, and then taking derivatives of each MI with respect to kinematic invariants and/or masses. The result of the differentiation is given in terms of FI of the same integral family. Then one applies IBP reduction again, thus relating the derivatives of MI to MI of the same integral family. This procedure leads to a system of linear differential equations for the MI which can be solved when appropriate boundary terms are provided.

More specifically, consider an integral family  $F(\vec{v})$  and its basis of MI, which we will denote as  $\mathbf{G}(\vec{v})$ . The dependence on the kinematics is given by invariants formed by external momenta such as  $p_i^2$ ,  $(p_i + p_j)^2 = s_{ij}$ , and masses. To obtain DE with respect to these invariants, one can use the following formulas [41],

$$\frac{\partial}{\partial(p_i \cdot p_j)} \mathbf{G}(\vec{v}) = \sum [\mathbb{G}^{-1}]_{kj} p_k \cdot \partial_{p_i} \mathbf{G}(\vec{v}) \quad (3.1)$$

$$\frac{\partial}{\partial(p_i^2)} \mathbf{G}(\vec{v}) = \frac{1}{2} \sum [\mathbb{G}^{-1}]_{ki} p_k \cdot \partial_{p_i} \mathbf{G}(\vec{v}) \quad (3.2)$$

where  $\mathbb{G} = \{p_i \cdot p_j\}$  is a Gram matrix. After IBP reduction the right-hand side is expressed in terms of MI. The resulting system of DE can be written in the following form,

$$\frac{\partial}{\partial s_{ij}} \mathbf{G} = \mathbf{A}(\epsilon, \{s_{ij}\}) \mathbf{G} \quad (3.3)$$

In general, the matrix  $\mathbf{A}$  can be very complicated. In 2013 a remarkable observation was made [42] that has since revolutionised the field of multiloop calculations. The main idea is that one can look for a set of MI that can be expressed in terms of functions that exhibit certain special properties upon differentiation.

In order to properly discuss these function we must introduce the concept of the *degree of transcendentality*  $\mathcal{T}(f)$  of a function  $f$  [42].  $\mathcal{T}(f)$  is defined as the number of iterated integrals needed to define the function  $f$ , e.g.  $\mathcal{T}(\log) = 1, \mathcal{T}(Li_n) = n$ , where  $Li_n$  is the classical polylogarithm, defined as

$$Li_n(x) = \int_0^x \frac{Li_{n-1}(t)}{t} dt \quad (3.4)$$

Further properties of transcendental functions are

$$\mathcal{T}(f_1 \cdot f_2) = \mathcal{T}(f_1) + \mathcal{T}(f_2) \quad (3.5)$$

$$\mathcal{T}(\zeta(n)) = \mathcal{T}(\pi^n) = n \quad (3.6)$$

$$\mathcal{T}(r) = 0, \text{ for rational } r \quad (3.7)$$

The MI which will be of interest to us will be expressed in terms of uniformly transcendental (UT) functions. A function  $f$  which is expressed as a sum of terms is called UT when all summands have the same degree of transcendentality. Finally, we will call a function *pure*, if its degree of transcendentality is lowered by taking a derivative, i.e.  $\mathcal{T}(df) = \mathcal{T}(f) - 1$ . This last property implies that the coefficient of a pure function cannot be anything more than a rational number, otherwise upon differentiation it would contribute additional terms which would have greater degree of transcendentality than the remaining terms.

MI whose leading singularity is constant tend to be pure and UT [43]. Later we will have more to say about how to go looking for such special MI, but for now let us assume that we have such a basis. Their DE will be of *dlog* form, meaning that the integrand will be written as a logarithmic differential form. What this practically means is that if we start with a basis  $\mathbf{G}$  of MI and based in them, start looking for a *good* basis of MI,  $\mathbf{g}$ , we are essentially looking for a transformation matrix  $\mathbf{T}$ , which will take us from basis  $\mathbf{G}$  to basis  $\mathbf{g}$ .

$$\mathbf{g} = \mathbf{T}\mathbf{G} \quad (3.8)$$

Assuming now that basis  $\mathbf{G}$  satisfies the DE (3.3), the new basis  $\mathbf{g}$  will satisfy the DE

$$d\mathbf{g} = \epsilon \sum_a \mathbf{B}_a d \log(W_a(s_{ij})) \quad \mathbf{g} = \epsilon \tilde{\mathbf{B}} \quad (3.9)$$

This is the celebrated *dlog* form of the DE. The functions  $W_a$  are called *letters* and they form the *alphabet* associated with the DE. The DE in (3.9) is also known as a *canonical* DE and the basis  $\mathbf{g}$  that satisfies it is known as a *canonical or pure basis* of MI.

The matrices  $\mathbf{A}$ ,  $\tilde{\mathbf{B}}$  in (3.3) and (3.9) respectively, are connected through the transformation matrix  $\mathbf{T}$  from (3.8) in the following way,

$$\begin{aligned} \partial_{s_{ij}} \mathbf{g} &= \partial_{s_{ij}} (\mathbf{T}\mathbf{G}) = \partial_{s_{ij}} (\mathbf{T})\mathbf{G} + \mathbf{T}\mathbf{A}\mathbf{G} \\ &= \partial_{s_{ij}} (\mathbf{T})\mathbf{T}^{-1}\mathbf{g} + \mathbf{T}\mathbf{A}\mathbf{T}^{-1}\mathbf{g} \\ &= [\partial_{s_{ij}} (\mathbf{T})\mathbf{T}^{-1} + \mathbf{T}\mathbf{A}\mathbf{T}^{-1}]\mathbf{g} \\ &= \tilde{\mathbf{B}}\mathbf{g} \end{aligned} \quad (3.10)$$

Notice the difference in the structure of  $\mathbf{A}$ ,  $\tilde{\mathbf{B}}$  when comparing (3.3) and (3.9). First of all, the  $\epsilon$ -dependence is fully factorised in the canonical DE. Next, all kinematic dependence is included in the functions  $W_a$ , the letters of the alphabet, leaving the matrices  $\mathbf{B}_a$ , known as *residue matrices*. to consist solely of rational numbers.

In this canonical form, the system of DE can be iterated order by order in  $\epsilon$ , with suitably chosen boundary conditions. If this a canonical DE can be reached using only rational transformations, then the letters are of the form  $W_a = \chi - \chi_a$ , where  $\chi$  can be any of the kinematic variables and  $\chi_a$  are the locations of the singularities in the kinematic invariants.

In general the letters can also be algebraic functions of the kinematic invariants, e.g. they can include square roots. This complicates significantly their analytic integration, although several methods have been developed to deal with this issue. The mathematical structure of the set of letters, i.e. the alphabet, characterises the function class the solution can belong to. If the alphabet can be written in terms of rational functions, one can write the solution of the canonical DE in terms of a special class of functions known as *Multiple or Goncharov polylogarithms* (GPLs) [44]–[47]. These functions will play a major role in the results presented in the second part of this thesis, therefore the following section is devoted to their introduction and review of several of their important properties.

## 3.2 Special functions

GPLs appear in the results of many calculations in perturbative Quantum Field Theory. More specifically, they have been known to form part of the space of functions that arise in the solution of several FI. In this section we will show that GPLs are generalisations of the logarithm and the classical polylogarithm (3.4) and we will review several of their properties which will be of use in the calculations presented in the the second part of this thesis.

### 3.2.1 Definitions

Like classical polylogarithms, GPLs can be defined recursively for  $n \geq 0$  via the iterated integral

$$\mathcal{G}(a_1, \dots, a_n; z) = \int_0^z \frac{dt}{t - a_1} \mathcal{G}(a_2, \dots, a_n; z) \quad (3.11)$$

with  $\mathcal{G}(z) = \mathcal{G}(\cdot; z) = 1$ ,  $a_i \in \mathbb{C}$  are constants and  $z$  is a complex variable. In the special case where all  $a_i$ 's are zero, we define

$$\mathcal{G}(\vec{0}_n; z) = \frac{1}{n!} \log^n(z) \quad (3.12)$$

The vector  $\vec{a}_n = (a_1, \dots, a_n)$  is called the vector of singularities of the GPL and the number of elements  $n$  is called the weight of the GPL. Working in dimensional regularisation, we will need to obtain results in terms of GPLs up to weight  $2l$  for an  $l$ -loop amplitude. In general, it is not known if GPLs are transcendental, but we will assume that they are.

The definitions (3.11) and (3.12) show that GPLs contain the ordinary logarithm and the classical polylogarithm as special cases,

$$\mathcal{G}(\vec{a}_n; z) = \frac{1}{n!} \log^n \left( 1 - \frac{z}{a} \right) \quad (3.13)$$

$$\mathcal{G}(\vec{0}_{n-1}, 1; z) = -Li_n(z) \quad (3.14)$$

GPLs are part of the more general family of iterated integrals. The notation used in the mathematics literature is slightly different than the one used by physicists. In mathematics an iterated integral is defined as,

$$\mathcal{I}(a_0; a_1, \dots, a_n; a_{n+1}) = \int_{a_0}^{a_{n+1}} \frac{dt}{t - a_n} \mathcal{I}(a_0; a_1, \dots, a_{n-1}; t) \quad (3.15)$$

and  $\mathcal{I}(a_0; a_1) = 1$ . The functions defined in (3.11) and those of (3.15) are related by

$$\mathcal{G}(a_n, \dots, a_1; a_{n+1}) = \mathcal{I}(0; a_1, \dots, a_n; a_{n+1}) \quad (3.16)$$

Notice however the reversal of the arguments in the vector of singularities on the GPL.



### 3.2.2 Basic properties

From the integral representation (3.11) of GPLs, we can see that  $\mathcal{G}(a_1, \dots, a_n; z)$  is divergent whenever  $z = a_1$ . Similarly  $\mathcal{G}(a_1, \dots, a_n; z)$  is analytic at  $z = 0$  whenever  $a_n \neq 0$ .

If we consider the  $a_i$ 's to be constant, then the GPLs have branch cuts in the complex  $z$  plane at most extending from  $z = a_i$  to  $z = \infty$ . If the  $a_i$ 's are allowed to vary, the branch cut structure becomes much more complicated. Some specific examples are the following:

1.  $\mathcal{G}(\vec{a}_n; z) = \frac{1}{n!} \log^n \left(1 - \frac{z}{a}\right)$  has a simple branch cut in the complex  $z$  plane, extending from  $z = a$  to  $z = \infty$ .
2.  $\mathcal{G}(0, 1; z) = -Li_2(z)$  has a branch cut extending in the complex  $z$  plane from  $z = 1$  to  $z = \infty$ . The branch cut starting at  $z = 0$  is absent in this case.

If the rightmost index  $a_n$  of  $\vec{a}$  is non-zero, then the function  $\mathcal{G}(\vec{a}; z)$  is invariant under a rescaling of all its arguments, i.e. for any  $k \in \mathbb{C}^*$  we have

$$\mathcal{G}(k\vec{a}; kz) = \mathcal{G}(\vec{a}; z), \quad a_n \neq 0 \quad (3.17)$$

GPLs also satisfy the Hölder convolution, i.e. whenever  $a_1 \neq 1$  and  $a_n \neq 0$ , we have,  $\forall p \in \mathbb{C}^*$

$$\begin{aligned} \mathcal{G}(a_1, \dots, a_n; 1) &= \sum_{k=0}^n (-1)^k \mathcal{G}(1 - a_k, \dots, 1 - a_1; 1 - 1/p) \\ &\quad \times \mathcal{G}(a_{k+1}, \dots, a_n; 1/p) \end{aligned} \quad (3.18)$$

In the limiting case where  $p \rightarrow \infty$ , this identity becomes

$$\mathcal{G}(a_1, \dots, a_n; 1) = (-1)^n \mathcal{G}(1 - a_n, \dots, 1 - a_1; 1) \quad (3.19)$$

Relations of the above kind are called functional equations.

### 3.2.3 The shuffle algebra

An important property of all iterated integrals thus of GPLs too, is that the product of two GPLs defined with the same integration limits can be written as a linear combination of GPLs. We may generalise this and see that the product of GPLs with weights  $n_1$  and  $n_2$  can always be written as a sum of GPLs with weight  $n_1 + n_2$ ,

$$\mathcal{G}(a_1, \dots, a_{n_1}; z) \mathcal{G}(a_{n_1+1}, \dots, a_{n_1+n_2}; z) = \sum_{\sigma \in \Sigma(n_1, n_2)} \mathcal{G}(a_{\sigma(1)}, \dots, a_{\sigma(n_1+n_2)}; z) \quad (3.20)$$

where  $\Sigma(n_1, n_2)$  denotes the set of all shuffles of  $n_1 + n_2$  elements. This property turns the set of all GPLs into a *shuffle algebra*, i.e. a vector space equipped with the shuffle multiplication. The shuffle product preserves the weight of the GPLs and in this case the algebra is graded.

If  $a_n = 0$  in  $\mathcal{G}(a_1, \dots, a_n; z)$  we may use the shuffle algebra to rewrite  $\mathcal{G}(a_1, \dots, a_n; z)$  in terms of functions whose rightmost index of the vector of singularities is non-zero. E.g., for  $a \neq 0$

$$\begin{aligned} \mathcal{G}(a, 0, 0; z) &= \mathcal{G}(a; z) \mathcal{G}(0, 0; z) - \mathcal{G}(0, a, 0; z) - \mathcal{G}(0, 0, a; z) \\ &= \mathcal{G}(0, 0; z) \mathcal{G}(a; z) - \mathcal{G}(0, 0, a; z) - [\mathcal{G}(0, a; z) \mathcal{G}(0; z) - 2\mathcal{G}(0, 0, a; z)] \\ &= \mathcal{G}(0, 0; z) \mathcal{G}(a; z) + \mathcal{G}(0, 0, a; z) - \mathcal{G}(0, a; z) \mathcal{G}(0; z) \end{aligned} \quad (3.21)$$

### 3.3 Simplified differential equations approach

In this section we will introduce a variant of the DE method, known as the *Simplified Differential Equations approach* (SDE). The SDE approach [38] is an attempt to simplify and systemize, as much as possible, the derivation of the appropriate system of DE satisfied by the MI.

Any 1-loop integral can be written in the following form

$$G_{a_1, \dots, a_n}(\{p_j\}, \epsilon) = \int \left( \prod_{r=1}^l \frac{d^d k_r}{i\pi^{d/2}} \right) \frac{1}{D_1^{a_1} \dots D_n^{a_n}}, \quad D_i = (c_{ij}k_j + d_{ij}p_j)^2, \quad d = 4 - 2\epsilon \quad (3.22)$$

with matrices  $\{c_{ij}\}$  and  $\{d_{ij}\}$  determined by the topology and the momentum flow of the graph, and the denominators are defined in such a way that all scalar product invariants can be written as a linear combination of them. The exponents  $a_i$  are integers and may be negative in order to accommodate irreducible numerators. Through the use of (IBP) identities, any integral of the above form can be written as a linear combination of a finite subset of MI, with coefficients depending on the independent scalar products,  $s_{ij} = p_i \cdot p_j$ , and space-time dimension  $d$ .

In the SDE approach the external incoming momenta are parametrized linearly in terms of  $x$  as  $p_i(x) = p_i + (1-x)q_i$ , where the  $q_i$ 's are a linear combination of the momenta  $\{p_i\}$  such that  $\sum_i q_i = 0$ . If  $p_i^2 = 0$ , the parameter  $x$  captures the off-shell-ness of the external leg. The FI are now dependent on  $x$  through the external momenta:

$$G_{a_1, \dots, a_n}(\{s_{ij}\}, \epsilon; x) = \int \left( \prod_{r=1}^l \frac{d^d k_r}{i\pi^{d/2}} \right) \frac{1}{D_1^{a_1} \dots D_n^{a_n}}, \quad D_i = (c_{ij}k_j + d_{ij}p_j(x))^2 \quad (3.23)$$

By introducing the dimensionless parameter  $x$ , the array of MI,  $\mathbf{G}(\{s_{ij}\}, \epsilon; x)$ , which now depends on  $x$ , satisfies

$$\frac{\partial}{\partial x} \mathbf{G}(\{s_{ij}\}, \epsilon; x) = \mathbf{M}(\{s_{ij}\}, \epsilon; x) \mathbf{G}(\{s_{ij}\}, \epsilon; x) \quad (3.24)$$

a system of differential equations in one independent variable, where  $\mathbf{M}$  is a matrix whose elements are rational functions of the kinematics  $\{s_{ij} \equiv p_i \cdot p_j\}$ , of  $x$  and of  $\epsilon$ . The expected benefit of this approach is that the integration of the DE naturally captures the expressibility of MI in terms of GPLs and more importantly make the problem *independent of the number of kinematic scales* (independent invariants) involved. Note that as  $x \rightarrow 1$ , the original configuration of the loop integrals (3.22) is reproduced, which corresponds to a simpler one with one scale less.

The form (3.24) is such that MI with  $m$  denominators only depend on MI with at most  $m$  denominators. This structure of the DE makes it possible to first solve the MI with  $m_0 + 1$  denominators, then those with  $m_0 + 2$  denominators and so forth. In other words, in practice the DE may be solved in a *bottom - up* approach.

Let's consider the DE for a single MI. Assume that all MI with  $m' \leq m$  denominators are known and already expressed in the desired form, the meaning of which will become clear below. The DE of MI with  $m + 1$  denominators can be written schematically in the form:

$$\partial_x G_{m+1} = H(\{s_{ij}\}, \epsilon; x) G_{m+1} + \sum_{m' \geq m_0}^m R(\{s_{ij}\}, \epsilon; x) G_{m'} \quad (3.25)$$

i.e. the sum of a homogeneous and an inhomogeneous term. The functions  $H$  and  $R$  are rational functions of their arguments. Equation (3.25) can be solved with the variation of constants method by introducing the integrating factor  $S(\{s_{ij}\}, \epsilon; x)$ , which satisfies the differential equation  $\partial_x S = -SH$  (dropping the arguments of the functions for brevity):

$$\partial_x(SG_{m+1}) = S \sum_{m' \geq m_0}^m R(\{s_{ij}\}, \epsilon; x) G_{m'} \quad (3.26)$$

Equation (3.26) could now be straightforwardly expanded in  $\epsilon$  and integrated, provided that the right-hand side is free of singularities at  $x \rightarrow 0$ . If any such singularities are present, we need to determine the resummed part of the solution in this limit.

The right-hand side of (3.26) can be rewritten schematically as a sum of a *singular* and a *regular* term at  $x = 0$ :

$$S \sum_{m' \geq m_0}^m R(\{s_{ij}\}, \epsilon; x) G_{m'} = \sum_i x^{-1+\beta_i \epsilon} \tilde{I}_{sin}^{(i)}(\{s_{ij}\}, \epsilon) + \tilde{I}_{reg}(\{s_{ij}\}, \epsilon, x) \quad (3.27)$$

with  $\beta_i$  being typically rational numbers. The singular term is integrated exactly and the solution of (3.26) becomes:

$$SG_{m+1} = C(\{s_{ij}\}, \epsilon) + \sum_i \frac{x^{\beta_i \epsilon}}{\beta_i \epsilon} \tilde{I}_{sin}^{(i)}(\{s_{ij}\}, \epsilon) + \int_0^x dx' \tilde{I}_{reg}(\{s_{ij}\}, \epsilon, x') \quad (3.28)$$

where the first term  $C(\{s_{ij}\}, \epsilon)$  is a constant in  $x$  but may be dependent on the kinematical invariants. The rightmost term in (3.28) is safely expanded in  $\epsilon$  and expressed in terms of GPLs. To this end, the integrating factors  $S$  in (3.26) should be rational functions of  $x$  in the limit  $\epsilon \rightarrow 0$ . This is a *sufficient condition* for the chosen  $x$ -parametrization to result in a differential equation solvable in terms of GPLs.

An important feature of the SDE approach is that in many cases the *boundary terms* are naturally captured by the integrated singularities in the DE (3.28) themselves at  $x = 0$ , which is precisely the lower integration boundary of the GPLs. Simply put the integrated singular terms in (3.28) correctly describe the behaviour of  $SG_{m+1}$  as  $x \rightarrow 0$  and thus the constant  $C(\{s_{ij}\}, \epsilon)$  vanishes. Due to this fact, the SDE approach is well suited for directly and efficiently expressing the MI in terms of GPLs without the need for an independent evaluation of the MI at the boundary  $x = 0$ .

For the original MI  $G_{m+1}$ , the resummed part is defined as follows:

$$G_{m+1, res} = \frac{1}{S} \sum_i \frac{x^{\beta_i \epsilon}}{\beta_i \epsilon} \tilde{I}_{sin}^{(i)}(\{s_{ij}\}, \epsilon) \quad (3.29)$$

The integrand of the remaining integral in (3.28) is regular at the boundary  $x = 0$ . After expanding in  $\epsilon$  and performing partial fraction decomposition in  $x$ , the integral is directly expressible in terms of GPLs. Note that the integration boundary in (3.28) was chosen to be  $x = 0$  precisely in order to directly express the integrals in terms of GPLs. If another boundary point  $x = x_0$  is chosen, the integrals in (3.28) result in slightly more complicated expressions made of differences of GPLs. The SDE approach therefore directly expresses the MI in terms of a well defined functional basis of GPLs, *independently of the number of kinematic scales involved*.

When the DE are coupled, the homogeneous factor  $\mathbf{H}$  is a *matrix* and  $\mathbf{G}_{m+1}$  is a *vector* in (3.25). For all cases considered so far, proceeding in the same way as in the uncoupled case, the diagonal elements are used to determine the integrating factor matrix, namely the diagonal matrix  $\mathbf{S}_D$  satisfying  $\partial_x \mathbf{S}_D = -\mathbf{S}_D \mathbf{H}_D$ , where  $\mathbf{H}_D$  is the diagonal part of  $\mathbf{H}$ .

The homogeneous matrix  $\tilde{\mathbf{H}} \equiv \mathbf{S}_D (\mathbf{H} - \mathbf{H}_D) \mathbf{S}_D^{-1}$  of the reduced system of DE is then *strictly triangular matrix* at order  $\epsilon^0$  and the system becomes effectively uncoupled, and may be easily integrated order by order in  $\epsilon$ . Furthermore, singularities at  $x = 0$  in the inhomogeneous terms

are integrated to determine the re-summed part of the solutions in exactly the same way as in the uncoupled DE case.

In order to illustrate the above procedure for couples DE, let us consider the following example. Let us assume that we have a system of two coupled DE for the vector  $\mathbf{G}_{m+i} = (G_{m+1}, G_{m+2})$ ,

$$\partial_x \mathbf{G}_{m+i} = \mathbf{H}(\{s_{ij}\}, \epsilon; x) \mathbf{G}_{m+i} + \sum_{m' \geq m_0}^m R(\{s_{ij}\}, \epsilon; x) G_{m'}$$

with the matrix  $\mathbf{H}$  being  $\mathbf{H} = \mathbf{H}_D + \mathbf{H}_{ND}$ , where  $\mathbf{H}_D$  and  $\mathbf{H}_{ND}$  are its diagonal and non-diagonal parts respectively. The integrating factor  $\mathbf{S}_D$  is defined through  $\mathbf{H}_D$  as follows

$$\partial_x \mathbf{S}_D = -\mathbf{S}_D \mathbf{H}_D$$

Introducing  $\mathbf{S}_D$  in the DE results to

$$\begin{aligned} \partial_x (\mathbf{S}_D \mathbf{G}_{m+i}) &= \partial_x (\mathbf{S}_D) \mathbf{G}_{m+i} + \mathbf{S}_D (\partial_x \mathbf{G}_{m+i}) \\ &= -\mathbf{S}_D \mathbf{H}_D \mathbf{G}_{m+i} + \mathbf{S}_D (\mathbf{H} \mathbf{G}_{m+i} + \sum_{m' \geq m_0}^m R G_{m'}) \\ &= -\mathbf{S}_D \mathbf{H}_D \mathbf{G}_{m+i} + \mathbf{S}_D \mathbf{H} \mathbf{G}_{m+i} + \mathbf{S}_D \sum_{m' \geq m_0}^m R G_{m'} \\ &= \mathbf{S}_D (\mathbf{H} - \mathbf{H}_D) \mathbf{G}_{m+i} + \mathbf{S}_D \sum_{m' \geq m_0}^m R G_{m'} \\ &= \left[ \mathbf{S}_D (\mathbf{H} - \mathbf{H}_D) \mathbf{S}_D^{-1} \right] (\mathbf{S}_D \mathbf{G}_{m+i}) + \mathbf{S}_D \sum_{m' \geq m_0}^m R G_{m'} \\ &= \tilde{\mathbf{H}} (\mathbf{S}_D \mathbf{G}_{m+i}) + \mathbf{S}_D \sum_{m' \geq m_0}^m R G_{m'} \end{aligned}$$

as expected from the above discussion.

### 3.4 Expansion by regions

The main method for obtaining boundary terms for the solution of DE that we will use is that of expansion by regions [48]–[51]. Here we give a brief description of the method, which can be used in its own right to compute Feynman integrals.

FI can be considered as functions depending on kinematic invariants and masses. If these variables differ in scale, then one can expand a FI in ratios of large and small parameters. As a result, the integral is written as a series of simpler quantities than the original integral itself and it can be substituted by a sufficiently large number of terms of such an expansion. This is the essence of the method known as expansion by regions.

In the momentum representation of loop integrals the main steps of this method are:

1. Divide the space of the loop momenta into various regions and, in every region, expand the integrand in a Taylor series with respect to the parameters that are considered small there.
2. Integrate the integrand, expanded in the appropriate way in every region, over the whole integration domain of the loop momenta.

3. Set to zero any scaleless integral.

A geometric approach of this method was first introduced in [52]. In general it is more convenient to reveal all relevant regions and construct an algorithmic approach when one applies expansion by regions to the Feynman parameter representation (2.11) of a FI. Public implementations are available in [51], [53].

## 3.5 Computational framework

So far we have introduced the method of DE for the analytic computation of MI. In addition we saw that by using a pure basis of MI we can obtain a canonical DE whose form allows for a straightforward solution in terms of GPLs, a special class of iterated integrals, in the case where the alphabet of the canonical DE can be written in terms of rational functions of the kinematic invariants. We have also introduced the SDE approach which greatly simplifies the derivation of the DE satisfied by the chosen basis of MI. Also we saw that the method of expansion by regions can be utilised to provide boundary terms for the SDE approach in a straightforward manner.

In this section we will combine all the ideas and methods mentioned above and formulate a framework which will allow us to solve several multiscale-multiloop integral families, the results of which are presented in the second part of this thesis.

### 3.5.1 Simplified differential equations in canonical form

We will start with the assumption that we already have obtained a pure basis of MI. Then we proceed by introducing an  $x$ -parametrization and using the SDE approach we derive a canonical DE with respect to  $x$ . In the case where all letters of the alphabet are rational in  $x$  the canonical DE will be of the form

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{i=1}^{l_{max}} \frac{\mathbf{M}_i}{x - l_i} \right) \mathbf{g} \quad (3.30)$$

where  $\mathbf{g}$  is the pure basis,  $\mathbf{M}_i$  are the residue matrices corresponding to each letter  $l_i$  and  $l_{max}$  is the length of the alphabet. Notice here that we follow a definition for the letters which is different than the standard notation. As we saw previously, the  $d \log$  form of a system of canonical DE is given as

$$d\mathbf{g} = \epsilon \sum_a \mathbf{B}_a d \log (W_a(s_{ij})) \mathbf{g} = \epsilon \tilde{\mathbf{B}} \mathbf{g}$$

where the letters  $W_a(s_{ij})$  are rational or algebraic functions of the independent kinematic variables. The standard  $d \log$  form is equivalent to (3.30) for  $W_a = x - l_a$ . The kinematic dependence is entirely contained within the letters  $l_i$ , leaving the residue matrices  $\mathbf{M}_i$  to be solely constructed by rational numbers.

### 3.5.2 Boundary terms

In order to solve (3.30) we need to provide boundary terms. As discussed earlier, in the SDE approach we choose as boundary terms the asymptotic behaviour of the MI as  $x \rightarrow 0$  in order to obtain a straightforward representation of the solution in terms of GPLs. Since we are using a pure basis of MI, we need to obtain the  $x \rightarrow 0$  limit of each basis element.

To do so, we first exploit the canonical DE, which in the limit  $x \rightarrow 0$  takes the form

$$\partial_x \mathbf{g} = \epsilon \frac{1}{x} \mathbf{M}_1 \mathbf{g}_0 + \mathcal{O}(x^0) \quad (3.31)$$

where  $\mathbf{M}_1$  is the residue matrix for the letter  $l_1 = 0$ . The solution of (3.31) is of the form

$$\mathbf{g}_0 = \mathbf{S} e^{\mathbf{D} \log(x)} \mathbf{S}^{-1} \mathbf{b} \quad (3.32)$$

where the matrices  $\mathbf{S}$ ,  $\mathbf{D}$  are obtained through the Jordan decomposition of  $\mathbf{M}_1$ ,

$$\mathbf{M}_1 = \mathbf{S} \mathbf{D} \mathbf{S}^{-1} \quad (3.33)$$

and  $\mathbf{b} = \sum_{i=0}^k \epsilon^i b_0^{(i)}$  are the boundary constants we need to compute. With this information at hand, we define the *resummation* matrix  $\mathbf{R}$  as follows

$$\mathbf{R} = \mathbf{S} e^{\epsilon \mathbf{D} \log(x)} \mathbf{S}^{-1}. \quad (3.34)$$

The naming *resummation* matrix for  $\mathbf{R}$  comes from the fact that when acting on  $\mathbf{b}$ , it should correctly describe the  $\log(x)$  dependence of each basis element.

On the other hand, through IBP reduction, the elements of the canonical basis can be related to a set of FI  $\mathbf{G}$ ,

$$\mathbf{g} = \mathbf{T} \mathbf{G}. \quad (3.35)$$

Furthermore using the expansion by regions method as implemented in the `asy` code which is shipped along with `FIESTA4`, we can obtain information for the asymptotic behaviour of the Feynman integrals in terms of which we express the pure basis of Master integrals (3.35) in the limit  $x \rightarrow 0$ ,

$$G_i \Big|_{x \rightarrow 0} = \sum_j x^{b_j + a_j \epsilon} G_i^{(b_j + a_j \epsilon)} \quad (3.36)$$

where  $a_j$  and  $b_j$  are integers and  $G_i$  are the individual members of the basis  $\mathbf{G}$  of Feynman integrals in (3.35). Combining equations (3.32) and (3.35) yields

$$\mathbf{R} \mathbf{b} = \lim_{x \rightarrow 0} \mathbf{T} \mathbf{G} \Big|_{\mathcal{O}(x^{0+a_j \epsilon})} \quad (3.37)$$

where the right-hand side implies that, apart from the terms  $x^{a_i \epsilon}$  coming from (3.36), we expand around  $x = 0$ , keeping only terms of order  $x^0$ . Equation (3.37) allows us to determine all boundary constants  $\mathbf{b}$ .

More specifically, in the case where  $\mathbf{D}$  in (3.33) is non-diagonal, we will get logarithmic terms in  $x$  on the left-hand side of (3.37), in the form  $x^{a_j \epsilon} \log(x)$ . Since no such terms appear on the right-hand side of (3.37), a set of linear relations between elements of the array  $\mathbf{b}$  are obtained by setting the coefficient of  $x^{a_j \epsilon} \log(x)$  terms to zero. Furthermore, powers of  $x^{a_j \epsilon}$  that appear only on the left-hand side can also yield linear relations among elements of  $\mathbf{b}$ , by setting their coefficients to zero. We shall call these two sets of relations *pure*, since they are linear relations among elements of  $\mathbf{b}$  with rational numbers as coefficients. These pure relations account for the determination of a significant part of the two components of the boundary array. Finally for the undetermined elements of  $\mathbf{b}$ , several regions usually need to be calculated coming from (3.36), although as we will see later, in certain cases the pure relations can be enough to determine all boundary constants. The  $b_0^{(i)}$  terms, with  $i$  indicating the corresponding weight, consist of Zeta functions  $\zeta(i)$ , logarithms and GPLs of weight  $i$  which have as arguments rational functions of the underline kinematic variables but not of  $x$ .

The above described method is general and straightforward to apply in all cases where a pure basis is obtained. In practice however, one usually exploits known results for integral sectors which have already been computed before and are available in the literature. The solution of (3.30) after determining all boundary terms can be written up to weight four in the following compact form,

$$\mathbf{g} = \epsilon^0 \mathbf{b}_0^{(0)} + \epsilon \left( \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(0)} + \mathbf{b}_0^{(1)} \right)$$

$$\begin{aligned}
& + \epsilon^2 \left( \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(0)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(1)} + \mathbf{b}_0^{(2)} \right) \\
& + \epsilon^3 \left( \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(1)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(2)} + \mathbf{b}_0^{(3)} \right) \\
& + \epsilon^4 \left( \sum \mathcal{G}_{abcd} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{M}_d \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(1)} \right. \\
& \left. + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(2)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(3)} + \mathbf{b}_0^{(4)} \right) \tag{3.38}
\end{aligned}$$

were  $\mathcal{G}_{ab\dots} := \mathcal{G}(l_a, l_b, \dots; x)$  represent the GPLs. Our results are presented in such a way that each coefficient of  $\epsilon^k$  has transcendental weight  $k$ . If we assign weight  $-1$  to  $\epsilon$ , then (3.38) has uniform weight zero. Extending this solution to higher weights is trivial, assuming one has obtained the relevant boundary terms up to the desired weight.

### 3.5.3 Scale reduction

As it was noted previously, the introduction of the  $x$ -parameterisation effectively captures the off-shellness of one external particle. By taking the limit  $x \rightarrow 1$  we can obtain the solution to a family of FI with one scale less.

Assuming that we have an integral family with  $m$  external massive particles whose solution we have expressed in the form of (3.38), we can obtain the solution for a family with  $m - 1$  external masses through the  $x \rightarrow 1$  limit of the former.

Firstly, we will exploit the shuffle properties of GPLs to write solution (3.38) as an expansion in terms of  $\log(1 - x)$  as follows

$$\mathbf{g} = \sum_{n \geq 0} \epsilon^n \sum_{i=0}^n \frac{1}{i!} \mathbf{c}_i^{(n)} \log^i(1 - x) \tag{3.39}$$

with all  $\mathbf{c}_i^{(n)}$  being finite in the limit  $x \rightarrow 1$ . The next step is to define the regular part of (3.39) at  $x = 1$

$$\mathbf{g}_{reg} = \sum_{n \geq 0} \epsilon^n \mathbf{c}_0^{(n)} \tag{3.40}$$

and after setting  $x = 1$  explicitly in (3.40) we may define the truncated part of (3.39),

$$\mathbf{g}_{trunc} = \mathbf{g}_{reg}(x = 1) \tag{3.41}$$

Having done that, we utilise the residue matrix that corresponds to the letter  $\{1\}$ ,  $\mathbf{M}_2$ , and define the *resummation matrix*  $\tilde{\mathbf{R}}$  as follows

$$\tilde{\mathbf{R}} = \tilde{\mathbf{S}} e^{\epsilon \tilde{\mathbf{D}} \log(1-x)} \tilde{\mathbf{S}}^{-1} \tag{3.42}$$

were  $\tilde{\mathbf{S}}, \tilde{\mathbf{D}}$  are constructed through the Jordan decomposition of  $\mathbf{M}_2$ , i.e.  $\mathbf{M}_2 = \tilde{\mathbf{S}} \tilde{\mathbf{D}} \tilde{\mathbf{S}}^{-1}$ . The *resummation matrix*  $\tilde{\mathbf{R}}$  has terms of  $(1 - x)^{a_i \epsilon}$ , with  $a_i$  being the eigenvalues of  $\mathbf{M}_2$ . After setting all terms  $(1 - x)^{a_i \epsilon}$  equal to zero, we define the purely numerical matrix  $\tilde{\mathbf{R}}_0$ . Obtaining the  $x \rightarrow 1$  limit of (3.38) amounts to acting with  $\tilde{\mathbf{R}}_0$  on (3.41)

$$\mathbf{g}_{x \rightarrow 1} = \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc} \tag{3.43}$$

Up to now we have calculated the  $x \rightarrow 1$  limit of the basis of MI  $\mathbf{g}$  which fully characterises the integral family with  $m$  external massive legs. This special limit however should give us the solution for the integral family with  $m - 1$  external masses. In general when considering an

integral family with  $m - 1$  scales we anticipate that it will have fewer MI than the one with  $m$  scales. Therefore, if the integral family with  $m$  external masses, denoted as  $\mathbf{g}_m$ , has  $N_m$  MI, then  $\mathbf{g}_{m-1}$  is expected to have  $N_{m-1}$  MI, with  $N_m > N_{m-1}$ .

In order to determine which of the  $N_m$  integrals are the MI for the  $\mathbf{g}_{m-1}$  family, i.e. which of the  $N_m$  are linearly independent in the  $x \rightarrow 1$  limit, there are two ways to proceed:

1. Use IBP identities for the  $\mathbf{g}_{m-1}$  integral family.
2. Consider the properties of  $\tilde{\mathbf{R}}_0$  and study its action on the  $\mathbf{g}_m$  basis at its  $x \rightarrow 1$  limit.

Whereas an IBP reduction is a more straightforward path, it is interesting to study the  $\tilde{\mathbf{R}}_0$  matrix in more detail. It turns out that  $\tilde{\mathbf{R}}_0$  is an *idempotent* matrix. Idempotent matrices have the following properties, all of which are satisfied by  $\tilde{\mathbf{R}}_0$ :

1.  $\mathbf{X} = \mathbf{X}^2$
2. singular except the identity matrix  $\mathbf{I}$
3. eigenvalues of  $\mathbf{X} = 0, 1$
4.  $\text{Trace}(\mathbf{X}) = \text{Rank}(\mathbf{X})$
5.  $\mathbf{I} - \mathbf{X}$  also idempotent

Since  $\tilde{\mathbf{R}}_0 = \tilde{\mathbf{R}}_0^2$ , acting with  $\tilde{\mathbf{R}}_0$  on  $\mathbf{g}_{x \rightarrow 1}$  yields

$$\begin{aligned} \tilde{\mathbf{R}}_0 \mathbf{g}_{x \rightarrow 1} &= \tilde{\mathbf{R}}_0^2 \mathbf{g}_{trunc} \\ &= \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc} \\ &= \mathbf{g}_{x \rightarrow 1} \end{aligned} \tag{3.44}$$

This relation, solved as an equation for each row, produces relations that allow us to determine linearly independent basis elements for the  $\mathbf{g}_{m-1}$  family. It should be noted that the outcome of this method is influenced by the  $x$ -parametrization that one uses regarding the number of linearly independent integrals that one finds. So far we have used two different parametrizations in all published results, with one  $x$  and with two  $x$ 's<sup>1</sup>. Our results so far indicate that the choice of two  $x$ 's is the most optimal for the application of this method, since after defining the resummation matrix and obtaining its purely numerical form, (3.44) yields a number of linearly independent basis elements exactly equal to the number of MI of the problem with one scale less, i.e. we do not need to perform an IBP reduction to determine the new basis elements. This can also be seen by computing the rank of the numerical resummation matrix. Exploiting this fact drastically simplifies the process of extracting a canonical basis for the problem with one scale less, however it is still yet not clear why the two parametrizations yield so different results.

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<sup>1</sup>By one and two  $x$ 's we mean that in the first case, only one external momentum is parametrized as  $x p_i$ , whereas in the latter case we have two external momenta parametrized as  $x p_i$ .



# Chapter 4

## A pedagogical example: two-loop planar master integrals

In order to showcase the applicability of the computational framework developed in chapter 4 and clarify all arguments made there, we revisit the calculation of the planar family of two-loop MI with one off-shell leg. This integral family was solved two decades ago [54] and it was among the first results which exemplified the power of the DE method for multiloop calculations.

### 4.1 Canonical basis and DE

Our first task is to define the integral family which we will study. For the doublebox with one massive leg we will use the following configuration:

$$G_{a_1, \dots, a_9} = e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 + q_1)^{2a_2} (k_1 + q_{12})^{2a_3} (k_1 + q_{123})^{2a_4}} \times \frac{1}{k_2^{2a_5} (k_2 - q_1)^{2a_6} (k_2 - q_{12})^{2a_7} (k_2 - q_{123})^{2a_8} (k_1 + k_2)^{2a_9}} \quad (4.1)$$

with the kinematics being

$$S \equiv q_{12}^2, \quad T \equiv q_{23}^2, \quad m^2 \equiv q_2^2 \quad (4.2)$$

We use the abbreviations  $q_{ij} = q_i + q_j$  and  $q_{ijk} = q_i + q_j + q_k$  and similarly for  $p$  later. The top-sector diagram is shown in figure 4.1.

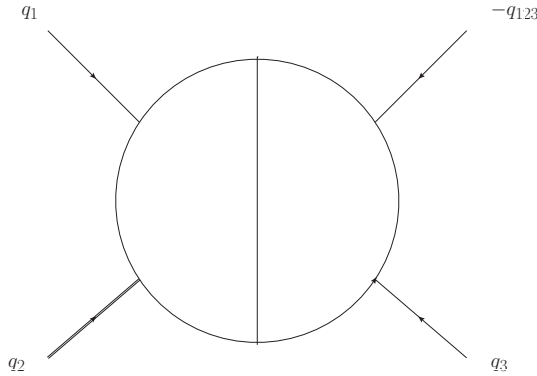


Figure 4.1: The doublebox graph with one massive leg. All momenta are taken to be incoming. The double line represents the massive particle.

We choose the following  $x$ -parametrisation for this family:

$$\begin{aligned} q_1 &= xp_1, & q_2 &= p_{12} - xp_1, & q_3 &= p_3, & q_4 &= -p_{123}, & p_i^2 &= 0, & \sum_i p_i &= 0, \\ s_{12} &\equiv p_{12}^2 = 2p_1p_2, & s_{23} &\equiv p_{23}^2 = 2p_2p_3, & S &= s_{12}, & T &= s_{23}x, & m^2 &= s_{12}(1-x) \end{aligned} \quad (4.3)$$

With this  $x$ -parametrisation the doublebox graph is depicted in figure 4.2 and (4.1) becomes

$$\begin{aligned} G_{a_1, \dots, a_9} &= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 + xp_1)^{2a_2} (k_1 + p_{12})^{2a_3} (k_1 + p_{123})^{2a_4}} \\ &\times \frac{1}{k_2^{2a_5} (k_2 - xp_1)^{2a_6} (k_2 - p_{12})^{2a_7} (k_2 - p_{123})^{2a_8} (k_1 + k_2)^{2a_9}} \end{aligned} \quad (4.4)$$

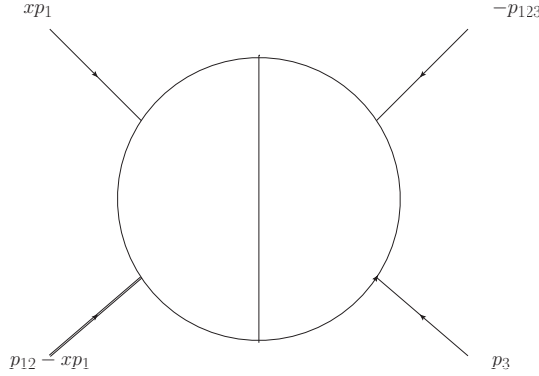


Figure 4.2: The doublebox graph with one massive leg in the SDE parametrisation.

Now that we have defined our integral family we use IBP identities, implemented in automated tools like KIRA and FIRE, to identify a pre-canonical basis  $\mathbf{G}$  of MI. Doing so yields 18 linearly independent MI for this family:

$$\begin{aligned} \mathbf{G}_1 &= \{ G_{0,0,1,0,1,0,0,0,1}, G_{0,1,0,0,0,0,1,0,1}, G_{0,1,0,0,0,0,0,1,1}, G_{0,1,1,0,1,0,0,0,1}, G_{1,0,1,0,0,0,0,1,1}, \\ &G_{0,1,1,0,0,0,0,1,1}, G_{0,1,0,0,1,0,1,0,1}, G_{1,0,1,0,1,0,1,0,0}, G_{0,1,1,0,1,0,1,0,0}, G_{1,1,1,0,0,0,0,1,1}, \\ &G_{1,1,0,0,0,0,1,1,1}, G_{0,1,1,0,1,0,0,1,2}, G_{0,1,1,0,1,0,0,1,1}, G_{0,1,1,0,1,0,1,0,1}, G_{0,1,0,0,1,0,1,1,1}, \\ &G_{0,1,1,0,1,0,1,1,1}, G_{1,1,1,0,1,0,1,1,1}, G_{1,1,1,-1,1,0,1,1,1} \} \end{aligned} \quad (4.5)$$

The next step is to identify a canonical basis by studying the leading singularity of the pre-canonical MI. This task can be performed by studying the maximal cuts of these integrals in their Baikov representation. Looking for integrals with constant leading singularity yields the following basis:

$$g_1 = -s_{12}\epsilon^2 G_{0,0,2,0,1,0,0,0,2} \quad (4.6)$$

$$g_2 = -s_{12}(x-1)\epsilon^2 G_{0,1,0,0,0,0,2,0,2} \quad (4.7)$$

$$g_3 = -s_{23}x\epsilon^2 G_{0,1,0,0,0,0,0,2,2} \quad (4.8)$$

$$g_4 = -s_{12}x\epsilon^3 G_{0,1,1,0,1,0,0,0,2} \quad (4.9)$$

$$g_5 = -s_{12}\epsilon^3 G_{1,0,1,0,0,0,0,1,2} \quad (4.10)$$

$$g_6 = \epsilon^3 (-s_{12}(x-1) - s_{23}x) G_{0,1,1,0,0,0,0,1,2} \quad (4.11)$$

$$g_7 = -s_{12}x\epsilon^3 G_{0,1,0,0,1,0,1,0,2} \quad (4.12)$$

$$g_8 = s_{12}^2\epsilon^2 G_{2,0,1,0,2,0,1,0,0} \quad (4.13)$$

$$g_9 = s_{12}^2(x-1)\epsilon^2 G_{0,2,1,0,2,0,1,0,0} \quad (4.14)$$

$$g_{10} = s_{12}s_{23}x\epsilon^3 G_{1,1,1,0,0,0,1,2} \quad (4.15)$$

$$g_{11} = x\epsilon^4(-s_{12} - s_{23})G_{1,1,0,0,0,0,1,1,1} \quad (4.16)$$

$$g_{12} = s_{12}s_{23}x\epsilon^3 G_{0,1,1,0,1,0,0,1,2} \quad (4.17)$$

$$g_{13} = \epsilon^4(-s_{12} - s_{23}x)G_{0,1,1,0,1,0,0,1,1} \quad (4.18)$$

$$g_{14} = -s_{12}x\epsilon^4 G_{0,1,1,0,1,0,1,0,1} \quad (4.19)$$

$$g_{15} = s_{12}s_{23}x\epsilon^3 G_{0,1,0,0,1,0,1,1,2} \quad (4.20)$$

$$g_{16} = s_{12}\epsilon^4(s_{12}(x-1) + s_{23}x)G_{0,1,1,0,1,0,1,1,1} \quad (4.21)$$

$$g_{17} = -s_{12}^2s_{23}x\epsilon^4 G_{1,1,1,0,1,0,1,1,1} \quad (4.22)$$

$$g_{18} = s_{12}^2x\epsilon^4 G_{1,1,1,-1,1,0,1,1,1} \quad (4.23)$$

which is expressed in terms of a different set of FI than the pre-canonical ones in (4.5), namely:

$$\begin{aligned} \mathbf{G}_2 = \{ & G_{0,0,2,0,1,0,0,0,2}, G_{0,1,0,0,0,0,2,0,2}, G_{0,1,0,0,0,0,0,2,2}, G_{0,1,1,0,1,0,0,0,2}, G_{1,0,1,0,0,0,0,1,2}, \\ & G_{0,1,1,0,0,0,0,1,2}, G_{0,1,0,0,1,0,1,0,2}, G_{2,0,1,0,2,0,1,0,0}, G_{0,2,1,0,2,0,1,0,0}, G_{1,1,1,0,0,0,0,1,2}, \\ & G_{1,1,0,0,0,0,1,1,1}, G_{0,1,1,0,1,0,0,1,2}, G_{0,1,1,0,1,0,0,1,1}, G_{0,1,1,0,1,0,1,0,1}, G_{0,1,0,0,1,0,1,1,2}, \\ & G_{0,1,1,0,1,0,1,1,1}, G_{1,1,1,0,1,0,1,1,1}, G_{1,1,1,-1,1,0,1,1,1} \} \end{aligned} \quad (4.24)$$

The two sets of integrals are connected of course through IBP identities.

The ultimate test that a basis of MI is indeed canonical is if it satisfies a canonical DE. We proceed therefore by differentiating (4.6) with respect to  $x$ , which yields,

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{a=1}^4 \frac{\mathbf{M}_a}{(x-l_a)} \right) \mathbf{g} \quad (4.25)$$

with  $\mathbf{g}$  being the array of the 18 canonical basis elements in (4.6),  $\mathbf{M}_a$  are the purely numerical residue matrices and  $x-l_a$  the letters of the *alphabet*, with  $l_a = \{0, 1, s_{12}/(s_{12} + s_{23}), -s_{23}/s_{12}\}$ .

$$\mathbf{M}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{3}{8} & 0 & -\frac{3}{4} & -3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & -\frac{1}{2} & -3 & 0 & 0 & 0 & 0 \\ -\frac{3}{8} & 0 & \frac{3}{4} & -\frac{3}{2} & 0 & \frac{5}{2} & 0 & 0 & 0 & 0 & 0 & \frac{1}{4} & -\frac{5}{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & -\frac{3}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ \frac{3}{4} & -\frac{3}{2} & -\frac{3}{4} & 3 & 0 & -3 & -3 & 0 & -2 & 0 & 0 & -\frac{1}{2} & -3 & 0 & 1 & 2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \end{pmatrix} \quad (4.26)$$



$$\mathbf{M}_4 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.29)$$

## 4.2 Boundary terms and solution

In order to find boundary terms for solving (4.25) we proceed by computing the *resummation* matrix  $\mathbf{R}$ , as discussed in (3.31)-(3.34). The non-zero parts of the matrix read,

$$\begin{aligned} R_{1,1} &= 1, R_{2,2} = 1, R_{3,3} = x^{-2\epsilon}, R_{4,4} = x^{-\epsilon}, R_{5,5} = 1, R_{6,3} = \frac{1}{4} - \frac{x^{-2\epsilon}}{4}, R_{6,6} = 1, R_{7,7} = x^{-\epsilon}, \\ R_{8,8} &= 1, R_{9,9} = 1, R_{10,3} = \frac{3}{4}(x^{-2\epsilon} - 1), R_{10,10} = 1, R_{11,11} = 1, R_{12,1} = -\frac{3}{4}x^{-2\epsilon}(x^\epsilon - 1), \\ R_{12,3} &= -\frac{3}{4}x^{-2\epsilon}(x^\epsilon - 1), R_{12,4} = -3x^{-2\epsilon}(x^\epsilon - 1), R_{12,6} = 3x^{-2\epsilon}(x^\epsilon - 1), \\ R_{12,12} &= \frac{1}{2}x^{-2\epsilon}(3x^\epsilon - 1), R_{12,13} = -3x^{-2\epsilon}(x^\epsilon - 1), R_{13,1} = -\frac{1}{8}x^{-2\epsilon}(x^\epsilon + 2x^{2\epsilon} - 3), \\ R_{13,3} &= \frac{1}{8}x^{-2\epsilon}(x^\epsilon - 1)(2x^\epsilon + 1), R_{13,4} = -\frac{3}{2}x^{-2\epsilon}(x^\epsilon - 1), R_{13,6} = \frac{1}{2}(x^\epsilon - 3)x^{-2\epsilon} + 1, \\ R_{13,12} &= \frac{1}{4}x^{-2\epsilon}(x^\epsilon - 1), R_{13,13} = -\frac{1}{2}x^{-2\epsilon}(x^\epsilon - 3), R_{14,14} = x^{2\epsilon}, R_{15,3} = -\frac{3}{2}x^{-2\epsilon}(x^\epsilon - 1), \\ R_{15,15} &= x^{-\epsilon}, R_{16,1} = \frac{1}{8}x^{-2\epsilon}((-6x^\epsilon + 5x^{3\epsilon} - 2)x^\epsilon + 3), R_{16,2} = -\frac{3}{4}(x^{2\epsilon} - 1), \\ R_{16,3} &= \frac{1}{8}x^{-2\epsilon}(x^\epsilon(6x^\epsilon - 5x^{3\epsilon} + 2) - 3), R_{16,4} = \frac{3}{2}x^{-2\epsilon}(-2x^\epsilon + x^{4\epsilon} + 1), \\ R_{16,6} &= 3 - \frac{1}{2}x^{-2\epsilon}(-2x^\epsilon + 5x^{4\epsilon} + 3), R_{16,7} = x^{-\epsilon} - x^{2\epsilon}, R_{16,9} = 1 - x^{2\epsilon}, \\ R_{16,12} &= -\frac{1}{4}x^{-2\epsilon}(-2x^\epsilon + x^{4\epsilon} + 1), R_{16,13} = -\frac{1}{2}x^{-2\epsilon}(2x^\epsilon + x^{4\epsilon} - 3), R_{16,15} = \frac{1}{3}x^{-\epsilon}(x^{3\epsilon} - 1), \\ R_{16,16} &= x^{2\epsilon}, R_{17,1} = -\frac{3}{8}x^{-2\epsilon}(x^\epsilon - 1)^2, R_{17,3} = \frac{9}{8}x^{-2\epsilon}(x^\epsilon - 1)^2, R_{17,4} = -\frac{3}{2}x^{-2\epsilon}(x^\epsilon - 1)^2, \\ R_{17,6} &= \frac{3}{2}x^{-2\epsilon}(x^\epsilon - 1)^2, R_{17,12} = \frac{1}{4}(x^{-2\epsilon} - 6x^{-\epsilon} + 5), R_{17,13} = -\frac{3}{2}x^{-2\epsilon}(x^\epsilon - 1)^2, \\ R_{17,15} &= 2x^{-\epsilon} - 2, R_{17,17} = 1, R_{18,4} = 2 - 2x^{-\epsilon}, R_{18,7} = x^{-\epsilon} - 1, R_{18,14} = x^{2\epsilon} - 1, R_{18,18} = 1 \end{aligned} \quad (4.30)$$

Having the  $\mathbf{R}$  matrix at hand, we can construct the left-hand side of (3.37). From the definition of the canonical basis we can extract the  $\mathbf{T}$  matrix and using expansion-by-regions construct the right-hand side of (3.37). As discussed there, this equation yields two sets of relations. The so-called pure relations are,

$$\begin{aligned} b_4 = 0, b_7 = 0, b_{10} = \frac{3b_3}{4}, b_{11} = 0, b_{13} = -\frac{b_1}{4} - \frac{b_3}{4} + b_6 + \frac{b_{12}}{2}, b_{14} = 0, b_{15} = \frac{3b_3}{2}, \\ b_{16} = -\frac{3b_1}{4} + \frac{3b_2}{4} + 3b_6 + b_9 + \frac{b_{12}}{2}, b_{17} = \frac{3b_3}{2} - \frac{b_{12}}{2}, b_{18} = 0 \end{aligned} \quad (4.31)$$

These results leave the following boundary terms undetermined,

$$\{b_1, b_2, b_3, b_5, b_6, b_8, b_9, b_{12}\} \quad (4.32)$$

However most of them involve integrals which are already computed using other methods, e.g. direct integration in the Feynman parameter representation, and are readily available in the literature, namely

$$b_1 = -\frac{e^{2\gamma\epsilon}(3\epsilon-2)(3\epsilon-1)(-s_{12})^{-2\epsilon}\Gamma(1-\epsilon)^3\Gamma(2\epsilon+1)}{\Gamma(3-3\epsilon)} \quad (4.33)$$

$$b_2 = -\frac{s_{12}e^{2\gamma\epsilon}(3\epsilon-2)(3\epsilon-1)(-s_{12})^{-2\epsilon-1}\Gamma(1-\epsilon)^3\Gamma(2\epsilon+1)}{\Gamma(3-3\epsilon)} \quad (4.34)$$

$$b_3 = -\frac{e^{2\gamma\epsilon}(3\epsilon-2)(3\epsilon-1)(-s_{23})^{-2\epsilon}\Gamma(1-\epsilon)^3\Gamma(2\epsilon+1)}{\Gamma(3-3\epsilon)} \quad (4.35)$$

$$b_5 = -\frac{e^{2\gamma\epsilon}(3\epsilon-1)(-s_{12})^{-2\epsilon}\Gamma(1-2\epsilon)\Gamma(1-\epsilon)^2\Gamma(\epsilon+1)\Gamma(2\epsilon+1)}{4\Gamma(2-3\epsilon)} \quad (4.36)$$

$$b_8 = \frac{s_{12}^2 e^{2\gamma\epsilon} (-s_{12})^{-2(\epsilon+1)} \Gamma(1-\epsilon)^4 \Gamma(\epsilon+1)^2}{\Gamma(1-2\epsilon)^2} \quad (4.37)$$

$$b_9 = -\frac{s_{12}^2 e^{2\gamma\epsilon} (-s_{12})^{-2(\epsilon+1)} \Gamma(1-\epsilon)^4 \Gamma(\epsilon+1)^2}{\Gamma(1-2\epsilon)^2} \quad (4.38)$$

This leaves only two boundary terms undetermined,  $b_6$  and  $b_{12}$ . From the second set of relations produced by (3.37) we have

$$b_6 = s_{12}\epsilon^3 G_{0,1,1,0,0,0,0,1,2}^0 + \frac{1}{4}A(3)s_{23}\epsilon^2 \quad (4.39)$$

$$\begin{aligned} b_{12} = & -\frac{1}{2}s_{12}s_{23}\epsilon^3 G_{0,1,1,0,1,0,0,1,2}^{-2\epsilon-1} - 3s_{12}\epsilon^4 G_{0,1,1,0,1,0,0,1,1}^{-2\epsilon} - 3s_{12}\epsilon^3 G_{0,1,1,0,0,0,0,1,2}^{-2\epsilon} \\ & - \frac{3}{4}A(3)s_{23}\epsilon^2 \end{aligned} \quad (4.40)$$

where  $A(3)$  is given by

$$A(3) = \frac{e^{2\gamma\epsilon}(3\epsilon-2)(3\epsilon-1)(-s_{23})^{-2\epsilon}\Gamma(1-\epsilon)^3\Gamma(2\epsilon+1)}{s_{23}\epsilon^2\Gamma(3-3\epsilon)} \quad (4.41)$$

This means that we have to compute the following four regions

$$\{G_{0,1,1,0,0,0,0,1,2}^0, G_{0,1,1,0,0,0,0,1,2}^{-2\epsilon}, G_{0,1,1,0,1,0,0,1,1}^{-2\epsilon}, G_{0,1,1,0,1,0,0,1,2}^{-2\epsilon-1}\} \quad (4.42)$$

These are easily computed in the Feynman parameter representation and their result reads

$$G_{0,1,1,0,0,0,0,1,2}^0 = \frac{\pi^2 e^{2\gamma\epsilon} (-s_{12})^{-2\epsilon} \csc(\pi\epsilon) \csc(2\pi\epsilon) \Gamma(-\epsilon)}{2s_{12}\Gamma(1-3\epsilon)} \quad (4.43)$$

$$G_{0,1,1,0,0,0,1,2}^{-2\epsilon} = \frac{e^{2\gamma\epsilon} (-s_{23})^{-2\epsilon} \Gamma(-\epsilon)^3 \Gamma(2\epsilon)}{6s_{12}\Gamma(-3\epsilon)} \quad (4.44)$$

$$G_{0,1,1,0,1,0,0,1,1}^{-2\epsilon} = \frac{e^{2\gamma\epsilon} (-s_{23})^{-2\epsilon} \Gamma(-\epsilon)^3 \Gamma(2\epsilon + 1) {}_3F_2(1, 1, 1 - \epsilon; 2 - 2\epsilon, 2\epsilon + 1; 1)}{4s_{12}(2\epsilon - 1)\Gamma(1 - 3\epsilon)} \\ - \frac{\pi^2 e^{2\gamma\epsilon} \epsilon {}_2F_1(1 - 3\epsilon, 1 - 2\epsilon; 2 - 4\epsilon; 1) (-s_{23})^{-2\epsilon} \csc^2(2\pi\epsilon) \Gamma(-\epsilon)^2}{s_{12}\Gamma(2 - 4\epsilon)} \quad (4.45)$$

$$G_{0,1,1,0,1,0,0,1,2}^{-2\epsilon-1} = \frac{3\pi^{5/2} 2^{2\epsilon} e^{2\gamma\epsilon} (-s_{23})^{-2\epsilon} \csc(\pi\epsilon) \csc(2\pi\epsilon) \Gamma(-\epsilon) {}_3F_2(1, -2\epsilon, -\epsilon; 1 - 2\epsilon, \epsilon + 1; 1)}{s_{12}s_{23}\Gamma(1 - 3\epsilon)\Gamma(\frac{1}{2} - \epsilon)\Gamma(\epsilon + 1)} \\ + \frac{2\pi^2 e^{2\gamma\epsilon} (-s_{23})^{-2\epsilon} \csc(\pi\epsilon) \csc(2\pi\epsilon) \Gamma(2\epsilon)}{s_{12}s_{23}} \quad (4.46)$$

We now have determined all necessary boundary terms. A nice by-product in this case is that all boundary terms are in closed form in  $\epsilon$ . This allows us to obtain their expansion in  $\epsilon$  up to any desired order. The hyper-geometric functions present in the boundary terms can be expanded to any order in  $\epsilon$  using the HypExp [55], [56] package.

In general, for more complicated integral families obtaining all boundary terms in closed form is a non-trivial task due to the large number and complexity of the regions that are required to be computed. In those cases we will use results which are already available in the literature.

For the problem at hand, we can readily obtain an expansion in  $\epsilon$  up to order  $\mathcal{O}(\epsilon^4)$ , which allows us to obtain solutions of (4.25) up to weight four. The full result of basis element  $g_{17}$  which involves the top-sector scalar integral reads,<sup>1</sup>

$$g_{17} = -1 + \epsilon \left( 2\mathcal{G}_{l_1} - 2\mathcal{G}_{l_2} + 2L_2 \right) \\ + \epsilon^2 \left( -4\mathcal{G}_{l_1, l_1} + \mathcal{G}_{l_1, l_2} + 3\mathcal{G}_{l_2, l_1} + \mathcal{G}_{l_3, l_1} - \mathcal{G}_{l_3, l_2} - 4L_2\mathcal{G}_{l_1} + 3L_2\mathcal{G}_{l_2} + L_2\mathcal{G}_{l_3} \right. \\ \left. + L_1\mathcal{G}_{l_2} - L_1\mathcal{G}_{l_3} - 2L_2^2 + \frac{\pi^2}{12} \right) \\ + \epsilon^3 \left( 8\mathcal{G}_{l_1, l_1, l_1} - 2\mathcal{G}_{l_1, l_1, l_2} + \mathcal{G}_{l_1, l_2, l_1} - 4\mathcal{G}_{l_1, l_2, l_2} - 3\mathcal{G}_{l_1, l_3, l_1} + 3\mathcal{G}_{l_1, l_3, l_2} - 6\mathcal{G}_{l_2, l_1, l_1} \right. \\ \left. + 2\mathcal{G}_{l_2, l_1, l_2} - 3\mathcal{G}_{l_2, l_2, l_1} + 4\mathcal{G}_{l_2, l_2, l_2} + 5\mathcal{G}_{l_2, l_3, l_1} - 5\mathcal{G}_{l_2, l_3, l_2} - 2\mathcal{G}_{l_3, l_1, l_1} + 2\mathcal{G}_{l_3, l_2, l_1} \right. \\ \left. - 2\mathcal{G}_{l_3, l_3, l_1} + 2\mathcal{G}_{l_3, l_3, l_2} + 8L_2\mathcal{G}_{l_1, l_1} + L_2\mathcal{G}_{l_1, l_2} - 3L_2\mathcal{G}_{l_1, l_3} - 6L_2\mathcal{G}_{l_2, l_1} - 3L_2\mathcal{G}_{l_2, l_2} \right. \\ \left. + 5L_2\mathcal{G}_{l_2, l_3} - 2L_2\mathcal{G}_{l_3, l_1} + 2L_2\mathcal{G}_{l_3, l_2} - 2L_2\mathcal{G}_{l_3, l_3} - 3L_1\mathcal{G}_{l_1, l_2} + 3L_1\mathcal{G}_{l_1, l_3} + 3L_1\mathcal{G}_{l_2, l_2} \right. \\ \left. - 5L_1\mathcal{G}_{l_2, l_3} + 2L_1\mathcal{G}_{l_3, l_3} - \frac{1}{6}\pi^2\mathcal{G}_{l_1} - \frac{1}{6}\pi^2\mathcal{G}_{l_2} + \frac{1}{3}\pi^2\mathcal{G}_{l_3} + 4L_2^2\mathcal{G}_{l_1} - 3L_2^2\mathcal{G}_{l_2} \right. \\ \left. - L_2^2\mathcal{G}_{l_3} - L_1^2\mathcal{G}_{l_2} + L_1^2\mathcal{G}_{l_3} + \frac{4L_2^3}{3} - \frac{\pi^2 L_2}{6} + \frac{43\zeta(3)}{6} \right) \\ + \epsilon^4 \left( -\frac{2L_2^4}{3} - \frac{8}{3}\mathcal{G}_{l_1}L_2^3 + 2\mathcal{G}_{l_2}L_2^3 + \frac{2}{3}\mathcal{G}_{l_3}L_2^3 - 8\mathcal{G}_{l_1, l_1}L_2^2 - \mathcal{G}_{l_1, l_2}L_2^2 + 3\mathcal{G}_{l_1, l_3}L_2^2 \right. \\ \left. + 6\mathcal{G}_{l_2, l_1}L_2^2 + 3\mathcal{G}_{l_2, l_2}L_2^2 - 5\mathcal{G}_{l_2, l_3}L_2^2 + 2\mathcal{G}_{l_3, l_1}L_2^2 - 2\mathcal{G}_{l_3, l_2}L_2^2 + 2\mathcal{G}_{l_3, l_3}L_2^2 + \frac{1}{6}\pi^2L_2^2 \right. \\ \left. + \frac{1}{3}\pi^2\mathcal{G}_{l_1}L_2 - \frac{1}{2}\pi^2\mathcal{G}_{l_2}L_2 + \frac{1}{6}\pi^2\mathcal{G}_{l_3}L_2 - 16\mathcal{G}_{l_1, l_1, l_1}L_2 - 2\mathcal{G}_{l_1, l_1, l_2}L_2 + 6\mathcal{G}_{l_1, l_1, l_3}L_2 \right. \\ \left. - 2\mathcal{G}_{l_1, l_2, l_1}L_2 - \mathcal{G}_{l_1, l_2, l_2}L_2 + 3\mathcal{G}_{l_1, l_2, l_3}L_2 + 6\mathcal{G}_{l_1, l_3, l_1}L_2 + 3\mathcal{G}_{l_1, l_3, l_2}L_2 - 3\mathcal{G}_{l_1, l_3, l_3}L_2 \right. \\ \left. + 12\mathcal{G}_{l_2, l_1, l_1}L_2 - 2\mathcal{G}_{l_2, l_1, l_3}L_2 + 6\mathcal{G}_{l_2, l_2, l_1}L_2 + 3\mathcal{G}_{l_2, l_2, l_2}L_2 - 5\mathcal{G}_{l_2, l_2, l_3}L_2 - 10\mathcal{G}_{l_2, l_3, l_1}L_2 \right)$$

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<sup>1</sup>We use the abbreviations  $L_1 = \log(-s_{12})$ ,  $L_2 = \log(-s_{23})$ ,  $\mathcal{G}_{l_a, l_b, \dots} := \mathcal{G}(l_a, l_b, \dots; x)$ .

$$\begin{aligned}
& + \mathcal{G}_{l_2, l_3, l_2} L_2 - \mathcal{G}_{l_2, l_3, l_3} L_2 + 4\mathcal{G}_{l_3, l_1, l_1} L_2 + 2\mathcal{G}_{l_3, l_1, l_2} L_2 - 4\mathcal{G}_{l_3, l_1, l_3} L_2 - 4\mathcal{G}_{l_3, l_2, l_1} L_2 \\
& - 2\mathcal{G}_{l_3, l_2, l_2} L_2 + 2\mathcal{G}_{l_3, l_2, l_3} L_2 + 4\mathcal{G}_{l_3, l_3, l_1} L_2 - 4\mathcal{G}_{l_3, l_3, l_2} L_2 + 4\mathcal{G}_{l_3, l_3, l_3} L_2 - \frac{43\zeta(3)L_2}{3} \\
& + \frac{2}{3}L_1^3\mathcal{G}_{l_2} + \frac{5}{6}\pi^2 L_1\mathcal{G}_{l_2} - \frac{2}{3}L_1^3\mathcal{G}_{l_3} - \frac{5}{6}\pi^2 L_1\mathcal{G}_{l_3} + \frac{1}{3}\pi^2\mathcal{G}_{l_1, l_1} + 3L_1^2\mathcal{G}_{l_1, l_2} - \frac{1}{3}\pi^2\mathcal{G}_{l_1, l_2} \\
& - 3L_1^2\mathcal{G}_{l_1, l_3} + \frac{1}{2}\pi^2\mathcal{G}_{l_1, l_3} - \frac{1}{2}\pi^2\mathcal{G}_{l_2, l_1} - 3L_1^2\mathcal{G}_{l_2, l_2} + \frac{1}{2}\pi^2\mathcal{G}_{l_2, l_2} + 5L_1^2\mathcal{G}_{l_2, l_3} + \frac{1}{6}\pi^2\mathcal{G}_{l_2, l_3} \\
& + \frac{1}{6}\pi^2\mathcal{G}_{l_3, l_1} - \frac{1}{6}\pi^2\mathcal{G}_{l_3, l_2} - 2L_1^2\mathcal{G}_{l_3, l_3} - \frac{2}{3}\pi^2\mathcal{G}_{l_3, l_3} + 6L_1\mathcal{G}_{l_1, l_1, l_2} - 6L_1\mathcal{G}_{l_1, l_1, l_3} + 9L_1\mathcal{G}_{l_1, l_2, l_2} \\
& - 3L_1\mathcal{G}_{l_1, l_2, l_3} - 9L_1\mathcal{G}_{l_1, l_3, l_2} + 3L_1\mathcal{G}_{l_1, l_3, l_3} - 4L_1\mathcal{G}_{l_2, l_1, l_2} + 2L_1\mathcal{G}_{l_2, l_1, l_3} - 11L_1\mathcal{G}_{l_2, l_2, l_2} \\
& + 5L_1\mathcal{G}_{l_2, l_2, l_3} + 9L_1\mathcal{G}_{l_2, l_3, l_2} + L_1\mathcal{G}_{l_2, l_3, l_3} - 2L_1\mathcal{G}_{l_3, l_1, l_2} + 4L_1\mathcal{G}_{l_3, l_1, l_3} + 2L_1\mathcal{G}_{l_3, l_2, l_2} \\
& - 2L_1\mathcal{G}_{l_3, l_2, l_3} - 4L_1\mathcal{G}_{l_3, l_3, l_3} - 16\mathcal{G}_{l_1, l_1, l_1, l_1} + 4\mathcal{G}_{l_1, l_1, l_1, l_2} - 2\mathcal{G}_{l_1, l_1, l_2, l_1} + 5\mathcal{G}_{l_1, l_1, l_2, l_2} \\
& + 6\mathcal{G}_{l_1, l_1, l_3, l_1} - 6\mathcal{G}_{l_1, l_1, l_3, l_2} - 2\mathcal{G}_{l_1, l_2, l_1, l_1} - \mathcal{G}_{l_1, l_2, l_1, l_2} - \mathcal{G}_{l_1, l_2, l_2, l_1} + 10\mathcal{G}_{l_1, l_2, l_2, l_2} + 3\mathcal{G}_{l_1, l_2, l_3, l_1} \\
& - 3\mathcal{G}_{l_1, l_2, l_3, l_2} + 6\mathcal{G}_{l_1, l_3, l_1, l_1} + 3\mathcal{G}_{l_1, l_3, l_2, l_1} - 9\mathcal{G}_{l_1, l_3, l_2, l_2} - 3\mathcal{G}_{l_1, l_3, l_3, l_1} + 3\mathcal{G}_{l_1, l_3, l_3, l_2} + 12\mathcal{G}_{l_2, l_1, l_1, l_1} \\
& - 2\mathcal{G}_{l_2, l_1, l_1, l_2} - 3\mathcal{G}_{l_2, l_1, l_2, l_2} - 2\mathcal{G}_{l_2, l_1, l_3, l_1} + 2\mathcal{G}_{l_2, l_1, l_3, l_2} + 6\mathcal{G}_{l_2, l_2, l_1, l_1} - \mathcal{G}_{l_2, l_2, l_1, l_2} + 3\mathcal{G}_{l_2, l_2, l_2, l_1} \\
& - 12\mathcal{G}_{l_2, l_2, l_2, l_2} - 5\mathcal{G}_{l_2, l_2, l_3, l_1} + 5\mathcal{G}_{l_2, l_2, l_3, l_2} - 10\mathcal{G}_{l_2, l_3, l_1, l_1} + \mathcal{G}_{l_2, l_3, l_2, l_1} + 9\mathcal{G}_{l_2, l_3, l_2, l_2} - \mathcal{G}_{l_2, l_3, l_3, l_1} \\
& + \mathcal{G}_{l_2, l_3, l_3, l_2} + 4\mathcal{G}_{l_3, l_1, l_1, l_1} - 2\mathcal{G}_{l_3, l_1, l_1, l_2} + 2\mathcal{G}_{l_3, l_1, l_2, l_1} - 2\mathcal{G}_{l_3, l_1, l_2, l_2} - 4\mathcal{G}_{l_3, l_1, l_3, l_1} + 4\mathcal{G}_{l_3, l_1, l_3, l_2} \\
& - 4\mathcal{G}_{l_3, l_2, l_1, l_1} + 2\mathcal{G}_{l_3, l_2, l_1, l_2} - 2\mathcal{G}_{l_3, l_2, l_2, l_1} + 2\mathcal{G}_{l_3, l_2, l_2, l_2} + 2\mathcal{G}_{l_3, l_2, l_3, l_1} - 2\mathcal{G}_{l_3, l_2, l_3, l_2} + 4\mathcal{G}_{l_3, l_3, l_1, l_1} \\
& - 4\mathcal{G}_{l_3, l_3, l_2, l_1} + 4\mathcal{G}_{l_3, l_3, l_3, l_1} - 4\mathcal{G}_{l_3, l_3, l_3, l_2} - \frac{43\mathcal{G}_{l_1}\zeta(3)}{3} + \frac{19\mathcal{G}_{l_2}\zeta(3)}{3} + 8\mathcal{G}_{l_3}\zeta(3) + \frac{\pi^4}{180} \quad (4.47)
\end{aligned}$$

### 4.3 From massive to massless

Taking the  $x \rightarrow 1$  limit in the case of the doublebox family with one massive leg is the only way to get a solution for the fully massless doublebox family using the computational framework that we have developed so far. This serves not only as way of obtaining a solution for a separate integral family but also as a non-trivial cross-check of our full solution, in case the massless family is known. For the case at hand, the massless doublebox has also been solved a long time ago, and a canonical basis was presented for it in [42].

To get the  $x \rightarrow 1$  limit, we follow at first the steps outlined in eqs. (3.39)-(3.42) in order to compute the truncated part of our solution at  $x = 1$  and the numerical *resummation* matrix  $\tilde{\mathbf{R}}_0$ .



$$\tilde{\mathbf{R}}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{3}{2} & 0 & 0 & 3 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{3}{8} & 0 & \frac{3}{4} & 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & \frac{3}{2} & 3 & 0 & 0 & 0 & 0 \\ \frac{1}{8} & 0 & \frac{1}{8} & -\frac{1}{2} & 0 & -\frac{1}{2} & 0 & 0 & 0 & 0 & 0 & -\frac{1}{4} & -\frac{1}{2} & 0 & 0 & 0 & 0 \\ -\frac{1}{4} & -\frac{1}{4} & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\frac{3}{4} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ \frac{3}{8} & \frac{3}{4} & \frac{3}{8} & \frac{3}{2} & 0 & \frac{3}{2} & 0 & 0 & 0 & 0 & 0 & \frac{3}{4} & \frac{3}{2} & 0 & -1 & 0 & 0 \\ -\frac{3}{4} & -\frac{3}{4} & 0 & -2 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & -1 & 0 & 1 & 2 & 2 & 1 \\ \frac{3}{8} & 0 & -\frac{3}{8} & \frac{1}{2} & 0 & -\frac{3}{2} & -1 & 0 & -1 & 0 & 0 & \frac{1}{4} & -\frac{3}{2} & -1 & -1 & -1 & 0 & 1 \end{pmatrix} \quad (4.48)$$

Then, according to (3.43), the  $x \rightarrow 1$  limit for the doublebox family with one massive leg is the result of  $\tilde{\mathbf{R}}_0$  acting on the truncated part of the solution  $\mathbf{g}$  at  $x = 1$ . As we have already discussed, this special limit allows us to obtain the massless doublebox family. In order to get the canonical basis for the massless family from the massive one, we exploit the fact that  $\tilde{\mathbf{R}}_0$  is an idempotent matrix, and through (3.44) we obtain the following relations

$$\tilde{g}_2 = 0 \quad (4.49)$$

$$\tilde{g}_4 = -\frac{\tilde{g}_1}{2} \quad (4.50)$$

$$\tilde{g}_6 = -\frac{\tilde{g}_3}{2} \quad (4.51)$$

$$\tilde{g}_9 = 0 \quad (4.52)$$

$$\tilde{g}_{12} = \frac{3}{2}(\tilde{g}_1 + \tilde{g}_3 - 4\tilde{g}_{13}) \quad (4.53)$$

$$\tilde{g}_{14} = \frac{1}{4}(-\tilde{g}_1 - 4\tilde{g}_7) \quad (4.54)$$

$$\tilde{g}_{16} = \frac{1}{4}(3\tilde{g}_1 + 3\tilde{g}_3 - 12\tilde{g}_{13} - 4\tilde{g}_{15}) \quad (4.55)$$

where we denote as  $\tilde{g}_i$  the  $x \rightarrow 1$  limit of the  $i$ -th basis element. This operation leaves 11 integrals that can form the basis of the massless doublebox, namely

$$\{\tilde{g}_1, \tilde{g}_3, \tilde{g}_5, \tilde{g}_7, \tilde{g}_8, \tilde{g}_{10}, \tilde{g}_{11}, \tilde{g}_{13}, \tilde{g}_{15}, \tilde{g}_{17}, \tilde{g}_{18}\} \quad (4.56)$$

However as is it known, or as one can easily find out using KIRA[29] or FIRE[28], the massless doublebox family has 8 MI. In this particular case, the resulting formulas are compact enough and one can easily see that the following identities hold

$$\tilde{g}_7 = \tilde{g}_5 \quad (4.57)$$

$$\tilde{g}_{13} = \tilde{g}_{11} \quad (4.58)$$

$$\tilde{g}_{15} = \tilde{g}_{10} \quad (4.59)$$

This leaves exactly 8 linearly independent MI that form the basis for the massless doublebox, namely

$$s_{12} (-\epsilon^2) G_{0,0,2,0,1,0,0,0,2} \quad (4.60)$$

$$s_{23} (-\epsilon^2) G_{0,1,0,0,0,0,0,2,2} \quad (4.61)$$

$$s_{12} (-\epsilon^3) G_{1,0,1,0,0,0,0,1,2} \quad (4.62)$$

$$s_{12}^2 \epsilon^2 G_{2,0,1,0,2,0,1,0,0} \quad (4.63)$$

$$s_{12} s_{23} \epsilon^3 G_{1,1,1,0,0,0,0,1,2} \quad (4.64)$$

$$(-s_{12} - s_{23}) \epsilon^4 G_{1,1,0,0,0,0,1,1,1} \quad (4.65)$$

$$s_{12}^2 s_{23} (-\epsilon^4) G_{1,1,1,0,1,0,1,1,1} \quad (4.66)$$

$$s_{12}^2 \epsilon^4 G_{1,1,1,-1,1,0,1,1,1} \quad (4.67)$$

Relations (4.49) and (4.57) can also be verified using IBP identities.

All the results presented here have been cross-checked against results available in the literature and against numerical results obtained by `pySecDec`[57] and `FIESTA`[58].

## 4.4 Comparison with the standard approach

It is interesting to compare the solution presented here with the one obtained using the standard DE method, i.e. by differentiating with respect to all kinematic invariants. A canonical basis of MI for the doublebox with one off-shell leg was first presented in [59]. There, an alphabet of six letters was found, involving two variables constructed out of ratios of kinematic variables. In our analysis we obtained an alphabet with four letters. This *reduction* in the number of letters has been observed to all cases where the SDE approach has been applied so far, however the origin of this behaviour has yet to be determined.

# Part II

## Results

# Chapter 5

## Planar three-loop master integrals for the ladder-box topology

In this chapter we revisit the calculation of the so-called three-loop ladder-box topology with one off-shell leg, whose MI contribute to scattering amplitudes concerning for example a vector boson decaying to 3-jets or  $gg \rightarrow H + jet$  in gluon fusion at N3LO. This chapter presents original research done in collaboration with D. D. Canko and is based mainly on [60], as well as on [61] for the section regarding the analytic continuation of our results.

### 5.1 Introduction

It has been twenty years since the calculation of the two-loop FI for  $2 \rightarrow 2$  processes involving massless propagators and one off-shell external particle [54], [62] which established the method of DE as a powerful technique for the analytic computation of multiloop FI. These studies developed an approach which in essence is still used today, i.e. using Integration-By-Parts (IBP) identities [26], [27] to identify a minimal set of FI, known as *master integrals* (MI), deriving DE for these integrals by differentiating with respect to kinematic invariants and, if present, internal masses, and then using IBP identities again to recast the derivatives of the MI in terms of MI of equal or lower number of propagators.

A few years ago, a first step was taken towards the extension of these results at the three-loop level, with the calculation of the so-called planar ladder-box topology involving massless propagators and one off-shell leg [59]. This calculation was made possible through the adoption of the by now established method of canonical DE [42]. In [42] an observation was made that one can choose a *good* basis of MI, such that the DE that they satisfy have only logarithmic singularities and the dimensional regulator  $\epsilon$  is fully factorised. The conjecture made in [42] was that FI with constant leading singularities [43] are good candidates for the construction of such a basis, which is known as a *pure basis* of MI.

In [59] a basis of 85 MI was obtained and a canonical DE was derived based on Magnus series expansions [63]. In this chapter, we will re-calculate the three-loop ladder-box topology using a variant of the standard DE method, known as the Simplified Differential Equations (SDE) approach [38]. Our results are given in terms of real-valued GPLs of up to weight six for Euclidean and physical regions of phase-space. We also present the solution of the massless ladder-box family as a special limit of the ladder-box family with one massive leg.

## 5.2 General set up

### 5.2.1 Integral families

We begin this section by defining the integral family that will be treated in this chapter. For the sake of brevity we will call F1 the ladder-box topology 5.1.

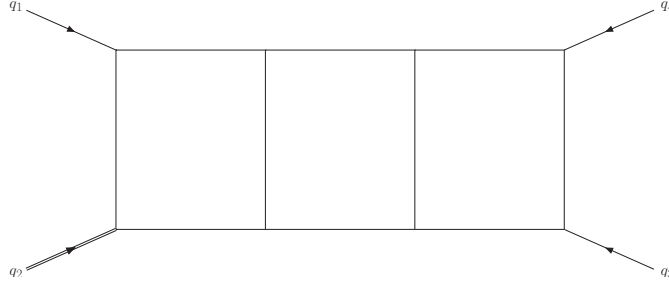


Figure 5.1: The F1 top-sector diagram. The double line represents the massive particle and all external momenta are taken to be incoming.

The corresponding FI are defined through<sup>1</sup>

$$G_{a_1 \dots a_{15}}^{F1} := \int \left( \prod_{l=1}^3 e^{\gamma_E \epsilon} \frac{d^d k_l}{i\pi^{d/2}} \right) \frac{(k_1 + q_{123})^{-2a_{11}} (k_2 + q_{123})^{-2a_{12}}}{(k_1 + q_{12})^{2a_1} (k_2 + q_{12})^{2a_2} (k_3 + q_{12})^{2a_3} (k_1 - k_2)^{2a_4}} \times \frac{(k_2 + q_1)^{-2a_{13}} (k_3 + q_1)^{-2a_{14}} (k_1 - k_3)^{-2a_{15}}}{(k_2 - k_3)^{2a_5} (k_3 + q_{123})^{2a_6} k_1^{2a_7} k_2^{2a_8} k_3^{2a_9} (k_1 + q_1)^{2a_{10}}} \quad (5.1)$$

with  $a_i$  being integers and  $a_i \leq 0$  for  $i = 11, \dots, 15$ . The external momenta of the considered families obey the following kinematics:  $\sum_{i=1}^4 q_i = 0$ ,  $q_2^2 = m^2$ ,  $q_i^2 = 0$  for  $i = 1, 3, 4$  and  $S_{12} = (q_1 + q_2)^2$ ,  $S_{23} = (q_2 + q_3)^2$ ,  $S_{13} = m^2 - S_{12} - S_{23}$ .

In this chapter we employ the SDE approach [38] for the analytic computation of family F1. To do so we parametrise the external momenta by introducing a dimensionless parameter  $x$  in the following manner

$$q_1 = xp_1, \quad q_2 = p_1 + p_2 - xp_1, \quad q_3 = p_3, \quad q_4 = p_4 \quad (5.2)$$

where the new momenta  $p_i$  are all massless. This parametrisation produces the following mapping for the kinematic invariants between the two momentum configurations

$$S_{12} = s_{12}, \quad S_{23} = s_{23}x, \quad m^2 = s_{12}(1 - x) \quad (5.3)$$

with  $s_{12} = (p_1 + p_2)^2$ ,  $s_{23} = (p_2 + p_3)^2$ .

### 5.2.2 Scattering kinematics

When considering the analytic solution of multiloop FI in dimensional regularisation, one usually solves these integrals in the Euclidean region, where all FI are free of branch cuts, and then analytically continues the results to the physical regions of phase-space. This is the approach that we will follow as well.

At first, by studying the second Symanzik polynomial [64] for the top-sector integral<sup>2</sup> of family F1 in its Feynman parameter representation, we can identify the Euclidean region in terms of the kinematic variables  $S_{12}$ ,  $S_{23}$ ,  $m^2$  such that

$$S_{12} < 0, \quad S_{23} < 0, \quad m^2 < 0. \quad (5.4)$$

<sup>1</sup>Where we use the abbreviation  $q_{12} = q_1 + q_2$  and  $q_{123} = q_1 + q_2 + q_3$ .

<sup>2</sup>By top-sector we mean the integrals with  $a_i = 1$  for  $i = 1, \dots, 10$  and  $a_i = 0$  for  $i = 11, \dots, 15$  in (5.1).

For scattering kinematics we have three physical regions when considering  $2 \rightarrow 2$  processes with one massive particle. For convenience we will denote them as the  $s$ ,  $t$  and  $u$  channels appropriately:

$$\text{s-channel : } m^2 > 0, \quad S_{12} \geq m^2, \quad S_{23} \leq 0, \quad S_{13} \leq 0 \quad (5.5)$$

$$\text{t-channel : } m^2 > 0, \quad S_{12} \leq 0, \quad S_{23} \geq m^2, \quad S_{13} \leq 0 \quad (5.6)$$

$$\text{u-channel : } m^2 > 0, \quad S_{12} \leq 0, \quad S_{23} \leq 0, \quad S_{13} \geq m^2. \quad (5.7)$$

Since we will use the SDE approach for the solution of (5.1), we would like to have the corresponding limits for each region of phase-space expressed in terms of the  $x$ ,  $s_{12}$ ,  $s_{23}$  variables. The mapping of (5.3) allows us to do so, although for reasons that will become clear at a later stage, we define the ratio  $y = \frac{s_{23}}{s_{12}}$  and use the variables  $x$ ,  $y$ ,  $s_{12}$ . Our approach therefore will be to compute all MI in terms of real-valued GPLs in the Euclidean region

$$0 < x < 1, \quad s_{12} < 0, \quad 0 < y < 1 \quad (5.8)$$

and then, using tools such as `HyperInt`[65] and `PolyLogTools`[66], analytically continue our solutions in the physical regions

$$\text{s-channel : } 0 < x < 1, \quad s_{12} > 0, \quad -1 \leq y \leq 0 \quad (5.9)$$

$$\text{t-channel : } 1 < x, \quad s_{12} < 0, \quad y \leq -1 \quad (5.10)$$

$$\text{u-channel : } 1 < x, \quad s_{12} < 0, \quad y \geq 0. \quad (5.11)$$

Performing the reduction to MI using modern IBP tools such as `FIRE6` [28] and `KIRA2` [29], we found for this family a set of 83 MI in contrast with [59], where a set of 85 MI was presented. The two extra MI contained in the set of 85 MI were found to be equal from IBP relations with two other integrals of the same set, namely  $\mathcal{T}_7 = \mathcal{T}_8$  and  $\mathcal{T}_{45} = \mathcal{T}_{46}$  of [59]. These relations can also be verified by checking the solutions for the corresponding basis elements, as presented in [59].

### 5.3 Canonical differential equations

Having a canonical basis for the studied family [59] we obtained a DE with respect to  $x$  which is of canonical form

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{i=1}^4 \frac{\mathbf{M}_i}{x - l_i} \right) \mathbf{g} \quad (5.12)$$

where  $\mathbf{g}$  is the pure basis and  $\mathbf{M}_i$  are the residue matrices corresponding to each letter  $l_i$ . All kinematic dependence is included in the letters  $l_i$ , leaving the matrices  $\mathbf{M}_i$  to consist solely of rational numbers. We have found an alphabet consisting of the four following letters

$$l_1 = 0, \quad l_2 = 1, \quad l_3 = \frac{1}{1+y}, \quad l_4 = -\frac{1}{y}. \quad (5.13)$$

The simplicity of the alphabet (5.13) in  $x$  allows for a straightforward solution of (5.12) in terms of GPLs. The solution can be written in the following compact form up to weight six:

$$\begin{aligned} \mathbf{g} = & \epsilon^0 \mathbf{b}_0^{(0)} + \epsilon \left( \sum \mathcal{G}_i \mathbf{M}_i \mathbf{b}_0^{(0)} + \mathbf{b}_0^{(1)} \right) + \epsilon^2 \left( \sum \mathcal{G}_{ij} \mathbf{M}_i \mathbf{M}_j \mathbf{b}_0^{(0)} + \sum \mathcal{G}_i \mathbf{M}_i \mathbf{b}_0^{(1)} + \mathbf{b}_0^{(2)} \right) + \dots \\ & + \epsilon^6 \left( \mathbf{b}_0^{(6)} + \sum \mathcal{G}_{ijklmn} \mathbf{M}_i \mathbf{M}_j \mathbf{M}_k \mathbf{M}_l \mathbf{M}_m \mathbf{M}_n \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{ijklm} \mathbf{M}_i \mathbf{M}_j \mathbf{M}_k \mathbf{M}_l \mathbf{M}_m \mathbf{b}_0^{(1)} \right. \\ & \left. + \sum \mathcal{G}_{ijkl} \mathbf{M}_i \mathbf{M}_j \mathbf{M}_k \mathbf{M}_l \mathbf{b}_0^{(2)} + \sum \mathcal{G}_{ijk} \mathbf{M}_i \mathbf{M}_j \mathbf{M}_k \mathbf{b}_0^{(3)} + \sum \mathcal{G}_{ij} \mathbf{M}_i \mathbf{M}_j \mathbf{b}_0^{(4)} + \sum \mathcal{G}_i \mathbf{M}_i \mathbf{b}_0^{(5)} \right) \end{aligned} \quad (5.14)$$

were  $\mathcal{G}_{ab\dots} := \mathcal{G}(l_a, l_b, \dots; x)$  represent the GPLs. The  $\mathbf{b}_0^{(i)}$  terms represent the boundary terms that need to be determined, with  $i$  indicating the corresponding weight, and consist of Zeta functions  $\zeta(i)$  and logarithms  $\{\log(-s_{12}), \log(y)\}$  of weight  $i$ . Our results are presented in such a way that each coefficient of  $\epsilon^i$  has transcendental weight  $i$ . If we assign weight  $-1$  to  $\epsilon$ , then (5.14) has uniform weight zero.

### 5.3.1 Boundary terms

In general we need to calculate the  $x \rightarrow 0$  limit of each pure basis element. Our first step is to exploit the canonical SDE at the limit  $x \rightarrow 0$  and define through it the resummation matrix

$$\mathbf{R} = \mathbf{S}e^{\mathbf{D}\log(x)}\mathbf{S}^{-1} \quad (5.15)$$

where the matrices  $\mathbf{S}$ ,  $\mathbf{D}$  are obtained through the Jordan decomposition<sup>3</sup> of the residue matrix for the letter  $l_1 = 0$ ,  $\mathbf{M}_1$ ,

$$\mathbf{M}_1 = \mathbf{S}\mathbf{D}\mathbf{S}^{-1}. \quad (5.16)$$

On the other hand, through IBP reduction, the elements of the pure basis can be related to a set of FI  $\mathbf{G}$ ,

$$\mathbf{g} = \mathbf{T}\mathbf{G}. \quad (5.17)$$

Furthermore using the expansion by regions method [51] as implemented in the `asy` code which is shipped along with `FIESTA4` [58], we can obtain information for the asymptotic behaviour of the FI in terms of which we express the pure basis of MI (5.17) in the limit  $x \rightarrow 0$ ,

$$G_i \underset{x \rightarrow 0}{=} \sum_j x^{b_j + a_j \epsilon} G_i^{(b_j + a_j \epsilon)} \quad (5.18)$$

where  $a_j$  and  $b_j$  are integers and  $G_i$  are the individual members of the basis  $\mathbf{G}$  of FI in (5.17). This analysis allows us to construct the following relation

$$\mathbf{R}\mathbf{b} = \lim_{x \rightarrow 0} \mathbf{T}\mathbf{G} \Big|_{\mathcal{O}(x^{0+a_j \epsilon})} \quad (5.19)$$

where the right-hand side implies that, apart from the terms  $x^{a_i \epsilon}$  coming from (5.18), we expand around  $x = 0$ , keeping only terms of order  $x^0$ . Equation (5.19) allows us in principle to determine all boundary constants  $\mathbf{b} = \sum_{i=0}^6 \epsilon^i \mathbf{b}_0^{(i)}$ .

More specifically, equation (5.19) produces two kinds of relations. The first one, called *pure relations* in [60], is in the form of linear relations with numerical rational coefficients between boundary terms  $\mathbf{b}$  and the second one is in the form of linear relations that contain boundary terms  $\mathbf{b}$  and region-integrals  $G_i^{(b_j + a_j \epsilon)}$  in the Feynman parameter representation.

The *pure relations* usually determine the boundary terms for the top-sector basis elements, which are the most non-trivial to compute since they involve the most complicated region-integrals. For the case of family F1 these *pure relations* for the three top-sector basis elements are

$$b_{81} = -\frac{b_1}{18} - \frac{7b_2}{18} - \frac{2b_7}{3} + \frac{b_{12}}{2} + \frac{b_{13}}{12} + \frac{2b_{16}}{3} + 2b_{32} - b_{39} + b_{41} \quad (5.20)$$

$$b_{82} = 0 \quad (5.21)$$

$$b_{83} = 0. \quad (5.22)$$

---

<sup>3</sup>For an earlier use of the Jordan decomposition method see [67], [68].

Similar relations are obtained for 59 basis elements in total, leaving the following basis elements undetermined,

$$\{b_1, b_2, b_3, b_4, b_5, b_6, b_7, b_8, b_9, b_{12}, b_{13}, b_{16}, b_{17}, b_{18}, b_{19}, b_{20}, b_{27}, b_{29}, b_{32}, b_{39}, b_{41}, b_{44}, b_{51}, b_{56}\}. \quad (5.23)$$

Out of those boundary terms, 11 of them are known from the massless solution,

$$\{b_1, b_2, b_3, b_4, b_5, b_6, b_7, b_{17}, b_{18}, b_{19}, b_{44}\} \quad (5.24)$$

leaving the following 13 genuinely unknown boundary terms to be determined,

$$\{b_8, b_9, b_{12}, b_{13}, b_{16}, b_{20}, b_{27}, b_{29}, b_{32}, b_{39}, b_{41}, b_{51}, b_{56}\} \quad (5.25)$$

The second kind of relations allow us to compute the above from expressions such as

$$b_{41} = G_{41}^{-3\epsilon} s_{12} \epsilon^5 + b_2/9 - b_{13}/12 - 2b_{16}/3. \quad (5.26)$$

Thus the problem of computing the remaining boundary terms is reduced to the calculation of the following 13 region-integrals

$$\{G_8^{\text{hard}}, G_9^{\text{hard}}, G_{12}^{\text{hard}}, G_{13}^{\text{hard}}, G_{16}^{\text{hard}}, G_{20}^{\text{hard}}, G_{27}^{\text{hard}}, G_{29}^{\text{hard}}, G_{51}^{\text{hard}}, G_{56}^{\text{hard}}\}, \quad (5.27)$$

$$\{G_{32}^{-3\epsilon}, G_{39}^{-3\epsilon}, G_{41}^{-3\epsilon}\}. \quad (5.28)$$

where with "hard" we denote the contribution from the  $x^0$  region.

From the set of the asymptotic limits the calculation of the hard limits was performed in momentum space with the use of the method of expansion-by-regions and IBP reduction. The SDE parametrization of the propagators makes it significantly easier in this case. In fact, the hard asymptotic limits are equal to some of the known MI and thus plugging them back into the relations between boundaries and asymptotic limits we found some extra relations between boundaries.

Regarding the  $x^{-3\epsilon}$  limits, we employed a strategy depending on the Feynman - parameter representation of the integrals under consideration, as well as a technique of integrating out bubble subintegrals inspired by [69]. For the case in point, the three integrals whose regions we want to compute, contain bubble subintegrals, i.e. each one can be written as a two-loop integral with a bubble insertion. As explained in [69], one can always integrate out bubble subintegrals and obtain a lower loop integral with some powers shifted by  $\epsilon$ . More specifically we have

$$\int \frac{d^d k}{i\pi^{d/2}} \frac{1}{(k^2)^{a_1} ((k+p)^2)^{a_2}} = \frac{\Gamma(a-d/2)\Gamma(d/2-a_1)\Gamma(d/2-a_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(d-a)} (p^2)^{d/2-a} \quad (5.29)$$

where  $a = a_1 + a_2$ . For the cases that we are interested in,  $a_1 = 2$  and  $a_2 = 1$ , and according to [69], after integrating out the bubble subintegral we arrive at a two-loop integral with one index shifted from 1 to  $1 + \epsilon$ .

In the following, we explain in detail the computation of the required region for  $G_{32}$ . The remaining regions can be computed in a similar manner.  $G_{32}$  can be written as

$$G_{32} = \int \frac{d^d k_1 d^d k_2 d^d k_3}{(i\pi^{d/2})^3} \frac{e^{3\epsilon\gamma_E}}{k_2^2 (k_1 - k_2)^2 (k_2 - k_3)^2 (k_1 + p_{12})^2 (k_1 + xp_1)^2 (k_3 + p_{123})^4}. \quad (5.30)$$

The bubble subintegral is

$$\int \frac{d^d k_3}{i\pi^{d/2}} \frac{1}{(k_2 - k_3)^2 (k_3 + p_{123})^4}. \quad (5.31)$$



By making the shift  $k_3 \rightarrow k - p_{123}$  we may write it as in (5.29). What is left is a two-loop integral with five propagators. The departure from the usual case is the fact that one propagator is raised to the power of  $1 + \epsilon$ . If one tries to find the regions contributing to the  $x \rightarrow 0$  limit of this integral we see that there are two regions, namely  $(x^0, x^{-3\epsilon})$  as for the full three-loop integral. We are interested in the  $x^{-3\epsilon}$  region, which now is significantly less complicated than the one resulting from the full three-loop integral analysis. After performing the necessary integrations, we may assemble the final result by multiplying the result of the bubble integration, namely (5.29) for  $a_1 = 2$  and  $a_2 = 1$ , with the result of the two-loop region and expand up to the desired power in the dimensional regulator.

The above steps allow us to fix all remaining boundary terms in a purely analytical way. Interestingly, we find that a general ansatz for all boundary terms can be constructed,

$$\begin{aligned}
b_i = & c(i, 0) + \epsilon \log(y)c(i, 1) + \epsilon^2 \left( \frac{1}{2} \log^2(y)c(i, 2, 2) + \frac{1}{6} \pi^2 c(i, 2, 1) \right) \\
& + \epsilon^3 \left( \frac{1}{6} \log^3(y)c(i, 3, 2) + \frac{1}{6} \pi^2 \log(y)c(i, 3, 1) + \zeta(3)c(i, 3, 3) \right) \\
& + \epsilon^4 \left( \zeta(3) \log(y)c(i, 4, 4) + \frac{1}{24} \log^4(y)c(i, 4, 3) + \frac{1}{12} \pi^2 \log^2(y)c(i, 4, 2) + \frac{1}{90} \pi^4 c(i, 4, 1) \right) \\
& + \epsilon^5 \left( \frac{1}{2} \zeta(3) \log^2(y)c(i, 5, 5) + \frac{1}{120} \log^5(y)c(i, 5, 3) + \frac{1}{36} \pi^2 \log^3(y)c(i, 5, 2) \right. \\
& \left. + \frac{1}{90} \pi^4 \log(y)c(i, 5, 1) + \zeta(5)c(i, 5, 6) + \frac{1}{6} \pi^2 \zeta(3)c(i, 5, 4) \right) \\
& + \epsilon^6 \left( \frac{1}{6} \zeta(3) \log^3(y)c(i, 6, 6) + \log(y) \left( \frac{1}{6} \pi^2 \zeta(3)c(i, 6, 5) + \zeta(5)c(i, 6, 8) \right) + \frac{1}{720} \log^6(y)c(i, 6, 4) \right. \\
& \left. + \frac{1}{144} \pi^2 \log^4(y)c(i, 6, 3) + \frac{1}{180} \pi^4 \log^2(y)c(i, 6, 2) + \zeta(3)^2 c(i, 6, 7) + \frac{1}{945} \pi^6 c(i, 6, 1) \right)
\end{aligned} \tag{5.32}$$

where we have multiplied by  $(-s_{12})^{(3\epsilon)}$  and expanded up to  $\epsilon^6$  to make the ansatz more compact.

## 5.4 Massless three-loop ladder-box

It is interesting to see how we can extract the pure basis and solution for the massless three-loop ladder-box using our results from the massive one. An important feature of the SDE approach is that by correctly taking the  $x \rightarrow 1$  limit [60], [70] of the solution of a specific integral family with  $n$  scales, one can arrive at the solution of the corresponding family with  $n - 1$  scales. In this particular case, taking the  $x \rightarrow 1$  limit of the one-mass ladder-box will yield the solution for the massless one.

### 5.4.1 The $x \rightarrow 1$ limit

Taking the  $x \rightarrow 1$  limit of the one-mass three-loop ladder-box amounts to performing the following manipulations. First, we rewrite our solution as an expansion in  $\log(1 - x)$  in the following form [60]

$$\mathbf{g} = \sum_{n \geq 0} \epsilon^n \sum_{i=0}^n \frac{1}{i!} \mathbf{c}_i^{(n)} \log^i(1 - x) \tag{5.33}$$

where all coefficients  $\mathbf{c}_i^{(n)}$  are finite in the limit  $x \rightarrow 1$ . This can be straightforwardly achieved, starting from the original solution (5.14) and transporting all letters  $l = 1$  of GPLs to the right, according to their known shuffle properties. Having done that, we may define the regular part

of  $\mathbf{g}$  at  $x = 1$  as

$$\mathbf{g}_{reg} = \sum_{n \geq 0} \epsilon^n \mathbf{c}_0^{(n)} \quad (5.34)$$

and through  $\mathbf{g}_{reg}$ , the truncated part of  $\mathbf{g}$  as

$$\mathbf{g}_{trunc} = \mathbf{g}_{reg}(x = 1). \quad (5.35)$$

If we return to the canonical DE (5.12) and single out the part singular at  $x = 1$ , then the full solution of the problem can be written schematically as follows

$$\mathbf{g} = e^{\epsilon \mathbf{M}_1 \log(1-x)} \mathbf{g}_{reg}. \quad (5.36)$$

Because  $\mathbf{M}_1$  is by definition a square matrix, we can always find its Jordan matrix decomposition

$$\mathbf{M}_1 = \mathbf{S}_1 \mathbf{D}_1 \mathbf{S}_1^{-1}. \quad (5.37)$$

We may then define the resummation matrix  $\tilde{\mathbf{R}}$  as follows

$$\tilde{\mathbf{R}} = e^{\epsilon \mathbf{M}_1 \log(1-x)} = \mathbf{S}_1 e^{\epsilon \mathbf{D}_1 \log(1-x)} \mathbf{S}_1^{-1}. \quad (5.38)$$

It is clear from (5.36) that when (5.38) acts on (5.34) we get the full solution of the problem. The resummation matrix  $\tilde{\mathbf{R}}$  has terms  $(1-x)^{a_i \epsilon}$ , with  $a_i$  the eigenvalues of  $\mathbf{M}_1$ . Setting these terms equal to zero results in a purely numerical matrix  $\tilde{\mathbf{R}}_0$

$$\tilde{\mathbf{R}} \rightarrow \tilde{\mathbf{R}}_0. \quad (5.39)$$

Now, finding the  $x \rightarrow 1$  limit of the original solution (5.14) amounts to  $\tilde{\mathbf{R}}_0$  acting on  $\mathbf{g}_{trunc}$ .

$$\mathbf{g}_{x \rightarrow 1} = \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc}. \quad (5.40)$$

## 5.4.2 From massive to massless

Remember that our goal is to find a pure basis for the massless three-loop ladder-box. From the massive one, the result of

$$\lim_{x \rightarrow 1} \mathbf{g}(x)$$

is an array of 83 pure basis elements. If we look at this result from the perspective of the massless three-loop ladder-box, some of these basis elements will be the 26 basis elements for the massless three-loop ladder-box and the rest will be reducible to the 26 massless basis elements or zero. We may distinguish them using IBP relations but first we may exploit an interesting feature of the  $\tilde{\mathbf{R}}_0$  matrix in order to simplify the procedure.

It turns out that  $\tilde{\mathbf{R}}_0$  is an *idempotent* matrix. Idempotent matrices have the following properties, all of which are satisfied by  $\tilde{\mathbf{R}}_0$ :

1.  $\mathbf{X} = \mathbf{X}^2$
2. singular except the identity matrix  $\mathbf{I}$
3. eigenvalues of  $\mathbf{X} = 0, 1$
4.  $\text{Trace}(\mathbf{X}) = \text{Rank}(\mathbf{X})$
5.  $\mathbf{I} - \mathbf{X}$  also idempotent

Since  $\tilde{\mathbf{R}}_0 = \tilde{\mathbf{R}}_0^2$ , if we act with  $\tilde{\mathbf{R}}_0$  on  $\mathbf{g}_{x \rightarrow 1}$  yields

$$\begin{aligned}\tilde{\mathbf{R}}_0 \mathbf{g}_{x \rightarrow 1} &= \tilde{\mathbf{R}}_0^2 \mathbf{g}_{trunc} \\ &= \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc} \\ &= \mathbf{g}_{x \rightarrow 1}.\end{aligned}\tag{5.41}$$

This relation, solved as an equation for each row, will yield the relations between the reducible pure basis elements and the massless basis elements as well as those who are equal to zero. We found 36 relations, which is expected since the rank of the purely numerical resummation matrix is 36, e.g.<sup>4</sup>

$$\tilde{g}_{24} = 0,\tag{5.42}$$

$$\tilde{g}_{49} = \frac{1}{2}(2\tilde{g}_{35} - \tilde{g}_{33}),\tag{5.43}$$

$$\begin{aligned}\tilde{g}_{80} &= \frac{1}{36}(4\tilde{g}_1 - 6\tilde{g}_4 - 48\tilde{g}_5 + 192\tilde{g}_{10} + 128\tilde{g}_{14} - 72\tilde{g}_{15} - 96\tilde{g}_{22} \\ &\quad - 12\tilde{g}_{33} - 192\tilde{g}_{36} + 3\tilde{g}_{40} - 12\tilde{g}_{42} - 9\tilde{g}_{43} - 8\tilde{g}_{48} - 24\tilde{g}_{53} \\ &\quad - 12\tilde{g}_{55} + 36\tilde{g}_{72} - 6\tilde{g}_{75} - 108\tilde{g}_{76} - 12\tilde{g}_{77}).\end{aligned}\tag{5.44}$$

The resulting relations can be verified in two ways.

1. Using IBP relations.
2. Using the analytic expressions for the  $x \rightarrow 1$  limit.

These 36 relations leave 47 basis elements as potential candidates for the 26 basis elements of the massless three-loop ladder-box, namely

$$\{\tilde{g}_1, \tilde{g}_2, \tilde{g}_4, \tilde{g}_5, \tilde{g}_6, \tilde{g}_7, \tilde{g}_{10}, \tilde{g}_{14}, \tilde{g}_{15}, \tilde{g}_{17}, \tilde{g}_{18}, \tilde{g}_{19}, \tilde{g}_{22}, \tilde{g}_{30}, \tilde{g}_{31}, \tilde{g}_{33}, \tilde{g}_{35}, \tilde{g}_{36}, \tilde{g}_{37}, \tilde{g}_{38}, \tilde{g}_{40}, \tilde{g}_{42}, \tilde{g}_{43}, \tilde{g}_{44}, \tilde{g}_{46}, \tilde{g}_{48}, \tilde{g}_{53}, \tilde{g}_{55}, \tilde{g}_{58}, \tilde{g}_{59}, \tilde{g}_{62}, \tilde{g}_{63}, \tilde{g}_{64}, \tilde{g}_{65}, \tilde{g}_{66}, \tilde{g}_{67}, \tilde{g}_{68}, \tilde{g}_{69}, \tilde{g}_{70}, \tilde{g}_{71}, \tilde{g}_{72}, \tilde{g}_{75}, \tilde{g}_{76}, \tilde{g}_{77}, \tilde{g}_{81}, \tilde{g}_{82}, \tilde{g}_{83}\}$$

To distinguish among them we may perform an IBP reduction. Since we want to extract the basis elements for the massless three-loop ladder-box from the basis elements of the massive one, we first substitute each  $\tilde{b}_i$  with its corresponding  $g_i$  and we set  $x = 1$  explicitly. We now have a set of 47 pure basis elements written in terms of certain FI. Via IBP reduction, we may reduce these FI to a set of MI for the massless three-loop ladder-box, and we can see that there are 26 linearly independent pure basis elements.

### 5.4.3 Pure basis for the massless three-loop ladder-box

The resulting pure basis for the massless three-loop ladder-box in terms of the ones from the massive three-loop ladder-box are

$$\{\tilde{g}_1, \tilde{g}_2, \tilde{g}_4, \tilde{g}_5, \tilde{g}_6, \tilde{g}_7, \tilde{g}_{17}, \tilde{g}_{18}, \tilde{g}_{19}, \tilde{g}_{30}, \tilde{g}_{31}, \tilde{g}_{35}, \tilde{g}_{36}, \tilde{g}_{37}, \tilde{g}_{44}, \tilde{g}_{53}, \tilde{g}_{55}, \tilde{g}_{62}, \tilde{g}_{63}, \tilde{g}_{64}, \tilde{g}_{65}, \tilde{g}_{68}, \tilde{g}_{69}, \tilde{g}_{81}, \tilde{g}_{82}, \tilde{g}_{83}\}$$

which can be written in terms of 26 MI as follows

$$\begin{aligned}g_1^0 &= s_{12}\epsilon^3 G_{0,0,2,2,2,0,1,0,0,0,0,0,0,0}, \\ g_2^0 &= s_{23}\epsilon^3 G_{0,0,0,2,2,1,0,0,0,2,0,0,0,0}, \\ g_3^0 &= s_{12}^2\epsilon^3 G_{0,2,2,1,0,0,2,0,1,0,0,0,0,0},\end{aligned}$$

---

<sup>4</sup>In the following we use the notation  $\tilde{g}_i$  to indicate the  $x \rightarrow 1$  limit of the corresponding  $g_i$ .

$$\begin{aligned}
g_4^0 &= s_{12}\epsilon^3(2\epsilon + 1)G_{0,1,0,1,1,0,2,0,2,0,0,0,0,0,0}, \\
g_5^0 &= s_{12}\epsilon^4G_{1,0,0,2,1,2,1,0,0,0,0,0,0,0,0}, \\
g_6^0 &= s_{12}\epsilon^4G_{0,1,0,2,1,2,1,0,0,0,0,0,0,0,0}, \\
g_7^0 &= s_{12}^3\epsilon^3G_{2,2,2,0,0,0,1,1,1,0,0,0,0,0,0}, \\
g_8^0 &= s_{12}(1 - 2\epsilon)\epsilon^4G_{1,0,1,2,1,0,1,0,1,0,0,0,0,0,0}, \\
g_9^0 &= s_{12}^2\epsilon^4G_{2,1,0,0,1,2,1,1,0,0,0,0,0,0,0}, \\
g_{10}^0 &= s_{12}s_{23}\epsilon^4G_{1,0,0,2,1,2,1,0,0,1,0,0,0,0,0}, \\
g_{11}^0 &= \epsilon^5(-s_{12} - s_{23})G_{0,1,0,1,1,2,1,0,0,1,0,0,0,0,0}, \\
g_{12}^0 &= s_{12}s_{23}\epsilon^4G_{0,1,0,2,1,2,0,1,0,1,0,0,0,0,0}, \\
g_{13}^0 &= \frac{1}{4}s_{12}\epsilon^3\left(\frac{4\epsilon(2\epsilon - 1)G_{0,1,0,2,1,2,-1,1,0,1,0,0,0,0,0}}{\epsilon - 1} + G_{0,0,0,2,2,1,0,0,0,2,0,0,0,0,0}\right), \\
g_{14}^0 &= \epsilon^5(-s_{12} - s_{23})G_{0,0,1,1,2,1,1,0,0,1,0,0,0,0,0}, \\
g_{15}^0 &= s_{12}\epsilon^6G_{1,0,1,1,1,1,1,1,0,0,0,0,0,0,0}, \\
g_{16}^0 &= -s_{12}^2\epsilon^5G_{1,0,1,1,1,1,0,2,0,1,0,0,0,0,0}, \\
g_{17}^0 &= s_{12}s_{23}\epsilon^5G_{1,0,1,2,1,1,0,1,0,1,0,0,0,0,0}, \\
g_{18}^0 &= s_{12}^2s_{23}\epsilon^5G_{1,1,0,1,1,2,1,1,0,1,0,0,0,0,0}, \\
g_{19}^0 &= s_{12}^2\epsilon^5(2\epsilon - 1)G_{1,1,0,1,1,1,1,1,0,1,0,0,0,0,0}, \\
g_{20}^0 &= -s_{12}\epsilon^6(s_{12} + s_{23})G_{1,0,1,1,1,1,1,1,0,1,0,0,0,0,0}, \\
g_{21}^0 &= s_{12}^2s_{23}\epsilon^5G_{1,0,1,1,2,1,1,1,0,1,0,0,0,0,0}, \\
g_{22}^0 &= s_{12}^2\epsilon^5(2\epsilon - 1)G_{1,0,1,1,1,1,1,0,1,1,0,0,0,0,0}, \\
g_{23}^0 &= s_{12}^2s_{23}\epsilon^5G_{1,0,1,1,2,1,1,0,1,1,0,0,0,0,0}, \\
g_{24}^0 &= s_{12}^3s_{23}\epsilon^6G_{1,1,1,1,1,1,1,1,1,1,0,0,0,0,0}, \\
g_{25}^0 &= -s_{12}^3\epsilon^6G_{1,1,1,1,1,1,1,1,1,1,-1,0,0,0,0}, \\
g_{26}^0 &= -s_{12}^3\epsilon^6G_{1,1,1,1,1,1,1,1,1,1,0,-1,0,0,0}.
\end{aligned} \tag{5.45}$$

The chosen normalisation of the FI is

$$G_{a_1, \dots, a_{15}}(\{p_j\}, \varepsilon) = (-s_{12})^{3\varepsilon} \int \left( \prod_{l=1}^3 \frac{d^d k_l}{i\pi^{d/2}} \right) \frac{e^{3\varepsilon\gamma_E}}{D_1^{a_1} \dots D_{15}^{a_{15}}} \quad \text{with} \quad d = 4 - 2\varepsilon \tag{5.46}$$

with the propagators being the  $x \rightarrow 1$  limit of (5.1).

## 5.5 Results

### 5.5.1 Analytic continuation

As already mentioned, our results are expressed in terms of GPLs up to weight six and thus can be numerically computed at high precision using automated tools, like `GinaC` [71]. The weight  $W=1 \dots 6$  is identified as the number of letters  $l_i$  in  $\mathcal{G}(l_i, \dots; x)$ . For the evaluations to be fast and efficient the GPLs should not contain letters  $l_i$  along the integration path connecting the origin and the argument  $x$ , i.e.  $l_i \notin [0, x]$ . Although this holds true in the Euclidean region, this is not the case in the physical regions anymore. One can get over this problem by using fibration-basis techniques [65], [66] for changing appropriately the arguments of GPLs at each physical region and making them real-valued. We followed this procedure using `HyperInt` [65], aiming to obtain results in terms of real-valued GPLs which can be efficiently evaluated numerically, thus making them well-suited for phenomenological applications.

Regions	Letters	Argument	Letters	Argument
Euclidean	$\{0, 1, -1/y, 1/(1+y)\}$	$x$	–	–
s-channel	$\{0, 1, -1/y, 1/(1+y)\}$	$x$	–	–
t-channel	$\{0, 1, 1+y, -y\}$	$1/x$	$\{0, 1\}$	$-1/y$
u-channel	$\{0, 1, 1+y, -y\}$	$1/x$	$\{0, -1\}$	$y$

Table 5.1: Structure of GPLs appearing in each of the 4 kinematic regions.

In order to make more clear the form of our solutions, we present in table 5.1 the arguments and the letters of the GPLs in the Euclidean and each of the physical regions after using `HyperInt`. Note that prior to the use of fibration-basis techniques, no GPLs with arguments depending on  $y$  are present. However, casting each GPL in a fibration basis which contains real-valued GPLs and explicit imaginary terms, produces GPLs with  $y$ -dependent argument as well.

In table 5.2 we provide an analysis regarding the number of GPLs that appear in each transcendental weight, for each kinematic region. In the same table we quote also the total number of GPLs and the timing for their numerical evaluation using `GinaC`. The number of GPLs is the same for the Euclidean and the s-channel due to the fact that the GPLs of the Euclidean region are already real valued in the s-channel and thus their is no need of using fibration-basis techniques for them.

Regions	$W = 1$	$W = 2$	$W = 3$	$W = 4$	$W = 5$	$W = 6$	Total	Timings (sec)
Euclidean	4	14	50	124	367	692	1251	39.0225769
s-channel	4	14	50	124	367	692	1251	39.2172529
t-channel	6	18	58	155	419	603	1259	62.0567800
u-channel	5	16	54	147	403	572	1197	55.1049640

Table 5.2: Number of GPLs per transcendental weight and per kinematic region, and timings for the numerical evaluation of the total GPLs. The quoted timings are obtained using the `Ginsh` command of `PolyLogTools`, running 1-core in a personal laptop (i7 processor, 8-core, 16GB RAM).

## 5.5.2 Validation

For the validation of our results we have performed various numerical checks in the Euclidean and physical regions. More specifically, for the Euclidean region we compared numerically every MI of each family with `pySecDec` [57] and `Fiesta` [58] and the analytic results of `mastrolia` for the point

$$s_{12} \rightarrow -7, y \rightarrow 3/7, x \rightarrow 1/4 \quad (5.47)$$

finding perfect agreement within the numerical accuracy provided by these programs.

Regarding our results for physical regions, obtaining numerical results for all MI using `pySecDec` or `Fiesta` can be rather challenging, and in some cases even impossible. To that end, in order to check that the analytic continuation was correct, we determined a specific set of low-sector MI (with up to 7 propagators), which contained the total set of GPLs at each region and we numerically compared them with `pySecDec` and `Fiesta` for the points

$$\text{s-channel : } s_{12} \rightarrow 2, y \rightarrow -1/2, x \rightarrow 1/4 \quad (5.48)$$

$$\text{t-channel : } s_{12} \rightarrow -2, y \rightarrow -3/2, x \rightarrow 5/3 \quad (5.49)$$

$$\text{u-channel : } s_{12} \rightarrow -2, y \rightarrow 3/2, x \rightarrow 5/3. \quad (5.50)$$

After properly choosing the branch of the analytic continuation, i.e. fixing the values of the auxiliary functions  $\{\delta(1/x), \delta(-1/y), \delta(y)\}$  either equal to 1 or -1 coming from `HyperInt`, perfect agreement was found for every MI that we checked.

Analytic checks were performed against [69] at the limit  $x \rightarrow 1$  in the Euclidean regions. The variable  $y = \frac{s_{23}}{s_{12}}$  introduced earlier is equal to the dimensionless variable  $x = \frac{t}{s}$  used therein.

# Chapter 6

## Pentagon integrals to arbitrary order in the dimensional regulator

We analytically calculate one-loop five-point MI, *pentagon integrals*, with up to one off-shell leg to arbitrary order in the dimensional regulator in  $d = 4 - 2\epsilon$  space-time dimensions. A pure basis of MI is constructed for the pentagon family with one off-shell leg, satisfying a single-variable canonical differential equation in the SDE approach. The relevant boundary terms are given in closed form, including a hypergeometric function which can be expanded to arbitrary order in the dimensional regulator using the `Mathematica` package `HypExp` [56]. Thus one can obtain solutions of the canonical differential equation in terms of GPLs of arbitrary transcendental weight. As a special limit of the one-mass pentagon family, we obtain a fully analytic result for the massless pentagon family in terms of pure and universally transcendental functions. For both families we provide explicit solutions in terms of GPLs up to weight four. This chapter is based on original research that first appeared in [72].

### 6.1 Introduction

The study of one-loop five-point Feynman diagrams, known as pentagon integrals, has a long history. Their calculation has been treated using various methods and techniques, with results presented in several different forms. In [73], analytic results for pentagon integrals with up to one massive leg were given in  $d = 4 - 2\epsilon$  space-time dimensions in terms of transcendental functions of up to weight two. In [74], the pentagon integral with fully massless legs was studied in  $d = 6 - 2\epsilon$  space-time dimensions in the multi-Regge limit and analytic expressions up to  $\mathcal{O}(\epsilon^2)$  were obtained. Analytic results in terms of Appell hypergeometric functions and Gauss hypergeometric functions were obtained in [75] for the pentagon with massless internal and external lines. First results in  $d = 4 - 2\epsilon$  space-time dimensions in terms of GPLs [44] of up to weight three (or  $\mathcal{O}(\epsilon)$ ) were obtained in [38] for the pentagon with up to one off-shell leg. One-fold integral representations were obtained in [76] in arbitrary space-time dimensions for the massless pentagon and in [77] for the pentagon with one off-shell leg in  $d = 6 - 2\epsilon$  space-time dimensions. More recently the massless pentagon has been implemented as part of the so-called *pentagon functions* up to weight four in [78], [79] and numerical results up to weight four in terms of generalised power-series expansion for the pentagon with one off-shell leg were presented in [80] for various phase-space points.

In this chapter we analytically calculate pentagon integrals with up to one off-shell leg in  $d = 4 - 2\epsilon$  space-time dimensions and express them in terms of GPLs of higher weights. We start with the pentagon with one massive leg and employ the method of differential equations in its modern, canonical incarnation [42], in conjunction with the SDE approach (SDE) [38]. This is achieved by constructing a *pure basis* of MI [40] for the pentagon with one massive

leg family. We find that all relevant boundary terms required for the solution of the canonical differential equation are given in closed form. This allows us to straightforwardly express our results in terms of GPLs of arbitrary transcendental weight. Having the solution of the pentagon with one off-shell leg at hand, we can obtain in an algorithmic way a fully analytical solution for the massless pentagon by taking the  $x \rightarrow 1$  limit of the former result, with  $x$  being a dimensionless parameter that is introduced in the SDE approach. This is a special feature of the SDE approach first described in [38], [81] and in more details in [60].

With a mind to phenomenological applications of our results, we present explicit solutions up to transcendental weight four. Our results are complementary to [82], where analytic expressions for all two-loop planar pentabox families with one massive leg were recently presented. The combination of these results provides a key ingredient for the calculation of two-loop planar amplitudes for  $W+2$  jets production at the LHC [83], [84].

## 6.2 Construction of a pure basis

We define the pentagon family with one off-shell leg as

$$G_{a_1 a_2 a_3 a_4 a_5} = \int \frac{d^d k_1}{i\pi^{(d/2)}} \frac{e^{\epsilon\gamma_E}}{\mathcal{D}_1^{a_1} \mathcal{D}_2^{a_2} \mathcal{D}_3^{a_3} \mathcal{D}_4^{a_4} \mathcal{D}_5^{a_5}} \quad (6.1)$$

with

$$\begin{aligned} \mathcal{D}_1 &= -(k_1)^2, \quad \mathcal{D}_2 = -(k_1 + q_1)^2, \quad \mathcal{D}_3 = -(k_1 + q_1 + q_2)^2 \\ \mathcal{D}_4 &= -(k_1 + q_1 + q_2 + q_3)^2, \quad \mathcal{D}_5 = -(k_1 + q_1 + q_2 + q_3 + q_4)^2. \end{aligned} \quad (6.2)$$

The kinematics consist of the massive momentum  $\{q_3, q_3^2 = m^2\}$  and four massless momenta  $\{q_i, q_i^2 = 0, \text{ for } i = 1, 2, 4, 5\}$ . In the SDE notation, we parametrise the external momenta by inserting a dimensionless variable  $x$  in the following way<sup>1</sup>

$$q_1 = xp_1, \quad q_2 = xp_2, \quad q_3 = p_{123} - xp_{12}, \quad q_4 = -p_{123}, \quad q_5 = -p_{1234} \quad (6.3)$$

where all  $p_i$  momenta are now massless. The kinematics of the two momentum configurations are connected as follows<sup>2</sup>

$$\begin{aligned} m^2 &= (x-1)(S_{12}x - S_{45}), \quad s_{12} = S_{12}x^2, \quad s_{23} = S_{23}x - S_{45}x + S_{45}, \\ s_{34} &= x(S_{12}(x-1) + S_{34}), \quad s_{45} = S_{45}, \quad s_{51} = S_{51}x. \end{aligned} \quad (6.4)$$

For reasons that will become clear shortly, we also define the square root of the Gram determinant of the external momenta as

$$\Delta_5 = \sqrt{\det[q_i \cdot q_j]}. \quad (6.5)$$

Using FIRE6 [28] for the IBP reduction we find that we need 13 MI to completely describe the vector space which consists of all FI that are included in (6.1). For the construction of the pure basis, the only non-trivial basis element is that of the top sector. The remaining basis elements can be constructed through the knowledge of the leading singularities of the relevant one-loop integrals. For the construction of the top sector basis element we follow the consensus developed in [80], [85], expressed here in the language of the Baikov representation of FI [86], [87]. More specifically, we choose as a candidate top sector basis element the following

$$\epsilon^2 \frac{\mathcal{P}_{11111}}{\Delta_5} \tilde{G}_{11111} \quad (6.6)$$

<sup>1</sup>We use the abbreviations  $p_{ij} = p_i + p_j$  and  $p_{ijk} = p_i + p_j + p_k$  and similarly for  $q$  later.

<sup>2</sup>We use the abbreviations  $s_{ij} = q_{ij}^2$ ,  $S_{ij} = p_{ij}^2$ .



where  $\mathcal{P}_{11111}$  is the Baikov polynomial of  $G_{11111}$  and  $\tilde{G}_{11111}$  is the integrand of  $G_{11111}$ . By studying the maximal cut of (6.6) in the Baikov representation [88], we can see that it has the desired properties of being pure and universally transcendental. This result is a strong indicator that the uncut (6.6) will satisfy a canonical differential equation. This is due to the fact that as shown in [40], since cut and uncut integrals satisfy the same system of IBP identities and hence the same system of differential equations, if one is looking for a system of canonical differential equations, then the same canonical differential equations have to be satisfied both by the cut and the uncut integrals. Therefore, a pure master integral of uniform weight that satisfies a canonical differential equation, has to preserve these properties on its maximal cut. Thus, when one has identified an integral, or a combination of integrals, which in its maximal cut is expressed in terms of pure functions of uniform weight, then this integral, or combination of integrals, is a strong candidate for an element of the desired pure basis.

In [80], a pure basis for the pentagon family with one off-shell leg is given in the ancillary files. The top sector basis element (6.6) is the same as the one given in [80], albeit in a different notation.

For convenience we choose to express our pure basis in terms of specific FI in the form

$$\mathbf{g} = \mathbf{T}\mathbf{G} \quad (6.7)$$

where  $\mathbf{g}$  is the pure basis,  $\mathbf{G}$  is our specific choice of FI and  $\mathbf{T}$  is the matrix that connects the two bases. The pure basis  $\mathbf{g}$  is

$$g_1 = x\epsilon S_{51} G_{0,2,0,0,1} \quad (6.8)$$

$$g_2 = x\epsilon ((x-1)S_{12} + S_{34}) G_{0,0,2,0,1} \quad (6.9)$$

$$g_3 = x^2\epsilon S_{12} G_{2,0,1,0,0} \quad (6.10)$$

$$g_4 = \epsilon S_{45} G_{2,0,0,1,0} \quad (6.11)$$

$$g_5 = \epsilon (xS_{23} - xS_{45} + S_{45}) G_{0,2,0,1,0} \quad (6.12)$$

$$g_6 = (x-1)\epsilon (xS_{12} - S_{45}) G_{0,0,2,1,0} \quad (6.13)$$

$$g_7 = x^3\epsilon^2 S_{12} S_{51} G_{1,1,1,0,1} \quad (6.14)$$

$$g_8 = x\epsilon^2 S_{45} S_{51} G_{1,1,0,1,1} \quad (6.15)$$

$$g_9 = x\epsilon^2 ((x-1)S_{12} + S_{34}) S_{45} G_{1,0,1,1,1} \quad (6.16)$$

$$g_{10} = x\epsilon^2 (-xS_{23}S_{34} + (x-1)S_{45}S_{34} - (x-1)S_{45}S_{51} + (x-1)S_{12}(x(-S_{23} + S_{45} + S_{51}) - S_{45})) G_{0,1,1,1,1} \quad (6.17)$$

$$g_{11} = x\epsilon^2 (S_{12} - S_{45}) G_{1,0,1,1,0} \quad (6.18)$$

$$g_{12} = x^2\epsilon^2 S_{12} (xS_{23} - xS_{45} + S_{45}) G_{1,1,1,1,0} \quad (6.19)$$

$$g_{13} = \frac{x\epsilon^2}{32\sqrt{\hat{\Delta}}} \left( A_1 G_{0,1,1,1,1} + A_2 G_{1,0,1,1,1} + A_3 G_{1,1,0,1,1} + A_4 G_{1,1,1,0,1} + A_5 G_{1,1,1,1,0} + A_6 G_{1,1,1,1,1} \right) \quad (6.20)$$

with

$$\hat{\Delta} = S_{12}^2 (S_{23} - S_{51})^2 + (S_{23}S_{34} + S_{45}(S_{51} - S_{34}))^2 + 2S_{12} (S_{34}S_{45}S_{23} + (S_{34} + S_{45})S_{51}S_{23} - S_{23}^2S_{34} + S_{45}(S_{34} - S_{51})S_{51}) \quad (6.21)$$

and

$$A_1 = (S_{12}S_{23} - S_{34}S_{23} + S_{34}S_{45} - (S_{12} + S_{45})S_{51}) \times (S_{34}(S_{23}x - S_{45}x + S_{45}) + S_{45}S_{51}(x-1) - S_{12}(x-1)((-S_{23} + S_{45} + S_{51})x - S_{45})) \quad (6.22)$$

$$A_2 = S_{45}(S_{34}(S_{23}S_{34} + S_{45}(S_{51} - S_{34})) - S_{12}^2(S_{23} - S_{51})(x-1))$$

$$+ S_{12} (S_{23}S_{34}(x-2) + S_{34}(-(S_{45} + 2S_{51})x + S_{45} + S_{51}) - S_{45}S_{51}(x-1)) \quad (6.23)$$

$$A_3 = -S_{45}S_{51} (S_{12} (S_{23}(2x-1) - 2(S_{45} + S_{51})x + 2S_{45} + S_{51}) + S_{23}S_{34} + S_{45}(S_{51} - S_{34})) \quad (6.24)$$

$$A_4 = S_{12}S_{51}(-x) (S_{23}S_{34}x - S_{45}S_{34}(x-2) + 2S_{12}S_{45}(x-1) + S_{45}S_{51}(x-2) + S_{12}(S_{51} - S_{23})x) \quad (6.25)$$

$$A_5 = S_{12}x(S_{34}S_{23}^2x + S_{45}^2(S_{34} - S_{51})(x-1) + S_{23}S_{45}(-2S_{34}x + S_{51}(x-2) + S_{34}) + S_{12}(S_{23}^2(-x) + (S_{45} + S_{51})S_{23}x + S_{45}S_{51}(x-1) - S_{45}S_{23})) \quad (6.26)$$

$$A_6 = -2S_{12}S_{45}S_{51}x (S_{34}(S_{23}x - S_{45}x + S_{45}) + S_{45}S_{51}(x-1) - S_{12}(x-1)((-S_{23} + S_{45} + S_{51})x - S_{45})). \quad (6.27)$$

The particular choice of FI in terms of which the above pure basis is written is the following

$$\mathbf{G} = \{G_{0,2,0,0,1}, G_{0,0,2,0,1}, G_{2,0,1,0,0}, G_{2,0,0,1,0}, G_{0,2,0,1,0}, G_{0,0,2,1,0}, G_{1,1,1,0,1}, G_{1,1,0,1,1}, G_{1,0,1,1,1}, G_{0,1,1,1,1}, G_{1,0,1,1,0}, G_{1,1,1,1,0}, G_{1,1,1,1,1}\}. \quad (6.28)$$

## 6.3 Results

The ultimate check that a candidate pure basis of MI has the desired properties is the derivation of its differential equation [42]. In the SDE approach [38], we derive differential equations with respect to the dimensionless parameter  $x$ , regardless of the number of scales of the problem. In this particular case, the candidate pure basis which was constructed in the previous section leads to the following canonical differential equation

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{i=1}^{11} \frac{\mathbf{M}_i}{x - l_i} \right) \mathbf{g} \quad (6.29)$$

where  $\mathbf{g}$  is the array of 13 pure MI,  $\mathbf{M}_i$  are the residue matrices which consist solely of rational numbers and  $l_i$  are the letters of the alphabet. The alphabet of the pentagon family with one off-shell leg has the following 11 letters,

$$\begin{aligned} l_1 &\rightarrow 0, l_2 \rightarrow \frac{S_{12} - S_{34}}{S_{12}}, l_3 \rightarrow \frac{S_{45}}{S_{45} - S_{23}}, l_4 \rightarrow 1, l_5 \rightarrow \frac{S_{45}}{S_{12}}, l_6 \rightarrow \frac{S_{12} - S_{34} + S_{51}}{S_{12}}, \\ l_7 &\rightarrow \frac{S_{45}}{-S_{23} + S_{45} + S_{51}}, l_8 \rightarrow \frac{S_{45}}{S_{34} + S_{45}}, l_9 \rightarrow \frac{S_{12} + S_{23}}{S_{12}}, \\ l_{10} &\rightarrow \frac{\sqrt{\Delta} + S_{12}S_{23} - S_{23}S_{34} - 2S_{12}S_{45} + S_{34}S_{45} - S_{12}S_{51} - S_{45}S_{51}}{2S_{12}(S_{23} - S_{45} - S_{51})}, \\ l_{11} &\rightarrow \frac{-\sqrt{\Delta} + S_{12}S_{23} - S_{23}S_{34} - 2S_{12}S_{45} + S_{34}S_{45} - S_{12}S_{51} - S_{45}S_{51}}{2S_{12}(S_{23} - S_{45} - S_{51})} \end{aligned} \quad (6.30)$$

with  $\Delta$  being

$$\begin{aligned} \Delta &= (S_{23}S_{34} + S_{45}(S_{51} - S_{34}) + S_{12}(-S_{23} + 2S_{45} + S_{51}))^2 \\ &\quad - 4S_{12}S_{45}(S_{12} - S_{34} + S_{51})(-S_{23} + S_{45} + S_{51}). \end{aligned} \quad (6.31)$$

Notice that here we follow [60], [81], [82] for the definition of the letters of the alphabet, which is different from the standard notation [45]–[47]. Usually the so-called d log form of a system of canonical differential equations is given as  $d\mathbf{g}(\vec{x}, \epsilon) = \epsilon \left( \sum_i \mathbf{M}_i d \log W_i(\vec{x}) \right) \mathbf{g}(\vec{x}, \epsilon)$ , where the alphabet  $W_i(\vec{x})$  is in terms of rational or algebraic functions of the independent variables. The standard d log form is equivalent to (6.29) for  $W_i(\vec{x}) = x - l_i$ .

This differential equation can be solved through recursive iterations up to the desired order in the dimensional regulator  $\epsilon$ . The only further input that is required are the boundary terms. In the SDE approach, we choose as a lower integration boundary  $x = 0$ , so that the result can be expressed directly in terms of GPLs. Thus the necessary boundary terms are given by the limit  $x \rightarrow 0$  of our chosen basis of MI.

Using the methods described in chapter 3, we define the *resummation matrix*  $\mathbf{R}$  as follows

$$\mathbf{R} = \mathbf{S}e^{\mathbf{D}\log(x)}\mathbf{S}^{-1} \quad (6.32)$$

where  $\mathbf{D}$ ,  $\mathbf{S}$  are defined through the Jordan decomposition<sup>3</sup> of the residue matrix corresponding to the letter  $\{0\}$ ,  $\mathbf{M}_1$ ,

$$\mathbf{M}_1 = \mathbf{S}\mathbf{D}\mathbf{S}^{-1} \quad (6.33)$$

Furthermore, using the expansion-by-regions method [51] we obtain information for the  $x \rightarrow 0$  limit of the FI in terms of which we express the pure basis of MI (6.7),

$$G_i = \sum_j x^{b_j+a_j\epsilon} G_i^{(b_j+a_j\epsilon)}. \quad (6.34)$$

where  $a_j$  and  $b_j$  are integers and  $G_i$  are the individual members of the basis  $\mathbf{G}$  of FI in (6.7), by making use of the publicly available FIESTA4 [58] code. As explained in chapter 3, we can construct the relation

$$\mathbf{R}\mathbf{b} = \lim_{x \rightarrow 0} \mathbf{T}\mathbf{G} \Big|_{\mathcal{O}(x^{0+a_j\epsilon})} \quad (6.35)$$

where  $\mathbf{b} = \sum_{i=0}^n \epsilon^i \mathbf{b}_0^{(i)}$  are the boundary terms that we need to compute. The right-hand-side of (6.35) implies that, apart from the terms  $x^{a_i\epsilon}$  coming from (6.34), we expand around  $x = 0$ , keeping only terms of order  $x^0$ . From (6.35) we can straightforwardly obtain all but one boundary terms without any further computation. This is due to the fact that all but one boundary terms are either given in terms of two-point functions or zero. The seventh basis element requires the computation of the leading region for  $G_{11101}$  which corresponds to  $G_7^{-3-2\epsilon}$  in the notation of (6.34). Through its Feynman parametrization this region can be computed in terms of a hypergeometric function. All boundary terms in closed form are as follows

$$\mathbf{b}_1 = \frac{e^{\gamma_E\epsilon} (-S_{51})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.36)$$

$$\mathbf{b}_2 = \frac{e^{\gamma_E\epsilon} (S_{12} - S_{34})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.37)$$

$$\mathbf{b}_3 = \frac{e^{\gamma_E\epsilon} (-S_{12})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.38)$$

$$\mathbf{b}_4 = \frac{e^{\gamma_E\epsilon} (-S_{45})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.39)$$

$$\mathbf{b}_5 = \frac{e^{\gamma_E\epsilon} (-S_{45})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.40)$$

$$\mathbf{b}_6 = \frac{e^{\gamma_E\epsilon} (-S_{45})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.41)$$

$$\mathbf{b}_7 = - \frac{e^{\gamma_E\epsilon} \epsilon (-S_{12})^{-\epsilon} \Gamma(-\epsilon)^2 \Gamma(\epsilon+1) {}_2F_1 \left( 1, -\epsilon; 1-\epsilon; \frac{S_{12}-S_{34}+S_{51}}{S_{51}} \right)}{\Gamma(-2\epsilon)} \quad (6.42)$$

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<sup>3</sup>For an earlier use of the Jordan decomposition method see also [67], [68]. We thank Prof. P. Mastrolia for bringing these references to our attention.

$$b_8 = \frac{2e^{\gamma_E \epsilon} (-S_{51})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.43)$$

$$b_9 = \frac{e^{\gamma_E \epsilon} (-S_{12})^{-\epsilon} (2(-S_{12})^\epsilon - (S_{12} - S_{34})^\epsilon) (S_{12} - S_{34})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.44)$$

$$b_{10} = \frac{2e^{\gamma_E \epsilon} (S_{12} - S_{34})^{-\epsilon} ((S_{12} - S_{34})^\epsilon - (-S_{51})^\epsilon) (-S_{51})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.45)$$

$$b_{11} = 0 \quad (6.46)$$

$$b_{12} = \frac{e^{\gamma_E \epsilon} (-S_{12})^{-\epsilon} \Gamma(1-\epsilon)^2 \Gamma(\epsilon+1)}{\Gamma(1-2\epsilon)} \quad (6.47)$$

$$b_{13} = 0. \quad (6.48)$$

Using standard algorithms as implemented in e.g. `Mathematica`, and with the additional help of the public package `HypExp` [56] for the series expansion of the hypergeometric function, we can obtain exact expressions for all boundary terms up to arbitrary order in  $\epsilon$ . Therefore we can trivially obtain solutions of (6.29) in terms of GPLs up to arbitrary weight.

In this particular work, we present explicit results up to weight four, which can be written in compact form as

$$\begin{aligned} \mathbf{g} = & \epsilon^0 \mathbf{b}_0^{(0)} + \epsilon \left( \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(0)} + \mathbf{b}_0^{(1)} \right) \\ & + \epsilon^2 \left( \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(0)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(1)} + \mathbf{b}_0^{(2)} \right) \\ & + \epsilon^3 \left( \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(1)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(2)} + \mathbf{b}_0^{(3)} \right) \\ & + \epsilon^4 \left( \sum \mathcal{G}_{abcd} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{M}_d \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(1)} \right. \\ & \left. + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(2)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(3)} + \mathbf{b}_0^{(4)} \right) \end{aligned} \quad (6.49)$$

$$\mathcal{G}_{ab\dots} := \mathcal{G}(l_a, l_b, \dots; x)$$

with the generalisation to higher orders in  $\epsilon$  being straightforward.

## 6.4 Massless pentagon family

Using the methods described in chapter 3, we can readily obtain a pure basis of 11 MI for the massless pentagon family from the  $x \rightarrow 1$  limit of (6.49). The results are by construction in terms of GPLs up to weight four, however following the arguments of the last section, we can obtain results in terms of GPLs of arbitrary weight.

To be more specific, the  $x \rightarrow 1$  limit of the solution for the pentagon with one off-shell leg can be given by the following formula

$$\mathbf{g}_{x \rightarrow 1} = \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc} \quad (6.50)$$

with  $\tilde{\mathbf{R}}_0$  being a purely numerical matrix which is constructed from the resummation matrix

$$\tilde{\mathbf{R}} = \tilde{\mathbf{S}} e^{\epsilon \tilde{\mathbf{D}} \log(1-x)} \tilde{\mathbf{S}}^{-1} \quad (6.51)$$

after setting all terms of  $(1-x)^{a_i \epsilon}$  in  $\tilde{\mathbf{R}}$  equal to zero<sup>4</sup>. The matrices  $\tilde{\mathbf{S}}, \tilde{\mathbf{D}}$  are constructed through the Jordan decomposition of the residue matrix corresponding to the letter  $\{1\}$ , which in this case is  $\mathbf{M}_4$ , i.e.  $\mathbf{M}_4 = \tilde{\mathbf{S}} \tilde{\mathbf{D}} \tilde{\mathbf{S}}^{-1}$ .

<sup>4</sup>Here  $a_i = \{-1, 0\}$  are the eigenvalues of  $\mathbf{M}_4$ .

The second input in (6.50),  $\mathbf{g}_{trunc}$ , is just the regular part of the solution (6.49) at  $x \rightarrow 1$  where we have set  $x = 1$  explicitly [60].

## 6.5 Numerical checks

We have performed various numerical checks of our results. Firstly, for the pentagon family with one leg off-shell we compared our results with `pySecDec` [57] for the Euclidean point

$$S_{12} \rightarrow -2, S_{23} \rightarrow -3, S_{34} \rightarrow -5, S_{45} \rightarrow -7, S_{51} \rightarrow -11, x \rightarrow \frac{1}{4} \quad (6.52)$$

For numerical results in physical regions, we refer to the detailed discussion in section 7.5 of chapter 7. Using the methods described therein, we managed to analytically continue our results for the pentagon family with one-off shell leg and compare with the numerical results of [80] for all the physical points that are provided there.

For the massless pentagon family, we have performed numerical checks against `pySecDec` [57] for the Euclidean point

$$S_{12} \rightarrow -2, S_{23} \rightarrow -3, S_{34} \rightarrow -5, S_{45} \rightarrow -7, S_{51} \rightarrow -11 \quad (6.53)$$

For the numerical evaluation of the relevant GPLs, we utilised `Ginac` [71], [89] through the `Mathematica` interface provided by `PolyLogTools` [66]. The latter package was also used extensively for the manipulation of the resulting GPLs. For all checks that were carried out we report excellent agreement.

## 6.6 Conclusions

In this chapter we have presented the analytic calculation of pentagon integrals with up to one off-shell leg in  $d = 4 - 2\epsilon$  space-time dimensions in terms of GPLs of higher weights. We constructed a candidate pure basis of MI for the pentagon family with one off-shell leg following the ideas of [80], [85] and we verified that it satisfies a canonical differential equation [42] in the SDE approach [38].

We have demonstrated that all relevant boundary terms are either zero or given in closed form. This allows one to straightforwardly obtain analytic solutions of the canonical differential equation for the pentagon family with one off-shell leg in terms of GPLs [44] of arbitrary transcendental weight. As a by-product of this result, we were able to obtain analytic expressions for the massless pentagon family in terms of GPLs, as well as a pure basis of MI, after taking the  $x \rightarrow 1$  limit of the former result in an algorithmic way [60].

# Chapter 7

## Two-loop planar Penta-Box master integrals with one massive leg

We present analytic expressions in terms of polylogarithmic functions for all three families of planar two-loop five-point Master Integrals with one off-shell leg. The calculation is based on the Simplified Differential Equations approach. The results are relevant to the study of many  $2 \rightarrow 3$  scattering processes of interest at the LHC, especially for the leading-color  $W + 2$  jets production. This chapter is based on original research done in collaboration with D.D. Canko and C. G. Papadopoulos and appeared first in [82].

### 7.1 Introduction

As we advance on the third decade of the 21st century, the established Standard Model of Particle Physics faces serious and interesting challenges from the domains of Cosmology and Astrophysics. One of those challenges for example is the particle nature of Dark Matter, and whether its dynamics can be described through the introduction of one or several new particles, thus imposing the need to extend our understanding of Particle Physics. The major experiments of Particle Physics however, spearheaded by the LHC program at CERN, have yet to reveal any clear signs of New Physics that would require the extension of the established Standard Model.

To make progress in the current situation, a *precision* [6] program has been initiated, in part because it is clear by now that any New Physics at the LHC data will appear in the form of small deviations from theoretical predictions, but also due to the increased precision of the accumulated experimental data. Thus the need arises for equally precise theoretical predictions, in order to be able to exploit the full discovery potential of the LHC and its future High Luminosity upgrade.

From a theoretical standpoint, it is estimated that the LHC Run 3 and the High Luminosity Run scheduled to commence after it, will require at least Next-to-Next-to-Leading-Order (NNLO) corrections for the QCD dominated processes [90]–[92]. A major ingredient of these higher order perturbative corrections is the calculation of the relevant scattering amplitudes for specific scattering processes, and within these amplitudes, complicated two-loop Feynman Diagrams need to be computed. Through the Feynman rules of quantum field theory, we can relate these two-loop Feynman Diagrams to two-loop Feynman Integrals, which are the topic of this contribution.

The current frontier in two-loop calculations is in  $2 \rightarrow 3$  scattering processes. For massless external particles and massless internal propagators, all planar [81] and non-planar Feynman Integrals have been calculated [93]. First results for  $2 \rightarrow 3$  scattering processes involving one massive external particle for planar topologies were presented in [81] a few years ago, with

the full list of all two-loop planar Feynman Integrals relevant to  $2 \rightarrow 3$  scattering processes with one off-shell leg appearing recently using a numerical approach [80]. Here, we will present analytic results for all planar two-loop Feynman Integrals with one off-shell leg in terms of polylogarithmic functions up to transcendental weight four [82].

## 7.2 Integral families and kinematics

There are three families of Master Integrals, labelled as  $P_1$ ,  $P_2$  and  $P_3$ , see Fig. 7.1, associated to planar two-loop five-point amplitudes with one off-shell leg. We adopt the definition of the scattering kinematics following [80], where external momenta  $q_i$ ,  $i = 1 \dots 5$  satisfy  $\sum_1^5 q_i = 0$ ,  $q_1^2 \equiv p_{1s}$ ,  $q_i^2 = 0$ ,  $i = 2 \dots 5$ , and the six independent invariants are given by  $\{q_1^2, s_{12}, s_{23}, s_{34}, s_{45}, s_{15}\}$ , with  $s_{ij} := (q_i + q_j)^2$ .

In the SDE approach [38] the momenta are re-parametrized by introducing a dimensionless variable  $x$ , as follows

$$q_1 \rightarrow p_{123} - xp_{12}, \quad q_2 \rightarrow p_4, \quad q_3 \rightarrow -p_{1234}, \quad q_4 \rightarrow xp_1 \quad (7.1)$$

where the new momenta  $p_i$ ,  $i = 1 \dots 5$  satisfy now  $\sum_1^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 1 \dots 5$ , whereas  $p_{i\dots j} := p_i + \dots + p_j$ . The set of independent invariants is given by  $\{S_{12}, S_{23}, S_{34}, S_{45}, S_{51}, x\}$ , with  $S_{ij} := (p_i + p_j)^2$ . The explicit mapping between the two sets of invariants is given by

$$\begin{aligned} q_1^2 &= (1-x)(S_{45} - S_{12}x), \quad s_{12} = (S_{34} - S_{12}(1-x))x, \quad s_{23} = S_{45}, \quad s_{34} = S_{51}x, \\ s_{45} &= S_{12}x^2, \quad s_{15} = S_{45} + (S_{23} - S_{45})x \end{aligned} \quad (7.2)$$

and as usual the  $x = 1$  limit corresponds to the on-shell kinematics.

The corresponding Feynman Integrals are defined through

$$\begin{aligned} G_{a_1 \dots a_{11}}^{P_1} &:= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 + q_1)^{2a_2} (k_1 + q_{12})^{2a_3} (k_1 + q_{123})^{2a_4}} \\ &\times \frac{1}{k_2^{2a_5} (k_2 + q_{123})^{2a_6} (k_2 + q_{1234})^{2a_7} (k_1 - k_2)^{2a_8} (k_1 + q_{1234})^{2a_9} (k_2 + q_1)^{2a_{10}} (k_2 + q_{12})^{2a_{11}}}, \end{aligned} \quad (7.3)$$

$$\begin{aligned} G_{a_1 \dots a_{11}}^{P_2} &:= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 - q_{1234})^{2a_2} (k_1 - q_{234})^{2a_3} (k_1 - q_{34})^{2a_4}} \\ &\times \frac{1}{k_2^{2a_5} (k_2 - q_{34})^{2a_6} (k_2 - q_4)^{2a_7} (k_1 - k_2)^{2a_8} (k_2 - q_{1234})^{2a_9} (k_2 - q_{234})^{2a_{10}} (k_1 - q_4)^{2a_{11}}}, \end{aligned} \quad (7.4)$$

$$\begin{aligned} G_{a_1 \dots a_{11}}^{P_3} &:= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 + q_2)^{2a_2} (k_1 + q_{23})^{2a_3} (k_1 + q_{234})^{2a_4}} \\ &\times \frac{1}{k_2^{2a_5} (k_2 + q_{234})^{2a_6} (k_2 - q_1)^{2a_7} (k_1 - k_2)^{2a_8} (k_1 - q_1)^{2a_9} (k_2 + q_2)^{2a_{10}} (k_2 + q_{23})^{2a_{11}}}, \end{aligned} \quad (7.5)$$

where  $q_{i\dots j} := q_i + \dots + q_j$ .

The  $P_1$  family consists of 74 Master integrals. For  $P_2$  and  $P_3$  the corresponding numbers are 75 and 86. This can easily be verified using standard IBP reduction software, such as FIRE6 [28] and KIRA [29], [94]. The top-sector integrals are shown in Fig. 7.1.

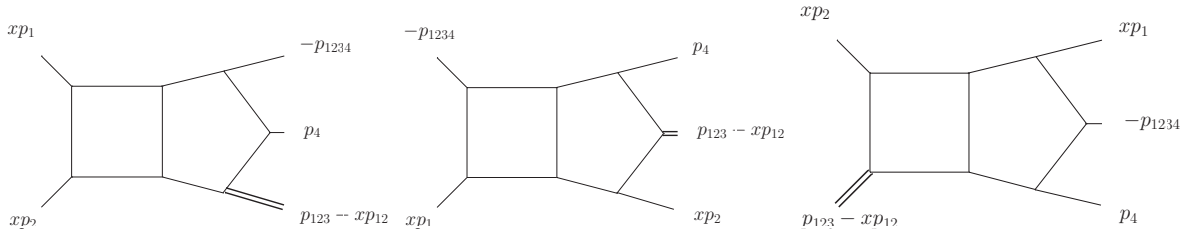


Figure 7.1: The two-loop diagrams representing the top-sector of the planar pentabox family  $P_1$ ,  $P_2$  and  $P_3$ . All external momenta are incoming.

### 7.3 Canonical basis and Differential Equations

In order to express all integrals given by Eqs.(7.3-7.5), the easiest way is to define a basis that satisfy a canonical differential equation. By basis we mean a combination of Feynman Integrals with coefficients depending on the set of invariants and the dimensionality of space-time  $d = 4 - 2\epsilon$ . Let us assume that such a basis is known, then the DE is written in general as

$$d\vec{g} = \epsilon \sum_a d \log(W_a) \tilde{M}_a \vec{g} \quad (7.6)$$

where  $\vec{g}$  represents a vector containing all elements of the canonical basis,  $W_a$  are functions of the kinematics and  $\tilde{M}_a$  are matrices independent of the kinematical invariants, whose matrix elements are pure rational numbers. Notice that Eq. (7.6) is a multi-variable equation and in the case under consideration the differentiation is understood with respect to the six-dimensional array of independent kinematical invariants,  $\{q_1^2, s_{12}, s_{23}, s_{34}, s_{45}, s_{15}\}$ . Since  $W_a$  are in general algebraic functions of the kinematical invariants a straightforward integration of Eq. (7.6) in terms of generalized poly-logarithms is not an easy task.

In the SDE approach though, Eq. 7.6 takes the much simpler form

$$\frac{d\vec{g}}{dx} = \epsilon \sum_b \frac{1}{x - l_b} M_b \vec{g} \quad (7.7)$$

where  $M_b$  are again rational matrices independent of the kinematics, and the so-called letters,  $l_b$ , are independent of  $x$ , depending only on the five invariants,  $\{S_{12}, S_{23}, S_{34}, S_{45}, S_{51}\}$ . Notice that the number of letters in  $x$  is generally smaller than the number of letters in Eq.(7.6). Since the Eq. (7.7) is a Fuchsian system of ordinary differential equations, it is straightforwardly integrated in terms of Goncharov poly-logarithms,  $\mathcal{G}(l_{b_1}, l_{b_2}, \dots; x)$ .

Over the last years much effort has been devoted to construct the canonical basis, or at least an educated guess of it, and then verify the form of Eq. 7.6 through standard differentiation and IBP reduction. We refer to section 4 of reference [80] for a thorough discussion of relevant work in the literature. In principle the knowledge of the canonical basis is enough within the SDE approach to derive the form of the corresponding canonical differential equation, Eq. (7.7), by explicitly differentiating with respect to  $x$  and using IBP identities to express the resulting combinations of Feynman integrals in terms of basis elements. In fact, as we will show later, since the matrices entering in Eq. (7.7) are independent of the kinematics, one can use solutions of IBP identities derived by assigning integer values to the kinematics, except  $x$ . Using nowadays packages such as FIRE6 and KIRA the above-mentioned IBP-reduction becomes a computationally trivial exercise. Notice that there is no need to use rational reconstruction methods, as far as the derivation of Eq. (7.7) is concerned.

Knowing from reference [80], the explicit form of the matrices  $\tilde{M}_a$  and of the letters  $W_a$  in terms of the variables  $p_{1s}, s_{12}, s_{23}, s_{34}, s_{45}, s_{15}$  ( $p_{1s} \equiv q_1^2$ ), in Eq. (7.6), we simply derive the data



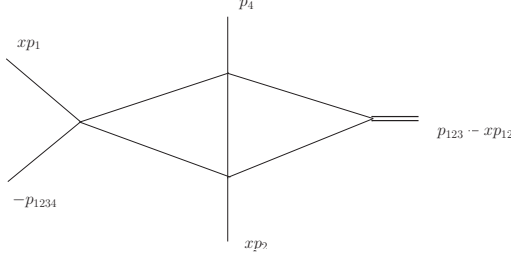


Figure 7.2: The two-loop diagram representing the decoupling basis element.

needed in Eq. (7.7), based on the following identity,

$$\sum_a \frac{d \log(W_a)}{dx} \tilde{M}_a \equiv \sum_b \frac{1}{x - l_b} M_b \quad (7.8)$$

making use of Eq. (7.2). For  $P_2$  and  $P_3$  families Eq. (7.8) is applicable after eliminating a special element basis whose leading singularity is proportional to a non-rationalizable square root in terms of  $x$ . The corresponding integral is shown in Fig. 7.2 and it is the same for the two families. It is already known from the double-box families with two off-shell legs [95],  $P_{23}$ . Since our task is to evaluate all basis elements up to  $\mathcal{O}(\epsilon^4)$  and since the basis element expansion of the above integral starts at  $\mathcal{O}(\epsilon^4)$ , it effectively decouples from the differential equation Eq. (7.7).

The alphabet for the three planar families considered in this chapter consists of 32 letters in total, namely

$$\begin{aligned} l_1 &\rightarrow 0, l_2 \rightarrow 1, l_3 \rightarrow \frac{S_{12} + S_{23}}{S_{12}}, l_4 \rightarrow 1 - \frac{S_{34}}{S_{12}}, l_5 \rightarrow \frac{S_{45}}{S_{12}}, l_6 \rightarrow -\frac{S_{45}}{S_{23} - S_{45}}, \\ l_7 &\rightarrow \frac{S_{45} - S_{23}}{S_{12}}, l_8 \rightarrow \frac{S_{45}}{S_{34} + S_{45}}, l_9 \rightarrow -\frac{S_{51}}{S_{12}}, l_{10} \rightarrow \frac{S_{12} - S_{34} + S_{51}}{S_{12}}, \\ l_{11} &\rightarrow \frac{S_{45}}{-S_{23} + S_{45} + S_{51}}, l_{12} \rightarrow \frac{\sqrt{\Delta_1} + S_{12}S_{23} - S_{23}S_{34} + S_{34}S_{45} - S_{12}S_{51} - S_{45}S_{51}}{2S_{12}S_{23} + 2S_{12}S_{34} - 2S_{12}S_{51}}, \\ l_{13} &\rightarrow \frac{\sqrt{\Delta_1} + S_{12}S_{23} - S_{23}S_{34} - 2S_{12}S_{45} + S_{34}S_{45} - S_{12}S_{51} - S_{45}S_{51}}{2S_{12}S_{23} - 2S_{12}S_{45} - 2S_{12}S_{51}}, \\ l_{14} &\rightarrow \frac{-\sqrt{\Delta_1} - S_{23}S_{34} + S_{34}S_{45} - S_{45}S_{51} - S_{12}(S_{51} - S_{23})}{2S_{12}(S_{23} + S_{34} - S_{51})}, \\ l_{15} &\rightarrow \frac{-\sqrt{\Delta_1} - S_{23}S_{34} + S_{34}S_{45} - S_{45}S_{51} - S_{12}(-S_{23} + 2S_{45} + S_{51})}{2S_{12}(S_{23} - S_{45} - S_{51})}, l_{16} \rightarrow \frac{S_{12}S_{45} - \sqrt{\Delta_2}}{S_{12}S_{34} + S_{12}S_{45}}, \\ l_{17} &\rightarrow \frac{\sqrt{\Delta_2} + S_{12}S_{45}}{S_{12}S_{34} + S_{12}S_{45}}, l_{18} \rightarrow \frac{\sqrt{\Delta_3} + S_{12}S_{23} - S_{23}S_{34} - S_{12}S_{45} + S_{34}S_{45} - S_{12}S_{51} - S_{45}S_{51}}{2S_{12}S_{23} - 2S_{12}S_{45} - 2S_{12}S_{51}}, \\ l_{19} &\rightarrow \frac{-\sqrt{\Delta_3} - S_{23}S_{34} + S_{34}S_{45} - S_{45}S_{51} - S_{12}(-S_{23} + S_{45} + S_{51})}{2S_{12}(S_{23} - S_{45} - S_{51})}, l_{20} \rightarrow \frac{S_{45}}{S_{12} - S_{34}}, \\ l_{21} &\rightarrow -\frac{S_{45}}{S_{51}}, l_{22} \rightarrow \frac{-\sqrt{\Delta_1} - S_{12}S_{23} + S_{23}S_{34} - S_{34}S_{45} + S_{12}S_{51} + S_{45}S_{51}}{2S_{12}S_{51}}, \\ l_{23} &\rightarrow \frac{\sqrt{\Delta_1} + S_{23}S_{34} - S_{34}S_{45} + S_{45}S_{51} + S_{12}(S_{51} - S_{23})}{2S_{12}S_{51}}, \\ l_{24} &\rightarrow \frac{-\sqrt{\Delta_4} + S_{23}S_{34} - S_{34}S_{45} + S_{45}S_{51} + S_{12}(-S_{23} + S_{45} + S_{51})}{2S_{12}S_{51}}, \\ l_{25} &\rightarrow \frac{\sqrt{\Delta_4} + S_{23}S_{34} - S_{34}S_{45} + S_{45}S_{51} + S_{12}(-S_{23} + S_{45} + S_{51})}{2S_{12}S_{51}}, \end{aligned}$$

$$\begin{aligned}
l_{26} &\rightarrow \frac{-\sqrt{\Delta_1} + S_{23}S_{34} - S_{34}S_{45} + S_{45}S_{51} + S_{12}(-S_{23} + 2S_{45} + S_{51})}{2S_{12}(S_{12} - S_{34} + S_{51})}, \\
l_{27} &\rightarrow \frac{\sqrt{\Delta_1} + S_{23}S_{34} - S_{34}S_{45} + S_{45}S_{51} + S_{12}(-S_{23} + 2S_{45} + S_{51})}{2S_{12}(S_{12} - S_{34} + S_{51})}, \\
l_{28} &\rightarrow \frac{\sqrt{\Delta_5} + S_{12}S_{45}}{S_{12}(S_{45} - S_{23})}, l_{29} \rightarrow \frac{\sqrt{\Delta_5} - S_{12}S_{45}}{S_{12}(S_{23} - S_{45})}, l_{30} \rightarrow \frac{(S_{23} - S_{45})S_{45}}{S_{12}S_{23} + (S_{23} - S_{45})S_{45}}, \\
l_{31} &\rightarrow \frac{-2S_{45}^3 + 2S_{23}S_{45}^2 - S_{34}S_{45}^2 - S_{51}S_{45}^2 + S_{23}S_{34}S_{45} - S_{12}(S_{51} - S_{23})S_{45} - \sqrt{\Delta_6}}{2(S_{12}S_{23}(S_{34} + S_{45}) + (S_{23} - S_{45})S_{45}(S_{34} + S_{45}) - S_{12}S_{45}S_{51})}, \\
l_{32} &\rightarrow \frac{-2S_{45}^3 + 2S_{23}S_{45}^2 - S_{34}S_{45}^2 - S_{51}S_{45}^2 + S_{23}S_{34}S_{45} + S_{12}(S_{23} - S_{51})S_{45} + \sqrt{\Delta_6}}{2(S_{12}S_{23}(S_{34} + S_{45}) + (S_{23} - S_{45})S_{45}(S_{34} + S_{45}) - S_{12}S_{45}S_{51})} \quad (7.9)
\end{aligned}$$

with

$$\begin{aligned}
\Delta_1 &= S_{12}^2(S_{23} - S_{51})^2 + (S_{23}S_{34} + S_{45}(S_{51} - S_{34}))^2 \\
&\quad + 2S_{12}(S_{45}S_{51}S_{23} + S_{34}(S_{45} + S_{51})S_{23} - S_{23}^2S_{34} + S_{45}(S_{34} - S_{51})S_{51}), \quad (7.10)
\end{aligned}$$

$$\Delta_2 = S_{12}S_{34}S_{45}(-S_{12} + S_{34} + S_{45}), \quad (7.11)$$

$$\begin{aligned}
\Delta_3 &= S_{12}^2(-S_{23} + S_{45} + S_{51})^2 + (S_{23}S_{34} + S_{45}(S_{51} - S_{34}))^2 \\
&\quad - 2S_{12}(S_{23} - S_{45} - S_{51})(S_{23}S_{34} - S_{45}(S_{34} + S_{51})), \quad (7.12)
\end{aligned}$$

$$\begin{aligned}
\Delta_4 &= (S_{23}^2 - 2(S_{45} + S_{51})S_{23} + (S_{45} - S_{51})^2)S_{12}^2 + (S_{23}S_{34} + S_{45}(S_{51} - S_{34}))^2 \\
&\quad - 2(S_{34}S_{23}^2 + S_{45}S_{51}S_{23} - S_{34}(2S_{45} + S_{51})S_{23} + S_{45}(S_{34} - S_{51})(S_{45} - S_{51}))S_{12}, \quad (7.13)
\end{aligned}$$

$$\Delta_5 = S_{12}S_{23}(S_{12} + S_{23} - S_{45})S_{45}, \quad (7.14)$$

$$\Delta_6 = S_{45}^2\Delta_1. \quad (7.15)$$

Each family is characterised by a subset of the full set of letters. In  $P_1$  the following 19 letters appear,

$$\{l_1, l_2, l_3, l_4, l_5, l_6, l_7, l_8, l_9, l_{10}, l_{11}, l_{12}, l_{13}, l_{14}, l_{15}, l_{16}, l_{17}, l_{18}, l_{19}\}, \quad (7.16)$$

in  $P_2$  the following 25 letters appear,

$$\{l_1, l_2, l_3, l_4, l_5, l_6, l_7, l_8, l_9, l_{10}, l_{11}, l_{12}, l_{13}, l_{14}, l_{15}, l_{18}, l_{19}, l_{20}, l_{21}, l_{22}, l_{23}, l_{24}, l_{25}, l_{26}, l_{27}\}, \quad (7.17)$$

and finally in  $P_3$  the following 25 letters appear,

$$\{l_1, l_2, l_3, l_4, l_5, l_6, l_7, l_8, l_{10}, l_{11}, l_{13}, l_{15}, l_{20}, l_{21}, l_{22}, l_{23}, l_{24}, l_{25}, l_{26}, l_{27}, l_{28}, l_{29}, l_{30}, l_{31}, l_{32}\}. \quad (7.18)$$

## 7.4 Boundary conditions and analytic expressions

Obtaining boundary terms for the solution of the canonical SDE requires the computation of the  $x \rightarrow 0$  limit for all basis elements. Following the computational framework as described in chapter 3, we define the resummation matrix  $\mathbf{R}$  for each planar family. For families  $P_2$  and  $P_3$ , despite the fact that two basis elements effectively decouple and are already known in the literature, we calculate their boundary terms as well, since they contribute to other basis elements.

Through IBP reduction, we can express the pure basis  $\mathbf{g}$  in terms of a specific choice of MI  $\mathbf{G}$ ,

$$\mathbf{g} = \mathbf{T}\mathbf{G} \quad (7.19)$$

Using the method of expansion-by-regions, we can obtain information for the asymptotic behaviour of the Feynman integrals in terms of which we express the pure basis of Master integrals (7.19) in the limit  $x \rightarrow 0$ ,

$$G_i \underset{x \rightarrow 0}{=} \sum_j x^{b_j + a_j \epsilon} G_i^{(b_j + a_j \epsilon)} \quad (7.20)$$

where  $a_j$  and  $b_j$  are integers and  $G_i$  are the individual members of the basis  $\mathbf{G}$  of Feynman integrals in (7.19). We thus arrive at

$$\mathbf{Rb} = \lim_{x \rightarrow 0} \mathbf{TG} \Big|_{\mathcal{O}(x^{0+a_j \epsilon})} \quad (7.21)$$

where the right-hand side implies that, apart from the terms  $x^{a_i \epsilon}$  coming from (7.20), we expand around  $x = 0$ , keeping only terms of order  $x^0$ . Notice that since the left-hand side of the equation contains pure functions with rational coefficients that are independent of the underlying kinematics  $\vec{S} := \{S_{12}, S_{23}, S_{34}, S_{45}, S_{51}\}$ , the determination of the matrix  $\mathbf{T}$ , as a function of  $x$  and  $d$ , is based on solutions of IBP identities, using integer values for  $\vec{S}$ . This results to a significant reduction in complexity and CPU time, taking into account that several basis elements are given in terms of Baikov polynomials,  $\mu_{11}$ ,  $\mu_{22}$ ,  $\mu_{12}$ , and containing FI with up to fourth power of irreducible inverse propagators.

As indicated in chapter 3, Eq. (7.21) is a powerful framework allowing to determine all boundary constants  $\mathbf{b}$ . First of all in the case the left-hand side contains a logarithmic term in  $x$ , a set of linear relations between elements of the array  $\mathbf{b}$  are obtained by setting the coefficient of  $\log(x)$  to zero. Secondly, powers of  $x^{a \epsilon}$  that appear only in the left-hand side do also produce relations among elements of  $\mathbf{b}$ . These two sets of relations account for the determination of a significant part of the components of the boundary array. The last set of equations requires the determination of some regions of Master Integrals,  $G_i^{(j)}$ , in the limit  $x \rightarrow 0$ . Expressions of these integral-regions in terms of Feynman parameters are obtained using `SDExpandAsy` in `FIESTA4` [58]. Their calculation is straightforwardly achieved either by direct integration in Feynman-parameter space and then by using `HypExp` [55], [56] to expand the resulting  ${}_2F_1$  hypergeometric functions, or in a very few cases, by Mellin-Barnes techniques using the `MB` [96], [97], `MBSums` [98] and `XSummer` [99] packages<sup>1</sup>. All the boundary values are analytically expressed in terms of poly-logarithmic functions, namely logarithms and Goncharov poly-logarithms as functions of the reduced kinematical variables  $\{S_{12}, S_{23}, S_{34}, S_{45}, S_{51}\}$ .

Although the above described method is general and straightforward, in practice many of the components of  $\mathbf{b}$  are obtained by exploiting the known representations of the elements of the canonical basis as given in the double-box families [95], [100].

After obtaining all boundary terms, the solution of the canonical SDE can be written in the following compact form up to order  $\mathcal{O}(\epsilon^4)$

$$\begin{aligned} \mathbf{g} &= \epsilon^0 \mathbf{b}_0^{(0)} + \epsilon \left( \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(0)} + \mathbf{b}_0^{(1)} \right) \\ &+ \epsilon^2 \left( \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(0)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(1)} + \mathbf{b}_0^{(2)} \right) \\ &+ \epsilon^3 \left( \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(1)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(2)} + \mathbf{b}_0^{(3)} \right) \\ &+ \epsilon^4 \left( \sum \mathcal{G}_{abcd} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{M}_d \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(1)} \right) \end{aligned}$$

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<sup>1</sup>The in-house `Mathematica` package `Gsuite`, that automatically process the `MBSums` output through `XSummer`, written by A. Kardos, is used.

$$+ \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(2)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(3)} + \mathbf{b}_0^{(4)} \quad (7.22)$$

$$\mathcal{G}_{ab\dots} := \mathcal{G}(l_a, l_b, \dots; x).$$

In order to get an idea of the actual structure of the solutions, we give explicit results for the non-zero top-sector basis element for each family up to order  $\mathcal{O}(\epsilon^1)$ ,

$$g_{72}^{P1} = \frac{3}{2} + \epsilon \left[ \mathcal{G} \left( \frac{S_{45}}{S_{12}}; x \right) - \mathcal{G} \left( \frac{S_{12} - S_{34}}{S_{12}}; x \right) - 3\mathcal{G}(0; x) + \mathcal{G}(1; x) - \log(S_{12} - S_{34}) - 2\log(-S_{51}) \right], \quad (7.23)$$

$$g_{73}^{P2} = \epsilon \left[ 3\mathcal{G} \left( \frac{S_{12} + S_{23}}{S_{12}}; x \right) - 3\mathcal{G} \left( \frac{S_{12} - S_{34}}{S_{12}}; x \right) - 3\mathcal{G} \left( \frac{S_{45}}{S_{12}}; x \right) + 3\mathcal{G}(1; x) - 3\log(S_{12} - S_{34}) + 3\log(-S_{51}) \right], \quad (7.24)$$

$$g_{84}^{P3} = \frac{1}{2} + \epsilon \left[ \frac{5}{2}\mathcal{G} \left( \frac{S_{45}}{S_{12}}; x \right) - \frac{3}{2}\mathcal{G} \left( \frac{S_{12} - S_{34}}{S_{12}}; x \right) - \frac{5}{2}\mathcal{G} \left( -\frac{S_{45}}{S_{23} - S_{45}}; x \right) - 2\mathcal{G}(0; x) + \frac{5}{2}\mathcal{G}(1; x) - \log(-S_{12}) - \frac{3}{2}\log(S_{12} - S_{34}) + \frac{3}{2}\log(-S_{51}) \right]. \quad (7.25)$$

## 7.5 Numerical Results and Validation

In order to numerically evaluate the solution given in Eq. (7.22), Goncharov poly-logarithms up to weight 4 need to be computed. To understand the complexity of the expressions at hand, we present in Table 7.1, the number of poly-logarithmic functions entering in the solution. In parenthesis we give the corresponding number for the non-zero top-sector basis elements. The weight  $W=1 \dots 4$  is identified as the number of letters  $l_a$  in GP  $\mathcal{G}(l_a, \dots; x)$ .

Family	W=1	W=2	W=3	W=4
$P_1 (g_{72})$	17 (14)	116 (95)	690 (551)	2740 (2066)
$P_2 (g_{73})$	25 (14)	170 (140)	1330 (1061)	4950 (3734)
$P_3 (g_{84})$	22 (12)	132 (90)	1196 (692)	4566 (2488)

Table 7.1: Number of GPLs entering in the solution, as explained in the text.

The computation of GPLs is performed using their implementation in `Ginac`. This implementation is capable to evaluate the GPLs at an arbitrary precision. The computational cost to numerically evaluate a GPL function, depends of course on the number of significant digits required as well as on their weight and finally on their structure, namely how many of its letters, Eq. (7.7), satisfy  $l_b \in [0, x]$ . We refer to reference [71] for more details.

For the following Euclidean point

$$S_{12} \rightarrow -2, S_{23} \rightarrow -3, S_{34} \rightarrow -5, S_{45} \rightarrow -7, S_{51} \rightarrow -11, x \rightarrow \frac{1}{4} \quad (7.26)$$

all GPL functions with real letters are real, namely no letter is in  $[0, x]$ , and moreover the boundary terms are by construction all real. The result is given in Table 7.2 with timings, running the `GiNaC` Interactive Shell `ginsh`, given by 1.9, 3.3, and 2 seconds for  $P_1$ ,  $P_2$  and  $P_3$

$P_1$	$g_{72}$	$\epsilon^0$ : 3/2 $\epsilon^1$ : -2.2514604753379400332169314784961 $\epsilon^2$ : -17.910593443812320786572184851867 $\epsilon^3$ : -26.429770706459534336624681550003 $\epsilon^4$ : 21.437938934510558345847354772412
$P_2$	$g_{73}$	$\epsilon^1$ : 2.8124788185742741402751457351382 $\epsilon^2$ : 5.4813042746593704203645729908938 $\epsilon^3$ : 11.590234540689191439870956817546 $\epsilon^4$ : -5.9962816226829136730734255754596
$P_3$	$g_{84}$	$\epsilon^0$ : 1/2 $\epsilon^1$ : 3.2780415861887284967738281876762 $\epsilon^2$ : 0.11455863130537720411162743574627 $\epsilon^3$ : -16.979642659429606120982671925458 $\epsilon^4$ : -48.101985355625914648042310964575

Table 7.2: Numerical results for the non-zero top sector element of each family with 32 significant digits.

respectively and for a precision of 32 significant digits. As can be seen also from Table 7.1, the timing for the evaluation of all GPs in a family, is of the same order as its top-sector element.

In order to obtain results for scattering kinematics, we need to properly analytically continue the GPs and logarithms involved in our solution. In general, the kinematic variables  $p_{1s}$  and  $s_{ij}$ , acquire an infinitesimal imaginary part [101]. This means that  $S_{ij}$  as well as the parameter  $x$ , through Eq. (7.1), acquire also an infinitesimal imaginary part, i.e.  $S_{ij} \rightarrow S_{ij} + i\delta_{ij}\eta$ ,  $x \rightarrow x + i\delta_x\eta$ , with  $\eta \rightarrow 0$  [81], [95]. Notice that Eq. (7.1) implies that for a given assignment of the kinematic variables  $p_{1s}$  and  $s_{ij}$ , there are two solutions in  $S_{ij}$  and  $x$ . In general  $\delta_{ij}$  and  $\delta_x$  should also satisfy the analyticity constraints stemming from the one-scale integrals, known in closed form in  $\epsilon$ . These integrals are proportional to  $(-s_{ij})^{n\epsilon}$ ,  $(-p_{1s})^{n\epsilon}$ ,  $n = -1, -2$ , and must be consistently expressed in terms of  $S_{ij}$  and  $x$ , through the following equations:

$$\begin{aligned}
(-s_{34})^{-\epsilon} &= (-S_{51})^{-\epsilon} x^{-\epsilon} \\
(-s_{45})^{-\epsilon} &= (-S_{12})^{-\epsilon} x^{-4\epsilon} \\
(-s_{15})^{-\epsilon} &= (-S_{45})^{-\epsilon} \left(1 - \frac{S_{45} - S_{23}}{S_{45}} x\right)^{-\epsilon} \\
(-p_{1s})^{-\epsilon} &= (1 - x)^{-\epsilon} (-S_{45})^{-\epsilon} \left(1 - \frac{S_{12}}{S_{45}} x\right)^{-\epsilon} \\
(-s_{12})^{-\epsilon} &= x^{-\epsilon} (S_{12} - S_{34})^{-\epsilon} \left(1 - \frac{S_{12}}{S_{12} - S_{34}} x\right)^{-\epsilon}, \tag{7.27}
\end{aligned}$$

which constrain the values of  $\delta_{ij}$  and  $\delta_x$ .

In Table 7.3 we present results for all top-sector integrals at  $W = 4$ , for the first physical point provided in reference [80], namely

$$s_{12} \rightarrow -\frac{22}{5}, \quad s_{15} \rightarrow \frac{249}{50}, \quad s_{23} \rightarrow \frac{241}{25}, \quad s_{34} \rightarrow -\frac{377}{100}, \quad s_{45} \rightarrow \frac{13}{50}, \quad p_{1s} \rightarrow \frac{137}{50}. \tag{7.28}$$

The timings, running the GiNaC Interactive Shell `ginsh`, are 5.95 (2.33), 11.98 (4.94) and 8.49 (3.32) seconds for  $P_1$ ,  $P_2$  and  $P_3$  respectively, for  $N_{digits} = 32$  (16). We have also compared our results for all families, all basis elements and all physical points with those of reference [80] and found perfect agreement to the precision used, ( $N_{digits} = 16, 32$ ). We also checked our

results, not only at the level of basis elements but also at the level of Master Integrals, against FIESTA4 [58] and found agreement within the numerical integration errors provided by it.

$P_1$	$g_{72}$	29.802763651793108812023893217593 +i 273.86627846266515113913295225572
mzz	$I_3$	29.802763651793108812023893217593 +i 273.86627846266515113913295225572
$P_2$	$g_{73}$	44.162165744735300867233118554183 -i 46.218746133850339969944403077557
zmz	$I_3$	44.162165744735300867233118554183 -i 46.218746133850339969944403077557
$P_3$	$g_{84}$	11.908529680841593329567378444341 -i 143.83838235097336513553728991658
zzz	$I_3$	11.908529680841593329567378444341 -i 143.83838235097336513553728991658

Table 7.3: Numerical results for the non-zero top sector element of each family at weight 4 with 32 significant digits. The notation  $I_i$  is used in accordance with Table 2 of [80].

For the other physical points, beyond the first one, the number of letters in  $[0, x]$  is not anymore zero. As a consequence the running time is increasing, up to two orders of magnitude, with the last physical point being the worst case, as for this point the number of letters in  $[0, x]$  amounts to 19 out of a total of 24 letters involved in the non-zero top-sector basis elements. It is therefore worthwhile to thoroughly investigate the structure of the analytic result, with the aim to provide alternative representations in terms of Goncharov poly-logarithmic functions that are manifestly real-valued and thus much faster to compute. Notice that, from the structure of the analytic representation studied in this chapter (see for instance Table 7.1), the computational time is entirely determined by the  $W = 4$  functions. Therefore, as experience shows [70], [78], [79], [102], the use of one-dimensional integral representations at  $W = 4$ , may lead to a significant reduction in CPU time.

## 7.6 Conclusions and outlook

In this chapter we have presented analytic expressions in terms of poly-logarithmic functions, Goncharov Polylogarithms, of all planar two-loop five-point integrals with a massive external leg. This has been achieved by using the Simplified Differential Equations approach and the data for the canonical basis provided in reference [80]. Moreover, the necessary boundary values of all basis elements have been computed, based mainly on the form of the canonical differential equation, Eq. (7.7) and, in few cases, on the expansion by regions approach. The ability to straightforwardly compute the boundary values at  $x = 0$  and to even more straightforwardly express the solution in terms of Goncharov Polylogarithms, is based on the unique property of the SDE approach that the scattering kinematics is effectively simplified and rationalized with respect to  $x$ , in noticeable contradistinction with the standard differential equation approach, where such an analytic realisation of the solution is prohibitively difficult.

Obviously, the next step, is to extend the work of this chapter in the case of the remaining five non-planar families, shown in Fig. 8.1. Since on top of the planar penta-box families presented in this chapter, we have already computed the pure-function solutions in SDE approach, for all double-box families, planar and non-planar, with up to two external massive legs, we expect that the construction of the canonical basis of the few remaining non-planar Master Integrals will be plausible in the near future. Having the corresponding equation, Eq. (7.7), for the

non-planar families, it should be straightforward to extend the work of this chapter and to complete the full list of two-loop five-point Feynman Integrals with one massive external leg. We remind that within the SDE approach, having the analytic representations of two-loop five-point Master Integrals with one massive external leg in terms of Goncharov poly-logarithmic functions, allows also to straightforwardly obtain the result for massless external legs in terms of Goncharov poly-logarithmic functions, by taking the limit  $x = 1$  [70], [81] and making use of the resummed matrix corresponding to  $l_b = 1$  term in Eq. (7.7). In summary, when this next step is completed, a library of all two-loop Master Integrals with internal massless particles and up to five (four) external legs, among which one (two) massive legs will be provided: this will constitute a significant milestone towards the knowledge of the full basis of two-loop Feynman Integrals.

We have also shown how to obtain numerical results for all kinematic configurations, including Euclidean and physical regions. With regard to the expected progress in the calculation of  $2 \rightarrow 3$  scattering process [83], [102], [103], it would be desirable to adapt our results in different kinematic regions, using for instance fibration-basis techniques [65], [66].

# Chapter 8

## Two-loop non-planar Hexa-Box master integrals with one massive leg

Based on the Simplified Differential Equations approach, we present results for the two-loop non-planar hexa-box families of master integrals. We introduce a new approach to obtain the boundary terms and establish a one-dimensional integral representation of the master integrals in terms of Generalised Polylogarithms, when the alphabet contains non-factorisable square roots. The results are relevant to the study of NNLO QCD corrections for  $W$ ,  $Z$  and Higgs-boson production in association with two hadronic jets. This chapter is based on original research which appeared first in [104], done in collaboration with A. Kardos, C.G. Papadopoulos, A.V. Smirnov and C. Wever.

### 8.1 Introduction

The computation of higher order corrections to Standard Model (SM) scattering processes and their comparison against data coming from collider experiments remains one of the best approaches for the study of Nature at its most fundamental level. The discovery of the Higgs boson at the LHC [4], [5] solidified the mathematical consistency of the SM of Particle Physics as our best fundamental description of Nature. In the absence of any clear signals for physics beyond the SM, a detailed study of the properties of the Higgs boson along with a scrutinization of key SM processes have spearheaded the endeavour to advance our understanding of Particle Physics [6].

The upcoming High Luminosity upgrade of the LHC will provide us with experimental data of unprecedented precision. Making sense of the data and exploiting the machine's full potential will require theoretical predictions of equally high precision. In recent years, the theoretical community has made tremendous effort to meet the challenge of performing notoriously difficult perturbative calculations in Quantum Field Theory. The current precision frontier for the QCD dominated processes studied at the LHC lies at the Next-to-Next-to-Leading-Order (NNLO) for massless  $2 \rightarrow 3$  scattering with one off-shell external particle [90], [105].

A typical NNLO calculation involves, among other things, the computation of two-loop Feynman diagrams [106]. The established method for performing such calculations is by solving first-order differential equations (DE) satisfied by the relevant Feynman integrals (FI) [34]–[37]. Working within dimensional regularisation in  $d = 4 - 2\epsilon$  dimensions, allows the derivation of linear relations in the form of Integration-By-Parts (IBP) identities satisfied by these integrals [26], which allows one to obtain a minimal and finite set of FI for a specific scattering process, known as master integrals (MI).

It has been conjectured that FI with constant leading singularities in  $d$  dimensions satisfy a simpler class of DE [40], known as canonical DE [42]. A basis of MI satisfying canonical DE



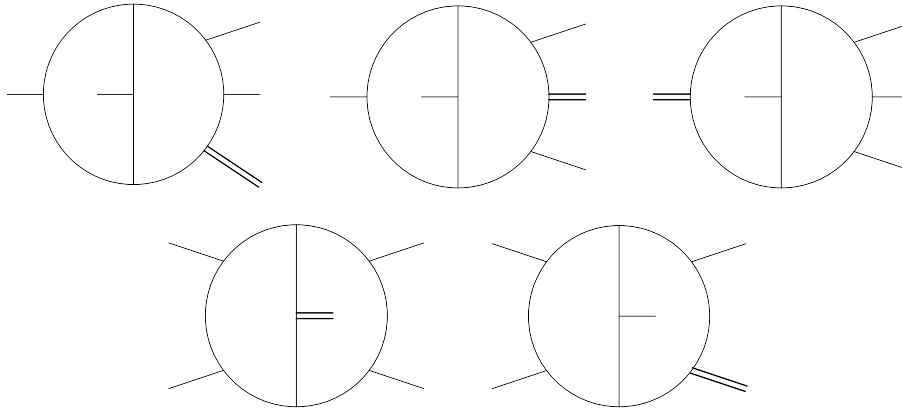


Figure 8.1: The five non-planar families with one external massive leg. The first row corresponds to the so-called hexabox topologies, whereas the diagrams of the second row are known as double-pentagons. We label them as follows:  $N_1$  (top left),  $N_2$  (top middle),  $N_3$  (top right),  $N_4$  (bottom left),  $N_5$  (bottom right). All diagrams have been drawn using Jaxodraw [115].

is known as a pure basis. The study of the special functions which appear in the solutions of such DE has provided a deeper understanding of their mathematical properties. These special functions often admit a representation in the form of Chen iterated integrals [107]. For a large class of FI, their result can be written in terms of a well studied class of special functions, known as Multiple of Goncharov polylogarithms (GPLs) [44]–[47]. Several computational tools have been developed for their algebraic manipulation [66] and numerical evaluation [71], [108].

For the case of two-loop five-point MI with one massive leg, pure bases of MI have been recently presented in [80] for the planar topologies, which we will call *one-mass pentaboxes*, and more recently in [109] for some of the non-planar topologies, which we will call *one-mass hexaboxes*. All one-mass pentaboxes have been computed both numerically [80], using generalised power-series expansions [110], [111], as well as analytically in terms of GPLs [82], by employing the Simplified Differential Equations (SDE) approach [38]. Recently, analytic results were also obtained in the form of Chen iterated integrals and have been implemented into the so-called *one-mass pentagon functions* [112], similar to the two-loop five-point massless results [78], [79]. These results, along with fully analytic solutions for the relevant one-loop integral family [72], have lead to the production of the first phenomenological studies at the leading-colour approximation for  $2 \rightarrow 3$  scattering processes involving one massive particle at the LHC [84], [113], [114]. For the one-mass hexabox topologies, numerical results were first presented in [70], using a method which emulates the Feynman parameter technique, for one of the non-planar integral families. All three integral families were treated numerically in [109] using the same methods as in [80].

In this chapter, we employ the SDE approach and obtain semi-analytic results for all one-mass hexaboxes, using the pure bases presented in [109]. More specifically, we obtain fully analytic expressions in terms of GPLs of up to weight 4 for the first non-planar family, denoted as  $N_1$  in figure 8.1. For families  $N_2$  and  $N_3$ , we obtain analytic results for the unknown non-planar integrals up to weight 2, whereas for weights 3 and 4 we introduce a one-fold integral representation in terms of GPLs allowing for a straightforward numerical evaluation of our expressions.

## 8.2 Hexabox integral families

There are three non-planar families of MI that correspond to the one-mass hexabox topologies, labelled as  $N_1$ ,  $N_2$  and  $N_3$ , see figure 8.1. We adopt the definition of the scattering kinematics

following [109], where external momenta  $q_i$ ,  $i = 1 \dots 5$  satisfy  $\sum_1^5 q_i = 0$ ,  $q_1^2 \equiv p_{1s}$ ,  $q_i^2 = 0$ ,  $i = 2 \dots 5$ , and the six independent invariants are given by  $\{q_1^2, s_{12}, s_{23}, s_{34}, s_{45}, s_{15}\}$ , with  $s_{ij} := (q_i + q_j)^2$ .

In the SDE approach [38] the momenta are parametrized by introducing a dimensionless variable  $x$ , as follows

$$q_1 \rightarrow p_{123} - xp_{12}, \quad q_2 \rightarrow p_4, \quad q_3 \rightarrow -p_{1234}, \quad q_4 \rightarrow xp_1 \quad (8.1)$$

where the new momenta  $p_i$ ,  $i = 1 \dots 5$  satisfy now  $\sum_1^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 1 \dots 5$ , whereas  $p_{i\dots j} := p_i + \dots + p_j$ . The set of independent invariants is given by  $\{S_{12}, S_{23}, S_{34}, S_{45}, S_{51}, x\}$ , with  $S_{ij} := (p_i + p_j)^2$ . The explicit mapping between the two sets of invariants is given by

$$\begin{aligned} q_1^2 &= (1-x)(S_{45} - S_{12}x), \quad s_{12} = (S_{34} - S_{12}(1-x))x, \quad s_{23} = S_{45}, \quad s_{34} = S_{51}x, \\ s_{45} &= S_{12}x^2, \quad s_{15} = S_{45} + (S_{23} - S_{45})x \end{aligned} \quad (8.2)$$

and as usual the  $x = 1$  limit corresponds to the on-shell kinematics.

The corresponding Feynman Integrals are defined through

$$\begin{aligned} F_{a_1 \dots a_{11}}^{N_1} &:= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 + q_1)^{2a_2} (k_1 + q_{12})^{2a_3} (k_1 + q_{123})^{2a_4}} \\ &\times \frac{1}{(k_1 + k_2 + q_{1234})^{2a_5} (k_1 + k_2)^{2a_6} k_2^{2a_7} (k_2 + q_4)^{2a_8} (k_2 + q_1)^{2a_9} (k_1 + q_4)^{2a_{10}} (k_2 + q_{12})^{2a_{11}}}, \end{aligned} \quad (8.3)$$

$$\begin{aligned} F_{a_1 \dots a_{11}}^{N_2} &:= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 - q_{1234})^{2a_2} (k_1 - q_{234})^{2a_3} (k_1 - q_{34})^{2a_4}} \\ &\times \frac{1}{(k_1 + k_2 - q_4)^{2a_5} (k_1 + k_2)^{2a_6} k_2^{2a_7} (k_2 + q_3)^{2a_8} (k_2 - q_{1234})^{2a_9} (k_1 + q_3)^{2a_{10}} (k_2 - q_{234})^{2a_{11}}}, \end{aligned} \quad (8.4)$$

$$\begin{aligned} F_{a_1 \dots a_{11}}^{N_3} &:= e^{2\gamma_E \epsilon} \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{1}{k_1^{2a_1} (k_1 + q_2)^{2a_2} (k_1 + q_{23})^{2a_3} (k_1 + q_{234})^{2a_4}} \\ &\times \frac{1}{(k_1 + k_2 + q_{1234})^{2a_5} (k_1 + k_2)^{2a_6} k_2^{2a_7} (k_2 + q_1)^{2a_8} (k_2 + q_2)^{2a_9} (k_1 + q_1)^{2a_{10}} (k_2 + q_{23})^{2a_{11}}}, \end{aligned} \quad (8.5)$$

where  $q_{i\dots j} := q_i + \dots + q_j$ .

Using FIRE6 [28] we found that the  $N_1$  family consists of 86 MI out of which 10 MI are genuinely new, the rest being known from the one-mass planar pentabox [82] or the non-planar double-box families [95]. For  $N_2$  and  $N_3$  the corresponding numbers are 86, 13 and 135, 21.

## 8.2.1 Pure bases and simplified canonical differential equations

We adopt the pure bases presented in [109]. As was the case for the pure bases of the planar families presented in [80], a d log form of the relevant differential equations was achieved, whose alphabet involves several square roots of the kinematic invariants  $\{q_1^2, s_{12}, s_{23}, s_{34}, s_{45}, s_{15}\}$ . More specifically, the following six square roots that appear in the alphabets of the one-mass hexabox integral families are

$$r_1 = \sqrt{\lambda(p_{1s}, s_{23}, s_{45})} \quad (8.6)$$

$$r_2 = \sqrt{\lambda(p_{1s}, s_{24}, s_{35})} \quad (8.7)$$

$$r_3 = \sqrt{\lambda(p_{1s}, s_{25}, s_{34})} \quad (8.8)$$

$$r_4 = \sqrt{\det \mathbb{G}(q_1, q_2, q_3, q_4)} \quad (8.9)$$

$$r_5 = \sqrt{\Sigma_5^{(1)}} \quad (8.10)$$

$$r_6 = \sqrt{\Sigma_5^{(2)}} \quad (8.11)$$

with  $\lambda(x, y, z) = x^2 - 2xy - 2xz + y^2 - 2yz + z^2$  representing the Källén function,  $\mathbb{G}(q_1, q_2, q_3, q_4) = \{2q_i \cdot q_j\}$  being the the Gram matrix of the external momenta, and  $\Sigma_5^{(1)}$ ,  $\Sigma_5^{(2)}$  are the polynomials

$$\begin{aligned} \Sigma_5^{(1)} &= s_{12}^2 (s_{15} - s_{23})^2 + (s_{23}s_{34} + (s_{15} - s_{34})s_{45})^2 \\ &\quad + 2s_{12} (-s_{45}s_{15}^2 + s_{23}s_{34}s_{15} + (s_{23} + s_{34})s_{45}s_{15} + s_{23}s_{34}(s_{45} - s_{23})) \end{aligned} \quad (8.12)$$

$$\begin{aligned} \Sigma_5^{(2)} &= (s_{12}(p_{1s} - s_{15} + s_{23}) - s_{23}s_{34})^2 + s_{45}^2 (p_{1s} - s_{15} + s_{34})^2 \\ &\quad - 2s_{45}(s_{34}((s_{12} + s_{23})p_{1s} - s_{15}s_{23} - s_{12}(s_{15} + s_{23})) + s_{12}(p_{1s} - s_{15})(p_{1s} - s_{15} + s_{23}) + s_{23}s_{34}^2). \end{aligned} \quad (8.13)$$

For topology  $N_1$ , the square roots  $r_1$  and  $r_4$  appear in its alphabet given in [109]. Introducing the dimensionless variable  $x$  rationalises these two roots through the mapping of (8.2). This allows us to derive a SDE in canonical form for  $N_1$ ,

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{i=1}^{l_{max}} \frac{\mathbf{M}_i}{x - l_i} \right) \mathbf{g} \quad (8.14)$$

where  $\mathbf{g}$  is the pure basis of  $N_1$ ,  $\mathbf{M}_i$  are the residue matrices corresponding to each letter  $l_i$  and  $l_{max}$  is the length of the alphabet, which for  $N_1$  is  $l_{max} = 21$ . It is interesting to note here the significant reduction in the number of letters in comparison with the alphabet of  $N_1$  given in [109], where the relevant length of the alphabet is 39. The form of (8.14) allows for a direct iterative solution order-by-order in  $\epsilon$  in terms of GPLs, assuming that the relevant boundary terms are obtained.

For topologies  $N_2$  and  $N_3$ , the square roots appearing in their respective alphabets [109] are  $\{r_1, r_2, r_4, r_5\}$  and  $\{r_1, r_3, r_4, r_6\}$ . In general all the square roots with the exception of  $\{r_5, r_6\}$  can be rationalised using either the mapping given in (8.2) or a variant of it [38], [82]. Nevertheless, in order to write an equation in the form of (8.14) a *simultaneous* rationalisation of all square roots is necessary. In fact, the mapping (8.2) allows for the rationalisation of  $r_1$  and  $r_4$  in terms of  $x$ , but this is not the case for  $\{r_2, r_3, r_5, r_6\}$ . It is thus not possible to achieve a canonical SDE in the form of (8.14) for families  $N_2$  and  $N_3$  using the parametrisation (8.1). This does not mean that the basis elements cannot be cast in the form of GPLs, but just that such a representation is not straightforwardly obtained based on the simple equation (8.14). The more general form of the SDE takes the form:

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{a=1}^{l_{max}} \frac{dL_a}{dx} \mathbf{M}_a \right) \mathbf{g} \quad (8.15)$$

where most of the  $L_a$  are simple rational functions of  $x$ , as in (8.14), whereas the rest are algebraic functions of  $x$  involving the non-rationalisable square roots.

A detailed analysis of (8.15) reveals that these non-rationalisable square roots start appearing at weight two. In practise this means that we can use the mapping (8.2) and solve the respective canonical DE for  $N_2$  and  $N_3$  by integrating with respect to  $x$  up to weight one in terms of ordinary logarithms. For weight two, analytic expressions in terms of GPLs can

be achieved due to the fact that the non-rationalisable square roots  $\{r_2, r_3, r_5, r_6\}$  appear decoupled in the DE. In fact, most of the basis elements are straightforwardly expressed in terms of GPLs by integrating the corresponding DE. For the rest, an educated ansatz can be constructed involving only specific weight-two GPLs, which are identified by inspecting the DE in each case where square roots  $\{r_2, r_3, r_5, r_6\}$  appear, modulo the boundary terms that one needs to compute. Thus analytic expressions in terms of GPLs up to weight two are obtained for all elements belonging in these families.

To further elaborate on this point let us analyse a rather simple case of a 3-point integral sector with three off-shell legs, that appears in both  $N_2$  and  $N_3$  families. This sector comprises two basis elements and the DE satisfied by those elements includes also two-point MI that are known in closed form. For instance, in  $N_2$ , the 3-point integrals appear as basis elements number 10 and 11 (see the ancillary file). The element 10 at weight 2,  $g_{10}^{(2)}$ , can straightforwardly be obtained by integrating the (8.15) and it is expressible in terms of GPLs in the form  $\mathcal{G}(a, b; x)$  where  $a, b$  are independent of  $x$ . On the contrary the element 11 at weight 2,  $g_{11}^{(2)}$ , is obtained by construction of an ansatz. Let us mention that all elements in question, except those involving the square roots  $\{r_5, r_6\}$ , namely element 73 in  $N_2$  and 114 in  $N_3$ , are known in terms of GPLs up to weight 4 [82], [95], based though on different variants of the parametrization (8.1). For instance element 11 of  $N_2$  is given as

$$g_{11}^{(2)} = 8 \left( 2\mathcal{G}(0, -y) \left( \mathcal{G}(1, y) - \mathcal{G}\left(\frac{\tilde{S}_{45}}{\tilde{S}_{12}}, y\right) \right) + 2\mathcal{G}\left(0, \frac{\tilde{S}_{45}}{\tilde{S}_{12}}, y\right) - \mathcal{G}(1, y) \log\left(\frac{\tilde{S}_{45}}{\tilde{S}_{12}}\right) \right. \\ \left. + \log\left(\frac{\tilde{S}_{45}}{\tilde{S}_{12}}\right) \mathcal{G}\left(\frac{\tilde{S}_{45}}{\tilde{S}_{12}}, y\right) - 2\mathcal{G}(0, 1, y) \right) \quad (8.16)$$

where the new parametrization of the external momenta is given by

$$q_1 \rightarrow \tilde{p}_{123} - y\tilde{p}_{12}, \quad q_2 \rightarrow y\tilde{p}_2, \quad q_3 \rightarrow -\tilde{p}_{1234}, \quad q_4 \rightarrow y\tilde{p}_1 \quad (8.17)$$

with the new momenta  $\tilde{p}_i$ ,  $i = 1 \dots 5$  satisfying as usual,  $\sum_1^5 \tilde{p}_i = 0$ ,  $\tilde{p}_i^2 = 0$ ,  $i = 1 \dots 5$ , with  $\tilde{p}_{i\dots j} := \tilde{p}_i + \dots + \tilde{p}_j$ . The set of independent invariants is given by  $\{\tilde{S}_{12}, \tilde{S}_{23}, \tilde{S}_{34}, \tilde{S}_{45}, \tilde{S}_{51}, y\}$ , with  $\tilde{S}_{ij} := (\tilde{p}_i + \tilde{p}_j)^2$ . The explicit mapping between the two sets of invariants is given by

$$q_1^2 = (1 - y)(\tilde{S}_{45} - \tilde{S}_{12}y), \quad s_{12} = \tilde{S}_{45}(1 - y) + \tilde{S}_{23}y, \quad s_{23} = -y(\tilde{S}_{12} - \tilde{S}_{34} + \tilde{S}_{51}), \\ s_{34} = \tilde{S}_{51}y, \quad s_{45} = y(\tilde{S}_{23} - \tilde{S}_{45} - \tilde{S}_{51}), \quad s_{15} = y(\tilde{S}_{34} - \tilde{S}_{12}(1 - y)). \quad (8.18)$$

Notice that the result of (8.16) is obtained through SDE approach in the parametrization of (8.17). By identifying  $f_- = y$  and  $f_+ = y\frac{\tilde{S}_{12}}{\tilde{S}_{45}}$ , which in terms of (8.2) are given as

$$f_{\pm} = \frac{S_{45} + x(-S_{23} - S_{34} + 2S_{51} + S_{12}x) \pm r_2}{2(S_{12} - S_{34} + S_{51})x}$$

we can write the DE for this element in the simple and compact form

$$\frac{d}{dx}g_{11}^{(2)} = -8 \left( \text{dlog}\left(\frac{f_+ - 1}{f_- - 1}\right) \log(f_- f_+) - \text{dlog}\left(\frac{f_+}{f_-}\right) \log((f_- - 1)(f_+ - 1)) \right).$$

The form of the DE makes the determination of the ansatz rather straightforward, with the result

$$g_{11}^{(2)} = -8 \left( -\log(f_- f_+) \left( \mathcal{G}(1, f_-) - \mathcal{G}(1, f_+) \right) + 2\mathcal{G}(0, 1, f_-) - 2\mathcal{G}(0, 1, f_+) \right). \quad (8.19)$$

Concerning the other non-rationalisable square root in the family  $N_2$ ,  $r_5$ , it also appears for the first time at weight 2 in the basis element 73 only (see the ancillary file), which is one of the new integrals to be calculated. Following the same procedure as for the element 11, namely writing the corresponding DE in a similar form, we find that the expression at weight 2 is similar to that of (8.19),

$$g_{73}^{(2)} = 16 \log(f_- f_+) \left( \mathcal{G}(1, f_-) - \mathcal{G}(1, f_+) \right) - 32 \left( \mathcal{G}(0, 1, f_-) - \mathcal{G}(0, 1, f_+) \right) \quad (8.20)$$

with

$$f_{\pm} = \frac{S_{45} (2S_{12}x - S_{34}x + S_{51}) + x (S_{23}S_{34} - S_{12}S_{23} + xS_{12}S_{51}) \pm r_5}{2S_{45} (S_{12} - S_{34} + S_{51})}$$

Regarding family  $N_3$ , there are two 3-point integral sectors with three off-shell legs that involve square root  $r_4$ , which is not rationalised in terms of  $x$  by (8.1), and consist of elements 12, 13 and 16, 17. Similarly to element 11 of family  $N_2$ , elements 12 and 16 cannot be expressed in terms of GPLs through a straightforward integration of their respective DE. However, we can achieve a GPL representation for them at weight 2 similar to (8.19), where now the  $f_-$ ,  $f_+$  functions involve the square root  $r_4$  instead of  $r_2$ . Square root  $r_6$  appears for the first time at weight 2 in element 114 similarly to the way square root  $r_5$  appears in element 73 in the  $N_2$  family, allowing us to obtain an expression at weight 2 as in (8.20), with the  $f_-$ ,  $f_+$  functions involving  $r_6$  instead of  $r_5$ .

Studying basis elements that are known in terms of GPLs up to weight 4, proved useful in constructing an educated ansatz for the unknown integrals at weight 2. It would be very interesting to further pursue this direction, with the aim to establish a systematic way to construct representations in terms of GPLs for weights higher than 2. This will allow to extend the SDE approach to cases where the letters  $L_a$  in (8.15) assume a general algebraic form. Constructing analytic expressions in terms of GPLs beyond weight 2 by applying a more general procedure following the ideas of [116], [117] is also possible, but it requires a significant amount of resources and it might well result to a proliferation of GPLs. A more practical and direct approach, introducing a one-dimensional integral representation will be presented in detail in section 8.4.

### 8.3 Boundary terms

In this section we will describe the analytic computation of all necessary boundary terms in terms of GPLs with rational functions of the underline kinematic invariants  $S_{ij}$  up to weight 4. We perform this task for all three non-planar families.

Our main approach is the one introduced in [82] and elaborated in detail in [60]. In general we need to calculate the  $x \rightarrow 0$  limit of each pure basis element. At first we exploit the canonical SDE at the limit  $x \rightarrow 0$  and define through it the resummation matrix

$$\mathbf{R} = \mathbf{S} e^{\epsilon \mathbf{D} \log(x)} \mathbf{S}^{-1} \quad (8.21)$$

where the matrices  $\mathbf{S}$ ,  $\mathbf{D}$  are obtained through the Jordan decomposition of the residue matrix for the letter  $l_1 = 0$ ,  $\mathbf{M}_1$ ,

$$\mathbf{M}_1 = \mathbf{S} \mathbf{D} \mathbf{S}^{-1}. \quad (8.22)$$

Secondly, we can relate the elements of the pure basis to a set of MI  $\mathbf{G}$  through IBP reduction,

$$\mathbf{g} = \mathbf{T} \mathbf{G}. \quad (8.23)$$

Using the expansion by regions method [51] as implemented in the `asy` code which is shipped along with `FIESTA4` [58], we can obtain the  $x \rightarrow 0$  limit of the MI in terms of which we express the pure basis (8.23),

$$G_i \underset{x \rightarrow 0}{=} \sum_j x^{b_j + a_j \epsilon} G_i^{(b_j + a_j \epsilon)} \quad (8.24)$$

where  $a_j$  and  $b_j$  are integers and  $G_i$  are the individual members of the basis  $\mathbf{G}$  of MI in (8.23). This analysis allows us to construct the following relation

$$\mathbf{Rb} = \lim_{x \rightarrow 0} \mathbf{TG} \Big|_{\mathcal{O}(x^{0+a_j \epsilon})} \quad (8.25)$$

where the right-hand side implies that, apart from the terms  $x^{a_i \epsilon}$  coming from (8.24), we expand around  $x = 0$ , keeping only terms of order  $x^0$ . Equation (8.25) allows us in principle to determine all boundary constants  $\mathbf{b} = \sum_{i=0}^6 \epsilon^i \mathbf{b}_0^{(i)}$ .

More specifically, in the case where  $\mathbf{D}$  in (8.22) is non-diagonal, we will get logarithmic terms in  $x$  on the left-hand side of (8.25), in the form  $x^{a_j \epsilon} \log(x)$ . Since no such terms appear on the right-hand side of (8.25), a set of linear relations between elements of the array  $\mathbf{b}$  are obtained by setting the coefficient of  $x^{a_j \epsilon} \log(x)$  terms to zero. Furthermore, powers of  $x^{a_j \epsilon}$  that appear only on the left-hand side can also yield linear relations among elements of  $\mathbf{b}$ , by setting their coefficients to zero. We shall call these two sets of relations *pure*, since they are linear relations among elements of  $\mathbf{b}$  with rational numbers as coefficients. These pure relations account for the determination of a significant part of the two components of the boundary array. Finally for the undetermined elements of  $\mathbf{b}$ , several region-integrals  $G_i^{(b_j + a_j \epsilon)}$  usually need to be calculated coming from (8.24). Their calculation is straightforwardly achieved either by direct integration in Feynman-parameter space and then by using `HypExp` [55], [56] to expand the resulting  ${}_2F_1$  hypergeometric functions, or in a very few cases, by Mellin-Barnes techniques using the `MB` [96], [97], `MBSums` [98] and `XSummer` [99] packages<sup>1</sup>. The  $\mathbf{b}_0^{(i)}$  terms, with  $i$  indicating the corresponding weight, consist of Zeta functions  $\zeta(i)$ , logarithms and GPLs of weight  $i$  which have as arguments rational functions of the underline kinematic variables  $\{S_{12}, S_{23}, S_{34}, S_{45}, S_{51}\}$ .

This approach was efficient enough for the determination of all boundary terms for families  $N_1$  and  $N_2$ . Specifically for family  $N_1$ , where a canonical SDE can be achieved (8.14), we can write a solution in terms of GPLs up to weight 4 in the following compact form

$$\begin{aligned} \mathbf{g} &= \epsilon^0 \mathbf{b}_0^{(0)} + \epsilon \left( \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(0)} + \mathbf{b}_0^{(1)} \right) \\ &+ \epsilon^2 \left( \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(0)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(1)} + \mathbf{b}_0^{(2)} \right) \\ &+ \epsilon^3 \left( \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(1)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(2)} + \mathbf{b}_0^{(3)} \right) \\ &+ \epsilon^4 \left( \sum \mathcal{G}_{abcd} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{M}_d \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(1)} \right. \\ &\left. + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(2)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(3)} + \mathbf{b}_0^{(4)} \right) \end{aligned} \quad (8.26)$$

were  $\mathcal{G}_{ab\dots} := \mathcal{G}(l_a, l_b, \dots; x)$  represent the GPLs. These results are presented in such a way that each coefficient of  $\epsilon^i$  has transcendental weight  $i$ . If we assign weight  $-1$  to  $\epsilon$ , then (8.26) has uniform weight zero.

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<sup>1</sup>The in-house `Mathematica` package `Gsuite`, that automatically process the `MBSums` output through `XSummer` is used.

For family  $N_3$ , eq. (8.25) resulted in a proliferation of region-integrals, more than 200, that one would have to calculate in order to obtain boundary terms for several higher-sector basis elements. More specifically, in order to obtain the following boundary terms

$$\{b_{101}, b_{103}, b_{104}, b_{106}, b_{113}, b_{117}, b_{118}, b_{124}, b_{125}, b_{126}, b_{130}, b_{131}, b_{132}, b_{133}\} \quad (8.27)$$

one would have to calculate 208 region-integrals, with 17 of them having seven Feynman parameters to be integrated, making their direct integration highly non-trivial. For all basis elements apart from (8.27) we were able to obtain boundary terms through (8.25).

To reduce the number of region-integrals for the computation of (8.27) we have investigated a different approach. The idea is rather simple and straightforward. The pure basis elements can be written in general as follows:

$$g = C \int \frac{d^d k_1}{i\pi^{d/2}} \frac{d^d k_2}{i\pi^{d/2}} \frac{P(\{D_i\}, \{S_{ij}, x\})}{\prod_{i \in \tilde{S}} D_i^{a_i}} \quad (8.28)$$

where  $D_i$ ,  $i = 1 \dots 11$ , represent the inverse scalar propagators,  $\tilde{S}$  the set of indices corresponding to a given sector,  $S_{ij}, x$  the kinematic invariants,  $P$  is a polynomial,  $a_i$  are positive integers and  $C$  a factor depending on  $S_{ij}, x$ . This form is usually decomposed in terms of FI,  $F_i$ ,

$$g = C \sum c_i(\{S_{ij}, x\}) F_i$$

with  $c_i$  being polynomials in  $S_{ij}, x$ . The limit  $x = 0$ , is then obtained, after IBP reduction, through Feynman parameter representation of the individual MI, as described in the previous paragraphs. An alternative approach, would be to build-up the Feynman parameter representation for the whole basis element, by considering the integral in (8.28) as a tensor integral and making use of the formulae from the references [118], [119], to bring it in its Feynman parameter representation. Then, by using the expansion by regions approach [51], [58], we determine the regions<sup>2</sup> in the limit  $x = 0$ . Rescaling the Feynman parameters by appropriate powers of  $x$ , keeping the leading power in  $x$ , we then obtain the final result that can be written as follows:

$$b = \sum_I N_I \int \prod_{i \in S_I} dx_i U_I^{a_i} F_I^{b_i} \Pi_I$$

where  $I$  runs over the set of contributing regions,  $U_I$  and  $F_I$  are the limits of the usual Symanzik polynomials,  $\Pi_I$  is a polynomial in the Feynman parameters,  $x_i$ , and the kinematic invariants  $S_{ij}$ , and  $S_I$  the subset of surviving Feynman parameters in the limit. In this way a significant reduction of the number of regions to be calculated is achieved. Notice that in contrast to the approach described in the previous paragraphs, only the regions  $x^{-2\epsilon}$  and  $x^{-4\epsilon}$  contribute to the final result. Moreover, this approach overpasses the need for an IBP reduction of the basis elements in terms of MI.

## 8.4 Integral representation

After obtaining all boundary terms in section 8.3 and constructing analytic expressions for families  $N_2$  and  $N_3$  up to  $\mathcal{O}(\epsilon^2)$  in terms of GPLs up to weight two, we will now introduce an one-fold integral representation for  $\mathcal{O}(\epsilon^3)$  and  $\mathcal{O}(\epsilon^4)$ . This representation will allow us to obtain numerical results through direct numerical integration [78], [120].

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<sup>2</sup>Only the corresponding scalar integral of (8.28) determines the regions.

**Weight 3:** The differential equation (8.15) can be written in the form:

$$\partial_x g_I^{(3)} = \sum_a (\partial_x \log L_a) \sum_J c_{IJ}^a g_J^{(2)} \quad (8.29)$$

where  $a$  runs over the set of contributing letters,  $I, J$  run over the set of basis elements,  $c_{IJ}^a$  are  $\mathbb{Q}$ -number coefficients read off from the matrices  $\mathbf{M}_a$  and  $g_J^{(2)}$  are the basis elements at weight 2, known in terms of GPLs. Since the lower limit of integration corresponds to  $x = 0$ , we need to subtract the appropriate term so that the integral is explicitly finite. This is achieved as follows:

$$\partial_x g_I^{(3)} = \sum_a \frac{l_a}{x} \sum_J c_{IJ}^a g_{J,0}^{(2)} + \left( \sum_a (\partial_x \log L_a) \sum_J c_{IJ}^a g_J^{(2)} - \sum_a \frac{l_a}{x} \sum_J c_{IJ}^a g_{J,0}^{(2)} \right) \quad (8.30)$$

where  $g_{I,0}^{(2)}$  are obtained by expanding  $g_I^{(2)}$  around  $x = 0$  and keeping terms up to order  $\mathcal{O}(\log(x)^2)$ , and  $l_a \in \mathbb{Q}$  are defined through

$$\partial_x \log L_a = \frac{l_a}{x} + \mathcal{O}(x^0). \quad (8.31)$$

The DE (8.30) can now be integrated from  $x = 0$  to  $x = \bar{x}$ , and the result is given by

$$g_I^{(3)} = g_{I,\mathcal{G}}^{(3)} + b_I^{(3)} + \int_0^{\bar{x}} dx \left( \sum_a (\partial_x \log L_a) \sum_J c_{IJ}^a g_J^{(2)} - \sum_a \frac{l_a}{x} \sum_J c_{IJ}^a g_{J,0}^{(2)} \right) \quad (8.32)$$

with  $b_I^{(3)}$  being the boundary terms at  $\mathcal{O}(\epsilon^3)$  and

$$g_{I,\mathcal{G}}^{(3)} = \int_0^{\bar{x}} dx \sum_a \frac{l_a}{x} \sum_J c_{LJ}^a g_{J,0}^{(2)} \Big|_{\mathcal{G}} \quad (8.33)$$

with the subscript  $\mathcal{G}$ , indicating that the integral is represented in terms of GPLs (see ancillary file), following the convention

$$\int_0^{\bar{x}} dx \frac{1}{x} \mathcal{G} \left( \underbrace{0, \dots, 0}_n; x \right) = \mathcal{G} \left( \underbrace{0, \dots, 0}_{n+1}; \bar{x} \right). \quad (8.34)$$

**Weight 4:** At weight 4, the differential equation (8.15) can be written in the form:

$$\partial_x g_I^{(4)} = \sum_a (\partial_x \log L_a) \sum_J c_{IJ}^a g_J^{(3)} \quad (8.35)$$

which after doubly-subtracting, in order to obtain integrals that are explicitly finite as in (8.30), is written as

$$\partial_x g_I^{(4)} = \sum_a \partial_x (\log L_a - LL_a) \sum_J c_{IJ}^a g_J^{(3)} + \sum_a \partial_x (LL_a) \sum_J c_{IJ}^a (g_J^{(3)} - g_{J,0}^{(3)}) + \sum_a \frac{l_a}{x} \sum_J c_{IJ}^a g_{J,0}^{(3)} \quad (8.36)$$

where  $LL_a$  are obtained by expanding  $\log(L_a)$  around  $x = 0$  and keeping terms up to order  $\mathcal{O}(\log(x))$ , and

$$g_{I,0}^{(3)} = g_{I,\mathcal{G}}^{(3)} + b_I^{(3)}. \quad (8.37)$$



Now, by integrating by parts and using (8.30) we can write the final result as follows:

$$\begin{aligned}
g_I^{(4)} = & g_{I,\mathcal{G}}^{(4)} + b_I^{(4)} + \left( \sum_a \log L_a \sum_J c_{IJ}^a g_J^{(3)} \right) - \left( \sum_a LL_a \sum_J c_{IJ}^a g_{J,0}^{(3)} \right) \\
& - \int_0^{\bar{x}} dx \sum_a (\log L_a - LL_a) \sum_J c_{IJ}^a \sum_b \frac{l_b}{x} \sum_K c_{JK}^b g_{K,0}^{(2)} \\
& - \int_0^{\bar{x}} dx \sum_a \log L_a \sum_J c_{IJ}^a \left( \sum_b (\partial_x \log L_b) \sum_K c_{JK}^b g_K^{(2)} - \sum_b \frac{l_b}{x} \sum_K c_{JK}^b g_{K,0}^{(2)} \right) \quad (8.38)
\end{aligned}$$

with  $a, b$  running over the set of contributing letters,  $I, J, K$  running over the set of basis elements,  $b_I^{(4)}$  being the boundary terms at  $\mathcal{O}(\epsilon^4)$  and

$$g_{I,\mathcal{G}}^{(4)} = \int_0^{\bar{x}} dx \left( \sum_a \frac{l_a}{x} \sum_J c_{IJ}^a g_{J,0}^{(3)} \right) \Big|_{\mathcal{G}} \quad (8.39)$$

where the subscript  $\mathcal{G}$  indicates that the integral is represented in terms of GPLs (see ancillary file), following (8.34).

**Implementation:** We have implemented the final formulae (8.32) and (8.38) in a `Mathematica` notebook included in the ancillary file. We use `NIntegrate` to perform the one-dimensional integrals appearing in the (8.32) and (8.38), after expressing all weight-2 functions in terms of classical polylogarithms following reference [121]. For the evaluation of the terms expressed as GPLs, (8.33) and (8.39), we use `GiNaC` [71], [89] as implemented in `PolyLogTools` [66]. We have checked against basis elements known in terms of GPLs up to weight 4, that with this setup, we can obtain numerical results with 32 digit-precision. For kinematic configurations where there are no singularities in the domain of integration  $(0, \bar{x})$ , we have checked the new basis elements against numerical results provided by the authors of reference [109] and found full agreement. For kinematic configurations with singularities in the domain of integration, we use the standard  $i\epsilon$ -prescription and obtain again full agreement. The performance of this simple implementation is quite encouraging: in all cases a few hundreds of evaluations of the integrand are enough to achieve the 32 digit-precision. Notice that the integrand expressions involve logarithms and classical polylogarithms  $\text{Li}_2$ , that are evaluated using very little CPU time, even within our simple `Mathematica` setup without any optimisation. We plan to address an optimised implementation, in line with references [79], [112], in a forthcoming publication.

## 8.5 Conclusions

The frontier of precision calculations at NNLO currently concerns  $2 \rightarrow 3$  scattering process involving massless propagators and one massive external particle. At the level of FI, all planar two-loop MI have been recently computed through the solution of canonical DE both numerically [80], via generalised power series expansions, and analytically in terms of GPLs up to weight 4 [82], using the SDE approach [38]. More recently, results in terms of Chen iterated integrals were presented and implemented in the so-called pentagon functions [112].

Concerning the two-loop non-planar topologies, these can be classified into the three so-called hexabox topologies and two so-called double-pentagons, see figure 8.1. One of the hexabox topologies, denoted as  $N_1$  in figure 8.1, was calculated numerically a few years ago using an approach which introduces a Feynman parameter and uses analytic results for the sub-topologies that are involved [70]. More recently, pure bases for the three hexabox topologies

satisfying DE in  $d \log$  form were presented in reference [109] and solved numerically using the same methods as in [80].

In this chapter we addressed the calculation of the three two-loop hexabox topologies,  $N_1$ ,  $N_2$ ,  $N_3$  in figure 8.1, using the SDE approach. For the  $N_1$  family results up to weight 4 in terms of GPLs are obtained. For the  $N_2$  and  $N_3$  families we have established an one-dimensional integral representation involving up to weight-2 GPLs. This allows to extend the scope of the SDE approach when non-factorisable square roots appear in the alphabet. We have also introduced a new approach to compute the boundary terms directly for the basis elements, that significantly reduces the complexity of the problem. With these new developments, we hope to complete the full set of five-point one-mass two-loop MI families in the near future and provide a solid implementation for their numerical evaluation.

# Chapter 9

## Multiscale pentagon integrals involving internal masses

We study several multiscale one-loop five-point families of Feynman integrals. More specifically, we employ the SDE approach to obtain results in terms of GPLs of up to transcendental weight four for families with two and three massive external legs and massless propagators, as well as with one massive internal line and up to two massive external legs. This is the first time this computational approach is applied to cases involving internal masses. This chapter is based on original research which first appeared in [122].

### 9.1 Introduction

In recent years the field of precision calculations in collider physics has emerged as a vibrant and fruitful line of research in our attempt to understand Nature at its most fundamental level [6]. The basic principle of this research endeavour is to have very precise experimental measurements of cross sections for Standard Model scattering processes compared against theoretical predictions of equally high precision and search for any deviations between them. Should any such deviations be established, their analysis and physical explanation would require New Physics, giving us an idea of what lies beyond the Standard Model.

The ever increasing demand for highly precise theoretical predictions for scattering processes relevant to LHC searches poses a challenge in our ability to perform higher order calculations in perturbative Quantum Field Theory [90]. Multiloop scattering amplitudes play a fundamental role in such calculations, encoding within their mathematical structure key information concerning the nature of particle interactions. One major aspect of the calculation of multiloop scattering amplitudes is the calculation of the relevant Feynman diagrams that are involved, which can be associated through the corresponding Feynman rules to the so-called Feynman integrals. In the following we will use the notion of *diagrams* and *integrals* interchangeably.

The standard approach for the calculation of these integrals involves obtaining a complete set of MI through the use of Integration-By-Part identities [26], constructing a pure basis of MI [40] and then deriving and solving differential equations in canonical form [42]. This approach has yielded numerous results [123], in part due to the fact that we have a solid understanding of the special class of functions, known as multiple or GPLs [44]–[47], in terms of which many Feynman integrals can be expressed. In more complicated cases however, this class of functions is not enough and important steps have been made in getting a better understanding of a more general class of functions, Elliptic integrals [124]–[130], which appear in solutions of multiloop Feynman integrals with many scales, especially when several internal masses are introduced.

When considering multiloop Feynman integrals involving many external particles, the current frontier lies at two-loop five-point integrals with up to one off-shell leg and massless internal

lines. For the fully massless case, all MI are by now known up to transcendental weight four [78], [81], [85], [93], [131]–[133] and their solutions have been implemented in a fast C++ library known as *pentagon functions* [79]. When one of the external particles is considered off-shell, the planar topologies have been recently solved using two different computational approaches for the solution of canonical differential equations, numerically [80] and analytically [82]. The numerical calculation was performed using a generalised power-series method [110], [111], while the analytical solution was achieved through the use of the SDE approach [38], with the results given in terms of GPLs of up to transcendental weight four. These results are relevant to many  $2 \rightarrow 3$  scattering processes studied experimentally at the LHC, e.g.  $W + 2$  jets production. For the computation of the relevant scattering amplitudes, one-loop five-point Feynman integrals with one off-shell leg also have to be known up to transcendental weight four [72]. These results were recently used for the calculation of two-loop QCD corrections to  $Wb\bar{b}$  production [84]. First results for one of the non-planar topologies have also appeared using a numerical approach [70]. More recently the three *hexabox* topologies were calculated in [109] using the same approach as in [80].

While staying at the level of five-point Feynman integrals, at some point we will have to introduce internal masses and consider more than one massive external particle. Judging from the level of complexity of the so far accumulated results, these Feynman integrals are expected to be highly non-trivial to be solved using current approaches, especially the genuine two-loop ones. To that end, we believe that it is instructive to consider first the relevant one-loop five-point Feynman integrals with more than one off-shell leg and/or with internal masses. The interest of these Feynman integrals is twofold. From a more formal point of view, it is interesting to see what kind of functions appear as solutions of the relevant canonical differential equations and study their structure. This will give us a glimpse of the minimum mathematical complexities and difficulties we should expect when we consider their two-loop counterparts. From a phenomenological standpoint, these one-loop integrals will be required for the computation of two-loop corrections for  $2 \rightarrow 3$  scattering processes involving more than one massive external particle and/or internal massive particles.

In line with the arguments presented above, we consider in this chapter the analytical calculation of several multiscale one-loop five-point Feynman integrals. More specifically, we present analytical results in terms of GPLs of up to transcendental weight four for families with two and three off-shell legs and massless internal lines, as well as for families with one massive propagator and up to two external massive particles. Our calculation is based on the SDE approach [38] which introduces an external dimensionless parameter  $x$  in such a way that captures the off-shellness of one massive leg. The system of canonical differential equations is constructed by differentiating a pure basis of MI in terms of  $x$ , regardless of the number of scales involved in the problem. One special feature of this approach is that by taking the limit of  $x \rightarrow 1$  [81] for a family with  $n$  massive legs, we can obtain the result for a family with  $n - 1$  massive legs in an algorithmic way [60]. In Figure 9.1 we present the families of Feynman integrals computed through the solution of SDE in canonical form, while in Figure 9.2 we present the families of integrals computed through the  $x \rightarrow 1$  limit.

The rest of our chapter is structured as follows: in section 9.2 we introduce basic notation and the kinematic configuration for each of the studied families of Feynman integrals, in section 9.3 we construct pure bases and derive and solve SDE in canonical form for all integral families depicted in Figure 9.1, we present some of the resulting alphabets in  $x$  and study their structure, and solve all integral families depicted in Figure 9.2 through the  $x \rightarrow 1$  limit in terms of GPLs of up to transcendental weight four. In section 9.4 we provide an analysis of our results, as well as numerical checks for Euclidean points and in section 9.6 we summarise our findings and discuss their key features. To the best of our knowledge these families have never before been considered in the literature, thus their solution constitutes an original contribution. This is

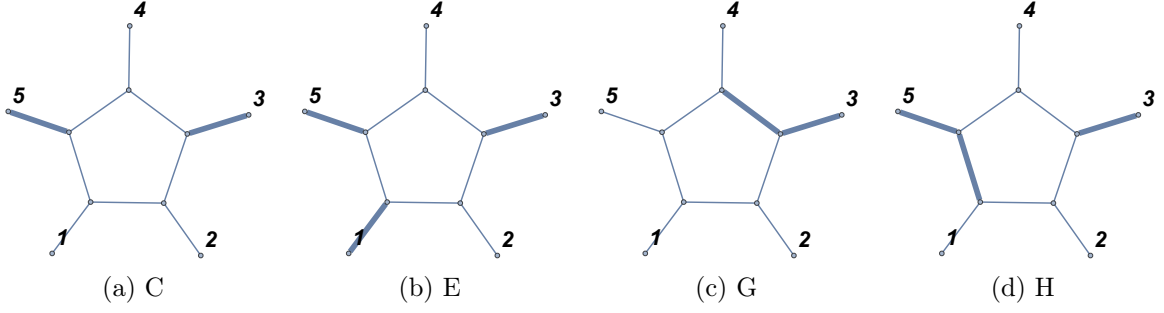


Figure 9.1: Top-sector diagrams for families computed with the SDE approach. All external particles are incoming. Bold external (internal) lines represent massive particles.

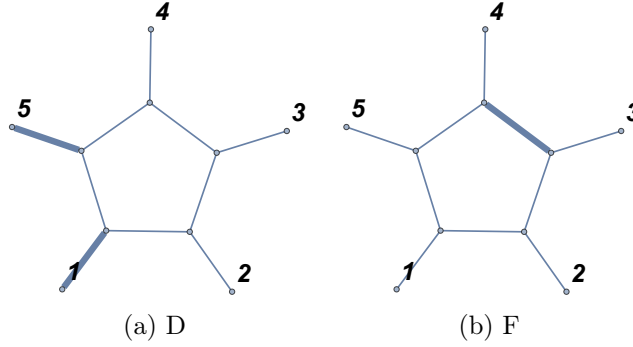


Figure 9.2: Top-sector diagrams for families computed through the  $x \rightarrow 1$  limit. All external particles are incoming. Bold external (internal) lines represent massive particles.

also the first time that a calculation with the SDE approach involving MI with internal masses is reported. Along with this chapter we provide all of our results in ancillary files. Explicit weight-three expressions for the top-sector basis elements of families  $C$  and  $H$  are given in appendix 9.5.

## 9.2 Notation and kinematics

The integral families are defined through the following parametrization,

$$G_{a_1 a_2 a_3 a_4 a_5} = \int \frac{d^d k_1}{i\pi^{(d/2)}} \frac{e^{\epsilon\gamma E}}{\mathcal{D}_1^{a_1} \mathcal{D}_2^{a_2} \mathcal{D}_3^{a_3} \mathcal{D}_4^{a_4} \mathcal{D}_5^{a_5}}, \quad d = 4 - 2\epsilon \quad (9.1)$$

with

$$\begin{aligned} \mathcal{D}_1 &= (k_1)^2 - n_1 m^2, \quad \mathcal{D}_2 = (k_1 + q_1)^2, \quad \mathcal{D}_3 = (k_1 + q_1 + q_2)^2 \\ \mathcal{D}_4 &= (k_1 + q_1 + q_2 + q_3)^2 - n_4 m^2, \quad \mathcal{D}_5 = (k_1 + q_1 + q_2 + q_3 + q_4)^2. \end{aligned} \quad (9.2)$$

For the families  $C$ ,  $D$  and  $E$  we have  $n_1 = n_4 = 0$ , for the families  $F$  and  $G$   $n_1 = 0, n_4 = 1$  and finally for the family  $H$   $n_1 = 1, n_4 = 0$ . The kinematics for the families depicted in Figure 9.1 is as follows,

- $C\&H$ :  $\sum_{i=1}^5 q_i = 0$ ,  $q_i^2 = 0$ ,  $i = 1, 2, 4$ ,  $q_3^2 = m_3^2$ ,  $q_5^2 = m_5^2$
- $E$ :  $\sum_{i=1}^5 q_i = 0$ ,  $q_i^2 = 0$ ,  $i = 2, 4$ ,  $q_1^2 = \bar{m}_1^2$ ,  $q_3^2 = m_3^2$ ,  $q_5^2 = m_5^2$
- $G$ :  $\sum_{i=1}^5 q_i = 0$ ,  $q_i^2 = 0$ ,  $i = 1, 2, 4, 5$ ,  $q_3^2 = m_3^2$ .

We introduce the following  $x$ -parametrization<sup>1</sup>

$$q_1 = xp_1, \quad q_2 = xp_2, \quad q_3 = p_{123} - xp_{12}, \quad q_4 = p_4, \quad q_5 = -p_{1234}. \quad (9.3)$$

The kinematics in this underline momentum parametrization is

- $C\&H$ :  $\sum_{i=1}^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 1, 2, 3, 4$ ,  $p_5^2 = m_5^2$
- $E$ :  $\sum_{i=1}^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 2, 3, 4$ ,  $p_1^2 = m_1^2$ ,  $p_5^2 = m_5^2$
- $G$ :  $\sum_{i=1}^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 1, 2, 3, 4, 5$ .

Introducing (9.3) results in a mapping between the kinematic invariants in the original momentum parametrization,  $q_i$ , and the underline momentum parametrization  $\{x, p_i\}$  for each of the families  $C, E, G, H$ .<sup>2</sup>

$$\begin{aligned} C\&H : m_3^2 &= (x-1)(S_{12}x - S_{45}), \quad s_{12} = S_{12}x^2, \quad s_{23} = S_{23}x - S_{45}x + S_{45} \\ s_{34} &= m_5^2(-x) + m_5^2 + x(S_{12}(x-1) + S_{34}), \quad s_{45} = S_{45}, \quad s_{15} = m_5^2(-x) + m_5^2 + S_{15}x \\ E : s_{12} &= S_{12}x^2, \quad s_{23} = x(m_1^2(x-1) + S_{23}) - S_{45}x + S_{45}, \\ s_{34} &= m_5^2(-x) + m_5^2 + x(S_{12}(x-1) + S_{34}), \quad s_{45} = S_{45}, \\ s_{15} &= x(m_1^2(x-1) + S_{15}) + m_5^2(-x) + m_5^2, \quad \bar{m}_1^2 = m_1^2x^2, \quad m_3^2 = (x-1)(S_{12}x - S_{45}) \\ G : s_{12} &= S_{12}x^2, \quad s_{23} = S_{23}x - S_{45}x + S_{45}, \quad s_{34} = x(S_{12}(x-1) + S_{34}), \quad s_{45} = S_{45}, \\ s_{15} &= S_{15}x, \quad m_3^2 = (x-1)(S_{12}x - S_{45}). \end{aligned} \quad (9.4)$$

For the families depicted in Figure 9.2 their definition through (9.1)&(9.2) is obtained by taking (9.3) and setting  $x = 1$ , and their kinematic configuration is effectively the one produced by the underline momentum parametrization of the families through which we will calculate them with the  $x \rightarrow 1$  limit, therefore we have

- $D$  ( $x \rightarrow 1$  of  $E$ ):  $\sum_{i=1}^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 2, 3, 4$ ,  $p_1^2 = m_1^2$ ,  $p_5^2 = m_5^2$
- $F$  ( $x \rightarrow 1$  of  $G$ ):  $\sum_{i=1}^5 p_i = 0$ ,  $p_i^2 = 0$ ,  $i = 1, 2, 3, 4, 5$ .

### 9.3 Differential equations and pure solutions

In this section we will describe the analytical calculation of the integral families considered in this chapter. We will construct pure bases for the families  $C, E, G, H$  and use the SDE approach [38] to compute them in terms of GPLs. We will show how to obtain boundary terms [60], [82] for these canonical differential equations and present explicit results up to transcendental weight four. A discussion on the structure of the alphabets in  $x$  for families  $C$  and  $H$  is also provided, along with their explicit expressions.

We will also show how by taking the  $x \rightarrow 1$  limit of the analytic solution of families  $E$  and  $G$ , one can obtain in an algorithmic way analytic results in terms of GPLs for the families  $D$  and  $F$  respectively. Additionally, this procedure will allow us to obtain pure bases for the

<sup>1</sup>We use the abbreviations  $p_{ij} = p_i + p_j$  and  $p_{ijk} = p_i + p_j + p_k$  and similarly for  $q$  later.

<sup>2</sup>We use the abbreviations  $s_{ij} = q_{ij}^2$ ,  $S_{ij} = p_{ij}^2$ .

families  $D$  and  $F$  in a straightforward manner [60]. The results presented here for these last two families are up to transcendental weight four as well.

It is important to note that introducing one internal mass does not appear to have any effect on the efficiency of the methods that have been developed for the determination of boundary terms, as well as taking the  $x \rightarrow 1$  limit within the SDE approach.

### 9.3.1 Families $C, E, G, H$

Constructing pure bases for the families  $C, E, G, H$  is by now a trivial exercise. Following the reasoning of [80], [85], the top sector basis element at the *integrand* level is of the form

$$\epsilon^2 \frac{\mathcal{P}_{11111}}{\sqrt{\Delta_5}} \tilde{G}_{11111} \quad (9.5)$$

where  $\mathcal{P}_{11111}$  is the Baikov polynomial corresponding to the top sector *integral*  $G_{11111}$  for each family,  $\tilde{G}_{11111}$  is the top sector *integrand* of each family and  $\Delta_5 = \det[q_i \cdot q_j]$  is the Gram determinant of the external momenta. The remaining pure basis elements can be constructed through the study of the leading singularities of their corresponding diagrams [40]. Using Azurite [30] and KIRA2 [29] we identify 15, 18, 16 and 18 MI for the families  $C, E, G, H$  respectively.

When considering five-point scattering, a number of square roots of the kinematic invariants enter the differential equations of the corresponding pure bases. These square roots originate from leading singularities of triangles with three massive legs<sup>3</sup> which are represented by square roots of the Källén function  $\lambda(x, y, z) = x^2 - 2xy - 2xz + y^2 - 2yz + z^2$  and from square roots of the Gram determinants of the five-point external momenta. The existence of these square roots poses a challenge if one wishes to solve the differential equations analytically in terms of GPLs.

For the families considered in this subsection the following square roots appear:

$$r_1 = \sqrt{\lambda(s_{12}, m_3^2, s_{45})} \quad (9.6)$$

$$r_2 = \sqrt{\lambda(s_{12}, s_{34}, m_5^2)} \quad (9.7)$$

$$r_3 = \sqrt{\lambda(\bar{m}_1^2, s_{23}, s_{45})} \quad (9.8)$$

$$r_4 = \sqrt{\lambda(\bar{m}_1^2, m_5^2, s_{15})} \quad (9.9)$$

$$r_5 = \sqrt{\Delta_5^C} = \sqrt{\Delta_5^H} \quad (9.10)$$

$$r_6 = \sqrt{\Delta_5^E} \quad (9.11)$$

$$r_7 = \sqrt{\Delta_5^G}. \quad (9.12)$$

We should note at this point that not all square roots appear in every family at the same time. More specifically, in families  $C$  and  $H$  we encounter  $r_1, r_2, r_5$ , in family  $E$   $r_1, r_2, r_3, r_4, r_6$  and in family  $G$   $r_1, r_7$ .

If one tries to compute these families using the standard differential equations approach, i.e. by differentiating with respect to all kinematic invariants, then the algebraic structure of the alphabet (i.e. the square roots appearing as letters) of the canonical differential equation for each family prohibits a straightforward solution in terms of GPLs. In order to achieve a result

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<sup>3</sup>For all integral families considered in this chapter the most complicated triangle Feynman integrals are the ones with fully massive legs and one massive propagator. This one internal mass however has no effect in the calculation of the leading singularity of the corresponding integral.

in such a form we need to find a way to deal with these square roots. Several ideas have been put forward recently that are able to circumvent this problem and provide solutions in terms of GPLs [116], [134]–[136] for specific cases, however a universal method to treat the problem of square roots appearing in the alphabet of canonical differential equations for multiscale families of Feynman integrals is still missing.

It turns out that for the families  $C, E, G, H$  the  $x$ -parametrization introduced in (9.3) and the resulting mapping of the kinematic invariants (9.4) rationalises all square roots with respect to  $x$ . This allows us to obtain a canonical differential equation in  $x$  for each of the four families considered in this subsection,

$$\partial_x \mathbf{g} = \epsilon \left( \sum_{i=1}^{l_{max}} \frac{\mathbf{M}_i}{x - l_i} \right) \mathbf{g} \quad (9.13)$$

where  $\mathbf{g}$  is the pure basis for each family,  $\mathbf{M}_i$  are the residue matrices corresponding to each letter  $l_i$  and  $l_{max}$  is the length of the alphabet<sup>4</sup>. The kinematic dependence is entirely contained within the letters  $l_i$ , leaving the residue matrices  $\mathbf{M}_i$  to be solely constructed by rational numbers. The length of the alphabet for each of the four families considered in this subsection is  $l_{max}^C = 14$ ,  $l_{max}^E = 19$ ,  $l_{max}^G = 22$ ,  $l_{max}^H = 30$ . The explicit form of the alphabet for each of the four families is provided in the ancillary files that accompany this chapter. In the next subsection we will study more closely some of these alphabets.

In order to solve (9.13) we need to provide boundary terms. We will follow closely the computational framework developed in [60], [82] for the determination of the relevant boundary terms. We start with the residue matrix corresponding to the letter  $\{0\}$ ,  $\mathbf{M}_1$  and through its Jordan Decomposition we rewrite it as follows,

$$\mathbf{M}_1 = \mathbf{S} \mathbf{D} \mathbf{S}^{-1}. \quad (9.14)$$

Then we define the *resummation matrix*  $\mathbf{R}$  as follows

$$\mathbf{R} = \mathbf{S} e^{\epsilon \mathbf{D} \log(x)} \mathbf{S}^{-1}. \quad (9.15)$$

The next step is to use IBP identities to write the pure basis  $\mathbf{g}$  in the following form

$$\mathbf{g} = \mathbf{T} \mathbf{G}. \quad (9.16)$$

The list of Feynman integrals  $\mathbf{G}$  is also provided in electronic form. Furthermore, using the expansion-by-regions method [51] implemented in the `asy` code which is shipped along with `FIESTA4` [58], we can obtain information for the asymptotic behaviour of the Feynman integrals in terms of which we express the pure basis of MI (9.16) in the limit  $x \rightarrow 0$ ,

$$G_i \underset{x \rightarrow 0}{=} \sum_j x^{b_j + a_j \epsilon} G_i^{(b_j + a_j \epsilon)} \quad (9.17)$$

where  $a_j$  and  $b_j$  are integers and  $G_i$  are the individual members of the basis  $\mathbf{G}$  of Feynman integrals in (9.16). As explained in [82], we can construct the relation

$$\mathbf{R} \mathbf{b} = \lim_{x \rightarrow 0} \mathbf{T} \mathbf{G} \Big|_{\mathcal{O}(x^{0+a_j \epsilon})} \quad (9.18)$$

where  $\mathbf{b} = \sum_{i=0}^n \epsilon^i \mathbf{b}_0^{(i)}$  are the boundary terms that we need to compute. The right-hand-side of (9.18) implies that, apart from the terms  $x^{a_i \epsilon}$  coming from (9.17), we expand around  $x = 0$ , keeping only terms of order  $x^0$ .

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<sup>4</sup>Note here that we are following the notation of [60], [72], [82] when talking about the *letters* of the *alphabet*.



Equation (9.18) allows us to fix all the necessary boundary terms without the need of any further computation for the families  $C, E, H$  while for family  $G$  a few regions had to be computed. Similarly to [72], the resulting boundary terms for all of the four families considered in this subsection are in closed form, including some  ${}_2F_1$  Hypergeometric functions which can be easily expanded to arbitrary powers of the dimensional regulator using HypExp [56]. Therefore we are able to trivially obtain solutions of (9.13) for the families  $C, E, G, H$  in terms of GPLs of arbitrary weight.

In this chapter we present explicit results for the families  $C, E, G, H$  in terms of GPLs of up to transcendental weight four, which can be written in the following compact form,

$$\begin{aligned}
\mathbf{g} = & \epsilon^0 \mathbf{b}_0^{(0)} + \epsilon \left( \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(0)} + \mathbf{b}_0^{(1)} \right) \\
& + \epsilon^2 \left( \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(0)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(1)} + \mathbf{b}_0^{(2)} \right) \\
& + \epsilon^3 \left( \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(1)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(2)} + \mathbf{b}_0^{(3)} \right) \\
& + \epsilon^4 \left( \sum \mathcal{G}_{abcd} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{M}_d \mathbf{b}_0^{(0)} + \sum \mathcal{G}_{abc} \mathbf{M}_a \mathbf{M}_b \mathbf{M}_c \mathbf{b}_0^{(1)} \right. \\
& \left. + \sum \mathcal{G}_{ab} \mathbf{M}_a \mathbf{M}_b \mathbf{b}_0^{(2)} + \sum \mathcal{G}_a \mathbf{M}_a \mathbf{b}_0^{(3)} + \mathbf{b}_0^{(4)} \right)
\end{aligned} \tag{9.19}$$

were  $\mathcal{G}_{ab\dots} := \mathcal{G}(l_a, l_b, \dots; x)$  represent the GPLs. The  $b_0^{(i)}$  terms, with  $i$  indicating the corresponding weight, consist of Zeta functions  $\zeta(i)$ , logarithms and GPLs of weight  $i$  which have as arguments rational functions of the underline kinematic variables  $S_{ij}$ .

Our results are presented in such a way that each coefficient of  $\epsilon^k$  has transcendental weight  $k$ . If we assign weight  $-1$  to  $\epsilon$ , then (9.19) has uniform weight zero. The closed-form expressions of the boundary terms trivialise the extension of (9.19) to higher transcendental weights (or higher orders in  $\epsilon$ ).

### 9.3.2 The alphabet in $x$

It is instructive to have a closer look at the alphabets for some of these families and see what lessons can be learned. We will study the alphabets of families  $C$  and  $H$ . We choose these families because they have the same external kinematics but differ on the fact that family  $H$  has one internal mass. Thus it is interesting to see how the introduction of an internal mass effects the alphabet. The conclusions drawn from the study of these families' alphabets are similar to what can be learned from the alphabets of the rest of the families considered in this chapter.

#### Family $C$

The alphabet for this family is

$$\begin{aligned}
l_1 & \rightarrow 0, l_2 \rightarrow 1, l_3 \rightarrow \frac{m_5^2}{m_5^2 - S_{15}}, l_4 \rightarrow \frac{S_{12} + S_{23}}{S_{12}}, l_5 \rightarrow \frac{S_{12} + S_{15} - S_{34}}{S_{12}}, \\
l_6 & \rightarrow \frac{-\sqrt{\Delta_1} + m_5^2 + S_{12} - S_{34}}{2S_{12}}, l_7 \rightarrow \frac{\sqrt{\Delta_1} + m_5^2 + S_{12} - S_{34}}{2S_{12}}, l_8 \rightarrow \frac{m_5^2 - S_{45}}{m_5^2 - S_{15} + S_{23} - S_{45}}, \\
l_9 & \rightarrow \frac{m_5^2 - S_{45}}{m_5^2 - S_{34} - S_{45}}, l_{10} \rightarrow \frac{S_{45}}{S_{12}}, l_{11} \rightarrow \frac{S_{45}}{S_{45} - S_{23}}, l_{12} \rightarrow \frac{m_5^2 S_{12} - S_{45} S_{12} + S_{34} S_{45}}{m_5^2 S_{12} - S_{12} S_{45}},
\end{aligned}$$

$$\begin{aligned}
l_{13} &\rightarrow -\frac{\sqrt{\Delta_2} - 2m_5^2 S_{12} - m_5^2 S_{23} + S_{15} S_{12} - S_{23} S_{12} + 2S_{45} S_{12} + S_{23} S_{34} + S_{15} S_{45} - S_{34} S_{45}}{2S_{12} (m_5^2 - S_{15} + S_{23} - S_{45})}, \\
l_{14} &\rightarrow \frac{\sqrt{\Delta_2} + 2m_5^2 S_{12} + m_5^2 S_{23} - S_{15} S_{12} + S_{23} S_{12} - 2S_{45} S_{12} - S_{23} S_{34} - S_{15} S_{45} + S_{34} S_{45}}{2S_{12} (m_5^2 - S_{15} + S_{23} - S_{45})}.
\end{aligned} \tag{9.20}$$

We notice that two square roots appear,  $\sqrt{\Delta_1}$ ,  $\sqrt{\Delta_2}$ , where  $\Delta_1$ ,  $\Delta_2$  are given by the following expressions

$$\Delta_1 = -2m_5^2 (S_{12} + S_{34}) + (m_5^2)^2 + (S_{12} - S_{34})^2, \tag{9.21}$$

$$\begin{aligned}
\Delta_2 &= (m_5^2 S_{23} - S_{34} S_{23} + (S_{34} - S_{15}) S_{45})^2 + S_{12}^2 (S_{15} - S_{23})^2 \\
&\quad + 2S_{12} (m_5^2 S_{23} (S_{15} - S_{23} - 2S_{34}) - S_{45} S_{15}^2 + S_{23} S_{34} S_{15} + (S_{23} + S_{34}) S_{45} S_{15} \\
&\quad + S_{23} S_{34} (S_{45} - S_{23})).
\end{aligned} \tag{9.22}$$

These square roots are directly associated with  $r_2$  and  $r_5$  respectively. We would expect a third square root to appear, namely  $r_1$ , as mentioned in the previous subsection. However, after introducing the  $x$ -parametrization (9.3),  $r_1$  is rational in all variables. More specifically, if we express these square roots using the first set of relations from (9.4), we get

$$r_1 = (S_{12} - S_{45}) x \tag{9.23}$$

$$r_2 = \sqrt{\Delta_1} x \tag{9.24}$$

$$r_5 = \sqrt{\Delta_2} x^2. \tag{9.25}$$

The structure of this alphabet is similar in terms of its complexity with the alphabet for the one-mass pentagon studied in [72]. The difference of course is the presence of an additional square root of the *underline kinematic variables*  $S_{ij}$  in the present case.

### Family $H$

The alphabet for this family is

$$\begin{aligned}
l_1 &\rightarrow 0, l_2 \rightarrow 1, l_3 \rightarrow \frac{m^2}{S_{12}}, l_4 \rightarrow -\frac{\sqrt{m^2}}{\sqrt{S_{12}}}, l_5 \rightarrow \frac{\sqrt{m^2}}{\sqrt{S_{12}}}, l_6 \rightarrow \frac{S_{12} + S_{23}}{S_{12}}, \\
l_7 &\rightarrow \frac{m_5^2 + S_{12} - S_{34} - \sqrt{\hat{\Delta}_1}}{2S_{12}}, l_8 \rightarrow \frac{m_5^2 + S_{12} - S_{34} + \sqrt{\hat{\Delta}_1}}{2S_{12}}, l_9 \rightarrow \frac{m^2 (m_5^2 + S_{12} - S_{34} - \sqrt{\hat{\Delta}_1})}{2m_5^2 S_{12}}, \\
l_{10} &\rightarrow \frac{m^2 (m_5^2 + S_{12} - S_{34} + \sqrt{\hat{\Delta}_1})}{2m_5^2 S_{12}}, l_{11} \rightarrow -\frac{m^2}{S_{23} - S_{45}}, l_{12} \rightarrow \frac{m_5^2 - S_{45}}{m_5^2 - S_{34} - S_{45}}, l_{13} \rightarrow \frac{m^2}{S_{45}}, \\
l_{14} &\rightarrow \frac{S_{45}}{S_{12}}, l_{15} \rightarrow -\frac{S_{45}}{S_{23} - S_{45}}, l_{16} \rightarrow \frac{-S_{12} m^2 - S_{12} S_{45} + \sqrt{\hat{\Delta}_2}}{2S_{12} (S_{23} - S_{45})}, l_{17} \rightarrow -\frac{S_{12} m^2 + S_{12} S_{45} + \sqrt{\hat{\Delta}_2}}{2S_{12} (S_{23} - S_{45})}, \\
l_{18} &\rightarrow -\frac{-m_5^2 m^2 + S_{34} m^2 + S_{45} m^2 - m_5^2 S_{12} + S_{12} S_{45} - S_{34} S_{45} + \sqrt{\hat{\Delta}_3}}{2S_{12} (m_5^2 - S_{45})}, \\
l_{19} &\rightarrow \frac{m_5^2 m^2 - S_{34} m^2 - S_{45} m^2 + m_5^2 S_{12} - S_{12} S_{45} + S_{34} S_{45} + \sqrt{\hat{\Delta}_3}}{2S_{12} (m_5^2 - S_{45})}, \\
l_{20} &\rightarrow \frac{m^2}{m_5^2 - S_{15}}, l_{21} \rightarrow \frac{m_5^2}{m_5^2 - S_{15}}, l_{22} \rightarrow \frac{m_5^2 - S_{45}}{m_5^2 - S_{15} + S_{23} - S_{45}}, l_{23} \rightarrow \frac{S_{12} + S_{15} - S_{34}}{S_{12}}, \\
l_{24} &\rightarrow \frac{m^2 (m_5^2 - S_{45})}{(m_5^2 - S_{15} + S_{23} - S_{45}) m^2 - m_5^2 S_{23} + S_{15} S_{45}}, l_{25} \rightarrow \frac{S_{12} m^2 + m_5^2 S_{12} - \sqrt{\hat{\Delta}_4}}{2S_{12} (m_5^2 - S_{15})},
\end{aligned}$$

$$\begin{aligned}
l_{26} &\rightarrow \frac{S_{12}m^2 + m_5^2 S_{12} + \sqrt{\hat{\Delta}_4}}{2S_{12}(m_5^2 - S_{15})}, \\
l_{27} &\rightarrow \frac{-S_{12}S_{15}m^2 + m_5^2 S_{23}m^2 + S_{12}S_{23}m^2 - S_{23}S_{34}m^2 - S_{15}S_{45}m^2 + S_{34}S_{45}m^2 + \sqrt{\hat{\Delta}_5}}{2S_{12}(m_5^2 S_{23} - S_{15}S_{45})}, \\
l_{28} &\rightarrow -\frac{S_{12}S_{15}m^2 - m_5^2 S_{23}m^2 - S_{12}S_{23}m^2 + S_{23}S_{34}m^2 + S_{15}S_{45}m^2 - S_{34}S_{45}m^2 + \sqrt{\hat{\Delta}_5}}{2S_{12}(m_5^2 S_{23} - S_{15}S_{45})}, \\
l_{29} &\rightarrow \frac{2m_5^2 S_{12} - S_{15}S_{12} + S_{23}S_{12} - 2S_{45}S_{12} + m_5^2 S_{23} - S_{23}S_{34} - S_{15}S_{45} + S_{34}S_{45} + \sqrt{\hat{\Delta}_6}}{2S_{12}(m_5^2 - S_{15} + S_{23} - S_{45})}, \\
l_{30} &\rightarrow -\frac{-2m_5^2 S_{12} + S_{15}S_{12} - S_{23}S_{12} + 2S_{45}S_{12} - m_5^2 S_{23} + S_{23}S_{34} + S_{15}S_{45} - S_{34}S_{45} + \sqrt{\hat{\Delta}_6}}{2S_{12}(m_5^2 - S_{15} + S_{23} - S_{45})}.
\end{aligned} \tag{9.26}$$

The first remark that we can make for this alphabet is that we have six square roots in the *underline kinematic variables*  $S_{ij}$ , namely  $\sqrt{\hat{\Delta}_i}$ ,  $i = 1, \dots, 6$ . The explicit expressions for the arguments of these square roots are as follows,

$$\hat{\Delta}_1 = -2m_5^2(S_{12} + S_{34}) + m_5^4 + (S_{12} - S_{34})^2, \tag{9.27}$$

$$\hat{\Delta}_2 = S_{12}(m^4 S_{12} + 4m^2 S_{23}(S_{12} + S_{23}) - 2m^2(S_{12} + 2S_{23})S_{45} + S_{12}S_{45}^2), \tag{9.28}$$

$$\begin{aligned}
\hat{\Delta}_3 &= m^4(-m_5^2 + S_{34} + S_{45})^2 + (m_5^2 S_{12} + (S_{34} - S_{12})S_{45})^2 \\
&\quad + 2m^2(m_5^2(-S_{12})(m_5^2 + S_{34}) + m_5^2(2S_{12} + S_{34})S_{45} - (S_{12} + S_{34})S_{45}^2 \\
&\quad + (S_{12} - S_{34})S_{34}S_{45}),
\end{aligned} \tag{9.29}$$

$$\hat{\Delta}_4 = S_{12}(m^4 S_{12} - 2m_5^2 m^2(S_{12} + 2S_{15} - 2S_{34}) + 4m^2 S_{15}(S_{12} + S_{15} - S_{34}) + m_5^4 S_{12}), \tag{9.30}$$

$$\hat{\Delta}_5 = m^4 \hat{\Delta}_6, \tag{9.31}$$

$$\begin{aligned}
\hat{\Delta}_6 &= (m_5^2 S_{23} - S_{23}S_{34} + (S_{34} - S_{15})S_{45})^2 + S_{12}^2(S_{15} - S_{23})^2 \\
&\quad + 2S_{12}(m_5^2 S_{23}(S_{15} - S_{23} - 2S_{34}) + S_{15}S_{23}S_{34} - S_{15}^2 S_{45} + S_{15}(S_{23} + S_{34})S_{45} \\
&\quad + S_{23}S_{34}(S_{45} - S_{23})).
\end{aligned} \tag{9.32}$$

In comparison with (9.20), we see the same two square roots associated with the leading singularities of the massive three-point functions,  $r_2$  and with the Gram determinant of the external momenta,  $r_5$ , namely

$$r_2 = \sqrt{\Delta_1} x = \sqrt{\hat{\Delta}_1} x \tag{9.33}$$

$$r_5 = \sqrt{\Delta_2} x^2 = \sqrt{\hat{\Delta}_6} x^2. \tag{9.34}$$

We have however four more square roots,  $\sqrt{\hat{\Delta}_2}$ ,  $\sqrt{\hat{\Delta}_3}$ ,  $\sqrt{\hat{\Delta}_4}$ ,  $\sqrt{\hat{\Delta}_5}$ , which involve the internal mass  $m^2$ , and are not directly associated with any leading singularities of any diagram from this family. We see therefore that the introduction of an internal mass has a major impact on the complexity of the resulting alphabet.

### Final remarks and comparison with other methods

We have seen that introducing an internal mass can significantly increase the complexity of the algebraic structure of an alphabet. It would be interesting to find an explanation for the appearance of the additional square roots in (9.26) which are not directly associated with a leading singularity. Normally, one would expect that the square roots that appear in the

alphabet also appear in the definition of the pure basis elements, although in the case of family  $H$  the extra square roots do not appear in the pure basis definition.

On a more general note, whenever the SDE approach has been applied in conjunction with a pure basis [60], [72], [82], we have observed a *reduction* in the number of letters that appear when compared with the alphabets that arise through the usual method of differential equations, i.e. when one differentiates with respect to all kinematic invariants. It would be interesting to see the structure of the alphabets for the families studied here when one uses the usual method of differential equations and whether this feature of alphabets in  $x$  with fewer letters still holds.

### 9.3.3 Families $D, F$

For these families we will obtain analytic expressions through the results of the families  $E$  and  $G$ . We will follow the procedure of taking the  $x \rightarrow 1$  limit of our solution for a family with  $n$  massive legs to obtain a pure basis and analytic solution of a family with  $n - 1$  massive legs, as described in detail in [60].

For families  $E$  and  $G$  we exploit the shuffle properties of GPLs to write their solution (9.19) as an expansion in terms of  $\log(1 - x)$  as follows

$$\mathbf{g} = \sum_{n \geq 0} \epsilon^n \sum_{i=0}^n \frac{1}{i!} \mathbf{c}_i^{(n)} \log^i(1 - x) \quad (9.35)$$

with all  $\mathbf{c}_i^{(n)}$  being finite in the limit  $x \rightarrow 1$ . The next step is to define the regular part of (9.35) at  $x = 1$

$$\mathbf{g}_{reg} = \sum_{n \geq 0} \epsilon^n \mathbf{c}_0^{(n)} \quad (9.36)$$

and after setting  $x = 1$  explicitly in (9.36) we may define the truncated part of (9.35),

$$\mathbf{g}_{trunc} = \mathbf{g}_{reg}(x = 1). \quad (9.37)$$

Having done that, we utilise the residue matrix that corresponds to the letter  $\{1\}$ ,  $\mathbf{M}_2$ , and define the *resummation matrix*  $\tilde{\mathbf{R}}$  as follows

$$\tilde{\mathbf{R}} = \tilde{\mathbf{S}} e^{\epsilon \tilde{\mathbf{D}} \log(1-x)} \tilde{\mathbf{S}}^{-1} \quad (9.38)$$

where  $\tilde{\mathbf{S}}, \tilde{\mathbf{D}}$  are constructed through the Jordan decomposition of  $\mathbf{M}_2$ , i.e.  $\mathbf{M}_2 = \tilde{\mathbf{S}} \tilde{\mathbf{D}} \tilde{\mathbf{S}}^{-1}$ . The *resummation matrix*  $\tilde{\mathbf{R}}$  has terms of  $(1 - x)^{a_i \epsilon}$ , with  $a_i$  being the eigenvalues of  $\mathbf{M}_2$ . After setting all terms  $(1 - x)^{a_i \epsilon}$  equal to zero, we define the purely numerical matrix  $\tilde{\mathbf{R}}_0$ . Obtaining the  $x \rightarrow 1$  limit of (9.19) amounts to acting with  $\tilde{\mathbf{R}}_0$  on (9.37)

$$\mathbf{g}_{x \rightarrow 1} = \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc}. \quad (9.39)$$

Up to now we have calculated the  $x \rightarrow 1$  limit for families  $E$  and  $G$ . This operation not only yields the result for a given family of MI with  $n$  massive legs at a special limit, but also allows us to obtain results for an independent family of MI with  $n - 1$  massive legs. In the case of family  $E$  for example, taking the  $x \rightarrow 1$  limit makes  $q_3$  to become massless through (9.3), thus yielding the kinematics for family  $D$ . However, having the  $x \rightarrow 1$  limit of  $E$  means that we have explicit solutions for the 18 pure basis elements of that family, whereas family  $D$  has 16 basis elements. This means that out of the 18 basis elements of family  $E$  at this limit, we need to find the 16 of them that form the pure basis and result for family  $D$ , i.e. at  $x \rightarrow 1$  only 16 of the 18 basis elements of family  $E$  should remain linearly independent. The same reasoning holds for family  $G$  which has 16 basis elements while family  $F$  has 15.

In order to find the pure bases for families  $D$  and  $F$  we can either use Integration-By-Part identities to do the reduction or follow the approach described in [60]. We shall use the latter method in the following.

In all cases that we have considered so far,  $\tilde{\mathbf{R}}_0$  is always an *idempotent* matrix which means that, among others, it has the following very useful property

$$\tilde{\mathbf{R}}_0^2 = \tilde{\mathbf{R}}_0. \quad (9.40)$$

Acting with  $\tilde{\mathbf{R}}_0$  on (9.39) and using (9.40) yields the following relation

$$\begin{aligned} \tilde{\mathbf{R}}_0 \mathbf{g}_{x \rightarrow 1} &= \tilde{\mathbf{R}}_0^2 \mathbf{g}_{trunc} \\ &= \tilde{\mathbf{R}}_0 \mathbf{g}_{trunc} \\ &= \mathbf{g}_{x \rightarrow 1}. \end{aligned} \quad (9.41)$$

This relation, solved as an equation for each row, produces relations that allow us to determine the linearly independent basis elements for families  $D$  and  $F$ . Therefore, applying (9.41) to the pure basis of  $E$  and  $G$  yields in an algorithmic way the pure bases for families  $D$  and  $F$ .

### 9.3.4 On the choice of integral families

The basic rule for choosing which five-point family to consider is to have the one-mass result [72] as a starting point and add masses, with the condition that their SDE in canonical form have alphabets rational in  $x$ , when one uses parametrization (9.3). If the resulting alphabet is not rational in  $x$ , then calculating the integral family through the  $x \rightarrow 1$  limit of another is considered. The exception to the above rule is the five-point family with one internal mass and massless external legs, which in the framework of the SDE can only be calculated through the  $x \rightarrow 1$  limit of its corresponding one-mass family.

More specifically, if one tries to calculate family  $D$  using (9.3) and deriving differential equations in  $x$ , then the resulting alphabet is not rational in  $x$ . Nevertheless, family  $D$  can be expressed in terms of GPLs through the  $x \rightarrow 1$  limit of family  $E$ . Apart from family  $E$  there is another family with massless propagators and three massive legs, the one which all three masses are adjacent. However, the alphabet of this family is not rational in  $x$ , if one uses (9.3) to parametrize it.

Introducing an internal mass allows for many more families to be considered. Apart from the ones presented in this chapter, a family with one internal mass and three massive legs (i.e. take family  $H$  and regard  $q_1$  as massive) was considered, however its alphabet in  $x$  is not rational using (9.3).

If the families with non-rational alphabets in  $x$  can be rationalised using a parametrization other than (9.3) remains an open question.

## 9.4 Validation

For all families computed in this chapter we have made heavy use of the `Mathematica` package `PolyLogTools` [66] for the manipulation of the resulting GPLs. As shown in (9.19), we provide explicit results up to order  $\mathcal{O}(\epsilon^4)$ . In Table 9.1 we provide an analysis of our results for each family, regarding the number of GPLs that appear in each transcendental weight, where the weight is counted as the number of  $l_i$  indices of  $\mathcal{G}(l_a, l_b, \dots; x)$ . These numbers are obtained by gathering all GPLs that appear up to order  $\mathcal{O}(\epsilon^4)$  in each integral family, and distinguishing them according to their corresponding weight. For comparison, we perform the same task for the top-sector basis element of each family.

A common feature of our results is that our solutions are dominated by the number of weight-four polylogarithmic functions. Due to the universally transcendental feature of our solutions, the  $\mathcal{O}(\epsilon^4)$  part is expected to be the most cumbersome to calculate numerically, since weight-four GPLs take longer to calculate than lower-weight ones. To avoid any misconceptions, it should be noted that each top-sector basis element starts from  $\mathcal{O}(\epsilon^3)$ , despite containing lower-weight polylogarithms.

In section 9.5 we present explicit formulas for the weight-three part of the pure top-sector basis elements of families  $C$  and  $H$  in order to give an idea of the structure and length of the resulting expressions, as well as the way the letters of the alphabets studied in subsection 9.3.2 are introduced in the relevant solutions.

Family	W=1	W=2	W=3	W=4	Total
$C$	9 (0)	54 (16)	204 (106)	605 (272)	872 (394)
$E$	13 (0)	87 (24)	349 (172)	1033 (432)	1482 (628)
$G$	21 (4)	163 (50)	878 (329)	2160 (884)	3222 (1267)
$H$	19 (0)	195 (42)	1527 (616)	5914 (2732)	7655 (3390)
$D$	11 (0)	83 (24)	393 (192)	1445 (656)	1932 (872)
$F$	19 (4)	151 (50)	872 (349)	2356 (1042)	3398 (1445)

Table 9.1: Number of GPLs entering the solution. Results for the respective top-sector basis elements are in parenthesis.

Regarding the validation of our results, we have performed numerical checks of our solution for each family against `pySecDec` [57] for Euclidean points. All GPLs have been computed numerically using the `Ginsh` command of `PolyLogTools` [66], as well as `handyG` [108], which is a Fortran implementation of the algorithms developed in [71]. For all checks that we have performed we have found perfect agreement. In Table 9.2 we also provide numerical results and timing for the top-sector basis element for each corresponding family. We include timings using `handyG` since we found that it is in general faster, although it is restrictive in its precision compared to `PolyLogTools`.

Top-Sector	Time (sec)	Result
$C$	0.146897	$-0.314547\epsilon^4 - 0.120811\epsilon^3$
$E$	0.248436	$-0.0332408\epsilon^4 - 0.0215131\epsilon^3$
$G$	0.475048	$-0.439003\epsilon^4 - 0.130267\epsilon^3$
$H$	1.89365	$-0.0165223\epsilon^4 - 0.0192393\epsilon^3$
$D$	2.15734	$-0.127286\epsilon^4 - 0.162439\epsilon^3$
$F$	0.730996	$-0.528266\epsilon^4 - 0.33331\epsilon^3$

Table 9.2: Numerical computation of GPLs using `handyG` with double precision. The computations were performed on a 1,6 GHz Intel Core i5 laptop using a single CPU core.

## 9.5 Explicit results at weight three

In this appendix we provide explicit results for families  $C$  and  $H$  for the weight-three part of each top-sector pure basis element. Assuming that each top-sector basis element is expressed in the following manner,

$$g_i^{\text{family}} = \sum_{w=3}^4 \epsilon^w \tilde{g}_{i,w}^{\text{family}} \quad (9.42)$$

we give the explicit expression for the  $\tilde{g}_{i,3}^{\text{family}}$  part. We introduce the following shorthand notations for brevity,

$$\mathcal{G}_{a,b,\dots} = \mathcal{G}(l_a, l_b, \dots; x) \quad (9.43)$$

$$L_1 = \log(-S_{12}), L_2 = \log(-S_{45}), L_3 = \log(-m_5^2), \quad (9.44)$$

$$L_4 = \log(m^2), L_5 = \log\left(\frac{m^2 - S_{45}}{m^2}\right), L_6 = \log\left(\frac{m^2 - m_5^2}{m^2}\right) \quad (9.45)$$

### 9.5.1 Top sector of family C

In the following formula note that letters  $l_i, i = \{6, 7, 13, 14\}$  contain square roots in the *underline kinematic variables*  $S_{ij}$ , as shown explicitly in (9.20).

$$\begin{aligned} \tilde{g}_{15,3}^C = & \frac{1}{4}L_1\mathcal{G}_{13,2} - \frac{1}{4}L_2\mathcal{G}_{13,2} + \frac{1}{4}L_1\mathcal{G}_{13,3} - \frac{1}{4}L_3\mathcal{G}_{13,3} - \frac{1}{4}L_1\mathcal{G}_{13,6} + \frac{1}{4}L_3\mathcal{G}_{13,6} - \frac{1}{4}L_1\mathcal{G}_{13,7} \\ & + \frac{1}{4}L_3\mathcal{G}_{13,7} - \frac{1}{4}L_2\mathcal{G}_{13,8} + \frac{1}{4}L_3\mathcal{G}_{13,8} + \frac{1}{4}L_2\mathcal{G}_{13,9} - \frac{1}{4}L_3\mathcal{G}_{13,9} + \frac{1}{4}L_1\mathcal{G}_{13,10} - \frac{1}{4}L_2\mathcal{G}_{13,10} \\ & - \frac{1}{4}L_1\mathcal{G}_{13,11} + \frac{1}{4}L_2\mathcal{G}_{13,11} - \frac{1}{4}L_1\mathcal{G}_{14,2} + \frac{1}{4}L_2\mathcal{G}_{14,2} - \frac{1}{4}L_1\mathcal{G}_{14,3} + \frac{1}{4}L_3\mathcal{G}_{14,3} + \frac{1}{4}L_1\mathcal{G}_{14,6} \\ & - \frac{1}{4}L_3\mathcal{G}_{14,6} + \frac{1}{4}L_1\mathcal{G}_{14,7} - \frac{1}{4}L_3\mathcal{G}_{14,7} + \frac{1}{4}L_2\mathcal{G}_{14,8} - \frac{1}{4}L_3\mathcal{G}_{14,8} - \frac{1}{4}L_2\mathcal{G}_{14,9} + \frac{1}{4}L_3\mathcal{G}_{14,9} \\ & - \frac{1}{4}L_1\mathcal{G}_{14,10} + \frac{1}{4}L_2\mathcal{G}_{14,10} + \frac{1}{4}L_1\mathcal{G}_{14,11} - \frac{1}{4}L_2\mathcal{G}_{14,11} + \frac{1}{2}\mathcal{G}_{13,2,1} + \frac{1}{2}\mathcal{G}_{13,3,1} + \frac{1}{4}\mathcal{G}_{13,3,3} \\ & - \frac{1}{4}\mathcal{G}_{13,3,6} - \frac{1}{4}\mathcal{G}_{13,3,7} - \frac{1}{4}\mathcal{G}_{13,4,2} - \frac{1}{4}\mathcal{G}_{13,4,10} + \frac{1}{4}\mathcal{G}_{13,4,11} - \frac{1}{4}\mathcal{G}_{13,5,3} + \frac{1}{4}\mathcal{G}_{13,5,6} \\ & + \frac{1}{4}\mathcal{G}_{13,5,7} - \frac{1}{2}\mathcal{G}_{13,6,1} - \frac{1}{2}\mathcal{G}_{13,7,1} + \frac{1}{4}\mathcal{G}_{13,8,3} - \frac{1}{4}\mathcal{G}_{13,8,11} + \frac{1}{4}\mathcal{G}_{13,9,2} - \frac{1}{4}\mathcal{G}_{13,9,6} \\ & - \frac{1}{4}\mathcal{G}_{13,9,7} + \frac{1}{4}\mathcal{G}_{13,9,10} + \frac{1}{2}\mathcal{G}_{13,10,1} - \frac{1}{2}\mathcal{G}_{13,11,1} + \frac{1}{4}\mathcal{G}_{13,11,2} + \frac{1}{4}\mathcal{G}_{13,11,10} - \frac{1}{4}\mathcal{G}_{13,11,11} \\ & - \frac{1}{4}\mathcal{G}_{13,12,2} + \frac{1}{4}\mathcal{G}_{13,12,6} + \frac{1}{4}\mathcal{G}_{13,12,7} - \frac{1}{4}\mathcal{G}_{13,12,10} - \frac{1}{2}\mathcal{G}_{14,2,1} - \frac{1}{2}\mathcal{G}_{14,3,1} - \frac{1}{4}\mathcal{G}_{14,3,3} \\ & + \frac{1}{4}\mathcal{G}_{14,3,6} + \frac{1}{4}\mathcal{G}_{14,3,7} + \frac{1}{4}\mathcal{G}_{14,4,2} + \frac{1}{4}\mathcal{G}_{14,4,10} - \frac{1}{4}\mathcal{G}_{14,4,11} + \frac{1}{4}\mathcal{G}_{14,5,3} - \frac{1}{4}\mathcal{G}_{14,5,6} \\ & - \frac{1}{4}\mathcal{G}_{14,5,7} + \frac{1}{2}\mathcal{G}_{14,6,1} + \frac{1}{2}\mathcal{G}_{14,7,1} - \frac{1}{4}\mathcal{G}_{14,8,3} + \frac{1}{4}\mathcal{G}_{14,8,11} - \frac{1}{4}\mathcal{G}_{14,9,2} + \frac{1}{4}\mathcal{G}_{14,9,6} \\ & + \frac{1}{4}\mathcal{G}_{14,9,7} - \frac{1}{4}\mathcal{G}_{14,9,10} - \frac{1}{2}\mathcal{G}_{14,10,1} + \frac{1}{2}\mathcal{G}_{14,11,1} - \frac{1}{4}\mathcal{G}_{14,11,2} - \frac{1}{4}\mathcal{G}_{14,11,10} \\ & + \frac{1}{4}\mathcal{G}_{14,11,11} + \frac{1}{4}\mathcal{G}_{14,12,2} - \frac{1}{4}\mathcal{G}_{14,12,6} - \frac{1}{4}\mathcal{G}_{14,12,7} + \frac{1}{4}\mathcal{G}_{14,12,10} \end{aligned} \quad (9.46)$$

### 9.5.2 Top sector of family H

In the following formula note that letters  $l_i, i = \{7, 8, 9, 10, 16, 17, 18, 19, 25, 26, 27, 28, 29, 30\}$  contain square roots in the *underline kinematic variables*  $S_{ij}$ , as shown explicitly in (9.26).

$$\begin{aligned} g_{18,3}^H = & \frac{1}{4}L_2\mathcal{G}_{27,3} - \frac{1}{4}L_4\mathcal{G}_{27,3} - \frac{1}{4}L_5\mathcal{G}_{27,3} - \frac{1}{4}L_3\mathcal{G}_{27,9} + \frac{1}{4}L_4\mathcal{G}_{27,9} + \frac{1}{4}L_6\mathcal{G}_{27,9} - \frac{1}{4}L_3\mathcal{G}_{27,10} \\ & + \frac{1}{4}L_4\mathcal{G}_{27,10} + \frac{1}{4}L_6\mathcal{G}_{27,10} - \frac{1}{4}L_2\mathcal{G}_{27,11} + \frac{1}{4}L_4\mathcal{G}_{27,11} + \frac{1}{4}L_5\mathcal{G}_{27,11} + \frac{1}{4}L_2\mathcal{G}_{27,13} - \frac{1}{4}L_4\mathcal{G}_{27,13} \\ & - \frac{1}{4}L_5\mathcal{G}_{27,13} - \frac{1}{4}L_2\mathcal{G}_{27,18} + \frac{1}{4}L_3\mathcal{G}_{27,18} + \frac{1}{4}L_5\mathcal{G}_{27,18} - \frac{1}{4}L_6\mathcal{G}_{27,18} - \frac{1}{4}L_2\mathcal{G}_{27,19} + \frac{1}{4}L_3\mathcal{G}_{27,19} \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{4}L_5\mathcal{G}_{27,19} - \frac{1}{4}L_6\mathcal{G}_{27,19} + \frac{1}{4}L_3\mathcal{G}_{27,20} - \frac{1}{4}L_4\mathcal{G}_{27,20} - \frac{1}{4}L_6\mathcal{G}_{27,20} + \frac{1}{4}L_2\mathcal{G}_{27,24} - \frac{1}{4}L_3\mathcal{G}_{27,24} \\
& - \frac{1}{4}L_5\mathcal{G}_{27,24} + \frac{1}{4}L_6\mathcal{G}_{27,24} - \frac{1}{4}L_2\mathcal{G}_{28,3} + \frac{1}{4}L_4\mathcal{G}_{28,3} + \frac{1}{4}L_5\mathcal{G}_{28,3} + \frac{1}{4}L_3\mathcal{G}_{28,9} - \frac{1}{4}L_4\mathcal{G}_{28,9} \\
& - \frac{1}{4}L_6\mathcal{G}_{28,9} + \frac{1}{4}L_3\mathcal{G}_{28,10} - \frac{1}{4}L_4\mathcal{G}_{28,10} - \frac{1}{4}L_6\mathcal{G}_{28,10} + \frac{1}{4}L_2\mathcal{G}_{28,11} - \frac{1}{4}L_4\mathcal{G}_{28,11} - \frac{1}{4}L_5\mathcal{G}_{28,11} \\
& - \frac{1}{4}L_2\mathcal{G}_{28,13} + \frac{1}{4}L_4\mathcal{G}_{28,13} + \frac{1}{4}L_5\mathcal{G}_{28,13} + \frac{1}{4}L_2\mathcal{G}_{28,18} - \frac{1}{4}L_3\mathcal{G}_{28,18} - \frac{1}{4}L_5\mathcal{G}_{28,18} + \frac{1}{4}L_6\mathcal{G}_{28,18} \\
& + \frac{1}{4}L_2\mathcal{G}_{28,19} - \frac{1}{4}L_3\mathcal{G}_{28,19} - \frac{1}{4}L_5\mathcal{G}_{28,19} + \frac{1}{4}L_6\mathcal{G}_{28,19} - \frac{1}{4}L_3\mathcal{G}_{28,20} + \frac{1}{4}L_4\mathcal{G}_{28,20} + \frac{1}{4}L_6\mathcal{G}_{28,20} \\
& - \frac{1}{4}L_2\mathcal{G}_{28,24} + \frac{1}{4}L_3\mathcal{G}_{28,24} + \frac{1}{4}L_5\mathcal{G}_{28,24} - \frac{1}{4}L_6\mathcal{G}_{28,24} + \frac{1}{4}L_5\mathcal{G}_{29,2} - \frac{1}{4}L_6\mathcal{G}_{29,7} - \frac{1}{4}L_6\mathcal{G}_{29,8} \\
& - \frac{1}{4}L_2\mathcal{G}_{29,12} + \frac{1}{4}L_3\mathcal{G}_{29,12} + \frac{1}{4}L_5\mathcal{G}_{29,14} - \frac{1}{4}L_5\mathcal{G}_{29,15} + \frac{1}{4}L_2\mathcal{G}_{29,18} - \frac{1}{4}L_3\mathcal{G}_{29,18} - \frac{1}{4}L_5\mathcal{G}_{29,18} \\
& + \frac{1}{4}L_6\mathcal{G}_{29,18} + \frac{1}{4}L_2\mathcal{G}_{29,19} - \frac{1}{4}L_3\mathcal{G}_{29,19} - \frac{1}{4}L_5\mathcal{G}_{29,19} + \frac{1}{4}L_6\mathcal{G}_{29,19} + \frac{1}{4}L_6\mathcal{G}_{29,21} + \frac{1}{4}L_2\mathcal{G}_{29,22} \\
& - \frac{1}{4}L_3\mathcal{G}_{29,22} - \frac{1}{4}L_2\mathcal{G}_{29,24} + \frac{1}{4}L_3\mathcal{G}_{29,24} + \frac{1}{4}L_5\mathcal{G}_{29,24} - \frac{1}{4}L_6\mathcal{G}_{29,24} - \frac{1}{4}L_5\mathcal{G}_{30,2} + \frac{1}{4}L_6\mathcal{G}_{30,7} \\
& + \frac{1}{4}L_6\mathcal{G}_{30,8} + \frac{1}{4}L_2\mathcal{G}_{30,12} - \frac{1}{4}L_3\mathcal{G}_{30,12} - \frac{1}{4}L_5\mathcal{G}_{30,14} + \frac{1}{4}L_5\mathcal{G}_{30,15} - \frac{1}{4}L_2\mathcal{G}_{30,18} + \frac{1}{4}L_3\mathcal{G}_{30,18} \\
& + \frac{1}{4}L_5\mathcal{G}_{30,18} - \frac{1}{4}L_6\mathcal{G}_{30,18} - \frac{1}{4}L_2\mathcal{G}_{30,19} + \frac{1}{4}L_3\mathcal{G}_{30,19} + \frac{1}{4}L_5\mathcal{G}_{30,19} - \frac{1}{4}L_6\mathcal{G}_{30,19} - \frac{1}{4}L_6\mathcal{G}_{30,21} \\
& - \frac{1}{4}L_2\mathcal{G}_{30,22} + \frac{1}{4}L_3\mathcal{G}_{30,22} + \frac{1}{4}L_2\mathcal{G}_{30,24} - \frac{1}{4}L_3\mathcal{G}_{30,24} - \frac{1}{4}L_5\mathcal{G}_{30,24} + \frac{1}{4}L_6\mathcal{G}_{30,24} + \frac{1}{4}\mathcal{G}_{27,3,2} \\
& - \frac{1}{4}\mathcal{G}_{27,3,4} - \frac{1}{4}\mathcal{G}_{27,3,5} + \frac{1}{4}\mathcal{G}_{27,3,14} + \frac{1}{4}\mathcal{G}_{27,9,4} + \frac{1}{4}\mathcal{G}_{27,9,5} - \frac{1}{4}\mathcal{G}_{27,9,7} - \frac{1}{4}\mathcal{G}_{27,9,8} \\
& + \frac{1}{4}\mathcal{G}_{27,10,4} + \frac{1}{4}\mathcal{G}_{27,10,5} - \frac{1}{4}\mathcal{G}_{27,10,7} - \frac{1}{4}\mathcal{G}_{27,10,8} - \frac{1}{4}\mathcal{G}_{27,11,15} + \frac{1}{4}\mathcal{G}_{27,13,2} - \frac{1}{4}\mathcal{G}_{27,13,4} \\
& - \frac{1}{4}\mathcal{G}_{27,13,5} + \frac{1}{4}\mathcal{G}_{27,13,14} - \frac{1}{4}\mathcal{G}_{27,16,2} + \frac{1}{4}\mathcal{G}_{27,16,4} + \frac{1}{4}\mathcal{G}_{27,16,5} - \frac{1}{4}\mathcal{G}_{27,16,14} + \frac{1}{4}\mathcal{G}_{27,16,15} \\
& - \frac{1}{4}\mathcal{G}_{27,17,2} + \frac{1}{4}\mathcal{G}_{27,17,4} + \frac{1}{4}\mathcal{G}_{27,17,5} - \frac{1}{4}\mathcal{G}_{27,17,14} + \frac{1}{4}\mathcal{G}_{27,17,15} - \frac{1}{4}\mathcal{G}_{27,18,2} + \frac{1}{4}\mathcal{G}_{27,18,7} \\
& + \frac{1}{4}\mathcal{G}_{27,18,8} - \frac{1}{4}\mathcal{G}_{27,18,14} - \frac{1}{4}\mathcal{G}_{27,19,2} + \frac{1}{4}\mathcal{G}_{27,19,7} + \frac{1}{4}\mathcal{G}_{27,19,8} - \frac{1}{4}\mathcal{G}_{27,19,14} + \frac{1}{4}\mathcal{G}_{27,20,21} \\
& + \frac{1}{4}\mathcal{G}_{27,24,15} - \frac{1}{4}\mathcal{G}_{27,24,21} - \frac{1}{4}\mathcal{G}_{27,25,4} - \frac{1}{4}\mathcal{G}_{27,25,5} + \frac{1}{4}\mathcal{G}_{27,25,7} + \frac{1}{4}\mathcal{G}_{27,25,8} - \frac{1}{4}\mathcal{G}_{27,25,21} \\
& - \frac{1}{4}\mathcal{G}_{27,26,4} - \frac{1}{4}\mathcal{G}_{27,26,5} + \frac{1}{4}\mathcal{G}_{27,26,7} + \frac{1}{4}\mathcal{G}_{27,26,8} - \frac{1}{4}\mathcal{G}_{27,26,21} + \frac{1}{4}\mathcal{G}_{27,29,2} - \frac{1}{4}\mathcal{G}_{27,29,7} \\
& - \frac{1}{4}\mathcal{G}_{27,29,8} + \frac{1}{4}\mathcal{G}_{27,29,14} - \frac{1}{4}\mathcal{G}_{27,29,15} + \frac{1}{4}\mathcal{G}_{27,29,21} + \frac{1}{4}\mathcal{G}_{27,30,2} - \frac{1}{4}\mathcal{G}_{27,30,7} - \frac{1}{4}\mathcal{G}_{27,30,8} \\
& + \frac{1}{4}\mathcal{G}_{27,30,14} - \frac{1}{4}\mathcal{G}_{27,30,15} + \frac{1}{4}\mathcal{G}_{27,30,21} - \frac{1}{4}\mathcal{G}_{28,3,2} + \frac{1}{4}\mathcal{G}_{28,3,4} + \frac{1}{4}\mathcal{G}_{28,3,5} - \frac{1}{4}\mathcal{G}_{28,3,14} \\
& - \frac{1}{4}\mathcal{G}_{28,9,4} - \frac{1}{4}\mathcal{G}_{28,9,5} + \frac{1}{4}\mathcal{G}_{28,9,7} + \frac{1}{4}\mathcal{G}_{28,9,8} - \frac{1}{4}\mathcal{G}_{28,10,4} - \frac{1}{4}\mathcal{G}_{28,10,5} + \frac{1}{4}\mathcal{G}_{28,10,7} \\
& + \frac{1}{4}\mathcal{G}_{28,10,8} + \frac{1}{4}\mathcal{G}_{28,11,15} - \frac{1}{4}\mathcal{G}_{28,13,2} + \frac{1}{4}\mathcal{G}_{28,13,4} + \frac{1}{4}\mathcal{G}_{28,13,5} - \frac{1}{4}\mathcal{G}_{28,13,14} + \frac{1}{4}\mathcal{G}_{28,16,2} \\
& - \frac{1}{4}\mathcal{G}_{28,16,4} - \frac{1}{4}\mathcal{G}_{28,16,5} + \frac{1}{4}\mathcal{G}_{28,16,14} - \frac{1}{4}\mathcal{G}_{28,16,15} + \frac{1}{4}\mathcal{G}_{28,17,2} - \frac{1}{4}\mathcal{G}_{28,17,4} - \frac{1}{4}\mathcal{G}_{28,17,5} \\
& + \frac{1}{4}\mathcal{G}_{28,17,14} - \frac{1}{4}\mathcal{G}_{28,17,15} + \frac{1}{4}\mathcal{G}_{28,18,2} - \frac{1}{4}\mathcal{G}_{28,18,7} - \frac{1}{4}\mathcal{G}_{28,18,8} + \frac{1}{4}\mathcal{G}_{28,18,14} + \frac{1}{4}\mathcal{G}_{28,19,2} \\
& - \frac{1}{4}\mathcal{G}_{28,19,7} - \frac{1}{4}\mathcal{G}_{28,19,8} + \frac{1}{4}\mathcal{G}_{28,19,14} - \frac{1}{4}\mathcal{G}_{28,20,21} - \frac{1}{4}\mathcal{G}_{28,24,15} + \frac{1}{4}\mathcal{G}_{28,24,21} + \frac{1}{4}\mathcal{G}_{28,25,4}
\end{aligned}$$



$$\begin{aligned}
& + \frac{1}{4}\mathcal{G}_{28,25,5} - \frac{1}{4}\mathcal{G}_{28,25,7} - \frac{1}{4}\mathcal{G}_{28,25,8} + \frac{1}{4}\mathcal{G}_{28,25,21} + \frac{1}{4}\mathcal{G}_{28,26,4} + \frac{1}{4}\mathcal{G}_{28,26,5} - \frac{1}{4}\mathcal{G}_{28,26,7} \\
& - \frac{1}{4}\mathcal{G}_{28,26,8} + \frac{1}{4}\mathcal{G}_{28,26,21} - \frac{1}{4}\mathcal{G}_{28,29,2} + \frac{1}{4}\mathcal{G}_{28,29,7} + \frac{1}{4}\mathcal{G}_{28,29,8} - \frac{1}{4}\mathcal{G}_{28,29,14} + \frac{1}{4}\mathcal{G}_{28,29,15} \\
& - \frac{1}{4}\mathcal{G}_{28,29,21} - \frac{1}{4}\mathcal{G}_{28,30,2} + \frac{1}{4}\mathcal{G}_{28,30,7} + \frac{1}{4}\mathcal{G}_{28,30,8} - \frac{1}{4}\mathcal{G}_{28,30,14} + \frac{1}{4}\mathcal{G}_{28,30,15} - \frac{1}{4}\mathcal{G}_{28,30,21} \\
& - \frac{1}{4}\mathcal{G}_{29,2,4} - \frac{1}{4}\mathcal{G}_{29,2,5} + \frac{1}{4}\mathcal{G}_{29,6,2} + \frac{1}{4}\mathcal{G}_{29,6,14} - \frac{1}{4}\mathcal{G}_{29,6,15} + \frac{1}{4}\mathcal{G}_{29,7,4} + \frac{1}{4}\mathcal{G}_{29,7,5} \\
& + \frac{1}{4}\mathcal{G}_{29,8,4} + \frac{1}{4}\mathcal{G}_{29,8,5} - \frac{1}{4}\mathcal{G}_{29,12,2} + \frac{1}{4}\mathcal{G}_{29,12,7} + \frac{1}{4}\mathcal{G}_{29,12,8} - \frac{1}{4}\mathcal{G}_{29,12,14} - \frac{1}{4}\mathcal{G}_{29,14,4} \\
& - \frac{1}{4}\mathcal{G}_{29,14,5} - \frac{1}{4}\mathcal{G}_{29,16,2} + \frac{1}{4}\mathcal{G}_{29,16,4} + \frac{1}{4}\mathcal{G}_{29,16,5} - \frac{1}{4}\mathcal{G}_{29,16,14} + \frac{1}{4}\mathcal{G}_{29,16,15} - \frac{1}{4}\mathcal{G}_{29,17,2} \\
& + \frac{1}{4}\mathcal{G}_{29,17,4} + \frac{1}{4}\mathcal{G}_{29,17,5} - \frac{1}{4}\mathcal{G}_{29,17,14} + \frac{1}{4}\mathcal{G}_{29,17,15} + \frac{1}{4}\mathcal{G}_{29,18,2} - \frac{1}{4}\mathcal{G}_{29,18,7} - \frac{1}{4}\mathcal{G}_{29,18,8} \\
& + \frac{1}{4}\mathcal{G}_{29,18,14} + \frac{1}{4}\mathcal{G}_{29,19,2} - \frac{1}{4}\mathcal{G}_{29,19,7} - \frac{1}{4}\mathcal{G}_{29,19,8} + \frac{1}{4}\mathcal{G}_{29,19,14} + \frac{1}{4}\mathcal{G}_{29,22,15} - \frac{1}{4}\mathcal{G}_{29,22,21} \\
& - \frac{1}{4}\mathcal{G}_{29,23,7} - \frac{1}{4}\mathcal{G}_{29,23,8} + \frac{1}{4}\mathcal{G}_{29,23,21} - \frac{1}{4}\mathcal{G}_{29,24,15} + \frac{1}{4}\mathcal{G}_{29,24,21} - \frac{1}{4}\mathcal{G}_{29,25,4} - \frac{1}{4}\mathcal{G}_{29,25,5} \\
& + \frac{1}{4}\mathcal{G}_{29,25,7} + \frac{1}{4}\mathcal{G}_{29,25,8} - \frac{1}{4}\mathcal{G}_{29,25,21} - \frac{1}{4}\mathcal{G}_{29,26,4} - \frac{1}{4}\mathcal{G}_{29,26,5} + \frac{1}{4}\mathcal{G}_{29,26,7} + \frac{1}{4}\mathcal{G}_{29,26,8} \\
& - \frac{1}{4}\mathcal{G}_{29,26,21} + \frac{1}{4}\mathcal{G}_{30,2,4} + \frac{1}{4}\mathcal{G}_{30,2,5} - \frac{1}{4}\mathcal{G}_{30,6,2} - \frac{1}{4}\mathcal{G}_{30,6,14} + \frac{1}{4}\mathcal{G}_{30,6,15} - \frac{1}{4}\mathcal{G}_{30,7,4} \\
& - \frac{1}{4}\mathcal{G}_{30,7,5} - \frac{1}{4}\mathcal{G}_{30,8,4} - \frac{1}{4}\mathcal{G}_{30,8,5} + \frac{1}{4}\mathcal{G}_{30,12,2} - \frac{1}{4}\mathcal{G}_{30,12,7} - \frac{1}{4}\mathcal{G}_{30,12,8} + \frac{1}{4}\mathcal{G}_{30,12,14} \\
& + \frac{1}{4}\mathcal{G}_{30,14,4} + \frac{1}{4}\mathcal{G}_{30,14,5} + \frac{1}{4}\mathcal{G}_{30,16,2} - \frac{1}{4}\mathcal{G}_{30,16,4} - \frac{1}{4}\mathcal{G}_{30,16,5} + \frac{1}{4}\mathcal{G}_{30,16,14} - \frac{1}{4}\mathcal{G}_{30,16,15} \\
& + \frac{1}{4}\mathcal{G}_{30,17,2} - \frac{1}{4}\mathcal{G}_{30,17,4} - \frac{1}{4}\mathcal{G}_{30,17,5} + \frac{1}{4}\mathcal{G}_{30,17,14} - \frac{1}{4}\mathcal{G}_{30,17,15} - \frac{1}{4}\mathcal{G}_{30,18,2} + \frac{1}{4}\mathcal{G}_{30,18,7} \\
& + \frac{1}{4}\mathcal{G}_{30,18,8} - \frac{1}{4}\mathcal{G}_{30,18,14} - \frac{1}{4}\mathcal{G}_{30,19,2} + \frac{1}{4}\mathcal{G}_{30,19,7} + \frac{1}{4}\mathcal{G}_{30,19,8} - \frac{1}{4}\mathcal{G}_{30,19,14} - \frac{1}{4}\mathcal{G}_{30,22,15} \\
& + \frac{1}{4}\mathcal{G}_{30,22,21} + \frac{1}{4}\mathcal{G}_{30,23,7} + \frac{1}{4}\mathcal{G}_{30,23,8} - \frac{1}{4}\mathcal{G}_{30,23,21} + \frac{1}{4}\mathcal{G}_{30,24,15} - \frac{1}{4}\mathcal{G}_{30,24,21} + \frac{1}{4}\mathcal{G}_{30,25,4} \\
& + \frac{1}{4}\mathcal{G}_{30,25,5} - \frac{1}{4}\mathcal{G}_{30,25,7} - \frac{1}{4}\mathcal{G}_{30,25,8} + \frac{1}{4}\mathcal{G}_{30,25,21} + \frac{1}{4}\mathcal{G}_{30,26,4} + \frac{1}{4}\mathcal{G}_{30,26,5} - \frac{1}{4}\mathcal{G}_{30,26,7} \\
& - \frac{1}{4}\mathcal{G}_{30,26,8} + \frac{1}{4}\mathcal{G}_{30,26,21}
\end{aligned} \tag{9.47}$$

## 9.6 Conclusions

The current frontier in the calculation of multiscale multiloop Feynman integrals for  $2 \rightarrow 3$  scattering processes relevant to LHC searches lies at two-loop five-point Feynman integrals with one off-shell leg and massless internal lines. As of this writing, results for all planar two-loop five-point MI have been obtained using a numerical [80], as well as an analytical approach [82]. Regarding the analytical results, all planar MI were expressed in terms of GPLs of up to transcendental weight four. These results, along with analytic results for the relevant one-loop five-point MI with one off-shell leg [72], were recently used to perform the first fully analytic calculation of a two-loop scattering amplitude for  $Wb\bar{b}$  production [84]. Furthermore, using a new method for calculating MI, the authors of [70] have computed numerically one of the non-planar two-loop five-point families. More recently, some of the authors of [80] presented the three *hexabox* topologies in [109] using the same techniques as in [80].

Looking ahead, at some point we will have to consider more complicated Feynman integrals,

involving more massive external particles and/or massive propagators. One of the expected challenges when considering such integrals is the introduction of many square roots in the alphabet of the resulting canonical differential equations. It remains a non-trivial exercise to find a universal way to handle these roots and achieve a result in terms of GPLs, however several ideas have been put forward in recent times [116], [134]–[136]. One should also keep in mind that even if a so-called *dlog* form of the differential equations is achieved, it does not guarantee that its solution will be in terms of GPLs [137].

In order to get a glimpse of the complexities that lie beyond the frontier of five-point scattering involving one off-shell leg and massless internal lines, in this chapter we studied families of one-loop five-point Feynman integrals with two and three massive external legs and massless propagators, as well as one-loop five-point families with one massive internal line and up to two massive external legs.

We used the SDE approach for the construction of canonical differential equations for pure bases of the families of Figure 9.1 and as a special limit we obtained results for the families of Figure 9.2. As it turned out, the parametrization (9.3) was enough to rationalise all square roots introduced in the alphabet of families  $C, E, G, H$  of Figure 9.1. For these families we were also able to obtain boundary terms for the canonical differential equations in closed form, allowing us to trivially derive solutions for these families in terms of GPLs of arbitrary transcendental weight.

For families  $D, F$  of Figure 9.2 we obtained analytic results through a special limit of our solutions for families  $E$  and  $G$  respectively. For all families studied in this chapter we provide explicit results in terms of GPLs of up to transcendental weight four.

Regarding the structure of the resulting alphabets in  $x$ , we saw that when one internal mass is introduced, square roots involving this mass arise, which are not present in the definition of the pure basis. Further study of these alphabets is required to pin-point the origin of these additional square roots, which we leave for future work. It is also interesting to explore in the future the structure of these alphabets when one employs the standard method of differential equations, i.e. differentiating with respect to all kinematic variables. A comparison between the two approaches might further elucidate the effectiveness of the SDE approach in providing solutions to multiscale Feynman integrals in terms of GPLs, as well as provide an idea of whether the representation of these integrals in terms of polylogarithmic functions is the best one for phenomenological applications.

# Epilogue

In this thesis we have presented analytic results for multiloop multiscale Feynman integrals regarding mostly NNLO virtual corrections to various  $2 \rightarrow 3$  scattering processes which are the subject of experimental studies at the LHC. We also presented a 3-loop calculation for one the planar families that are relevant to  $2 \rightarrow 2$  scattering processes with up to one external massive particle.

The frontier of precision calculations in perturbative QCD is rapidly expanding. Particularly in the subject of Feynman integrals, more and more analytical as well as numerical results are becoming available. Still, there are open problems to consider, such as the calculation of the two remaining 2-loop 5-point non-planar topologies with one off-shell leg, as well as the calculation of the as of yet unknown 3-loop 4-point non-planar topologies with one off-shell leg. These are important problems that need to be addressed in order to increase the precision of the theoretical predictions for key QCD scattering processes. It is the intent of the author to contribute to these outstanding problems in the near future.

The mathematical complexity of these problems poses a great challenge in our ability to provide solutions that are suited for fast and efficient evaluation at the level that is needed for phenomenological studies. The success of the past years gives us confidence that new methods and ideas will be developed, allowing us to overcome all issues that may currently seem insurmountable.

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It is a strange thing to write something personal after presenting tens of pages filled with mathematical statements, calculations and results, written in a language that is unreasonably effective in its ability to encode the laws of physics, yet it is devoid of any expression of human emotion. And yet it is us, humans, who do science, and behind every calculation, every scientific publication, there are real people leading real lives.

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