Diss. ETH No. 22916

# High precision determination of the Higgs production cross section in gluon fusion at $N^3LO$

A dissertation submitted to attain the degree

**Doctor of Sciences of ETH Zurich**

(Dr. sc. ETH)

presented by

**Falko Dulat**

Msc. Physics, ETH Zurich
born on 13.06.1987
citizen of Germany

accepted on the recommendation of:

**Prof. Charalampos Anastasiou**, examiner

**Prof. David Kosower**, co-examiner

**Prof. Zoltan Kunszt**, co-examiner

2015

# Abstract

Higgs physics at the LHC has entered the precision era after the discovery of the Higgs boson in 2012. One of the most important goals of LHC in the coming years is to determine whether the Higgs boson is the Higgs boson of the standard model, or whether it is a Higgs boson of some extension of the standard model. This requires high precision measurements of the properties of the Higgs boson. These measurements rely on accurate predictions of the Higgs cross section in the standard model. As such, the inclusive Higgs production cross section in the standard model is one of the most important theoretical inputs for Higgs physics at the LHC.

In this dissertation we present the calculation of the inclusive Higgs boson production cross section in gluon fusion at next-to-next-to-next-to-leading order in QCD. We describe the methods that have been developed in order to make this calculation possible. A lot of progress in recent perturbative calculations is due to an improved understanding of the multiple polylogarithms, the elementary functions that appear in the calculation of many cross sections. We outline several algorithms based on the modern understanding of the algebraic structure of multiple polylogarithms that are indispensable for the calculation of the integrals appearing in the Higgs cross section.

We show that using the method of differential equations, we are able to reduce the problem of calculating the Higgs cross section to the calculation of combined loop and phase space integrals in the soft limit. We describe our method for obtaining representations of integrals in the soft limit that are feasible for direct integration. In order to perform these integrals, we have developed an algorithm that allows us to perform integrals in the soft limit in a canonical way, by exploiting the algebraic structure of the multiple polylogarithms.

We apply these methods to calculate the contributions to the cross section that are due to the emission of three real partons into the final state as well as due to the emission of a single parton at two loops. We obtain thirty orders in the threshold expansion of gluon-fusion cross section. We discuss the phenomenology of this new result and show that this calculation leads to a dramatic reduction of the scale dependence down to 3%. We also compute the threshold resummation of our result to improve the behavior of potentially large threshold logarithms and show the phenomenological impact.

# Zusammenfassung

Die Higgs Physik am LHC befindet sich nach der Entdeckung des Higgs Teilchens im Jahre 2012 in einer Ära der Präzision. Eines der wichtigsten Ziele des LHC Programms in den kommenden Jahren ist es zu Bestimmen ob das entdeckte Higgs Boson das Higgs Boson des Standard Modells ist, oder ob es sich dabei um ein Higgs Boson einer Erweiterung des Standard Modells handelt. Dies erfordert hochpräzise Messungen der Eigenschaften des Higgs Bosons. Vorraussetzung für diese Messungen sind akkurate Vorhersagen der Eigenschaften des Higgs Bosons im Standard Modell. Folglich ist der inklusive Streuquerschnitt für die Produktion von Higgs Bosonen am LHC eine der wichtigsten theoretischen Vorhersagen für die Higgs Physik am LHC.

In dieser Dissertation präsentieren wir die Berechnung des inklusiven Streuquerschnitts für die Produktion von Higgs Bosonen via Gluonen-Fusion in nächst-nächst-nächst-führender Ordnung in QCD. Wir beschreiben die Methoden, welche entwickelt wurden um diese Rechnung zu ermöglichen. Ein grosser Teil des Fortschrittes in perturbativen Rechnungen der letzten Jahre ist auf ein besseres Verständniss der multiplen Polylogarithmen, der elementaren Funktionenklasse, welche viele Wirkungsquerschnitte beschreibt, zurückzuführen. Wir beschreiben mehrere Algorithmen, welche auf dem modernen Verständniss der algebraischen Strukturen, die den multiplen Polylogarithmen zugrunde liegen, basieren und für die Berechnung der im Streuquerschnitt auftretenden Integrale unersetzlich sind.

Wir zeigen mithilfe der Methode der Differentialgleichungen, wie das Problem der Berechnung des Wirkungsquerschnitts für die Produktion von Higgs Bosonen auf die Berechnung von Schleifenintegralen und Phasenrauminteralen im niederenergetischen Grenzbereich reduziert werden kann. Wir beschreiben unsere Methode um Darstellungen für Integrale im niederenergetischen Grenzbereich herzuleiten welche sich direkt integrieren lassen. Des Weiteren, haben wir haben einen Algorithmus entwickelt, welcher uns erlaubt diese Integrale im niederenergetischen Grenzwert durch Ausnutzung der algebraische Struktur der multiplen Polylogarithmen, kanonisch zu integrieren.

Wir wenden diese Methoden an, um die Beiträge zum Streuquerschnitt auszurechnen, welche durch die Emission von drei reellen Partonen in den Endzustand, sowie durch die Emission eines reellen Partons durch zwei Schleifen, hervorgerufen werden. Nachdem wir alle Resultate zusammenfügen erhalten wir den Wirkungsquerschnitt für die Produktion von Higgs Bosonen als Entwicklung um den Schwellenwert zu mehr als dreissig Ordnungen. Wir diskutieren die Phänomenologie dieses neuen Resultats und zeigen, dass diese Rechnung die Skalenabhängigkeit des Wirkungsquerschnitts auf etwa 3% reduziert. Weiterhin berechnen wir die Schwellenwertresummation unseres Resultats um das Verhalten von potentiell grossen Logarithmen zu verbesseren und demonstrieren den phänomenologischen Einfluss davon.

# Declaration

I declare that I have not previously submitted any material presented in this dissertation for any other degree at this or any other university.

The research presented in this thesis has been carried out in collaboration with C. Anastasiou, C. Duhr, E. Furlan, T. Gehrmann, F. Herzog and B. Mistlberger. Aspects of this dissertation have been published in the following publications

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, and Bernhard Mistlberger. "Soft triple-real radiation for Higgs production at N3LO". *JHEP* 1307 (2013)

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Franz Herzog, and Bernhard Mistlberger. "Real-virtual contributions to the inclusive Higgs cross section at $N^3LO$". *JHEP* 12 (2013)

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Thomas Gehrmann, Franz Herzog, and Bernhard Mistlberger. "Higgs boson gluon–fusion production at threshold in N$^3$LO QCD". *Phys. Lett.* B737 (2014)

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Thomas Gehrmann, Franz Herzog, and Bernhard Mistlberger. "Higgs boson gluon-fusion production beyond threshold in N$^3$LO QCD". *JHEP* 03 (2015)

- Falko Dulat and Bernhard Mistlberger. "Real-Virtual-Virtual contributions to the inclusive Higgs cross section at N3LO" (2014)

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Franz Herzog, and Bernhard Mistlberger. "Higgs Boson Gluon-Fusion Production in QCD at Three Loops". *Phys. Rev. Lett.* 114.21 (2015)

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Franz Herzog, and Bernhard Mistlberger. "Soft Expansion of Double-Real-Virtual Corrections to Higgs Production at N$^3$LO" (2015)

# Acknowledgements

There are many people that have greatly influenced me during my time as a PhD student and without whom I would have never been able to come this far.

First of all I would like to thank my supervisor Babis Anastasiou for all he has done for me. He first sparked my interest in particle theory with his particle physics phenomenology lecture back when I first came to ETH as a Master student. When I decided to pursue my interest in particle physics he believed in me and gave me the opportunity to do a PhD in his group. I am very grateful for this opportunity and have never regretted my decision. I would also like to thank him for being so patient with my constant interest in "useless" things such as $\mathcal{N} = 4$ super Yang-Mills while keeping me on the right track at the same time.

Special thanks go to my friend and mentor Claude Duhr from whom I have learned incredibly much. Without him, I would probably still be tinkering around with one-loop integrals. It is always a pleasure and a privilege to work with you!

I would also like to thank the whole particle theory group here at ETH. You have made these past years here an unforgettable experience and provided ample inspiration for better physics and distractions from physics whenever needed.

I would also especially like to thank my friend and fellow graduate Bernhard Mistlberger with whom I have spent countless hours discussing crazy ideas about physics and practical ideas on how to make these crazy ideas reality. It was a pleasure to work with you all these years.

Given the amount of papers I had the privilege of coauthoring during my PhD I would like to thank all my collaborators for their tireless work: Babis Anastasiou, Claude Duhr, Elisabetta Furlan, Franz Herzog, Achilleas Lazopoulos, Thomas Gehrmann and Bernhard Mistlberger.

At last I also would especially like to thank my girlfriend Gizem, who has supported me greatly, especially during these last months.

# Contents

# List of Figures

# List of Tables

CHAPTER 1

# INTRODUCTION

The experiments at the Large Hadron Collider (LHC) have been tremendously successful in the exploration of physics at the TeV scale. This remarkable achievement is the result of a strong interplay of experiments and theory. On one hand amazing experimental and technological advances were made, while on the other hand, there was extraordinary progress in perturbative QCD. In particular, the discovery of the Higgs boson [8, 9] is an incredible experimental success that has initiated an era of precision studies of the properties of the Higgs boson, where precise theory predictions for Higgs observables play an indispensable role. The increasing demand for precision predictions for the LHC has lead to a swift progress in theoretical calculations. Indeed, while next-to-leading order (NLO) computations have been completely automated, see e.g. [10, 11], including the matching to parton showers [12], progress in next-to-next-to-leading order (NNLO) is equally fast and impressive, with several important milestones for key processes at hadron colliders having recently been reached, see e.g. [13–15].

One of the most important goals of the Higgs physics program at the LHC in the coming years, is to determine whether the Higgs boson that has been observed is the Higgs boson of the standard model, or whether it is a Higgs boson of some extension of the standard model. The LHC can shed light on this question through precision measurements of the Higgs boson properties. By searching for deviations of the Higgs couplings from their predicted standard model values, the experiments at the LHC will be able to constrain the range of possible new physics models. Such studies require high precision predictions of the properties of the Higgs boson in the standard model. One ubiquitous ingredient of such predictions is the production cross section for the Higgs boson in the standard model. Unfortunately, the theory predictions for the inclusive cross section suffer from significant theoretical uncertainties. Scale variations at NNLO indicate that missing higher order effects are of the order of $\pm 9\%$ at LHC energies [16, 17]. The size of this uncertainty is comparable to the experimental uncertainty from LHC Run 1 [18, 19]. With the expected reduction of experimental uncertainty during the LHC Run 2, the theoretical uncertainty will be the dominant source of error on the extraction of Higgs observables. An update of the theoretical predictions is therefore imperative. It was therefore a logical next step to undertake efforts to compute the Higgs cross section at next-to-next-to-next-to-leading order ($\mathrm{N^3LO}$) in perturbative QCD. The cross section at $\mathrm{N^3LO}$ receives contributions from many different building blocks, all of which have been computed at least partially over the last years. The three-loop corrections to Higgs production in gluon-fusion have been obtained in ref. [20, 21], and the corrections from the emission of an additional parton at one or two loops were computed in ref. [2, 22–25]. In order to obtain a finite result, appropriate ultraviolet and infrared counterterms need to be included [26–34]. While all of these contributions had been computed in full generality, contributions from the emission of two partons at one loop and three partons at tree-level had only been computed as an expansion. In particular, for these contributions the first two terms in the expansion around threshold were obtained [1, 3, 35, 36], confirming previous results for terms of the cross section [37, 38] that are logarithmically enhanced in the threshold limit and resulting in the complete computation of the inclusive gluon-fusion cross section at $\mathrm{N^3LO}$ in the soft-virtual [3, 36, 39] and next-to-soft approximations [4]. Thanks to the universality of soft gluon emissions, these results have inspired a flurry of new results for QCD processes at $\mathrm{N^3LO}$ in the soft-virtual approximation [40–45].

Despite this progress and the exhaustive study of the soft-virtual approximation at $\mathrm{N^3LO}$, predictions derived from soft-virtual and next-to-soft approximations are unreliable at the current LHC energies, due to the slow convergence of the threshold expansion [4].

In ref. [6] we remedied this by presenting the inclusive Higgs production cross section in gluon-fusion at $\mathrm{N^3LO}$ in perturbative QCD. This constitutes the first ever complete calculation of a cross section at $\mathrm{N^3LO}$ at a hadron collider.

Many of the calculations contributing to the Higgs production cross section have been made possible by the rapid developments in the mathematics of scattering amplitudes in recent years, fueled in particular by the bustling field of amplitudes. One of the most important advances has been the systematic study of the so-called multiple polylogarithms, generalizations of the classical polylogarithms that were introduced by Goncharov [46]. These functions have been intensively studied both from the mathematical side [46–53] as well as from the perspective of physicists [54–60]. This has made many important mathematical advances available to the physics community leading to breakthroughs in the computation and study of scattering amplitudes [49, 54, 61–73].

Simultaneously, in recent years the study of differential equations has moved back into the focus of the amplitudes community [2, 5, 74–78] after they had first been introduced over fifteen years ago [79, 80] and used successfully for a variety of calculations [81–84]. New developments in recent years have lead to a flurry of new results being obtained using differential equations [2, 5, 13, 25, 85–96].

This thesis is organized as follows: in chapter 2 we review multiple polylogarithms in the context of general iterated integrals. We discuss the algebraic structures underlying these functions culminating in an analysis of the Hopf algebra structure. We then discuss several algorithms for the treatment of multiple polylogarithms, furnishing what we call the "coproduct calculus", based on the Hopf algebra structure of the multiple polylogarithms. These algorithms are crucial for the calculations presented in this thesis. In particular, we discuss the method of canonical integration and the iterative integration of parameter integrals in terms of multiple polylogarithms which has been developed by us in [1]. In chapter 3 we discuss our setup for calculating the integrals appearing in the different components of the cross section. We briefly describe the method of integration-by-parts reduction which allows us to express all integrals appearing an amplitude or cross section in terms of a small set of so-called master integrals. Afterwards, we discuss the derivation of differential equations for master integrals as well as the solution of these systems in terms of multiple polylogarithms. Finally, we analyze the boundary conditions required for the solution of the differential equations. This connects to chapter 4 where we discuss extensively the explicit calculation of boundary conditions. We derive the required loop integral and phase space integral parametrizations and discuss calculational tools like the Mellin-Barnes integrals that are required to evaluate the integrals explicitly. Furthermore, we introduce dimensional recurrence relations for combined loop and phase space integrals which provide important cross checks for the results of the explicit calculations. This chapter concludes the first part of the thesis which is concerned with calculational methods that are generally applicable. In the remainder of the thesis we discuss the application of these methods to the concrete example of the inclusive Higgs cross section in gluon-fusion at $\text{N}^3\text{LO}$. In chapter 5 we discuss the calculation of the first two terms in the threshold expansion of the so-called triple-real contributions, processes with three partons in the final state in addition to the Higgs boson. We explicitly calculate the soft integrals appearing in this contribution. In chapter 6 we present the calculation of the contributions with one parton in the final state, which are due to the square of one loop amplitudes. We calculate this part of the cross section using different methods in order to provide cross checks for the methods which will be used in the remaining contributions. In chapter 7 we calculate the parts of the cross section with one parton in the final state which are due to genuine two-loop amplitudes interfered with the corresponding tree level amplitudes. Here, we explicitly use the methods for solving differential equations discussed in chapter 3. Finally, in chapter 8 we combine all the different pieces and present the final result for the inclusive Higgs cross section at N$^3$LO. We show some phenomenological studies performed using our result and discuss its impact. We wrap up the thesis with our conclusions and future prospects in chapter 9.

## 1.1 Setup of the calculation

The gluon-fusion cross section is by far the most important production mode for Higgs bosons at the LHC. In the standard model the Higgs boson does not couple directly to gluons. As such gluon-fusion is a loop-induced process that is mediated by a virtual loop of fermions. The leading order cross section is shown in figure 1.1.

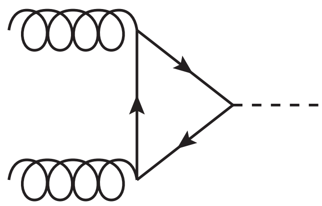


Figure 1.1: Leading order diagram for gluon-fusion

For Higgs bosons that are relatively light compared to the threshold of twice the mass of the quark running around the loop, the limit of infinitely heavy quarks yields a good approximation to the cross section [97, 98]. This approximation can be formalized in the language of an effective field theory. In this framework the heavy quarks are integrated out from the underlying field theory. In the Standard Model, this means that we integrate out the top quark, and obtain the effective Lagrangian,

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{QCD}^{n_f} - \frac{1}{4v} C_1 H G^{a,\mu\nu} G_{\mu\nu}^{a}, \tag{1.1}$$

where $G_{\mu\nu}^{a}$ denotes the gluonic field-strength tensor and $\mathcal{L}_{QCD}^{n_f}$ denotes the standard Lagrangian of quantum chromodynamics (QCD) with $n_f$ light quarks. The Wilson coefficient matches the effective theory to the Standard Model and has been computed in [99–101]. Higher-dimensional operators in the effective theory are suppressed by powers of $1/m_t$ and can be used to calculate finite-quark-mass effects of the cross section in an $1/m_t$ expansion [102–107].

In this thesis we will only concern ourselves with the leading term in the effective theory. The hadronic Higgs production cross section then takes the form

$$\sigma = \sum_{ij} \int \mathrm{d}x_1 \mathrm{d}x_2 f_i(x_1) f_j(x_2) \hat{\sigma}_{ij}(m_H^2, x_1 x_2 S), \tag{1.2}$$

where $\hat{\sigma}_{ij}$ is the partonic cross section for producing a Higgs boson from partons $i$ and $j$. $f_i(x_1)$ and $f_j(x_2)$ are the corresponding parton density functions (pdfs) and $S$ denotes the center of mass energy of the colliding protons. The partonic cross section can be expanded in the strong coupling constant $\alpha_s$, starting at order $\alpha_s^2$. The NLO corrections, proportional to $\alpha_s^3$, to the partonic cross section can be found in refs. [98, 108–113]. The NNLO corrections have been calculated in refs. [83, 114–116]. The goal of this thesis is to describe the calculation of the N$^3$LO corrections, i.e. the contribution to the cross section proportional to $\alpha_s^5$.

Before we discuss the actual calculation we will review some of the technologies that were required and in part developed for this calculation.

CHAPTER 2

# MULTIPLE POLYLOGARITHMS

The calculation of Feynman integrals is closely to the analysis of integrals over rational functions and of the transcendental functions that arise. Even the most basic Feynman integral evaluates to simple transcendental functions, the logarithms. Already at the one-loop level, in the computation of the box integral, one encounters the first generalization of the logarithm, the dilogarithm $\mathrm{Li}_2$.

Moving to more loops or more legs, Feynman diagrams yield more complicated generalizations, harmonic polylogarithms (HPLs), their two variable versions, the 2d-HPLs and so on. These classes of functions have been studied and complicated functional identities have been derived in order to enable computations involving them [59, 117, 118].

From the mathematical side, these functions have been studied extensively in the field of number theory and it has been long known [47] that the different generalizations of the logarithms are all subsets of a much larger class of functions. However it was only recently [49, 55, 56] that the results of the systematic study of the general class of functions, the multiple polylogarithms, have been exploited by the physics community. The multiple polylogarithms (MPLs) offer a plethora of beautiful structure that has aided remarkable advances in the study of scattering amplitudes [54, 62–72].

In the following we will describe the structure of the multiple polylogarithms, laying the groundwork for the methods that we employ in the calculations that are presented in later chapters of this thesis. The discussion of iterated integrals and of the multiple polylogarithms is based on reviews present in refs. [50, 56, 119, 120].

## 2.1 Iterated integrals

The multiple polylogarithms are a special case of the very general class of functions that form the so-called *iterated integrals*. Iterated integrals can be defined in terms of $\mathbb{K}$-valued 1-forms $\omega_1, \ldots, \omega_m$ on some smooth manifold $M$ over $\mathbb{K}$, where $\mathbb{K}$ is in practice usually $\mathbb{R}$ or $\mathbb{C}$. Writing

$$\int_\gamma \omega_i = \int_0^1 \mathrm{d}t \; \omega_i(t), \tag{2.1}$$

for the integral over $\omega_i$ along a piecewise smooth path $\gamma : [0,1] \to M$, parametrized by $t$, we can define the $m$-fold iterated integral as

$$\int_\gamma \omega_1 \ldots \omega_m = \int_0^1 \mathrm{d}t_1 \omega_1(t_1) \int_0^{t_1} \mathrm{d}t_2 \omega_2(t_2) \ldots \int_0^{t_{m-1}} \mathrm{d}t_m \omega_m(t_m). \tag{2.2}$$

Equivalently, we also allow for $\mathbb{K}$-linear combinations of the $\omega$. The empty iterated integral $\int_\gamma$ is just constant 1.

Already this very general definition of the iterated integrals allows for some useful properties. Any iterated integral $\int_\gamma \omega$ is invariant under reparametrizations of $\gamma$. Under reversal of the path of integration $\gamma \to \gamma^{-1} = \gamma(1-t)$, the iterated integrals transform as

$$\int_\gamma \omega_1 \ldots \omega_m = (-1)^m \int_{\gamma^{-1}} \omega_m \ldots \omega_1. \tag{2.3}$$

Two paths $\gamma_1, \gamma_2 : [0,1] \to M$ with $\gamma_2(0) = \gamma_1(1)$ can be concatenated such that the iterated integral obtained by first integrating along $\gamma_1$ and then along $\gamma_2$ is

$$\int_{\gamma_1\gamma_2} \omega_1 \ldots \omega_m = \sum_{i=0}^{m} \int_{\omega_1} \omega_1 \ldots \omega_i \int_{\gamma_2} \omega_{i+1} \ldots \omega_m. \tag{2.4}$$

The most notable property, which is used extensively, is the ***shuffle product***

$$\int_\gamma \omega_1 \ldots \omega_r \int_\gamma \omega_{r+1} \ldots \omega_{r+s} = \sum_{\sigma \in \Sigma(r,s)} \int_\gamma \omega_{\sigma(1)} \ldots \omega_{\sigma(r+s)}. \tag{2.5}$$

Here $\Sigma(r,s)$ is the set of all $(r,s)$ shuffles, i.e. permutations of $r+s$ elements which leave the ordering of the $\omega_1 \ldots \omega_r$ among each other and of the $\omega_{r+1} \ldots \omega_{r+s}$ among each other invariant. These permutations form a subset of the symmetric group $S_{r+s}$ given by

$$\Sigma(r,s) = \left\{ \sigma \in S_{r+s} : \sigma^{-1}(1) < \cdots < \sigma^{-1}(r) \;\wedge\; \sigma^{-1}(r+1) < \cdots < \sigma^{-1}(r+s) \right\}. \tag{2.6}$$

*Example.*

$$\int_\gamma \omega_1\omega_2 \int_\gamma \omega_3 = \int_\gamma \omega_1\omega_2\omega_3 + \int_\gamma \omega_1\omega_3\omega_2 + \int_\gamma \omega_3\omega_1\omega_2. \tag{2.7}$$

In general such iterated integrals will depend on the exact shape of the path $\gamma$, however it is possible to construct functions that only depend on the endpoints $\gamma(0)$ and $\gamma(1)$ of the path and on its homotopy class.

If $\omega$ is a single 1-form then the integral $\int_\gamma \omega$ does not depend on the shape of the path $\gamma$ if and only if $\omega$ is closed, i.e. $\mathrm{d}\omega = 0$. Such a function is referred to as a *homotopy functional* or as *homotopy invariant.*

*Example.*
Let $\omega$ be a 1-form on $\mathbb{R}^2$ given by

$$\omega = f(x,y)\mathrm{d}x + g(x,y)\mathrm{d}y. \tag{2.8}$$

Then in order for $\omega$ to be closed we need to have

$$\begin{aligned} \mathrm{d}\omega &= \mathrm{d}f \wedge \mathrm{d}x + \mathrm{d}g \wedge \mathrm{d}y \\ &= \left(\frac{\partial f}{\partial x}\mathrm{d}x + \frac{\partial f}{\partial y}\mathrm{d}y\right) \wedge \mathrm{d}x + \left(\frac{\partial g}{\partial x}\mathrm{d}x + \frac{\partial g}{\partial y}\mathrm{d}y\right) \wedge \mathrm{d}y \\ &= \left(\frac{\partial f}{\partial y} - \frac{\partial g}{\partial x}\right) \mathrm{d}x \wedge \mathrm{d}y = 0, \end{aligned} \tag{2.9}$$

i.e. $\partial_y f = \partial_x g$.

Homotopy invariant iterated integrals $\int_\gamma \omega$ with $\omega = \omega_1 \ldots \omega_m$ need to fulfill

$$\sum_{k=1}^{m} \omega_1 \ldots (\mathrm{d}\omega_k) \ldots \omega_m - \sum_{k=1}^{m-1} \omega_1 \ldots (\omega_k \wedge \omega_{k+1}) \ldots \omega_m = 0. \tag{2.10}$$

## 2.2 Multiple polylogarithms

Having discussed the properties of general iterated integrals, we can now specialize to the multiple polylogarithms. These are obtained by letting

$$M = \{(\sigma_1, \ldots, \sigma_n) \in \mathbb{C}^n : \sigma_i \neq \sigma_j, \quad \sigma_i \neq 0, 1\}. \tag{2.11}$$

The differential forms $\omega_i$ on $M$ are taken from the set

$$\Omega = \left\{ \frac{\mathrm{d}\sigma_i - \mathrm{d}\sigma_j}{\sigma_i - \sigma_j}, \frac{\mathrm{d}\sigma_i}{\sigma_i}, \frac{\mathrm{d}\sigma_i}{1-\sigma_i} \right\}. \tag{2.12}$$

For practical purposes it often suffices to consider $n-1$ of the $\sigma_i$ to be constant. In that case multiple polylogarithms degenerate to the so-called *hyperlogarithms* and we have the simpler differential forms

$$\omega_i = \mathrm{dlog}(z-\sigma_i) = \frac{\mathrm{d}z}{z-\sigma_i}, \tag{2.13}$$

where we have written $z$ for the non-constant $\sigma_i$ for clarity. For the remainder of this thesis this distinction is not relevant and we will usually refer to the functions as (multiple) polylogarithms even though technically we could restrict ourselves to hyperlogarithms.

The iterated integral is then written as

$$I(z_0,\sigma_1,\ldots,\sigma_n,z) = \int_\gamma \omega_n \ldots \omega_1, \tag{2.14}$$

for $\gamma(0) = z_0$ and $\gamma(1) = z$. The multiple polylogarithms are defined for $\gamma(0) = 0$ and one introduces the common notation

$$G(\sigma_n,\ldots,\sigma_1;z) = \int_\gamma \omega_n \ldots \omega_1, \tag{2.15}$$

for $\gamma(0) = 0$ and $\gamma(1) = z$. Note the reversal of the arguments between the two notations. The $\sigma_i$ are also referred to as indices. The length $n$ of the indices is called the *weight* of the multiple polylogarithm (MPL), corresponding to the number of integrations. The multiple polylogarithms are sometimes referred to as *Goncharov polylogarithms*, especially in the physics literature. For brevity we will often write the integrals directly in terms of the endpoints of the path

$$\int_{\gamma(0)}^{\gamma(1)} \omega = \int_0^1 \mathrm{d}t\; \omega(t). \tag{2.16}$$

The $I$ notation for generic basepoints (2.14) and the $G$ notation for the MPLs in eq. (2.15) can be related recursively using the path reversal and concatenation properties of the iterated integral. At weight 1, the result is simply

$$I(z_0,\sigma_1,z) = I(0,\sigma_1,z) - I(0,\sigma_1,z_0) = G(\sigma_1,z) - G(\sigma_1,z_0). \tag{2.17}$$

At higher weights one proceeds by iteration and obtains for example at weight 2,

$$\begin{aligned} I(z_0,\sigma_1,\sigma_2,z) &= \int_{z_0}^{z} \frac{\mathrm{d}t}{t-\sigma_2} I(z_0,\sigma_1,t) \overset{(2.17)}{=} \int_{z_0}^{z} \frac{\mathrm{d}t}{t-\sigma_2} \left(I(0,\sigma_1,t) - I(0,\sigma_1,z_0)\right) \\ &= G(\sigma_2,\sigma_1,z) + G(\sigma_1,z_0)\left(G(\sigma_2,z_0) - G(\sigma_2,z)\right) - G(\sigma_2,\sigma_1,z_0). \end{aligned} \tag{2.18}$$

At weight 3, we find

$$\begin{aligned}I(z_0,a_1,a_2,a_3,z) &= \int_{z_0}^{z}\frac{\mathrm{d}t}{t-\sigma_3}I(z_0,\sigma_1,\sigma_2,t)\\ &\overset{(2.18)}{=} G(\sigma_3,\sigma_2,\sigma_1,z)+G(\sigma_3,z)G(\sigma_1,\sigma_2,z_0)\\ &-G(\sigma_1,z_0)G(\sigma_3,\sigma_2,z)-G(\sigma_3,z_0)G(\sigma_1,\sigma_2,z_0)\\ &+G(\sigma_1,z_0)G(\sigma_3,\sigma_2,z_0)-G(\sigma_3,\sigma_2,\sigma_1,z_0).\end{aligned} \tag{2.19}$$

For higher weights we obtain corresponding, unwieldier expressions in a similar fashion that can be used to freely translate between the $I$ and $G$ notation. For the most part we will restrict ourselves to the $G$ notation, which is prevalent in the physics literature. However, in the later discussion of the Hopf algebra structure of the MPLs the $I$ notation is particularly useful.

Note the special case where all $\sigma_i$ are zero. In this case we use the vector notation $\vec{0}_n = \underbrace{(0,\ldots,0)}_{n\text{ times}}$ for brevity and define,

$$G(\vec{0}_n,z) = \frac{1}{n!}\log^n(z). \tag{2.20}$$

For $a \neq 0$ we have the following closed representations of certain MPLs,

$$\begin{aligned}G(\vec{a}_n,z) &= \frac{1}{n!}\log^n\left(1-\frac{z}{a}\right)\\ G(\vec{0}_{n-1},a,z) &= -\mathrm{Li}_n\left(\frac{z}{a}\right),\end{aligned} \tag{2.21}$$

where the $\mathrm{Li}_n$ are the classical polylogarithms. MPLs of the form $G(\vec{\sigma},\sigma_n,z)$ with $\sigma_n \neq 0$ are invariant under rescaling of all arguments,

$$G(\vec{\sigma},\sigma_n,z) = G(\vec{\sigma}k,\sigma_n k,zk) \quad k \in \mathbb{C}^*. \tag{2.22}$$

Convergent MPLs permit a representation in terms of multiple nested sums,

$$\begin{aligned}\mathrm{Li}_{m_1,\ldots,m_k}(x_1,\ldots,x_k) &= \sum_{n_1<n_2<\cdots<n_k}\frac{x_1^{n_1}x_2^{n_2}\ldots x_k^{n_k}}{n_1^{m_1}n_2^{m_2}\ldots n_k^{m_k}}\\ &= \sum_{n_k=1}^{\infty}\frac{x_k^{n_k}}{n_k^{m_k}}\sum_{n_{k-1}=1}^{n_k-1}\cdots\sum_{n_1=1}^{n_2-1}\frac{x_1^{n_1}}{n_1^{m_1}}.\end{aligned} \tag{2.23}$$

The Li functions are yet another notation for the same class of functions and are related to the $G$ notation through,

$$\mathrm{Li}_{m_1,\ldots,m_k}(x_1,\ldots,x_k) = (-1)^k G\left(\vec{0}_{m_k-1},\frac{1}{x_k},\ldots,\vec{0}_{m_1-1}\frac{1}{x_1\ldots x_k},1\right). \tag{2.24}$$

The number of summations $k$ is referred to as the *depth* of the multiple polylogarithm. The weight $w$ is compatible with the definition of the MPLs in terms of iterated integrals and can be computed as,

$$w = \sum_{i=1}^{k} m_i. \tag{2.25}$$

A certain specialization of the multiple polylogarithms deserves some attention due to its significance in many physical calculations. Letting $M = \mathbb{C} \setminus \{-1, 0, 1\}$ and $\mathbb{K} = \mathbb{C}$ as before, we obtain the so called harmonic polylogarithms (HPLs) [117] which are written as,

$$H(\vec{\sigma}, z) = (-1)^p G(\vec{\sigma}, z), \tag{2.26}$$

where $p$ is the number of elements of $\vec{\sigma}$ equal to $+1$. From the sum representation of the MPLs in eq. (6.77) it is apparent that the HPLs with indices 0 and 1 evaluated at 1 will yield multiple zeta values (MZVs),

$$\zeta(n_1, \ldots, n_r) = \mathrm{Li}_{n_1,\ldots,n_r}(1) = \sum_{0<k_1<\cdots<k_r} \frac{1}{k_1^{n_1} \ldots k_r^{n_r}}. \tag{2.27}$$

If we allow for all indices $-1, 0$ and 1 to be present we obtain the so called colored multiple zeta values (cMZVs),

$$\tilde{\zeta}(n_1, \ldots, n_r) = \mathrm{Li}_{n_1,\ldots,n_r}(1) = \sum_{0<k_1<\cdots<k_r} \frac{\mathrm{sign}(n_1)^{k_1} \ldots \mathrm{sign}(n_r)^{k_r}}{k_1^{|n_1|} \ldots k_r^{|n_r|}}. \tag{2.28}$$

MZVs and cMZVs have been studied extensively in mathematics and are of interest in different areas of physics, e.g. refs. [52, 60, 119, 121–126]. It can be shown that up to weight 7, all MZVs can be decomposed into the classical $\zeta$ values. For the applications presented in this thesis we can therefore restrict ourselves to classical $\zeta$ values. The cMZVs can also be decomposed so that, e.g. at weight one we obtain this way excatly one cMZV $\tilde{\zeta}(-1) = -\log(2)$. We have observed that cMZVs can appear in intermediate results of the Higgs cross section, while the final result is expressible in terms of MZVs.

## Shuffle regularization

The definition of the iterated integral over punctured manifolds immediately begs one question: What happens when the endpoint of integration approaches a point that is not in $M$?

In the case where the endpoint of the path of integration approaches a singularity, i.e., $\lim_{z\to\sigma_n} I(z_0, \sigma_1, \ldots, \sigma_n, z)$ we need a regularization prescription. In principle such a regularization introduces a dependence on the path, through the tangent of the path at the singular point [50]. However, it can be shown that this path dependence cancels in finite quantities, even if individual pieces need to be regulated in order to cancel spurious divergences, provided that the regularization prescription ensures that all pieces are regulated in the same way.

In practice we can always decompose the path of integration into piecewise straight lines such that we can define the regularization prescription explicitly by moving the endpoints of the path

$$\begin{aligned} I(z_0,\sigma_1,\ldots,\sigma_n,z) &\to \mathrm{Reg}_z I(z_0,\sigma_1,\ldots,\sigma_n,z) \\ &= \begin{cases} I(z_0(1+\varepsilon),\sigma_1,\ldots,\sigma_n,z(1-\varepsilon)), & \text{if } z_0 \neq 0, \\ I(\varepsilon,\sigma_1,\ldots,\sigma_n,z(1-\varepsilon)), & \text{if } z_0 = 0. \end{cases} \end{aligned} \tag{2.29}$$

This regularization prescription leaves convergent integrals invariant. Furthermore it preserves the shuffle product, so that we can use the shuffle identities to extract all divergences in terms of powers of logarithms. The idea is to use the shuffle product, to write the divergent parts of the iterated integral as a product of a power of a divergent logarithm and a finite MPL as well as less-divergent terms generated by the shuffle product. These less-divergent terms are then recursively also written in terms of lower powers of divergent logarithms. This way we arrive at a polynomial in $\log(\varepsilon)$ with finite coefficients. The regularized value of the MPL is then defined as the constant term of this polynomial.

*Example.*
Consider the multiple polylogarithm,

$$I(z_0(1+\varepsilon),\sigma_1,\sigma_2,\sigma_3,\sigma_3,\sigma_3(1-\varepsilon)), \tag{2.30}$$

exhibiting an endpoint divergence that is regulated by the prescription. First we would like to extract the divergent piece $I(z_0(1+\varepsilon),\sigma_3,\sigma_3,\sigma_3(1-\varepsilon))$. For brevity we write $z_0'$ for $z_0(1+\varepsilon)$ and $\sigma_3'$ for $\sigma_3(1-\varepsilon)$ and obtain

$$\begin{aligned} &I(z_0',\sigma_1,\sigma_2,\sigma_3,\sigma_3,\sigma_3') = I(z_0',\sigma_1,\sigma_2,\sigma_3')I(z_0',\sigma_3,\sigma_3,\sigma_3') \\ &- I(z_0',\sigma_1,\sigma_3,\sigma_3,\sigma_2,\sigma_3') - I(z_0',\sigma_3,\sigma_1,\sigma_3,\sigma_2,\sigma_3') - I(z_0',\sigma_3,\sigma_3,\sigma_1,\sigma_2,\sigma_3') \\ &- I(z_0',\sigma_1,\sigma_3,\sigma_2,\sigma_3,\sigma_3') - I(z_0',\sigma_3,\sigma_1,\sigma_2,\sigma_3,\sigma_3'). \end{aligned} \tag{2.31}$$

Having shuffled out the explicitly divergent piece $I(z_0',\sigma_3,\sigma_3,\sigma_3')$, we can see that the last two MPLs still end in $\sigma_3$ and thus need to be regulated as well. They are regulated by shuffling out the explicit divergence $I(z_0',\sigma_3,\sigma_3')$

so that we obtain

$$
\begin{aligned}
&I(z_0',\sigma_1,\sigma_2,\sigma_3,\sigma_3,\sigma_3') = I(z_0',\sigma_1,\sigma_2,\sigma_3')I(z_0',\sigma_3,\sigma_3,\sigma_3')\\
&- I(z_0',\sigma_1,\sigma_3,\sigma_2,\sigma_3')I(z_0',\sigma_3,\sigma_3') - I(z_0',\sigma_3,\sigma_1,\sigma_2,\sigma_3')I(z_0',\sigma_3,\sigma_3')\\
&+ I(z_0',\sigma_1,\sigma_3,\sigma_3,\sigma_2,\sigma_3') + I(z_0',\sigma_3,\sigma_1,\sigma_3,\sigma_2,\sigma_3') + I(z_0',\sigma_3,\sigma_3,\sigma_1,\sigma_2,\sigma_3').
\end{aligned}
\tag{2.32}
$$

In this expression only the terms $I(z_0',\sigma_3,\sigma_3,\sigma_3')$ and $I(z_0',\sigma_3,\sigma_3')$ are divergent and we can rewrite the regulated MPL as a polynomial in $\log(\varepsilon)$,

$$
\begin{aligned}
&I(z_0',\sigma_1,\sigma_2,\sigma_3,\sigma_3,\sigma_3') = \frac{1}{2}\log^2(\varepsilon)I(z_0,\sigma_1,\sigma_2,\sigma_3)\\
&- \log(\varepsilon)\Big[I(z_0,\sigma_1,\sigma_3,\sigma_2,\sigma_3) + I(z_0,\sigma_3,\sigma_1,\sigma_2,\sigma_3)\Big]\\
&+ I(z_0,\sigma_1,\sigma_3,\sigma_3,\sigma_2,\sigma_3) + I(z_0,\sigma_3,\sigma_1,\sigma_3,\sigma_2,\sigma_3) + I(z_0,\sigma_3,\sigma_3,\sigma_1,\sigma_2,\sigma_3).
\end{aligned}
\tag{2.33}
$$

We therefore obtain the regulated value of the MPL as

$$
\begin{aligned}
&\mathrm{Reg}_{\sigma_3} I(z_0,\sigma_1,\sigma_2,\sigma_3,\sigma_3,\sigma_3) =\\
&I(z_0,\sigma_1,\sigma_3,\sigma_3,\sigma_2,\sigma_3) + I(z_0,\sigma_3,\sigma_1,\sigma_3,\sigma_2,\sigma_3) + I(z_0,\sigma_3,\sigma_3,\sigma_1,\sigma_2,\sigma_3).
\end{aligned}
\tag{2.34}
$$

## 2.3 Algebraic structures of multiple polylogarithms

The multiple polylogarithms fulfill a plethora of complicated functional identities. A very well known one is the dilogarithm identity

$$
\mathrm{Li}_2(1-z) + \mathrm{Li}_2(z) = \zeta_2 - \log(z)\log(1-z). \tag{2.35}
$$

For simple polylogarithms of low weight some of these identities are known, however in general the functional identities of multiple polylogarithms are unknown. The derivation of these identities from the integral representation of multiple polylogarithms is not straightforward. Fortunately, there has been a considerable effort to study the relations between the multiple polylogarithms on a more abstract algebraic level. We have already encountered one simpler way to obtain functional identities. Recall the shuffle product defined in eq. (2.5). This is in fact the multiplication of a *graded algebra*, the so called shuffle algebra.

## The shuffle algebra of multiple polylogarithms

To understand the shuffle algebra, let us consider a set $A$ with an ordering relation $<$, as well as the free monoid $\mathfrak{A}$ generated by $A$, i.e. the set of all strings of zero or more elements in $A$. We refer to $A$ as alphabet, to its elements as letters and to the elements of $\mathfrak{A}$ consequently as words. $\mathfrak{A}$ is equipped with a map $\mu$ which concatenates two words $\mu(a,b) = ab$. We denote the empty word of length zero as $\varepsilon$, so that $\varepsilon w = w\varepsilon = w$. $\mathfrak{A}$ is equipped with a lexicographical ordering relation, induced by the relation $<$ on $A$. We can then obtain the shuffle algebra $\mathrm{Sh}_{\mathbb{K}}(A)$ by endowing the space $\mathbb{K}[A]$, i.e. the space spanned by polynomials of the letters in $A$ with coefficients in $\mathbb{K}$, with a shuffle product, defined recursively by

$$\begin{aligned} &xu \sqcup\!\sqcup\, yv = x(u \sqcup\!\sqcup\, yv) + y(xu \sqcup\!\sqcup\, v) && \forall x,y \in A,\ \forall u,v \in \mathfrak{A} \\ &\varepsilon \sqcup\!\sqcup\, w = w \sqcup\!\sqcup\, \varepsilon = w && \forall w \in \mathfrak{A}. \end{aligned} \tag{2.36}$$

This can also be written in terms of permutations, analogous to the formulation used in eq. (2.5),

$$w_1 \dots w_r \sqcup\!\sqcup\, w_{r+1} \dots w_{r+s} = \sum_{\sigma \in \Sigma(r,s)} w_{\sigma(1)} \dots w_{\sigma(r+s)}, \tag{2.37}$$

where $\Sigma(r,s)$ is defined in eq. (2.6). As we can see the shuffle product in eq. (2.36) preserves the length of the words and as such the shuffle algebra $\mathrm{Sh}_{\mathbb{K}(A)}$ is graded by the length of the words [50, 120],

$$\mathrm{Sh}_{\mathbb{K}}(A) = \bigoplus_{n=0}^{\infty} \mathrm{Sh}^n_{\mathbb{K}}(A) \tag{2.38}$$

We can see that this abstract definition of the shuffle algebra is compatible with the shuffle product given for the iterated integrals. Applied to the MPLs, the letters become the indices of the $G$ functions and the shuffle algebra can be used to rewrite the product of two or more $G$ functions with the same argument, e.g.

$$\begin{aligned} G(a,b,1)G(c,d,1) = G(a,b,c,d,1) + G(a,c,b,d,1) + G(a,c,d,b,1) \\ G(c,a,b,d,1) + G(c,a,d,b,1) + G(c,d,a,b,1). \end{aligned} \tag{2.39}$$

So far we have not gained anything new compared to the original definition of the iterated integrals. However, equipped with these formal definitions, we can define so-called *Lyndon words.* A Lyndon word is a non-empty word in $\mathfrak{A}$ that is smaller, with respect to the lexicographical ordering induced by the ordering operation $<$ on $A$, than any of its proper right factors,

$$\ell \text{ is a Lyndon word iff } \quad \forall u,v \in \mathfrak{A} \quad \ell = uv \text{ and } v \neq \varepsilon \Rightarrow \ell < v. \tag{2.40}$$

Or to say it differently, a Lyndon word $\ell$ is a word that cannot be factored into a product of two non-empty words, where the right factor is lexicographically smaller than $\ell$. We denote the set of all Lyndon words for a given alphabet $A$ by $\mathcal{L}(A)$. It can be shown that Lyndon words form a basis for the shuffle algebra

$$\mathrm{Sh}_{\mathbb{K}}(A) \simeq \mathbb{K}[\mathcal{L}(A)], \tag{2.41}$$

which means that we can compose any given word in $\mathfrak{A}$ modulo shuffles into a polynomial of Lyndon words with coefficients in $\mathbb{K}$ [50, 120]. For a given alphabet, the Lyndon words up to a definite length can be obtained using the Duval algorithm [127].

*Example.*
Suppose we have $A = \{w_0, w_1\}$ with $w_0 < w_1$. The Lyndon words up to length four are then

$$\mathcal{L}_4(A) = \{w_0, w_1, w_0w_1, w_0w_0w_1, w_0w_1w_1, w_0w_1w_1w_1, w_0w_0w_1w_1, w_0w_0w_0w_1\}, \tag{2.42}$$

and we can decompose for example the multiple polylogarithm $G(0, 1, 1, 0, z)$ into a polynomial over $\mathcal{L}_4(A)$ as,

$$G(0, 1, 1, 0, z) = G(0, z)G(0, 1, 1, z) - \frac{1}{2}G(0, 1, z)^2. \tag{2.43}$$

Such decompositions can be very useful as they reduce the number of functions that need to be studied at a given weight and provide a purely algebraic way of reducing certain functions of a higher weight in terms of functions of a lower weight.

## The stuffle algebra of multiple polylogarithms

The MPLs carry another algebraic structure, the so-called *stuffle* algebra, that is independent of the shuffle algebra. The stuffle algebra originates from the sum representation, eq. (6.77), of the multiple polylogarithms. To study the action of the stuffle product we define tuples,

$$\sigma_i = (m_i, x_i) \tag{2.44}$$

and a map $\mu$ between two tuples that acts as,

$$\mu(\sigma_i, \sigma_j) = \sigma_{i+j} = (m_i + m_j, x_i x_j), \tag{2.45}$$

so that we have

$$\mathrm{Li}_{\sigma_1,\ldots,\sigma_n} = \mathrm{Li}_{m_1,\ldots,m_n}(x_1, \ldots, x_n). \tag{2.46}$$

Then we can define the action of the stuffle algebra [50] as,

$$\mathrm{Li}_{\vec{\sigma}}\mathrm{Li}_{\vec{\sigma}'} = \mathrm{Li}_{\vec{\sigma}''}, \tag{2.47}$$

where $\vec{\sigma}''$ is obtained recursively as

$$\begin{aligned} \mu(\sigma\vec{\sigma},\sigma'\vec{\sigma}') = \sigma\mu(\vec{\sigma},\sigma'\vec{\sigma}') + \sigma'\mu(\sigma\vec{\sigma},\vec{\sigma}') + \mu(\sigma,\sigma')\mu(\vec{\sigma},\vec{\sigma}') \\ \mu(\sigma,1) = \sigma \quad \mu(1,\sigma) = \sigma. \end{aligned} \tag{2.48}$$

This stuffle product is generated by the products of nested sums, in the simplest case its origin can be understood easily from,

$$\mathrm{Li}_m(x)\mathrm{Li}_n(y) = \sum_{k\geq 1}\frac{x^k}{k^m}\sum_{k\geq 1}\frac{x^l}{l^n} = \left(\sum_{k<l} + \sum_{l<k} + \sum_{k=l}\right)\frac{x^k y^l}{k^m l^n}, \tag{2.49}$$

which is simply the decomposition of a two dimensional summation over $\mathbb{N}\times\mathbb{N}$ into two triangular regions $k<l$, $l<k$ and the boundary $k=l$ between them. For the simplest case of two polylogarithms of depth 1 we have e.g.,

$$\mathrm{Li}_1(x)\mathrm{Li}_2(y) = \mathrm{Li}_{1,2}(x,y) + \mathrm{Li}_{2,1}(y,x) + \mathrm{Li}_3(xy). \tag{2.50}$$

This stuffle product can be seen as the action of a generalization of the shuffle algebra, a so-called *quasi-shuffle algebra* [128–130]. Starting from the set of tuples $A$ equipped with an ordering relation $<$ that compares two elements of $A$ as

$$\sigma < \sigma' = m < m', \quad \forall\sigma = (m,x), \sigma' = (m',x') \in A, \tag{2.51}$$

we have the free monoid $\mathfrak{A}$ generated by $A$. Then we can obtain the quasi-shuffle algebra $\mathbb{Q}_{\mathbb{K}}(A)$ by endowing $\mathbb{K}[A]$ with a product

$$xu \circ yv = x(u\circ yv) + y(xu\circ v) + [x,y](u\circ v) \quad \forall x,y\in A,\ u,v\in\mathfrak{A}. \tag{2.52}$$

We can see that this algebra is a deformation of the shuffle algebra as defined in eq. (2.36), as such we obtain for

$$[x,y] = 0 \quad \forall x,y\in A, \tag{2.53}$$

the shuffle product. The stuffle algebra can be described by

$$[x,y] = \mu(x,y) \quad \forall x,y\in A. \tag{2.54}$$

## Algebras, coalgebras and Hopf algebras

Before we introduce the Hopf algebra of multiple polylogarithms, we should briefly remind ourselves of some basic algebraic structures. An *algebra* over a field $\mathbb{K}$ is a vector space $A$ over $\mathbb{K}$ that is equipped with an associative binary operation $\cdot : A\times A\to A$. This operation needs to be left and right distributive,

$$\begin{aligned} (u+v)\cdot w = u\cdot w + v\cdot w \quad \forall u,v,w\in A, \\ u\cdot(v+w) = u\cdot v + u\cdot w \quad \forall u,v,w\in A; \end{aligned} \tag{2.55}$$

furthermore, it needs to be compatible with scalar multiplication,

$$(ru)\cdot(sv) = (rs)(u\cdot v) \quad \forall u,v\in A,\ r,s\in\mathbb{K}. \tag{2.56}$$

In addition the algebra has a unit operation $\varepsilon$

$$\varepsilon\cdot u = u\cdot\varepsilon = u \quad \forall u\in A. \tag{2.57}$$

The unit element in $A$ can be identified with the unit element in $\mathbb{K}$, such that the unit operation is $\varepsilon : \mathbb{K} \to A$. We have already encountered a concrete example of an algebra, the shuffle algebra. In the case of the shuffle algebra, the binary operation is the shuffle product and the unit operation is simply the shuffle product with an empty word. We can see from the definition in eq. (2.36) that the operations fulfill the required properties.

The next structure that we require is the *coalgebra*. A coalgebra over a field $\mathbb{K}$ is a vector space $A$ over $\mathbb{K}$ equipped with a coassociative coaction, or *coproduct*, $\Delta : A \to A\otimes A$, and a unary map $\varepsilon : A \to \mathbb{K}$, the counit. Very loosely speaking, we can obtain a coalgebra from an algebra by reversing the maps that define the algebra. While the action of an algebra combines two elements in the vector space into one, the coaction of the coalgebra decomposes one element in the vector space into two. Of course we are free two iterate the decomposition of an object in $A$ by applying the coaction mutliple times. Coassociativity requires that the coaction fulfill,

$$(\mathrm{id}\otimes\Delta)\Delta = (\Delta\otimes\mathrm{id})\Delta, \tag{2.58}$$

stating that the order in which we iterate the decomposition does not matter.

*Example.*
Let us assume that $\mathbb{K} = \mathbb{Q}$ and $A = \mathfrak{A}$ is the free monoid generated by some alphabet, such that the coproduct $\Delta$ is simply the ordered deconcatenation, with the unit element 1 being the empty word, i.e.

$$\Delta(w_1w_2) = (w_1w_2)\otimes 1 + w_1\otimes w_2 + 1\otimes(w_1w_2) \quad \forall w_1,w_2\in A. \tag{2.59}$$

We iterate the comultiplication of e.g. a three letter word $w_1w_2w_3$ starting from

$$\Delta(w_1w_2w_3) = w_1w_2w_3\otimes 1 + 1\otimes w_1w_2w_3 + w_1w_2\otimes w_3 + w_1\otimes w_2w_3. \tag{2.60}$$

In the next step of the iteration we can either act with the coproduct on the first slot of the tensor product,

$$
\begin{aligned}
(\Delta \otimes \mathrm{id})\Delta(w_1w_2w_3) = {} & w_1w_2w_3 \otimes 1 \otimes 1 + 1 \otimes w_1w_2w_2 \otimes 1 + w_1w_2 \otimes w_3 \otimes 1 \\
& + w_1 \otimes w_2w_3 \otimes 1 + 1 \otimes 1 \otimes w_1w_2w_3 + 1 \otimes w_1w_2 \otimes w_3 \\
& + w_1w_2 \otimes 1 \otimes w_3 + w_1 \otimes w_2 \otimes w_3 + 1 \otimes w_1 \otimes w_2w_3 \\
& + w_1 \otimes 1 \otimes w_2w_3,
\end{aligned}
\tag{2.61}
$$

or alternatively on the second slot of the tensor product,

$$
\begin{aligned}
(\mathrm{id} \otimes \Delta)\Delta(w_1w_2w_3) = {} & w_1w_2w_3 \otimes 1 \otimes 1 + 1 \otimes 1 \otimes w_1w_2w_3 + 1 \otimes w_1w_2w_3 \otimes 1 \\
& + 1 \otimes w_1w_2 \otimes w_3 + 1 \otimes w_1 \otimes w_2w_3 + w_1w_2 \otimes 1 \otimes w_3 \\
& + w_1w_2 \otimes w_3 \otimes 1 + w_1 \otimes 1 \otimes w_2w_3 + w_1 \otimes w_2w_3 \otimes 1 \\
& + w_1 \otimes w_2 \otimes w_3.
\end{aligned}
\tag{2.62}
$$

We have colored the expressions to mark the origin of each term. As we can see, in both orderings we obtain the same result, as the coassociativity of the coaction demands.

Next we can combine the features of an algebra and a coalgebra into a single structure called a *bialgebra*. A bialgebra is consequently a vector space $A$ over $\mathbb{K}$ that is equipped with two maps, the associative multiplication $\cdot$ and the coassociative comultiplication $\Delta$. In general the multiplication and comultiplication will not be each others' inverse, however they are compatible with each other,

$$\Delta(u \cdot v) = \Delta(u) \cdot \Delta(v) \quad \forall u, v \in A. \tag{2.63}$$

The multiplication of the two coproduct terms is taken term by term in the tensor product, i.e.

$$(u_1 \otimes u_2) \cdot (v_1 \otimes v_2) = (u_1 \cdot v_1) \otimes (u_2 \cdot v_2). \tag{2.64}$$

We can turn a bialgebra into a *Hopf algebra* $\mathcal{H}$ by grading it by some weight $n$ such that

$$\mathcal{H} = \bigoplus_{n=0}^{\infty} \mathcal{H}_n. \tag{2.65}$$

The multiplication preserves the weight,

$$\mathcal{H}_m \cdot \mathcal{H}_n \subset \mathcal{H}_{n+m}, \tag{2.66}$$

as does the comultiplication,

$$\Delta(\mathcal{H}_n) \subset \bigoplus_{p+q=n} \mathcal{H}_p \otimes \mathcal{H}_q. \tag{2.67}$$

In addition a Hopf algebra is equipped with a so called antipode, a map $\mathcal{H} \to \mathcal{H}$, which however does not seem to have any practical significance, so we will not elaborate any further on it.

The action of the coproduct can be written as,

$$\Delta(x) = 1 \otimes x + x \otimes 1 + \Delta'(x) \quad \forall x \in \mathcal{H}, \tag{2.68}$$

where the reduced coproduct $\Delta'$ is defined as,

$$\Delta'(x) = \sum_{\substack{p+q=n \\ 1 \le p,q}} \Delta_{p,q}(x) \quad \forall x \in \mathcal{H}_n, \tag{2.69}$$

$\Delta_{p,q}$ is defined to be the part of the coproduct that yields elements in $\mathcal{H}_p \otimes \mathcal{H}_q$.

## The Hopf algebra of multiple polylogarithms

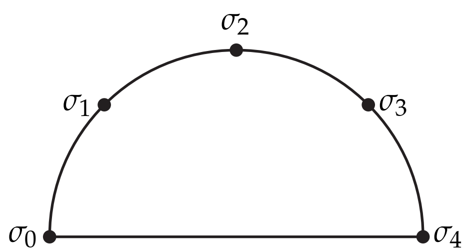
We are now in a position to introduce the Hopf algebra of multiple polylogarithms [48, 56]. The multiple polylogarithms equipped with the shuffle product form a Hopf algebra over $\mathbb{C}$ graded by their weight. The coproduct is defined as,

$$\begin{aligned} &\Delta I(\sigma_0, \sigma_1, \ldots, \sigma_n, z) = \\ &\sum_{0 \le i_1 < i_2 < \ldots i_{k+1} \le n} I(\sigma_0, \sigma_{i_1}, \ldots, \sigma_{i_k}, z) \otimes \left( \prod_{p=0}^{k} I(\sigma_{i_p}, \sigma_{i_p+1}, \ldots \sigma_{i_{p+1}-1}, \sigma_{i_{p+1}}) \right), \end{aligned} \tag{2.70}$$

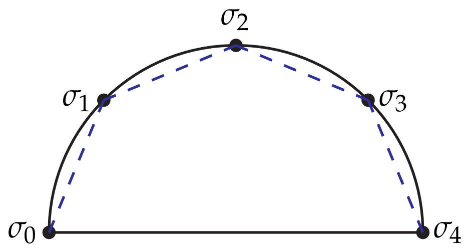
with $0 \le k \le n$. In this form the definition is valid only for generic $\sigma_i$ and in particular for $z$ not equal to any of the $\sigma_i$. In the non-generic case, when $z$ can approach any of the singular points the MPLs resulting from the coproduct need to be shuffle-regulated according to the prescription given in eq. (2.29).

In practice, the coproduct of a given MPL $I(\sigma_0, \sigma_1, \ldots, \sigma_n, \sigma_{n+1})$ is obtained by arranging the points $\sigma_i$ along a semi-circle. By connecting any subset of the points labeled $\sigma_1 \ldots \sigma_n$ in all possible ways with polygons, together with the points $\sigma_0$ and $\sigma_{n+1}$ one obtains the first entry of the coproduct. The second entry is obtained from the points that are not corners of the polygon.

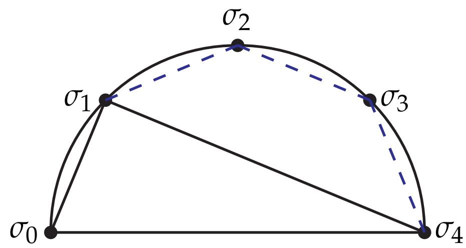
*Example.*
Consider the multiple polylogarithm $I(\sigma_0, \sigma_1, \sigma_2, \sigma_3, \sigma_4)$. We arrange the points $\sigma_0$ to $\sigma_4$ on a semi-circle



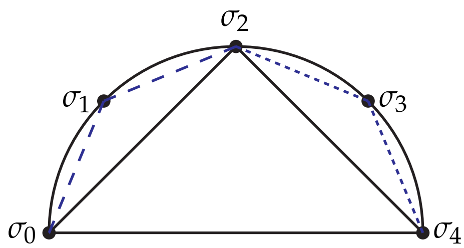
Now we draw all possible polygons that connect zero or more points from the set $\{\sigma_1, \sigma_2, \sigma_3\}$ with the base points $\sigma_0$ and $\sigma_4$ (solid black lines). The points on these polygons determine the first entry of the coproduct. The remaining points are also connected by polygons (dashed blue lines) and determine the second entry of the coproduct. Note that in the case of the second entry, disjoint polygons, in the sense that they are only joined by a vertex that belongs to the polygon for the first entry, can appear. In that case the coproduct contains a product of MPLs in the second entry.



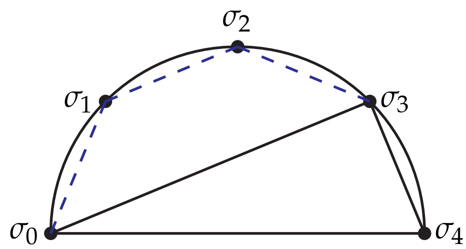
$1 \otimes I(\sigma_0, \sigma_1, \sigma_2, \sigma_3, \sigma_4)$



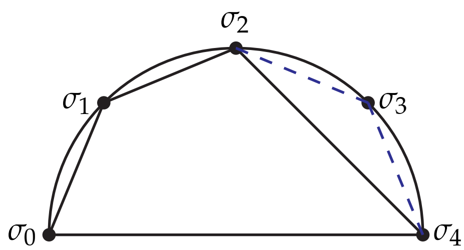
$I(\sigma_0, \sigma_1, \sigma_4) \otimes I(\sigma_1, \sigma_2, \sigma_3, \sigma_4)$



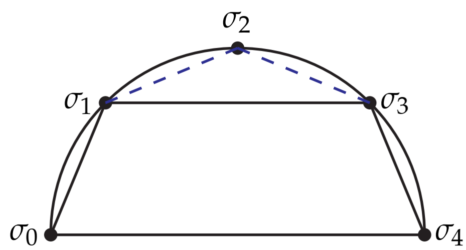
$I(\sigma_0, \sigma_2, \sigma_4) \otimes [I(\sigma_0, \sigma_1, \sigma_2) I(\sigma_2, \sigma_3, \sigma_4)]$



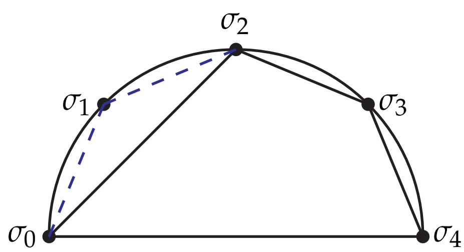
$I(\sigma_0, \sigma_3, \sigma_4) \otimes I(\sigma_0, \sigma_1, \sigma_2, \sigma_3)$



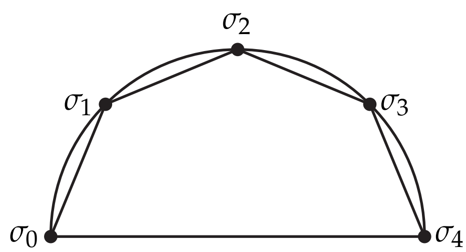
$I(\sigma_0, \sigma_1, \sigma_2, \sigma_4) \otimes I(\sigma_2, \sigma_3, \sigma_4)$



$I(\sigma_0, \sigma_1, \sigma_3, \sigma_4) \otimes I(\sigma_1, \sigma_2, \sigma_3)$



$I(\sigma_0, \sigma_2, \sigma_3, \sigma_4) \otimes I(\sigma_0, \sigma_1, \sigma_2)$



$I(\sigma_0, \sigma_1, \sigma_2, \sigma_3, \sigma_4) \otimes 1$

Using this procedure we can determine the coproduct and find

$$\begin{aligned}\Delta(I(\sigma_0,\sigma_1,\sigma_2,\sigma_3,\sigma_4)) &= I(\sigma_0,\sigma_1,\sigma_2,\sigma_3,\sigma_4)\otimes 1 + 1\otimes I(\sigma_0,\sigma_1,\sigma_2,\sigma_3,\sigma_4)\\ &+ I(\sigma_0,\sigma_1,\sigma_4)\otimes I(\sigma_1,\sigma_2,\sigma_3,\sigma_4) + I(\sigma_0,\sigma_2,\sigma_4)\otimes[I(\sigma_0,\sigma_1,\sigma_2)I(\sigma_2,\sigma_3,\sigma_4)]\\ &+ I(\sigma_0,\sigma_3,\sigma_4)\otimes I(\sigma_0,\sigma_1,\sigma_2,\sigma_3) + I(\sigma_0,\sigma_1,\sigma_2,\sigma_4)\otimes I(\sigma_2,\sigma_3,\sigma_4)\\ &+ I(\sigma_0,\sigma_1,\sigma_3,\sigma_4)\otimes I(\sigma_1,\sigma_2,\sigma_3) + I(\sigma_0,\sigma_2,\sigma_3,\sigma_4)\otimes I(\sigma_0,\sigma_1,\sigma_2).\end{aligned} \tag{2.71}$$

Using this semi-circle method the coproduct for any MPL can be determined. For the logarithm and the classical polylogarithms it is possible to write down the coproduct in a closed form

$$\begin{aligned}\Delta(\log^n(x)) &= \sum_{k=0}^{n}\binom{n}{k}\log^k(x)\otimes\log^{n-k}(x)\\ \Delta(\mathrm{Li}_n(x)) &= 1\otimes\mathrm{Li}_n(x) + \mathrm{Li}_n(x)\otimes 1 + \sum_{k=1}^{n-1}\mathrm{Li}_{n-k}(x)\otimes\frac{\log^k(x)}{k!}\end{aligned} \tag{2.72}$$

We observe that we obtain different entries of different components of the Hopf algebra after we act with the coproduct. In the example of the weight 3 MPL we found entries from the $\mathcal{H}_3\otimes\mathcal{H}_0$, $\mathcal{H}_0\otimes\mathcal{H}_3$, $\mathcal{H}_2\otimes\mathcal{H}_1$ and $\mathcal{H}_1\otimes\mathcal{H}_2$ components of $\mathcal{H}$. In fact a multiple polyogarithm of weight $n$ will be split into components of weight $p$ and $q$ with $p+q=n$, i.e. $(p,q)$ are all integer compositions of length 2 of $n$. It is therefore clear that the repeated application of the coproduct to a weight $n$ MPL stabilizes after $n-1$ iterations, or in other words, the coproduct will not produce new terms after $n-1$ iterations. After $n-1$ iterations we have reached the $\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_1$ component of the Hopf algebra which is irreducible as

$$\Delta(x) = x\otimes 1 + 1\otimes x \quad \forall x\in\mathcal{H}_1. \tag{2.73}$$

We refer to these irreducible elements of $\mathcal{H}_1\otimes\cdots\otimes\mathcal{H}_1$ as *elementary tensors.*

For practical purposes it is useful to look at subcomponents of the coproduct. We define the operator $\Delta_{w_1,\ldots,w_k}$,

$$\Delta_{w_1,\ldots,w_k}(\mathcal{H})\subset\mathcal{H}_{w_1}\otimes\cdots\otimes\mathcal{H}_{w_k} \tag{2.74}$$

i.e. the operator that picks out the $k$-fold tensor product terms from the $(k-1)$-fold application of the coproduct that lie inside the $\mathcal{H}_{w_1}\otimes\cdots\otimes\mathcal{H}_{w_k}$ component of the Hopf algebra.

Note that these definitions rely on the coassociativity of the coproduct. For example if we want to go to $\mathcal{H}_1\otimes\mathcal{H}_1\otimes\mathcal{H}_1$ starting from $\mathcal{H}_3$ it does not matter whether we use the path $\mathcal{H}_3\to\mathcal{H}_1\otimes\mathcal{H}_2\to\mathcal{H}_1\otimes\mathcal{H}_1\otimes\mathcal{H}_1$ or if we calculate $\mathcal{H}_3\to\mathcal{H}_2\otimes\mathcal{H}_1\to\mathcal{H}_1\otimes\mathcal{H}_1\otimes\mathcal{H}_1$, the result is the same. In practice we choose the latter, for reasons that will become clear later.

The maximal iteration of the coproduct $\Delta_{1,\ldots,1}$ is related to the so-called symbol map $\mathcal{S}$ that was introduced in refs. [49, 55]. One can see that

$$\mathcal{S} = \Delta_{1,\ldots,1} \mod \pi, \tag{2.75}$$

i.e. one can obtain the symbol from the maximal coproduct by dropping any terms proportional to any power of $\pi$. The literature on symbols uses a slightly different notation than the one introduced for the coproduct. We can compare the two notations using an example. Suppose we compute the coproduct of $\mathrm{Li}_3(z)$ and look at the $\Delta_{1,1,1}$ component,

$$\Delta_{1,1,1}(\mathrm{Li}_3(z)) = -G(1,z) \otimes G(0,z) \otimes G(0,z), \tag{2.76}$$

the corresponding symbol is,

$$\mathcal{S}(\mathrm{Li}_3(z)) = -(1-z) \otimes z \otimes z. \tag{2.77}$$

Recalling that $G(1,z) = \log(1-z)$ and $G(0,z) = \log(z)$, it becomes clear that we just drop the log and only write the argument in the tensor product when using the symbol notation. Since the maximal component of the coproduct can only contain logarithms in the slots of the tensor product, we will often also adopt the symbol notation for $\Delta_{1,\ldots,1}$. Note however, that while the symbol calculus only provides an equivalent expression for $\Delta_{1,\ldots,1}$, it does not provide equivalent objects for the other components of the coproduct. Using the coproduct we cannot only investigate $\Delta_{1,1,1}(\mathrm{Li}_3(z))$ in the above example, but we can also look at other components,

$$\begin{aligned} \Delta_{2,1}(\mathrm{Li}_3(z)) &= \mathrm{Li}_2(z) \otimes \log(z), \\ \Delta_{1,2}(\mathrm{Li}_3(z)) &= -\frac{1}{2}\log(1-z) \otimes \log^2(z), \end{aligned} \tag{2.78}$$

that might provide us with additional information about the function under investigation.

Not every element of $\mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_1$ lies in the image of the coaction, meaning that it is possible to write down a symbol that cannot be obtained by applying the symbol map to a linear combination of multiple polylogarithms of the appropriate weight. Conversely, that means that it is not possible to find a function corresponding to an arbitrary symbol. We therefore need to a criterion to decide whether a symbol has an associated function. This *integrability* criterion takes the following form. For a given symbol of weight $n$

$$S = \sum_{i_1,\ldots,i_n} c_{i_1,\ldots,i_n} \omega_{i_1} \otimes \cdots \otimes \omega_{i_n} \quad c_{i_1\ldots,i_n} \in \mathbb{K}, \tag{2.79}$$

to be integrable we have to demand that

$$\sum_{i_1,\ldots,i_n} c_{i_1,\ldots,i_n} \left(\mathrm{dlog}\ \omega_{i_j} \wedge \mathrm{dlog}\ \omega_{i_{j+1}}\right) \omega_{i_1} \otimes \ldots \omega_{i_{j-1}} \otimes \omega_{i_{j+2}} \otimes \omega_{i_{j+3}} \cdots \otimes \omega_{i_n} = 0, \tag{2.80}$$

which is nothing else than the requirement that the iterated integral generated by these dlog-forms be homotopy invariant, cf. eq. (2.10).

*Example.*
Let us consider the symbol of $G(x,y,z)$,

$$\begin{aligned}S = \Delta_{1,1}(G(x,y,z)) &= -y \otimes (x-z) + (x-z) \otimes (x-y) - (x-z) \otimes y \\ &- (y-z) \otimes (x-y) + (y-z) \otimes (x-z) - x \otimes (x-y) \\ &+ x \otimes y + y \otimes (x-y).\end{aligned} \tag{2.81}$$

This needs to satisfy

$$\begin{aligned}&- \mathrm{dlog}(y) \wedge \mathrm{dlog}(x-z) + \mathrm{dlog}(x-z) \wedge \mathrm{dlog}(x-y) \\ &- \mathrm{dlog}(x-z) \wedge \mathrm{dlog}(y) - \mathrm{dlog}(y-z) \wedge \mathrm{dlog}(x-y) \\ &+ \mathrm{dlog}(y-z) \wedge \mathrm{dlog}(x-z) - \mathrm{dlog}(x) \wedge \mathrm{dlog}(x-y) \\ &+ \mathrm{dlog}(x) \wedge \mathrm{dlog}(y) + \mathrm{dlog}(y) \wedge \mathrm{dlog}(x-y) = 0.\end{aligned} \tag{2.82}$$

We can bring the dlog-forms into a more manageable form by using,

$$\mathrm{dlog}(f(x,y,z)) = \sum_{\chi \in \{x,y,z\}} \frac{\partial \log(f(x,y,z))}{\partial \chi} \mathrm{d}\chi. \tag{2.83}$$

When we insert that relation and additionally exploit the antisymmetry of the wedge product we find,

$$\begin{aligned}&\mathrm{d}x \wedge \mathrm{d}y \left( -\frac{1}{(x-z)(y-z)} - \frac{1}{(x-y)(x-z)} + \frac{1}{(x-y)(y-z)} + \frac{1}{xy} \right. \\ &\left. + \frac{1}{x(x-y)} - \frac{1}{y(x-y)} \right) + \mathrm{d}x \wedge \mathrm{d}z \left( -\frac{1}{(x-y)(y-z)} + \frac{1}{(x-y)(x-z)} \right. \\ &\left. + \frac{1}{(x-z)(y-z)} \right) + \mathrm{d}y \wedge \mathrm{d}z \left( \frac{1}{(x-y)(y-z)} - \frac{1}{(x-y)(x-z)} \right. \\ &\left. - \frac{1}{(x-z)(y-z)} \right) = 0,\end{aligned} \tag{2.84}$$

where the coefficient of each wedge product needs to vanish separately. Simplifying the expression we find that this is indeed the case. Therefore the symbol $S$ is in fact integrable, which should not be surprising considering that we obtained it from a multiple polylogarithm in the first place.

The integrability criterion provides a very powerful tool to build functions from symbols. It has been used extensively in many impressive calculations in particular for scattering amplitudes in $\mathcal{N} = 4$ super Yang-Mills [65–67, 72, 73]. There it is often possible to determine the alphabet of the symbol that describes a scattering amplitude from first principles as well as certain conjectures, without actually computing the scattering amplitude. By writing down all possible linear combinations of elementary tensors of a given weight that can be built from the given symbol alphabet and demanding that the resulting symbol should satisfy the integrability condition as well as certain physical criterions it is often possible to uniquely determine the symbol of the amplitude.

At this point we should mention two more useful properties of the coproduct. At least conjecturally we have,

$$\begin{aligned} \Delta\left(\frac{\partial}{\partial x}F(x)\right) &= \left(\mathrm{id}\otimes\frac{\partial}{\partial x}\right)\Delta(F(x)), \\ \Delta(\mathcal{M}_{x=a}F(x)) &= (\mathcal{M}_{x=a}\otimes\mathrm{id})\,\Delta(F(x)). \end{aligned} \tag{2.85}$$

Here $\mathcal{M}_{x=a}$ computes the monodromy around $x = a$,

$$\mathcal{M}_{x=a}\log\omega = \begin{cases} 2\pi i, & \text{if } \omega|_{x=a} = 0, \\ 0, & \text{otherwise.} \end{cases} \tag{2.86}$$

This means that differential operators only act on the last component of the coproduct while monodromy operators only act on the first component. This also holds for the iterated coproduct. In particular, at the symbol level, the first entry of the elementary tensor encodes the information about the monodromy of the function, while the last entry encodes information about the derivatives.

This has profound implications for the structure of the symbol of a physical scattering amplitude. Physical amplitudes are only allowed to have branch cuts in certain variables, which is often discussed under the concept of *unitarity*. For example, a planar four-point integral cannot have a branch cut for $u \to 0$. Knowing how monodromy operators act on the symbol we can therefore conclude that $u$ will not appear in the first entry of the symbol of such an amplitude.

## The coproduct of multiple zeta values

Before we are ready to use the coproduct in actual computations we first have to investigate the coproduct of multiple zeta values. As we have seen before, cMZVs are HPLs evaluated at unit argument, cf. eq. (2.28). As such we should expect to be able to compute their coproduct. We can for example look at the coproduct of $\mathrm{Li}_2(z)$,

$$\Delta(\mathrm{Li}_2)(z) = 1\otimes\mathrm{Li}_2(z) + \mathrm{Li}_2(z)\otimes 1 - \log(1-z)\otimes\log(z); \tag{2.87}$$

taking the limit $z \to 1$ we obtain the coproduct of $\zeta_2$,

$$\Delta(\zeta_2) = 1\otimes\zeta_2 + \zeta_2\otimes 1. \tag{2.88}$$

Considering the closed form of the coproduct of $\mathrm{Li}_n$ in eq. (2.72) we should conclude that

$$\Delta(\zeta_n) = 1 \otimes \zeta_n + \zeta_n \otimes 1. \tag{2.89}$$

At this point we can observe that the classical zeta values, i.e. MZVs of depth 1, are primitives of the coproduct, i.e. they cannot be split into objects of lower weight.

Another observation however hints at a problem in our defintion of the Hopf algebra. For example for $\zeta_4$ we have,

$$\Delta(\zeta_4) = \zeta_4 \otimes 1 + 1 \otimes \zeta_4. \tag{2.90}$$

However, the even $\zeta$ values are not algebraically independent, as a matter of fact,

$$\zeta_4 = \frac{2}{5}\zeta_2^2. \tag{2.91}$$

This relation should of course also be respected by the coproduct,

$$\Delta(\zeta_4) = \frac{2}{5}\Delta(\zeta_2^2) = \frac{2}{5}(\zeta_2 \otimes 1 + 1 \otimes \zeta_2)^2 = \frac{2}{5}(1 \otimes \zeta_2^2 + \zeta_2^2 \otimes 1 + 2\zeta_2 \otimes \zeta_2). \tag{2.92}$$

This is a clear contradiction with eq. (2.90) due to the $\zeta_2 \otimes \zeta_2$ term, which furthermore would suggest that $\zeta_4$ is not a primitive of the coproduct.

One obvious way to avoid this inconsistency would be to only compute $\Delta$ mod $\zeta_2$. However, in that case the coproduct would lose all information about terms proportional to $\zeta_2$, which might be too big a price to pay.

Another, less destructive way to fix the inconsistency was suggested by Brown [51]. It consists of defining the coproduct of all even $\zeta$ values as

$$\Delta(\zeta_{2n}) = \zeta_{2n} \otimes 1. \tag{2.93}$$

With this definition the problem is solved,

$$\Delta(\zeta_4) = \frac{2}{5}\Delta(\zeta_2^2) = \frac{2}{5}(\zeta_2 \otimes 1)^2 = \frac{2}{5}\zeta_2^2 \otimes 1 = \zeta_4 \otimes 1. \tag{2.94}$$

As suggested by Duhr [56], this definition can also be extended to include $\pi$ into coproduct,

$$\Delta(\pi) = \pi \otimes 1. \tag{2.95}$$

This is compatible with the definition of the even $\zeta$ values,

$$\Delta(\zeta_2) = \frac{1}{6}\Delta(\pi^2) = \frac{1}{6}(\pi \otimes 1)^2 = \frac{1}{6}\pi^2 \otimes 1 = \zeta_2 \otimes 1. \tag{2.96}$$

The inclusion of terms proportional to $\pi$ into the Hopf algebra is important as it allows us to keep terms proportional to $i\pi$ which appear in the analytic continuation of logarithms.

These modifications also lead to a modification of the coalgebra structure of $\mathcal{H}$, the coproduct is changed from a map $\Delta : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}$ to a map

$$\Delta : \mathcal{H} \to \mathcal{H} \otimes \mathcal{H}^{\pi}, \tag{2.97}$$

where $\mathcal{H}^{\pi}$ is the Hopf algebra modulo powers of $\pi$, meaning that when computing the coproduct, we drop all terms proportional to $\pi$ in all slots of the tensor except for the first one.

## Coproduct calculus

With the algebraic foundation in place, we can now proceed to the core of the coproduct calculus that makes the coproduct useful for actual calculations involving multiple polylogarithms. Suppose that we have two functions $\mathcal{U}_w$ and $\mathcal{V}_w$ of equal weight $w$ that are equal modulo functional identities of the multiple polylogarithms, i.e. both expressions describe the same function but due to the complicated functional identities of the MPLs this equality is not manifest. It follows that their coproducts must be equal,

$$\Delta(\mathcal{U}_w) = \Delta(\mathcal{V}_w), \tag{2.98}$$

and in particular

$$\Delta'(\mathcal{U}_w) = \Delta'(\mathcal{V}_w). \tag{2.99}$$

As we have seen, the reduced coproduct $\Delta'$ of a weight $w$ MPL only involves MPLs of weight $w' < w$. This means that, while the functional identities to relate $\mathcal{U}_w$ and $\mathcal{V}_w$ are unknown, the identities at lower weight might be known, so that it will be possible to prove the equality of the coproducts in eq. (2.99). However, we should note that the equality (2.99) does not imply the equality (2.98) since we lose all information about the primitives of the coproduct at weight $w$. However, at least conjecturally we can state that, starting from a function $\mathcal{U}_w$ of weight $w$, if we can find a function $\mathcal{F}_w$, such that

$$\Delta'(\mathcal{F}_w) = \Delta'(\mathcal{U}_w), \tag{2.100}$$

then it follows that

$$\mathcal{U}_w = \mathcal{F}_w + \sum_{\rho} c_\rho P_\rho^{(w)}, \tag{2.101}$$

where the $P_\rho^{(w)}$ are the primitives of $\mathcal{H}_w$ with some coefficients $c_\rho \in \mathbb{Q}$.

In practice the primitives of $\mathcal{H}_w$ need to be determined for the given problem and usually turn out to be powers of $\pi$, $\zeta$ values as well as the Clausen function evaluated at roots of unity. The $c_\rho$ can then be determined by demanding that the functions $\mathcal{U}_w$ and $\mathcal{F}_w$ be equal in certain limits [53, 120]. Another, very powerful and flexible method for determining the $c_\rho$, which we use in practice, is to evaluate $\mathcal{U}_w - \mathcal{F}_w$ numerically at a few points. By calculating this difference numerically to sufficiently many digits (several tens of digits), we can use the PSLQ algorithm [131]. This algorithm can be used to decompose a number that is known with finite precision into a basis of transcendental numbers with rational coefficients. Of course this basis needs to be determined a priori, however the transcendental numbers that make up the basis are exactly the primitives of $\mathcal{H}_w$.

*Example.*
As an example we can try to reproduce the well known dilogarithm identity in eq. (2.35) using the coproduct. Or to phrase it differently, let us assume we would like to rewrite $\mathrm{Li}_2(1-z)$ in terms of $\mathrm{Li}_2(z)$. We start by computing the maximal coproduct, or symbol, of $\mathrm{Li}_2(1-z)$,

$$\Delta_{1,1}(\mathrm{Li}_2(1-z)) = -\log(z) \otimes \log(1-z). \tag{2.102}$$

Next, we would like to find a function $f(z)$ that has the same symbol. Knowing that,

$$\begin{aligned} \Delta_{1,1}(\mathrm{Li}_2(z)) &= -\log(1-z) \otimes \log(z), \\ \Delta_{1,1}(\log(z)\log(1-z)) &= \log(z) \otimes \log(1-z) + \log(1-z) \otimes \log(z), \end{aligned} \tag{2.103}$$

it is not hard to guess an ansatz for $f(z)$,

$$f(z) = -\mathrm{Li}_2(z) - \log(z)\log(1-z) + c\zeta_2. \tag{2.104}$$

By evaluating the difference $\mathrm{Li}_2(1-z) - f(z)$ at $z = 1$ we can easily determine the unknown coefficient $c$ of the primitive $\zeta_2$ and find,

$$\mathrm{Li}_z(1-z) = -\mathrm{Li}_2(z) - \log(z)\log(1-z) + \zeta_2. \tag{2.105}$$

*Example.*
In the same way we can try to determine whether we can write $\mathrm{Li}_2\left(1-\frac{1}{z}\right)$ in terms of functions with simpler arguments. First we compute the symbol

$$\Delta_{1,1}\left(\mathrm{Li}_2\left(1-\frac{1}{z}\right)\right) = z \otimes (1-z) - z \otimes z, \tag{2.106}$$

guessing an ansatz as before we can determine $f(z)$ so that,

$$\Delta_{1,1}(f(z)) = \Delta_{1,1}\left(\mathrm{Li}_2\left(1-\frac{1}{z}\right)\right), \tag{2.107}$$

to be

$$f(z) = \mathrm{Li}_2(z) - \frac{1}{2}\log^2(z) + \log(1-z)\log(z) + c\zeta_2 \tag{2.108}$$

Evaluating $\mathrm{Li}_2\left(1-\frac{1}{z}\right) - f(z)$ in the limit $z \to 1$ we find that,

$$\mathrm{Li}_2\left(1-\frac{1}{z}\right) = \mathrm{Li}_2(z) - \frac{1}{2}\log^2(z) + \log(1-z)\log(z) - \zeta_2. \tag{2.109}$$

*Example.*
Equipped with this knowledge we can look at higher weights, where the coproduct calculus really starts to shine. Suppose we would like to rewrite $\mathrm{Li}_3(1-z)$, in terms of $\mathrm{Li}_3(z)$. Again we start by computing the symbol

$$\Delta_{1,1,1}(\mathrm{Li}_3(1-z)) = -z \otimes (1-z) \otimes (1-z). \tag{2.110}$$

Once again we would like to find a function $f(z)$ such that,

$$\Delta_{1,1,1}(\mathrm{Li}_3(1-z)) = \Delta_{1,1,1}(f(z)). \tag{2.111}$$

Knowing that

$$\begin{aligned}
\Delta_{1,1,1}(\mathrm{Li}_3(z)) &= -(1-z) \otimes z \otimes z \\
\Delta_{1,1,1}(\mathrm{Li}_3(1-\frac{1}{z})) &= z \otimes (1-z) \otimes (1-z) - z \otimes (1-z) \otimes z \\
&\quad - z \otimes z \otimes (1-z) + z \otimes z \otimes z \\
\Delta_{1,1,1}(\log^3(z)) &= 6z \otimes z \otimes z \\
\Delta_{1,1,1}(\log^2(z)\log(1-z)) &= 2\left(z \otimes z \otimes (1-z) + z \otimes (1-z)z + (1-z) \otimes z \otimes z\right),
\end{aligned} \tag{2.112}$$

we can make an educated guess for $f(z)$

$$f(z) = -\mathrm{Li}_3(z) - \mathrm{Li}_3\left(1-\frac{1}{z}\right) + \frac{1}{6}\log^3(z) - \frac{1}{2}\log^2(z)\log(1-z). \tag{2.113}$$

Now that we have found a function $f(z)$ that yields the same symbol as $\mathrm{Li}_3(1-z)$, we should remind ourselves that this does not mean that the two functions are the same, it does not even mean that the other components of the coproduct are in general the same, due to the existence of primitives of the Hopf algebra. Looking at the $\mathcal{H}_1 \otimes \mathcal{H}_2$ component

$$\Delta_{1,2}\left(\mathrm{Li}_3(1-z) - f(z)\right) = 0, \tag{2.114}$$

we see that two functions have the same image under action of $\Delta_{1,2}$. This is however not surprising, considering that the most important primitives of $\mathcal{H}$, the $\zeta$ values, only appear in the first slot of the coproduct, as it was defined in eqs. (2.93) and (2.95).

That means we have to look at the $\mathcal{H}_2 \otimes \mathcal{H}_1$ component in order to learn something about the terms proportional to primitives of $\mathcal{H}_2$. Indeed, we see that

$$\begin{aligned}&\Delta_{2,1}\left(\mathrm{Li}_3(1-z)-f(z)\right)\\&=\left(\log(1-z)\log(z)-\frac{1}{2}\log^2(z)-\mathrm{Li}_2\left(1-\frac{1}{z}\right)+\mathrm{Li}_2(z)\right)\otimes\log(z)\\&+\left(\frac{1}{2}\log^2(z)+\mathrm{Li}_2\left(1-\frac{1}{z}\right)+\mathrm{Li}_2(1-z)\right)\otimes\log(1-z).\end{aligned} \tag{2.115}$$

Here we see the beauty of the coproduct calculus. The terms proportional to primitives of $\mathcal{H}$ can be determined using the identities for MPLs of lower weight. In this case we see that we need the identities for $\mathrm{Li}_2(1-z)$ and $\mathrm{Li}_2\left(1-\frac{1}{z}\right)$ that we determined analytically before. Plugging in eq. (2.105) and eq. (2.109) we find

$$\Delta_{2,1}\left(\mathrm{Li}_3(1-z)-f(z)\right)=\zeta_2\otimes\log(z). \tag{2.116}$$

Since $\zeta$ values can only appear in the first slot of the coproduct, it is easy to see that the term $\zeta_2\otimes\log z$ can only originate from a product term

$$\Delta_{2,1}(\zeta_2\log(z))=\zeta_2\otimes\log(z). \tag{2.117}$$

We can therefore improve our ansatz

$$\begin{aligned}\tilde{f}(z)=&-\mathrm{Li}_3(z)-\mathrm{Li}_3\left(1-\frac{1}{z}\right)+\frac{1}{6}\log^3(z)-\frac{1}{2}\log^2(z)\log(1-z)\\&+\zeta_2\log(z)+c\zeta_3.\end{aligned} \tag{2.118}$$

The only thing left to determine is the terms coming from primitives of $\mathcal{H}_3$, which at this point can only be a multiple of $\zeta_3$. We can determine the coefficient $c$ of $\zeta_3$ by evaluating the difference $\mathrm{Li}_3(1-z)-\tilde{f}(z)$ in the limit $z \to 1$ and find $c = 1$, so that we have

$$\begin{aligned}\mathrm{Li}_3(1-z) = -\mathrm{Li}_3(z) - \mathrm{Li}_3\left(1-\frac{1}{z}\right) + \frac{1}{6}\log^3(z) \\ - \frac{1}{2}\log^2(z)\log(1-z) + \zeta_2\log(z) + \zeta_3.\end{aligned} \tag{2.119}$$

In this way it is possible to successively derive functional identities for multiple polylogarithms.

While the example outlines the beauty of the coproduct calculus that enables us to derive functional identities as they are needed, on-the-fly, it should also hint at a few problems that can arise when using the method as above. The first and foremost problem with this approach is of course that it requires us to guess a function that produces the required symbol. While this is still rather trivial in the case of the classical polylogarithms, it gets significantly more complicated when dealing with “true” multiple polylogarithms, i.e. if we allow for multiple variables. It would therefore be preferable to have an algorithmic way to find a function that corresponds to a given symbol. The process of finding a function that reproduces a given symbol is also referred to as *integrating* the symbol. In the sections 2.4 and 2.5 we will outline two algorithms that enable us to integrate a given symbol.

Another problem is that we need to determine the primitives of $\mathcal{H}_n$ that can appear when we try to integrate a symbol of weight $n$. Which primitives appear at a given weight depends in general on the *alphabet* of the symbol that we are trying to integrate, i.e. on the set of entries of the different slots of the symbol. In the example above the symbol alphabet was $\{z, 1-z\}$, corresponding to the dlog-forms $\mathrm{dlog}(z)$ and $\mathrm{dlog}(1-z)$, i.e. potential singularities in the integration kernel at $z = 0$ and at $z = 1$. In this case, the only possible primitives turn out to be the $\zeta$ values[1] as well as $\pi$. This is not too surprising, when we recall that the MZVs are obtained from HPLs with indices 0 and 1 evaluated at unity. These HPLs however, are the MPLs with singularities at 0 and at 1, i.e. they are the functions with symbol alphabet $\{z, 1-z\}$.

Consequently, when we try to integrate a symbol with entries drawn from the alphabet $\{1+z, z, 1-z\}$, we should expect to find cMZVs as primitives, as the HPLs with indices $\{-1, 0, 1\}$, which yield cMZVs when evaluated at unity, are the functions corresponding to that symbol alphabet.

In these simple cases it is still possible to easily survey the primitives; however for larger and more complicated alphabets, determining the primitives requires greater care and effort[2].

[1] Classical $\zeta$ values up to weight 7, the first irreducible MZV appears at weight 8.

[2] and often also numerical experimentation with the PSQL algorithm.

## 2.4 Canonical integration

In this section we describe the method of *canonical integration*, which was first presented by us in ref. [1]. The algorithm was developed in order to bring MPLs to a canonical form, i.e. to find a transformation that takes a MPL of the form

$$G(f_1(x), f_2(x), \ldots, f_n(x), f_{n+1}(x)), \tag{2.120}$$

where the $f_i$ are linearly factorizeable rational functions, to a canonical form, so that the variable $x$ only appears in the last argument,

$$G(\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_n, x), \tag{2.121}$$

where the $\tilde{f}_i$ are independent of $x$ but in general will still depend on other variables.

The algorithm starts by calculating the symbol of the given MPL,

$$T = \Delta_{1,\ldots,1}\left(G(f_1(x_i), f_2(x_i), \ldots, f_n(x_i), f_{n+1}(x_i))\right) \tag{2.122}$$

depending on a set of variables $\{x_i\}$. In the first step it determines a function $\mathcal{G}(x_i)$ such that,

$$\Delta_{1,\ldots,1}(\mathcal{G}(x_i)) = T. \tag{2.123}$$

This function $\mathcal{G}$ will be expressed in terms of MPLs that are in a canonical form with respect to the $x_i$, i.e. the first variable $x_1$ will only appear in last argument of the MPLs. MPLs which are independent of $x_1$, will be put in a form where $x_2$ only appears in the last argument and so on. As such $\mathcal{G}$ is inherently not unique, but depends strongly on the ordering of the $x_i$.

We start by making the following observation about the symbol of a multiple polylogarithm: if the $a_i$ are independent of $x$, then the symbol of $G(a_1, \ldots, a_n; x)$ has exactly one term that contains $x$ in all its entries, and this term can be chosen to be of the form,

$$\mathcal{S}(G(a_1, \ldots, a_n; x)) = (a_n - x) \otimes \ldots \otimes (a_1 - x) + \ldots . \tag{2.124}$$

In order to prove this statement, we focus on the term in the total differential of $G(a_1, \ldots, a_n; x)$ proportional to $dx$,

$$\begin{aligned} dG(a_1, \ldots, a_n; x) &= G(a_2, \ldots, a_n; x)\, \frac{dx}{x - a_1} + \ldots \\ &= G(a_2, \ldots, a_n; x)\, d\log(a_1 - x) + \ldots , \end{aligned} \tag{2.125}$$

where the last step follows from

$$d\log(a_1 - x) = \frac{dx - da_1}{x - a_1}, \tag{2.126}$$

and where the dots indicate terms in the total differential that are independent of $dx$. The statement then follows recursively. Note that this statement is independent of whether the $a_i$ are zero or not.

Assume now that we are given an integrable symbol $T$ (which will correspond later to the symbol of the multiple polylogarithm we want to bring into canonical form) which is of uniform weight $w$ and has rational coefficients. If $T$ does not satisfy this last condition, we deal separately with the contributions of different weight and / or different rational-function prefactors. Let us suppose that the entries are drawn from a set $S$. Without loss of generality, we may assume $S$ to consist of irreducible polynomials in some variables $x_i$, $1 \leq i \leq n$, and for simplicity we assume for now that the polynomials are linear in *all* the $x_i$. Furthermore, we assume that we have fixed an ordering on the variables, which we will take in the following to be $(x_1, \ldots, x_n)$. For each variable $x_i$, we define a linear map $\phi_{x_i}$ which acts on elementary tensors $s$ by

$$\phi_{x_i}(s) = \begin{cases} G\left(-\frac{b_1}{a_1}, \ldots, -\frac{b_w}{a_w}; x_i\right), & \text{if } s = (a_w x_i + b_w) \otimes \ldots \otimes (a_1 x_i + b_1), \\ 0, & \text{otherwise}. \end{cases} \tag{2.127}$$

Morally speaking, the map $\phi_{x_i}$ assigns to $T$ the combination of multiple polylogarithms which will give the same terms that have $x_i$ in all entries through eq. (2.124).

Using the maps $\phi_{x_i}$, we can now formulate an algorithm that assigns to $T$ a multiple polylogarithm in the canonical form associated to the ordering of the variables $(x_1, \ldots, x_n)$. We start by defining a new symbol by subtracting off the contribution from $\phi_{x_1}(T)$,

$$T_1 = T - \mathcal{S}[\phi_{x_1}(T)]. \tag{2.128}$$

By construction, each term in the symbol $T_1$ has at least one entry that is independent of $x_1$. Next, concentrate on the terms of the form,

$$\sum_{(i_1,\ldots,i_w)} c_{i_1,\ldots,i_w}\, b_{i_1} \otimes (a_{i_2} x_1 + b_{i_2}) \otimes \ldots \otimes (a_{i_w} x_1 + b_{i_w})), \tag{2.129}$$

where by hypothesis the $b_{i_k}$ are independent of $x_1$. As we have subtracted of the contribution from $\phi_{x_1}(T)$, these terms cannot come from a multiple polylogarithm of the form $G(\ldots; x_1)$ of weight $w$, but it can only arise from the product

$$\begin{aligned} \log b_{i_1}\, G\left(-\frac{b_{i_w}}{a_{i_w}}, \ldots, -\frac{b_{i_2}}{a_{i_2}}; x_1\right) \to \\ \phi_{x_2}(b_{i_1})\, \phi_{x_1}\Big((a_{i_2} x_1 + b_{i_2}) \otimes \ldots \otimes (a_{i_w} x_1 + b_{i_w})\Big). \end{aligned} \tag{2.130}$$

It is easy to convince oneself that the difference

$$T_2 = T_1 - \sum_{(i_1,\ldots,i_w)} c_{i_1,\ldots,i_w}\, \mathcal{S}\left(\phi_{x_2}(b_{i_1})\, \phi_{x_1}\Big((a_{i_2} x_1 + b_{i_2}) \otimes \ldots \otimes (a_{i_w} x_1 + b_{i_w}))\Big)\right) \tag{2.131}$$

contains only terms for which at most $(w-2)$ entries depend on $x_1$. We can now go on and recursively subtract contributions with different multiplicities of $x_1$. Assume for example that we have subtracted all contributions where $x_1$ appears in more than $(w-r)$ entries, and that the resulting symbol is $T_r$. We can then concentrate on the terms

$$\sum_{(i_1,\dots,i_w)} c_{i_1,\dots,i_w}\, b_{i_1}\otimes\ldots\otimes b_{i_r}\otimes(a_{i_{r+1}}x_1+b_{i_{r+1}})\otimes\ldots\otimes(a_{i_w}x_1+b_{i_w}))\,. \quad (2.132)$$

It is easy to convince oneself that in the difference,

$$\begin{aligned} T_{r+1} &= T_r - \sum_{(i_1,\dots,i_w)} c_{i_1,\dots,i_w}\,\mathcal{S}\left[\phi_{x_2}\Big(b_{i_1}\otimes\ldots\otimes b_{i_r}\Big)\right.\\ &\left.\times\phi_{x_1}\Big((a_{i_{r+1}}x_1+b_{i_{r+1}})\otimes\ldots\otimes(a_{i_w}x_1+b_{i_w}))\Big)\right]\,, \end{aligned} \quad (2.133)$$

$x_1$ appears in at most $(w-r-1)$ entries. We continue this procedure until we reach $T_w$, which is independent of $x_1$, and we restart the algorithm with $T_w$ and $\phi_{x_2}$. We then repeat this procedure until we have exhausted all the integration variables, and the algorithm stops. The result of this algorithm is, by construction, a function of the form,

$$\sum_{(i_1,\dots,i_n)} c_{i_1,\dots,i_n}\, G(\vec{a}_{i_n};x_n)\ldots G(\vec{a}_{i_1};x_1)\,, \quad (2.134)$$

whose symbol is $T$ and such that the $\vec{a}_{i_k}$ are sequences of rational functions that are in the variables $x_k$, $k>i_k$, i.e., the sought-for canonical form for $T$.

At this point we have constructed a function $\mathcal{G}$ that agrees with the given function at the symbol level, i.e. the symbol,

$$\mathcal{S}(\delta)=0 \quad (2.135)$$

of the difference,

$$\delta = G(f_1(x_i),\ldots,f_n(x_i),f_{n+1}(x_i))-\mathcal{G}(x_i), \quad (2.136)$$

vanishes. However, as we have seen before, it would be wrong to conclude that the two functions are equal, due to the fact that we are still missing terms proportional to primitive elements of $\mathcal{H}$.

In the following we assume for simplicity that the function $\delta$ is real[3], so we do not need to worry about imaginary parts proportional to $i\pi$. Next we act with $\Delta_{2,1,\dots,1}$ on the difference, where $\Delta_{2,1,\dots,1}$ is the component of the iterated coproduct where the first component has weight two and all other components have weight one. Without loss of generality we can write,

$$\Delta_{2,1,\dots,1}(\delta) = \sum_{(i_1,\dots,i_{w-1})} c_{i_1,\dots,i_{w-1}}\, A_{i_1}\otimes\log a_{i_2}\otimes\ldots\otimes\log a_{i_{w-1}}\,, \quad (2.137)$$

[3]There is no obstacle to consider complex-valued functions. Imaginary parts can be extracted in exactly the same way using $\Delta_{1,\dots,1}$.

where the $a_{i_k}$ are irreducible polynomials and $A_{i_1}$ is a combination of multiple polylogarithms of weight two. Without loss of generality we can assume that we have collected all terms that have the same 'tail' $\log a_{i_2} \otimes \ldots \otimes \log a_{i_{w-1}}$, i.e., we can assume,

$$\log a_{i_2} \otimes \ldots \otimes \log a_{i_{w-1}} \neq \log a_{j_2} \otimes \ldots \otimes \log a_{j_{w-1}} \text{ if } (i_2, \ldots, i_{w-1}) \neq (j_2, \ldots, j_{w-1}) \,. \tag{2.138}$$

As we know that the symbol of the function vanishes, eq. (2.135), we necessarily conclude that $A_{i_1}$ is proportional to a primitive of $\mathcal{H}_2$, usually $\zeta_2$, i.e., $A_{i_1} = k_{i_1}\zeta_2$, for some rational number $k_{i_1}$. This rational number can easily be determined by evaluating $A_{i_1}$ numerically at a single point using any of the standard libraries to evaluate multiple polylogarithms [132–138], and running for example the PSLQ algorithm [131]. Equation (2.137) then takes the form,

$$\Delta_{2,1,\ldots,1}(\delta) = \sum_{(i_1,\ldots,i_{w-1})} c_{i_1,\ldots,i_{w-1}}\, k_{i_1}\, \zeta_2 \otimes \log a_{i_2} \otimes \ldots \otimes \log a_{i_{w-1}} . \tag{2.139}$$

Next we drop $\zeta_2$, i.e., we only keep the tail of each elementary tensor. If we also drop the log signs, we obtain a symbol associated with the terms proportional to $\zeta_2$,

$$\Delta_{2,1,\ldots,1}(\delta) \to \sum_{(i_1,\ldots,i_{w-1})} c_{i_1,\ldots,i_{w-1}}\, k_{i_1}\, a_{i_2} \otimes \ldots \otimes a_{i_{w-1}} \,. \tag{2.140}$$

Running the algorithm described at the beginning of this section on the symbol in eq. (2.140) we obtain a function $\mathcal{G}_2(\bar{x}_a, x_b, \ldots)$ of weight $w-2$ in canonical form such that,

$$\Delta_{2,1,\ldots,1}\left(\delta - \zeta_2\, \mathcal{G}_2(\bar{x}_a, x_b, \ldots)\right) = 0 \,. \tag{2.141}$$

We have in this way determined all the contributions proportional to $\zeta_2$, and the result is by construction in canonical form. We then repeat exactly the same exercise by acting with $\Delta_{3,1,\ldots,1}$ to determine the terms proportional to $\zeta_3$, and we continue in this way until we have exhausted all possibilities and the algorithms stops. As a result we obtain the expression of $G\left(f_1(x_i), \ldots, f_n(x_i), f_{n+1}(x_i)\right)$ in canonical form at *function level.*

This terminates the algorithm to bring multiple polylogarithms into the canonical form corresponding to a certain ordering of the variables.

*Example.*
Suppose we would like to rewrite the multiple polylogarithm

$$G\left(\frac{(1-x)(1+y)}{1-y}, 1, x\right) \tag{2.142}$$

in terms of multiple polylogarithms that depend on $x$ only in the last argument, i.e. we would like to bring it to a canonical form with respect to the ordering $\{x, y\}$ of the variables. We start by computing the symbol

$$\begin{aligned} T = \Delta_{1,1}&\left(G\left(\frac{(1-x)(1+y)}{1-y}, 1, x\right)\right) \\ &= (1-x)\otimes(1-y) + (1-x)\otimes(1+y-2x) \\ &- 2(1-x)\otimes(-2y+(1+y)x) \\ &+ (1+y)\otimes(1-y) - (1+y)\otimes(-2y+(1+y)x) \\ &- (1+y-2x)\otimes(1-y) + (1+y-2x)\otimes(-2y+(1+y)x). \end{aligned} \tag{2.143}$$

Now we can use the map $\phi_x$ to find MPLs corresponding to the elementary tensors with $x$ in every slot. The map $\phi_x$ will operate operate on the terms,

$$\begin{aligned} T|_{\phi_x} &= (1-x)\otimes(1+y-2x) - 2(1-x)\otimes(-2y+(1+y)x) \\ &\quad + (1+y-2x)\otimes(-2y+(1+y)x), \end{aligned} \tag{2.144}$$

yielding the MPLs,

$$\phi_x(T) = G\left(\frac{1+y}{2}, 1, x\right) - 2G\left(\frac{2y}{1+y}, 1, x\right) + G\left(\frac{2y}{1+y}, \frac{1+y}{2}, x\right). \tag{2.145}$$

Next we need to compute

$$T_1 = T - \mathcal{S}\left(\phi_x\left(T\right)\right) = 0, \tag{2.146}$$

which already happens to vanish, meaning that we have found a function

$$\mathcal{G} = \phi_x(T) = G\left(\frac{1+y}{2}, 1, x\right) - 2G\left(\frac{2y}{1+y}, 1, x\right) + G\left(\frac{2y}{1+y}, \frac{1+y}{2}, x\right), \tag{2.147}$$

that is equal to $G\left(\frac{(1-x)(1+y)}{1-y}, 1, x\right)$ at the symbol level. If we demand that $x, y \in (0, 1)$ we can convince ourselves that they in fact agree at the function level, by evaluating the difference

$$G\left(\frac{(1-x)(1+y)}{1-y}, 1, x\right) - \mathcal{G} \tag{2.148}$$

numerically. This means that we have found a representation for the original MPL in terms of MPLs that only depend on $x$ in the last argument.

To underline the fact that this representation depends on the ordering of the variables, let us find a representation for the reverse ordering $\{y, x\}$.

We now start by applying the map $\phi_y$ to $T$. This map will act on the terms,

$$\begin{aligned} T|_{\phi_y} &= (1+y) \otimes 1 - y - (1+y) \otimes (x - (2-x)y) \\ &\quad - (1-2x+y) \otimes (1-y) + (1-2x+y) \otimes x - (2-x)y, \end{aligned} \tag{2.149}$$

producing the MPLs,

$$\begin{aligned} \phi_y(T) &= G(1,-1,y) - G\left(\frac{x}{2-x}, -1, y\right) - G(1, 2x-1, y) \\ &\quad + G\left(\frac{x}{2-x}, 2x-1, y\right). \end{aligned} \tag{2.150}$$

Next we compute,

$$\begin{aligned} T_1 = T - \mathcal{S}(\phi_y(T)) &= -(1-2x) \otimes (1-x) - (1-2x) \otimes 1 - y \\ &+ (1-2x) \otimes (x-(2-x)y) + (1-x) \otimes (1-y) + (1-x) \otimes (1-2x+y) \\ &- 2(1-x) \otimes x - (2-x)y - x \otimes (1-2x) + 2x \otimes (1-x) \\ &- (1-y) \otimes (1-2x) + (1-y) \otimes (1-x) + (1-2x+y) \otimes (1-x) \\ &+ (x-(2-x)y) \otimes (1-2x) - 2(x-(2-x)y) \otimes (1-x), \end{aligned} \tag{2.151}$$

here we focus on elementary tensors of the form,

$$b_1 \otimes (a_2 y + b_2), \tag{2.152}$$

where the $a_i$ and $b_i$ are independent of $y$, so that we can act on the second slot with $\phi_y$ to obtain the functions,

$$\begin{aligned} \phi_y(T_1) &= -\log(1-2x) G(1,y) + \log(1-2x) G\left(\frac{x}{2-x}, y\right) \\ &\quad + \log(1-x) G(1,y) + \log(1-x) G(2x-1, y) \\ &\quad - \log(1-x) G\left(\frac{x}{2-x}, y\right). \end{aligned} \tag{2.153}$$

Computing

$$\begin{aligned} &T_2 = T_1 - \mathcal{S}(\phi_y(T_1)) = \\ &\quad (1-2x) \otimes x + (1-x) \otimes (1-2x) - 2(1-x) \otimes x, \end{aligned} \tag{2.154}$$

we observe that we have taken care of all $y$ dependent functions. The final step is therefore to apply $\phi_x$ to $T_2$, which yields,

$$\phi_x(T_2) = G\left(0, \frac{1}{2}, x\right) + G\left(\frac{1}{2}, 1, x\right) - 2G(0, 1, x). \tag{2.155}$$

We observe that

$$T_3 = T_2 - \mathcal{S}(\phi_x(T_2)) = 0, \tag{2.156}$$

vanishes, indicating that we have found a function,

$$\begin{aligned}\mathcal{G} = {} & G(1, -1, y) - G(1, 2x-1, y) - G\left(\frac{x}{2-x}, -1, y\right) \\ & + G\left(\frac{x}{2-x}, 2x-1, y\right) \\ & + G\left(0, \frac{1}{2}, x\right) - 2G(0, 1, x) + G\left(\frac{1}{2}, 1, x\right) \\ & + G(1, x)G(2x-1, y) + G(1, y)\left(G(1, x) - G\left(\frac{1}{2}, x\right)\right) \\ & + G\left(\frac{x}{2-x}, y\right)\left(G\left(\frac{1}{2}, x\right) - 2G(1, x)\right),\end{aligned} \tag{2.157}$$

that agrees with the original MPL at the symbol level. As before we demand that $x, y \in (0, 1)$ and convince ourselves numerically that they do in fact also agree at the function level.

## 2.5 Building polylogarithmic functions with a specific alphabet

For symbol alphabets that fulfill the linear reducibility criterion canonical integration provides an automatic way to associate a basis of functions to a given symbol. This basis is very useful if one intends to integrate a polylogarithmic expression over one of the variables appearing in the arguments of the polylogarithms, which we will exploit in section 2.6. However, often one would prefer to find a different basis, in particular one that expresses a given polylogarithmic function through a fixed basis of polylogarithms. Furthermore, one might be interested in finding a basis for the function space generated by an alphabet that is not linearly reducible. In this section we discuss an algorithm first presented in ref. [55] that enables us to build such bases.

The method is based on the observation that due to the plethora of functional identities the multiple polylogarithms up to a given weight can be expressed through a finite set of independent functions. A possible choice for these functions is given in table 2.1, which is of course by no means unique.

| Weight | Independent functions |
|---|---|
| 1 | $\log(x)$ |
| 2 | $\mathrm{Li}_2(x)$ |
| 3 | $\mathrm{Li}_3(x)$ |
| 4 | $\mathrm{Li}_4(x), \mathrm{Li}_{2,2}(x,y)$ |
| 5 | $\mathrm{Li}_5(x), \mathrm{Li}_{2,3}(x,y)$ |
| 6 | $\mathrm{Li}_6(x), \mathrm{Li}_{2,4}(x,y), \mathrm{Li}_{3,3}(x,y), \mathrm{Li}_{2,2,2}(x,y,z)$ |

Table 2.1: Independent functions of pure weight.

It should therefore be possible e.g. to express any linear combination of arbitrarily complicated multiple polylogarithms at weight 3 in terms of a linear combination of just $\mathrm{Li}_3$s with complicated arguments as well as products of lower weight functions. One motivation why it might be interesting to express multiple polylogarithms this way is the need for fast and easy numerical evaluation. By expressing MPLs through classical Lis, only a small set of functions, which furthermore have well known series expansions, need to be implemented efficiently to yield numerical results.

The goal of the algorithms is therefore to determine arguments for the functions given in table 2.1 so that we can find a linear combination of these functions with the determined arguments that will reproduce a given symbol.

Let us assume that we are given a symbol of weight $w$,

$$S = \sum_{i_1,\ldots,i_w} c_{i_1,\ldots,i_w} f_{i_1}(x_1,\ldots,x_m) \otimes \cdots \otimes f_{i_w}(x_1,\ldots,x_m), \tag{2.158}$$

where the sum runs over all elementary tensors that make up the symbol. The $f_i$ are rational functions of some the variables $x_j$. Then we can factor the $f_i$ over $\mathbb{Q}$ into multiplicatively independent polynomials $\pi_i = \pi_i(x_1,\ldots,x_m)$ and use the distributivity of the symbol to write $S$ as,

$$S = \sum_{i_1,\ldots,i_w} \tilde{c}_{i_1,\ldots,i_w} \pi_{i_1} \otimes \cdots \otimes \pi_{i_w}. \tag{2.159}$$

Let there be $K$ such irreducible factors $\pi_i$ and let us denote their set as $\mathcal{P} = \{\pi_1,\ldots,\pi_K\}$. Then we can define the set,

$$\overline{\mathcal{P}} = \mathcal{P} \cup \mathcal{P}', \tag{2.160}$$

where $\mathcal{P}'$ is the set of all irreducible factors that appear when factoring $\pi_i \pm \pi_j$, $1 \pm \pi_i$ over $\mathbb{Q}$ $\forall \pi_i, \pi_j \in \mathcal{P}$. Let us denote the elements of $\overline{\mathcal{P}}$ as $\overline{\pi}_i$.

We can now define functions,

$$f_{n_1,\ldots,n_K}(x_1,\ldots,x_m) = \pm \prod_{\overline{\pi}\in\overline{\mathcal{P}}} \overline{\pi}^{n_{\overline{\pi}}}(x_1,\ldots,x_m), \tag{2.161}$$

with $n_{\overline{\pi}} \in \mathbb{Z}$ and denote the set of these functions as $\mathcal{F}$.

If we assume for a moment that the given symbol $S$ is of weight $w = 1$, then it is of course completely trivial to find a function to reproduce this symbol. We could just write the ansatz,

$$T = \sum_{f \in \mathcal{F}} c_f \log(f) \tag{2.162}$$

Since the $\pi_i$ are multiplicatively independent, we can just compute $S - \mathcal{S}(T)$ and demand that the coefficients of all elementary tensors of the $\bar{\pi}_i$s vanish separately, which will yield a linear system of equations that can be solve to determine the $c_f$. This way we would obtain a function $T$ that has the symbol $S$. Of course it is no great feat to reproduce a weight 1 symbol, so let us consider higher weights and let us focus first on building the subset of functions that can be described in terms of classical polylogarithms, which is enough to completely determine functions of weight 2 and 3.

### Building classical polylogarithms

Recall that the symbol of a classical polylogarithm is

$$\mathcal{S}(\mathrm{Li}_n(x)) = -(1-x) \otimes x \otimes \cdots \otimes x. \tag{2.163}$$

If we were to ignore the first entry for a second, we could conclude that by writing down a linear combination of classical polylogarithms of the form

$$\sum_{f \in \mathcal{F}} c_f \mathrm{Li}_n(f), \tag{2.164}$$

we should be able to reproduce the given symbol $S$, after appropriately choosing the $c_i$. And while this may be true for the last $w-1$ entries of the elementary tensor, we can of course not forget about the first entry.

Therefore we have to refine the set of functions that can appear in the arguments. We need to require that the functions be drawn from the set,

$$\overline{\mathcal{F}} = \{f \in \mathcal{F} | \, (1-f) \in \mathcal{F}\} \subset \mathcal{F}. \tag{2.165}$$

In other words, we only allow such functions $f \in \mathcal{F}$ for which $1-f$ can be factored into elements of $\mathcal{F}$.

This way we ensure that all entries of the symbol of $\mathrm{Li}_n(\overline{f})$ factor into elements of $\overline{\mathcal{P}}\ \forall\ \overline{f} \in \overline{\mathcal{F}}$. We therefore only need to take a linear combination of the possible Lis

$$\tilde{T}_w = \sum_{f \in \overline{\mathcal{F}}} c_f \mathrm{Li}_w\left(f\right). \tag{2.166}$$

At this point we should note that a symbol of weight $w$ is of course not necessarily due only to functions of maximum weight $w$, but in general we also expect to see products of functions of lower weight. However, we can always proceed successively and build up the functions weight by weight, so that we can assume that we know all required functions at lower weights. It is possible to eliminate terms generated by products from the symbol by defining the operator $\Pi_w$ recursively in the weight $w$,

$$\Pi_w(a_1 \otimes \dots a_w) = \\ \frac{w-1}{w}\left([\Pi_{w-1}(a_1 \otimes \cdots \otimes a_{w-1})] \otimes a_w - [\Pi_{w-1}(a_2 \otimes \cdots \otimes a_w)] \otimes a_1\right), \tag{2.167}$$

with $\Pi_1 = \mathrm{id}$, which eliminates all shuffles from a given symbol,

$$\Pi_w\left(\mathcal{S}(f_p g_q)\right) = 0, \tag{2.168}$$

where $f_p, g_q$ are linear combinations of multiple polylogarithms of weight $p$ and $q$ respectively with $p + q = w$. See ref. [55] for a more detailed discussion.

To determine the coefficients $c_f$ we then compute,

$$\delta = \Pi_w\left(S - \mathcal{S}(\tilde{T}_w)\right), \tag{2.169}$$

after factoring the entries of the tensors in $\delta$ into the irreducible factors $\overline{\pi}$, we can demand that the coefficient of each elementary tensor in the $\overline{\pi}$ vanish separately, which will yield a system of linear equations for the $c_{\overline{f}}$ that can be solved with computational algebra methods in order to uniquely determine $\tilde{T}_w$. Thus we have a function

$$T_w = \tilde{T}_w + \text{products of lower weight}, \tag{2.170}$$

that reproduces the symbol $S$.

## Building polylogarithms of higher depth

Starting from weight 4 we need to include multiple polylogarithms of depth $> 1$, e.g. $\mathrm{Li}_{2,2}, \mathrm{Li}_{2,3}$, into the algorithm since they are independent of the classical polylogarithms. We therefore need to find $k$-tuples of arguments for a multiple polylogarithm of depth $k$. In order to simplify the discussion we first introduce yet another notation for multiple polylogarithms, defining

$$G_{m_1,\dots,m_k}(t_1,\dots,t_k) = G(\vec{0}_{m_1-1}, t_1, \dots, \vec{0}_{m_k-1}, t_k, 1), \tag{2.171}$$

so that,

$$\mathrm{Li}_{m_1,\dots,m_k}(x_1,\dots,x_k) = (-1)^k G_{m_k,\dots,m_1}\left(\frac{1}{x_k}, \dots, \frac{1}{x_1 \dots x_k}, 1\right) \tag{2.172}$$

which is essentially just a rearrangement of the arguments of the Lis. Since the arguments that we consider are all multiplicatively independent we are free to use these functions to simplify the discussion.

When we compute the symbol of a depth 2 MPL $\mathcal{S}(G_{2,2}(x,y))$ we find that the only terms appearing in the slots of the elementary tensors after factoring over $\mathbb{Q}$ are

$$\{x, 1-x, y, 1-y, x-y\}. \tag{2.173}$$

From this we learn that, whatever functions we plug in for the arguments $x$ and $y$, needs to fulfill at least the same criteria as in the depth-1 case. Consequently, we need to choose a tuple $(x,y)$ from $\overline{\mathcal{F}} \times \overline{\mathcal{F}}$, as we see that $x$ and $y$, as well as $1-x$ and $1-y$ need to factor again into irreducible factors $\bar{\pi}$. However, we see another term appearing in the symbol that did not exist at depth 1, $x-y$, meaning that we also need to require that the difference of both arguments factors into $\bar{\pi}$. We can therefore define a new class of functions for the arguments of MPLs of depth 2,

$$\overline{\mathcal{F}_2} = \{(f_1, f_2) \in \overline{\mathcal{F}} \times \overline{\mathcal{F}} | \, (f_1 - f_2) \in \mathcal{F}\} \subset \overline{\mathcal{F}} \times \overline{\mathcal{F}}. \tag{2.174}$$

If we consider the symbols of MPLs of depth $> 2$ and analyze the factors appearing in the elementary tensors, we notice that there are no new constraints beyond depth 2, i.e. the only constraint is that the pairwise differences of two arguments need to factor. E.g. at depth 3 we see that the factors appearing in the symbol $\mathcal{S}(G_{2,2,2}(x,y,z))$ are,

$$\{x, y, z, 1-x, 1-y, 1-z, x-y, x-z, y-z\}. \tag{2.175}$$

We can therefore, at least conjecturally, write down the set of functions for the arguments of MPLs of depth $d$,

$$\begin{aligned} \overline{\mathcal{F}_d} = &\{(f_1, \ldots, f_d) \in \overline{\mathcal{F}} \times \cdots \times \overline{\mathcal{F}} | \, (f_i - f_j) \in \mathcal{F} \; \forall \, 1 \le i < j \le d\} \\ &\subset \overline{\mathcal{F}} \times \cdots \times \overline{\mathcal{F}}. \end{aligned} \tag{2.176}$$

At this point we should mention a small complication: The set $\mathcal{F}$ is of course infinite. However, it turns out that, at least conjecturally, the sets $\overline{\mathcal{F}}$ and $\overline{\mathcal{F}}_d$ are finite. One can therefore successively enumerate members of $\mathcal{F}$ and test whether they also lie in $\overline{\mathcal{F}}$. In practice this can be done by grouping the members $f_{n_1,\ldots,n_K}$ of $\mathcal{F}$ according to $r = |n_1| + \cdots + |n_k|$. Next, we test all functions with $r = 1$ and successively increase $r$. We will observe that after a few iterations no new functions in $\overline{\mathcal{F}}$ will be found. At this point the iteration can be terminated and we have obtained the finite subset $\overline{\mathcal{F}}$. Since the functions that make up the tuples in $\overline{\mathcal{F}}_d$ must all be taken from $\overline{\mathcal{F}}$ it is trivial to find these sets once $\overline{\mathcal{F}}$ is known.

Of course this does not prove that there cannot be any new functions for large values of $r$ even if the algorithm has seemed to stabilize before. However, in practice this does not seem to happen. Furthermore, a non-exhaustive ansatz would not permit a solution for the coefficients in $\mathbb{Q}$. This way missing functions can easily be detected.

## 2.6 Iteratively integrating parametric integrals

Using the identities and algorithms for multiple polylogarithms discussed before, we can now state an algorithm that allows us to integrate certain classes of parametric integrals in terms of iterated integrals over multiple polylogarithms. This algorithm has been applied, in some variant or another, to the computation of Feynman integrals [69, 139–143] and we present an example of a very simple Feynman integral calculation using this algorithm as well in chapter 4.1. The algorithm has been extended and implemented in the `Maple` package `HyperInt` by Erik Panzer [144] in combination with an algorithm to regulate divergent parametric integrals.

Let us consider a generic parametric integral of the form,

$$\mathcal{I}(\{y_j\};\epsilon) = \int_0^\infty \left(\prod_{i=1}^{n} dx_i\right) \prod_{k=1}^{m} P_k(\{x_i\};\{y_j\})^{a_k+\epsilon\, b_k}\,, \tag{2.177}$$

where $a_k$ and $b_k$ are integers and the $P_k(\{x_i\};\{y_j\})$ are polynomials with integer coefficients, which we assume irreducible over $\mathbb{Z}$, i.e., they cannot be factorized into a product of non-constant polynomials of lower degree. We assume that the integration range is $[0,\infty]$ for each integration variable $x_i$. While many statements remain true for generic integration boundaries, in certain cases the algorithm we are going to describe breaks down, due to the appearance of boundary contributions. We can however always map a generic integration region $x_i \in [a,b]$ to $y_i \in [0,\infty]$ by the change of variable

$$y_i = \frac{x_i - b}{x_i - a}\,. \tag{2.178}$$

We furthermore assume that the integral is convergent for $\epsilon = 0$, and so we can expand in $\epsilon$ under the integration sign. Note that in the simplest divergent cases where the singularities in the integrand factorize we can reduce the problem to a convergent integral by subtracting the divergencies.

Our goal is to compute the coefficients of the Taylor expansion of $\mathcal{I}(\{y_j\};\epsilon)$ by integrating out the integration variables recursively one-by-one in terms of multiple polylogarithms.

Obviously, not every integral can be performed in this way. We will therefore first describe a sufficient condition, first obtained in ref. [139], to be satisfied by the integrand of $\mathcal{I}(\{y_j\};\epsilon)$ so that it can be integrated in terms of multiple polylogarithms.

### Denominator reduction

In this section we review (a variant of) the sufficient condition of ref. [139] to determine whether an integral can be performed recursively in terms of multiple polylogarithms. The main idea is that we need to determine an ordering of the integration variables such that at each step during the integration all the denominators are linear in the next integration variable. We start by defining the set $S$ of all the polynomials that are not monomials and that appear inside the integrand of eq. (2.177),

$$S = \Big\{P_k(\{x_i\};\{y_j\})\Big\}\,. \tag{2.179}$$

To start the integration, we have to assume that there is one integration variable, say $x_a$ such that all the element of $S$ are linear in $x_a$. In that case we may write,

$$P_k(\{x_i\};\{y_j\}) = Q_k^a(\{x_i\};\{y_j\})\,x_a + R_k^a(\{x_i\};\{y_j\})\,, \tag{2.180}$$

where $Q_k^a(\{x_i\};\{y_j\})$ and $R_k^a(\{x_i\};\{y_j\})$ are polynomials that are independent of $x_a$. Note that, after expansion in $\epsilon$, the integrand may also contain logarithms of the $P_k(\{x_i\};\{y_j\})$, which can be rewritten in terms of multiple polylogarithms,

$$\begin{aligned}\log P_k &= \log\Big(Q_k^a\,x_a + R_k^a\Big) = \log R_k^a + \log\left(1 + \frac{Q_k^a}{R_k^a}x_a\right)\\ &= \log R_k^a + G\left(-\frac{R_k^a}{Q_k^a};x_a\right)\,,\end{aligned} \tag{2.181}$$

where for clarity we have suppressed the arguments of the polynomials. Furthermore, we can use the shuffle algebra of multiple polylogarithms to replace every product of multiple polylogarithms by a sum. Thus we can assume without loss generality that the integration over $x_a$ takes the form,

$$\int_0^\infty \frac{dx_a}{(Q_1^a x_a + R_1^a)^{-a_1}\ldots(Q_m^a x_a + R_m^a)^{-a_m}}\,G(\vec{a};x_a)\,. \tag{2.182}$$

Partial fractioning the factors in the denominator, e.g.,

$$\frac{1}{(Q_k^a x_a + R_k^a)(Q_l^a x_a + R_l^a)} = \frac{1}{Q_k^a R_l^a - Q_l^a R_k^a}\left(\frac{1}{x_a + R_k^a/Q_k^a} - \frac{1}{x_a + R_l^a/Q_l^a}\right)\,, \tag{2.183}$$

we obtain a sum of integrals that can be reduced to the recursive definition of multiple polylogarithms, eq. (2.15). We can thus easily compute a primitive with respect to $x_a$, and then take the limits $x_a \to 0$ and $x_a \to \infty$. We will address the issue of limits in the next subsection.

We would like to iterate this procedure and integrate over the next variable. This is however only possible if inside the new integrand we can still find an integration variable in which all polynomials are linear. The polynomials appearing inside the integrand are $Q_k^a$ and $R_k^a$, which have been introduced through eq. (2.181) and (2.183), as well as the combinations $Q_k^a R_l^a - Q_l^a R_k^a$

introduced by partial fractioning. This last polynomial however need not necessarily be linear, even if the $Q_k^a$ and $R_k^a$ are. In order to proceed, it is therefore mandatory that all the $Q_k^a R_l^a - Q_l^a R_k^a$ factor into polynomials that are linear in a certain variable.

In ref. [139] a criterion was given that allows one to determine a priori whether the above procedure terminates, i.e., whether there is an ordering of the integration variables such that all the denominators stay linear at each integration step. We start by defining the set $S_{(x_a)}$ as the set of irreducible factors that appear inside the polynomials $Q_k^a$, $R_k^a$ and $Q_k^a R_l^a - Q_l^a R_k^a$. Then, if we can find an integration variable $x_b$ such that all the elements of $S_{(x_a)}$ are linear in $x_b$, we can restart the above procedure and integrate over $x_b$. If we iterate this procedure and are able to construct a sequence of sets of polynomials,

$$S_{(x_a)}, S_{(x_a,x_b)}, S_{(x_a,x_b,x_c)}, \ldots \tag{2.184}$$

such that in each set all the polynomials are linear in at least one integration variable, then we have found an ordering of the integration variables such that we can recursively integrate out all the integration variables in terms of multiple polylogarithms. We stress that this condition is sufficient, but not necessary: even if we fail to find a suitable sequence (2.184), the integral might still be expressible in terms of multiple polylogarithms (e.g., after a suitable change of variables). In addition, note that for the last integration step it is not necessary for the polynomials to be linear: we can then factor the polynomials into linear factors, whose roots involve algebraic expressions of the parameters $\{y_j\}$.

## Symbolic integration and denominator reduction

We now have a criterion to determine whether an integral of type (2.177) can be integrated in terms of multiple polylogarithm and we have already seen how to perform the first integration step. After we have taken the primitive with respect to some integration variable $x_a$ we still need to take the limits $x_a \to 0$ and $x_a \to \infty$ of the primitive. The limit $x_a \to 0$ can easily be computed because of the fact that,

$$\lim_{x\to 0} G(\vec{\omega}; x) = 0, \quad \text{for } \vec{\omega} \neq \vec{0}. \tag{2.185}$$

Of course it is possible that the primitive has spurious poles or logarithmic singularities at $x_a \to 0$. To deal with poles at $x_a = 0$, we expand the multiple polylogarithms around $x_a = 0$ using their series representation given in eq. (6.77). Logarithmic singularities at $x_a = 0$ can be easily extracted using shuffle regularization as described in section 2.2.

In order to obtain the limit $x_a \to \infty$ we define $\bar{x}_a = \frac{1}{x_a}$. Then we use canonical integration to rewrite the multiple polyloarithms appearing the primitive with respect to $x_a$ as multiple polylogarithms with argument $\bar{x}_a$. This reduces the problem to taking the limit $\bar{x} \to 0$.

The use of canonical integration to rewrite the multiple polylogarithms also guarantees that we can bring the integrand,

$$I_b = \lim_{x_a \to \infty} P_a - \lim_{x_a \to 0} P_a, \tag{2.186}$$

with $P_a$ being the primitive with respect to $x_a$, into a form where we can use once again the iterative definition of the multiple polylogarithms, eq. (2.15), in order to obtain the primitive $P_b$ with respect to the second integration variable $x_b$. At this point we proceed iteratively until all integration variables have been integrated out.

The only caveat to this procedure is that we need to be able to use canonical integration in order to bring the intermediate polylogarithms into a form that is suitable for taking the required limits or performing the next integration step. We will therefore argue now that the criterion of denominator reducibility is sufficient to guarantee that rewriting the intermediate multiple polylogarithms is always possible and that the above algorithm always converges if we can find a suitable order of integration variables. From now on we assume that we have found an ordering of the integration variables, which we take as $(x_1, \ldots, x_n)$ and we can find a sequence

$$S, S_{(x_1)}, S_{(x_1,x_2)}, S_{(x_1,x_2,x_3)}, \ldots \tag{2.187}$$

such that all the elements of $S_{(x_1,\ldots x_k)}$ are linear in $x_{k+1}$. We start by showing that under these hypotheses and after having integrated out $(x_1, \ldots, x_{k-1})$,

1. the symbol of the primitive with respect to $x_k$ has all its entries drawn from the set $\overline{S}_{(x_1,\ldots x_{k-1})} = \{x_k, \ldots, x_n\} \cup S_{(x_1,\ldots x_{k-1})}$.
2. the symbol of the function after integration over $x_k$, i.e., after taking the limits $x_k \to 0, \infty$ of the primitive, has all its entries drawn from $\widetilde{S}_{(x_1,\ldots x_k)} = \{x_{k+1}, \ldots, x_n\} \cup S_{(x_1,\ldots x_k)}$.

We start by proving the first statement, the second then immediately follows by taking the appropriate limits. As in the following we constantly switch between polynomials of the sets we just defined, and polynomials as entries of symbols, we introduce the notation $[P]$ to refer to $P$ as an entry of a symbol. Note that we then have the identities,

$$\begin{aligned} [P\,Q] &= [P] + [Q]\,, \\ [P/Q] &= [P] - [Q]\,, \\ [\pm 1] &= 0\,, \\ &\text{etc.} \end{aligned} \tag{2.188}$$

We proceed by iteration in the number $k$ of variables we have already integrated out. We start by analyzing what happens after the first integration. It is obvious from eqs. (2.181) and (2.183) that after the first integration the primitive only involves multiple polylogarithms $G(a_1, \ldots, a_w; x_1)$ with,

$$a_i \in \left\{0, -R_k^1/Q_k^1\right\} . \tag{2.189}$$

It is then easy to see (e.g., from the polygon approach to the symbol of ref. [145], or our description of the maximal coproduct in section 2.3) that the symbol can only have the following entries:

$$\begin{aligned}
&[x_k], [R_k^1] ,\\
&\left[-R_k^1/Q_k^1\right] = [R_k^1] - [Q_l^1] ,\\
&\left[1 + \frac{x_1\, Q_k^1}{R_k^1}\right] = [R_k^1 + Q_k^1\, x_1] - [R_k^1] = [P_k] - [R_k^1] ,\\
&\left[1 + \frac{Q_k^1\, R_l^1}{R_k^1\, Q_l^1}\right] = [Q_k^1\, R_l^1 - R_k^1\, Q_l^1] - [R_k^1] - [Q_l^1] .
\end{aligned} \tag{2.190}$$

The polynomials that appear inside the symbol are precisely those that appear in $S$ and $S_{(x_1)}$, which finishes the proof of the first statement for the first integration.

Next consider taking the limits $x_1 \to 0$ and $x_1 \to \infty$. By definition, $R_k^1$ and $Q_k^1$ are independent of the limit, so we only need to consider the limits of $[x_1]$ and $[P_k]$. $[x_1]$ will give rise to logarithmic singularities in the limit, and these terms must cancel if the integral is convergent. For $[P_k]$ we have,

$$\begin{aligned}
\lim_{x_1 \to 0} [P_k] &= [R_k^1] ,\\
\lim_{x_1 \to \infty} [P_k] &= \lim_{\bar{x}_1 \to 0} \{[\bar{x}_1\, R_k^1 + Q_k^1] - [\bar{x}_1]\} = [Q_k^1] + \lim_{\bar{x}_1 \to 0} [x_1] .
\end{aligned} \tag{2.191}$$

The logarithmic singularity in the last line must again cancel for convergent integrals, and so we see that the only polynomials that appear in the limit are those in $S_{(x_1)}$. This finishes the proof of the second statement for the first integration. We stress that it is important that the integration region is $[0, \infty]$, because otherwise we have to take into account effects coming from the integration boundaries.

Let us now suppose that the two statements are true for the first $r-1$ integrations. The set $S_{(x_1, \ldots, x_{r-1})}$ then consists of polynomials of the form $\tilde{P}_k = \tilde{Q}_k^r\, x_r + \tilde{R}_k^r$. Let us now compute the primitive with respect to $x_r$. We start by running the algorithm to bring the multiple polylogarithms in the integrand into canonical form. As this involves the application of the map $\phi_{x_r}$, we obtain multiple polylogarithms of the form $G(a_1, \ldots, a_w; x_r)$ with,

$$a_i \in \left\{0, -\tilde{R}_k^r/\tilde{Q}_k^r\right\} . \tag{2.192}$$

If we compute the primitive, we integrate over linear functions in $x_r$ from the set $S_{(x_1,\ldots,x_{r-1})}$, and it is easy to see that this does not change eq. (2.192). Using exactly the same argument as for the first integration, we see that these multiple polylogarithms only contribute terms to the symbols whose entries are drawn from $\overline{S}_{(x_1,\ldots x_{r-1})}$. In addition we have multiple polylogarithms that are independent of $x_r$, whose symbols involve those elements of $\widetilde{S}_{(x_1,\ldots x_{r-1})}$ that are independent of $x_r$. As these functions do not change if we take the primitive with respect to $x_r$, we see that they do not alter the conclusion. So the symbol of the primitive with respect to $x_r$ must have all its entries drawn from $\overline{S}_{(x_1,\ldots x_{r-1})}$. Taking the limits $x_r \to 0$ and $x_r \to \infty$ just as for the first integration then finishes the proof.

Having proved the two statements, we can show that our algorithm always terminates for the class of integrals we consider. More precisely, we have to show that our algorithm can always produce the canonical form for the next integration step. This is done by applying the map $\phi_{x_r}$, which requires all the entries in the symbol to be either independent of $x_r$ or linear in $x_r$. By construction, this condition is always fulfilled for the elements of $\widetilde{S}_{(x_1,\ldots x_{r-1})}$. It is easy to check that the same argument shows that the map $\phi_{x_{r+1}}$, which is called recursively by $\phi_{x_r}$ is well-defined, and so we can always find a canonical form for the integrand.

CHAPTER 3

# DIFFERENTIAL EQUATIONS FOR MASTER INTEGRALS

## 3.1 Reverse unitarity and integral reductions

Integrals over particle momenta are ubiquitous in the computation of multi-loop scattering amplitudes. They arise directly from internal loops in Feynman diagrams, which require the integration over the momentum of the internal virtual particle, as such they are referred to as *loop integrals*. Loop integrals suffer from infrared and ultraviolet divergences. These can be regulated using the framework of dimensional regularization, which promotes the internal loop momenta from four-dimensional Minkowski space to $d$-dimensional Minkowski space. With this in mind, we can write a general $n$-point $\ell$-loop integral with $m$ propagators as,

$$I^{\nu_1,\dots,\nu_m}(p_1,\dots,p_n) = \int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \mathcal{I}^{\nu_1,\dots,\nu_m}(k_1,\dots,k_\ell,p_1,\dots,p_n), \tag{3.1}$$

with the corresponding integrand,

$$\mathcal{I}^{\nu_1,\dots,\nu_m}(k_1,\dots,k_\ell,p_1,\dots,p_n) = \prod_i^m \left[\left(\sum_j \alpha_{ij}k_j + \sum_j \beta_{ij}p_j\right)^2 - m_i^2 - i0\right]^{-\nu_i}. \tag{3.2}$$

Here the $p_i$ are the external momenta, which are all assumed to be incoming, furthermore $m_i$ is the mass of the particle in the internal propagator $i$. The $i0$ denotes the Feynman prescription for the propagator. The $\alpha_{ij}$ and $\beta_{ij}$ can be determined by e.g. reading off the propagators from the corresponding Feynman diagram.

## Integral reductions

One of the most powerful techniques for the computation of multiloop scattering amplitudes is *integral reduction*. The basic idea of integral reduction techniques is to exploit relations that exist at the integral level in order to express the amplitude through a small set of integrals.

The most widely used integral reduction method [146–149] is known as *integration-by-parts* (IBP) reduction. The method builds on the observation that in dimensional regularization the integral of the total derivative, with respect to the loop momentum, vanishes, e.g.,

$$\int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{\partial}{\partial k_\mu} \frac{1}{k^2(k+p_1)^2(k+p_1+p_2)^2(k+p_1+p_2+p_3)^2} = 0. \tag{3.3}$$

In the following we shall consider a set of denominator factors $\mathcal{D}_i$ with,

$$\mathcal{D}_i = (\sum_j \alpha_{ij} k_j + \sum_j \beta_{ij} p_j)^2, \tag{3.4}$$

where $\alpha_{ij}, \beta_{ij} \in \mathbb{Z}$ can be read off from the propagators that appear in the associated loop integral. Then,

$$I(\nu_1, \ldots, \nu_m) = \int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \prod_{j=1}^{m} \mathcal{D}_j^{-\nu_j}, \tag{3.5}$$

is an $\ell$-loop integral with propagators $\mathcal{D}_i$. Note that the $\nu_i$ are arbitrary, in particular some of the $\nu_i$ can vanish, signaling that the corresponding propagator is pinched. Conventionally, we write the integrand corresponding to the integral $I(\nu_1, \ldots, \nu_m)$ as,

$$\mathcal{I}(\vec{\nu}) = \mathcal{I}(\nu_1, \ldots, \nu_m) = \prod_{j=1}^{m} \mathcal{D}_j^{-\nu_j}, \tag{3.6}$$

so that we have,

$$I(\nu_1, \ldots, \nu_m) = \int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \mathcal{I}(\nu_1, \ldots, \nu_m). \tag{3.7}$$

*Example.*
As an example we consider the scalar massless box at one loop. This

integral can be written by choosing the denominator factors $\mathcal{D}_i$ as,

$$\mathcal{T}_{\text{box}} = \{\mathcal{D}_i\}_{i=1\ldots4} = \{k^2, (k+p_1)^2, (k+p_1+p_2)^2, (k+p_1+p_2+p_3)^2\}, \tag{3.8}$$

so that $I_{\text{box}} = I(1,1,1,1)$.

Likewise, the triangle that is obtained by pinching the propagator $(k + p_1 + p_2 + p_3)^2$ from the box can be written as $I(1,1,1,0)$.

Equipped with this notation, we can now further examine the statement that the integral of the total derivative with respect to a loop momentum vanishes,

$$\int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \frac{\partial}{\partial k_l} \mathcal{I}(\nu_1, \ldots, \nu_m) = 0 \quad \forall \ l \in \{1, \ldots, \ell\} \tag{3.9}$$

We can act with the derivative under the integral sign and express the vanishing of the derivative with respect to $k_l^\mu$ as,

$$\int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \sum_{j=1}^{m} (-\nu_j) \left( \frac{\partial}{\partial k_{l,\mu}} \mathcal{D}_j \right) \oplus_j \mathcal{I}(\nu_1, \ldots, \nu_m) = 0. \tag{3.10}$$

Here we have defined the operator $\oplus_j$ which acts on the integrand by increasing the exponent $\nu_j$ by one, e.g.

$$\oplus_4 \mathcal{I}(1,1,1,0) = \mathcal{I}(1,1,1,1). \tag{3.11}$$

Equation (3.10) of course also holds true after contracting both sides with one of the external vectors $p_a^\mu$. If we contract both sides with the loop momentum $k_l$ we pick up an additional term proportional to

$$\partial_{k_{l,\mu}} k_l^\mu = d. \tag{3.12}$$

The scalar product $p_{a,\mu} \left( \frac{\partial}{\partial k_{l,\mu}} \mathcal{D}_j \right)$ will then contain two types of terms, products that involve loop momenta and products between two external momenta. The latter are constants with respect to the loop integration over the $k_l$ and can be ignored. The former require some more consideration.

By choosing the set of denominator factors $\{\mathcal{D}_i\}$ such that every possible scalar product $k_l^\mu p_{a\mu}$ and $k_l^\mu k_{l'\mu}$ can be uniquely expressed in terms of denominator factors and constants, the product $p_{a,\mu} \left( \frac{\partial}{\partial k_{l,\mu}} \mathcal{D}_j \right)$ can be written as a linear combination ratios of denominator factors with constant coefficients. Beyond one loop, this potentially requires the introducing of so-called ***irreducible numerators***, referring to factors $\mathcal{D}_i$, required for completeness, that only appear in the numerator. Such a complete set of denominators is referred to as ***topology***. Multiplying or dividing $\mathcal{I}(\vec{\nu})$ by a denominator $\mathcal{D}_i$ is of course expressible through the action of the operator $\oplus_i$ or its inverse $\ominus_i$, which decreases $\nu_i$ by one, so that we find,

$$\int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \sum_{j=1}^{m} (-\nu_j) \left( \sum_a c_{a,b} \prod_b \oplus_b^{p_{a,b}} \ominus_b^{m_{a,b}} \right) \mathcal{I}(\nu_1, \ldots, \nu_m) = 0. \tag{3.13}$$

Here the sum over $a$ enumerates the different terms obtained in decomposing the derivative in terms of denominator factors, $c_{a,b}$ captures constants with respect to the integration, such as the dimension $d$, scalar products between external momenta $p_i \cdot p_j$ as well as masses. Taking a step back we have therefore a relation between different integrals,

$$\sum_i \mathcal{C}_i I\left(\vec{\nu}_i\right) = 0, \tag{3.14}$$

where the $\mathcal{C}_i$ and the $\vec{\nu}_i$ can be determined from the above steps depending on the exact form of the denominators and the derivative being calculated.

*Example.*
Returning to the example of the one-loop massless box, we can first convince ourselves that $\mathcal{T}_{\text{box}}$ defined in eq. (3.8) does indeed fashion a topology. In the one-loop case it is straightforward to note that the only scalar products with the loop momentum that can appear in the derivative term are,

$$k \cdot k, \quad k \cdot p_1, \quad k \cdot p_2 \;\text{ and }\; k \cdot p_3. \tag{3.15}$$

By solving the system of equations given by the denominator factors $\mathcal{T}_{\text{box}}$ we can find the relations,

$$\begin{aligned}
k \cdot k &= \mathcal{D}_1 && (3.16)\\
k \cdot p_1 &= \frac{1}{2}\left(\mathcal{D}_2 - \mathcal{D}_1\right) && (3.17)\\
k \cdot p_2 &= \frac{1}{2}\left(\mathcal{D}_3 - \mathcal{D}_2 - s_{12}\right) && (3.18)\\
k \cdot p_3 &= \frac{1}{2}\left(\mathcal{D}_4 - \mathcal{D}_3 - s_{13} - s_{23}\right), && (3.19)\\
& && (3.20)
\end{aligned}$$

where we let $(p_i + p_j)^2 = s_{ij}$. Because all scalar products have been expressed through denominators and constants, $\mathcal{T}_{\text{box}}$ is indeed a topology. We can therefore find relations between different integrals. Writing $\mathcal{T}_{\text{box}}(\vec{\nu})$ for the integrand $\mathcal{I}(\vec{\nu})$ with the $\mathcal{D}_i$ taken from the set $\mathcal{T}_{\text{box}}$ and $T_{\text{box}}$ for the corresponding integral we can for example look at the relations generated by

$$\int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{\partial}{\partial k_\mu} k_\mu \mathcal{T}_{\text{box}}(1,1,1,0) = 0. \tag{3.21}$$

Going through the algebra we find,

$$\begin{aligned}
&\int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{\partial}{\partial k_\mu} k_\mu \mathcal{T}_{\text{box}}(1,1,1,0) \\
=&\int \frac{\mathrm{d}^d k}{(2\pi)^d} \left(d - 4 - s_{12} \oplus_3 - \oplus_2 \ominus_1 - \oplus_3 \ominus_1\right) \mathcal{T}_{\text{box}}(1,1,1,0) \\
=&(d-4) T_{\text{box}}(1,1,1,0) - s_{12} T_{\text{box}}(1,1,2,0) \\
&- T_{\text{box}}(0,2,1,0) - T_{\text{box}}(0,1,2,0) = 0.
\end{aligned} \tag{3.22}$$

By contracting the starting equation with different external vectors or loop momenta and considering different values for the $\vec{\nu}$, one can obtain large sets of these relations. They form an overconstrained system of equations for the integrals $I(\vec{\nu}_i)$. Such systems can be solved using different techniques, mostly commonly using the Laporta algorithm [146], a variation of Gauss elimination. There are a number of public codes that can automatically derive the above relations and solve the resulting systems [150–152]. As a result of this process one finds that the integrals $I(\vec{\nu}_i)$ in a specific topology can be expressed through a small set of integrals, which are referred to as *master integrals.*

*Example.*

Let us return to the example of the box topology. By deriving more relations such as in eq. (3.22) and solving the resulting system, we find that all integrals $T_{\text{box}}(\nu_i)$ can be written in terms of only three master integrals, for example

$$T_{\text{box}}(0,1,0,1), \quad T_{\text{box}}(1,0,1,0) \;\text{ and }\; T_{\text{box}}(1,1,1,1). \tag{3.23}$$

In particular, the triangle integral $T_{\text{box}}(1,1,1,0)$ can be expressed as

$$T_{\text{box}}(1,1,1,0) = \frac{2(d-3)}{(d-4)s_{12}} T_{\text{box}}(1,0,1,0). \tag{3.24}$$

The master integrals for a specific topology form a basis for the integrals appearing in that topology. We note that the choice of a basis and with that the choice of master integrals is of course not unique. Different programs can sometimes produce different bases of master integrals and one usually strives to choose the simplest integrals possible as master integrals. However, the criterion ‘simple’ is often not sufficiently constraining and while the method of IBP reduction has been known for almost thirty years [147, 153], the choice of an optimal basis is a topic of active research [76–78].

Looking at the result obtained in our example in eq. (3.24), we can observe one advantage of reducing integrals to master integrals, the triangle integral $T_{\text{box}}(1,1,1,0)$ has been reduced to a bubble integral, $T_{\text{box}}(1,0,1,0)$, which by virtue of having one less propagator, is simpler than the original integral. This shows one of the guiding principles of successfully using IBP reductions, by performing a reduction of complicated integrals to simpler integrals and furthermore by expressing many integrals through a small set of master integrals, the computation of the master integrals is drastically simpler than the computation of the original integrals.

Equipped with this powerful reduction technique, we will concern ourselves exclusively with the calculation of master integrals for the remainder of this thesis. Any multiloop amplitude that we might be interested in computing will be expressed in terms of a large number of integrals, however we can always reduce these integrals to a relatively small set of master integrals and need only to compute these master integrals. In fact we will from now on often drop the label "master" and refer to them generically as "integrals" knowing that they capture all information required.

## Reverse unitarity

The calculation of multiloop scattering amplitudes is dramatically simplified by using IBP reductions. However scattering amplitudes are but one ingredient in the calculation of cross sections. In particular, the calculation of inclusive cross section requires the integration over the phase-space of any unresolved external momenta,

$$\sigma_{\text{inclusive}} \propto \int d\Phi \, |\mathcal{A}|^2 \,. \tag{3.25}$$

Having simplified the calculation of the scattering amplitude $\mathcal{A}$, we shall now turn to the phase-space integral $\mathrm{d}\Phi$ using *reverse unitarity.*

While the method of reverse unitarity is completely general, only relying on the unitarity of the $S$-matrix of quantum field theory, it is instructive to consider a concrete set of phase-spaces. Therefore, we will consider phase-spaces for the scattering of two massless particles to one massive particle, which we denote suggestively as $H$, and $j = 3 \ldots N$ massless particles,

$$1 + 2 \to H + 3 + \cdots + N. \tag{3.26}$$

The cross section for a process in this class is written in terms of an integration over the momenta $p_j$ of the final state particles of the process specific scattering amplitude[1] $\mathcal{A}$,

$$\sigma = \int \mathrm{d}\Phi_{N-1}(p_3, \ldots, p_N) \left|\mathcal{A}(p_1, p_2, \{p_j\}, d)\right|^2 . \tag{3.27}$$

[1]We shall assume here, that $|\mathcal{A}|^2$ has been multiplied by the physical flux factor, as well as any required symmetry factors. However these are irrelevant for the following discussion.

The $d$-dimensional phase-space measure is here

$$\begin{aligned}&d\Phi_{N-1}(p_3,\dots,p_N)\\ =&(2\pi)^d\delta^{(d)}(p_{12}-p_H-p_{3\dots N})\frac{\mathrm{d}^d p_H}{(2\pi)^d}\delta^+(p_H^2-m^2)\prod_{j=3}^{N}\frac{\mathrm{d}^d p_j}{(2\pi)^d}\delta^+(p_j^2),\end{aligned} \tag{3.28}$$

where $\delta^+(p^2-m^2)=\delta(p^2-m^2)\theta(p^0)$ is the usual on-shell constraint for physical particles and we have used the abbreviations

$$p_{ij\dots}=p_i+p_j+\dots. \tag{3.29}$$

If we compare the integral measures for the external momenta $p_j$ to loop integrals we realize that the only difference is the on-shell constraint that leads to a potentially complicated integration contour. This can be alleviated using the Cutkosky cutting rules [154].

Using the Cutkosky rule in reverse, the method of reverse unitarity [83] exploits the duality between on-shell constraints and cut propagators,

$$\begin{aligned}\delta^+(p^2-m^2)\to\left[\frac{1}{p^2-m^2}\right]_c &\equiv\frac{1}{2\pi i}\mathrm{Disc}\frac{1}{p^2-m^2}\\ &=\frac{1}{2\pi i}\left(\frac{1}{p^2-m^2+i0}-\frac{1}{p^2-m^2-i0}\right).\end{aligned} \tag{3.30}$$

Using reverse unitarity we can therefore rephrase the phase-space integration in eq. (3.27) as an $(N-2)$-fold cut of the corresponding forward scattering amplitude,

$$\begin{aligned}\sigma=\int\frac{\mathrm{d}^d p_H}{(2\pi)^d}\prod_{j=3}^{N}\frac{\mathrm{d}^d p_j}{(2\pi)^d}(2\pi)^d\\ \times\delta^{(d)}(p_{12}-p_H-p_{3\dots N})\left[\frac{1}{p_H^2-m^2}\right]_c\prod_{j=3}^{N}\left[\frac{1}{p_j^2}\right]_c|\mathcal{A}|^2.\end{aligned} \tag{3.31}$$

Because the cut propagators can be differentiated in exactly the same way as regular (uncut) propagators with respect to their momenta,

$$\frac{\partial}{\partial p_\mu}\left(\left[\frac{1}{p^2}\right]_c\right)^\nu=-\nu\left(\left[\frac{1}{p^2}\right]_c\right)^{\nu+1}2p^\mu, \tag{3.32}$$

we can obtain the same IBP identities for phase-space integrals as for loop integrals. The systems of IBP identities for the phase-space integrals can be solved in the same way as for loop integrals, with the exception that cut propagators come with a simplifying constraint,

$$\left(\left[\frac{1}{p^2}\right]_c\right)^{-\nu}\to 0\quad\forall\ \nu=0,1,2,\dots, \tag{3.33}$$

because the integral will of course only develop a branch cut whose discontinuity we can take, if the integrand has the appropriate pole.

Combining the power of integration-by-parts reductions and reverse unitarity [83, 84, 155–157] we can therefore reduce not only loop integrals to a master integral basis but also reduce phase-space integrals to the respective phase-space master integrals. Once again, as in the loop-integral case, this will significantly reduce the complexity of the calculation as only the phase-space masters need to be determined.

## 3.2 Obtaining differential equations for master integrals

Let us consider an $n$-point $\ell$-loop integral with $m$ propagators, as we defined it in eq. (3.1),

$$\begin{aligned}&I^{\nu_1,\dots,\nu_m}(p_1,\dots,p_n,m_1,\dots,m_m) = \\ &\int \prod_{i=1}^{\ell} \frac{\mathrm{d}^d k_i}{(2\pi)^d} \mathcal{I}^{\nu_1,\dots,\nu_m}(k_1,\dots,k_\ell,p_1,\dots,p_n,m_1,\dots,m_m),\end{aligned} \tag{3.34}$$

with the integrand defined as before,

$$\begin{aligned}&\mathcal{I}^{\nu_1,\dots,\nu_m}(k_1,\dots,k_\ell,p_1,\dots,p_n,m_1,\dots,m_m) \\ &= \prod_i^m \left[\left(\sum_j \alpha_{ij}k_j + \sum_j \beta_{ij}p_j\right)^2 - m_i^2 - i0\right]^{-\nu_i} \\ &= \prod_i^m \mathcal{D}_i^{-\nu_i}.\end{aligned} \tag{3.35}$$

Here we have taken care to write out explicitly the dependence on all physical parameters $p_i^\mu$ and $m_i$. We can employ Lorentz invariance of the integral to rephrase the dependence on momenta in terms of the Mandelstam invariants

$$s_{ij} = (p_i + p_j)^2, \quad s_{ii} = p_i^2. \tag{3.36}$$

Note that because of momentum conservation,

$$\sum_{i=1}^n p_i^\mu = 0, \tag{3.37}$$

these Mandelstam invariants will in general not be independent, but we will have

$$\sum_{i<j} s_{ij} = \sum_i s_{ii}. \tag{3.38}$$

We can thus view the integrals as functions of the Mandelstam invariants $s_{ij}$ and masses $m_i$. This makes it only natural to consider derivatives of an integral with respect to any of these parameters.

### Differential equations with respect to internal masses

We start by considering derivatives with respect to internal masses. These are particularly simple and we can write down a closed expression for the derivative with respect to some mass $m$ as,

$$\begin{aligned}&\frac{\partial}{\partial m^2} I^{\nu_1,\ldots,\nu_n}(p_1,\ldots,p_n,m_1,\ldots,m_m)\\&=\sum_{j=1}^{m}\int\prod_{i=1}^{\ell}\frac{\mathrm{d}^d k_i}{(2\pi)^d}\frac{\partial\mathcal{D}_j}{\partial m^2}\frac{\partial}{\partial\mathcal{D}_j}\mathcal{I}^{\nu_1,\ldots,\nu_m}(k_1,\ldots,k_\ell,p_1,\ldots,p_n,m_1,\ldots,m_m),\end{aligned} \tag{3.39}$$

in terms of the increment $\oplus_i$ operators, defined in eq. (3.11), this can be written as,

$$\begin{aligned}&\frac{\partial}{\partial m^2} I^{\nu_1,\ldots,\nu_n}(p_1,\ldots,p_n,m_1,\ldots,m_m)\\&=\sum_{j=1}^{m}\int\prod_{i=1}^{\ell}\frac{\mathrm{d}^d k_i}{(2\pi)^d}\frac{\partial\mathcal{D}_j}{\partial m^2}(-\nu_j)\oplus_j\mathcal{I}^{\nu_1,\ldots,\nu_m}(k_1,\ldots,k_\ell,p_1,\ldots,p_n,m_1,\ldots,m_m).\end{aligned} \tag{3.40}$$

We can see that the action of derivatives with respect to external masses is similar to the action of the derivatives used to derive the integration-by-parts identities. As such it is not surprising that we can employ IBP reductions to reduce the integrals produced by the action of the derivative. For a set of master integrals $\{\mathcal{M}_i\}$, we will, obtain after reduction, for the derivative with respect to some internal mass $m$,

$$\frac{\partial}{\partial m^2}\mathcal{M}_\alpha=\sum_\beta \mathcal{C}_{\alpha\beta}(s_{ij},m_i,\epsilon)\mathcal{M}_\beta, \tag{3.41}$$

where the $\mathcal{C}_{\alpha\beta}$ are coefficients that are constant with respect to the loop momenta and the sum on the right runs over all master integrals. In particular there will be a term proportional to $\mathcal{M}_\alpha$ on the right-hand-side, in other words, we obtain a differential equation for $\mathcal{M}_\alpha$.

*Example.*
Let us consider as an example the triangle integral family defined by,

$$\mathcal{T}_{tri}=\{\mathcal{D}_i\}_{i=1\ldots3}=\{k^2-m^2,(k+p_1)^2-m^2,(k+p_1+p_2)^2-m^2\}. \tag{3.42}$$

By using integration-by-parts reductions on integrals within this topology, we find that there are three master integrals in the basis for this family.

One possible choice of basis is,

$$\mathcal{T}_{tri} \simeq \mathbb{F}(s, m, \epsilon)\Big[\{\mathcal{M}_i\}\Big], \tag{3.43}$$

where $s = (p_1 + p_2)^2$, with the master integrals

$$\{\mathcal{M}_i\}_{i=1\ldots3} = \{I(1,0,0), I(1,0,1), I(1,1,1)\}, \tag{3.44}$$

and where $\mathbb{F}$ is the field of rational functions, i.e. all integrals in the $\mathcal{T}_{tri}$ topology can be expressed as linear combinations of the three master integrals with coefficients that are rational functions of the dimensional regulator $\epsilon$ and of the scales of the problem $s$ and $m$. Equipped with this, we can derive the differential equations for the master integrals with respect to $m^2$. For the tadpole $\mathcal{M}_1 = I(1,0,0)$ we find

$$\partial_{m^2} I(1,0,0) = \frac{\partial \mathcal{D}_1}{\partial m^2}\frac{\partial I(1,0,0)}{\partial \mathcal{D}_1} = I(2,0,0). \tag{3.45}$$

We observe that the resulting integral $I(2,0,0)$ is no longer an element of the basis of master integrals. Consequently, we can find an IBP reduction for it

$$I(2,0,0) = \frac{1-\epsilon}{m^2} I(1,0,0), \tag{3.46}$$

so that we have the differential equation

$$\partial_{m^2}\mathcal{M}_1(m) = \frac{1-\epsilon}{m^2}\mathcal{M}_1(m). \tag{3.47}$$

For the bubble integral $\mathcal{M}_2 = I(1,0,1)$ we find

$$\partial_{m^2} I(1,0,1) = \frac{\partial \mathcal{D}_1}{\partial m^2}\frac{\partial I(1,0,1)}{\partial \mathcal{D}_1} + \frac{\partial \mathcal{D}_2}{\partial m^2}\frac{\partial I(1,0,1)}{\partial \mathcal{D}_2} = I(2,0,1) + I(1,0,2). \tag{3.48}$$

Once again we can IBP-reduce the integrals appearing on the right hand side,

$$\begin{aligned} I(2,0,1) &= -\frac{1-\epsilon}{m^2(4m^2-s)} I(1,0,0) + \frac{1-2\epsilon}{4m^2-s} I(1,0,1), \\ I(1,0,2) &= -\frac{1-\epsilon}{m^2(4m^2-s)} I(1,0,0) + \frac{1-2\epsilon}{4m^2-s} I(1,0,1), \end{aligned} \tag{3.49}$$

and obtain the differential equation

$$\partial_{m^2}\mathcal{M}_2(m) = -\frac{2(1-\epsilon)}{m^2(4m^2-s)}\mathcal{M}_1(m) + \frac{2-4\epsilon}{4m^2-s}\mathcal{M}_2(m). \tag{3.50}$$

Here we observe a general feature of the differential equations that we obtain for master integrals: The differential equations for different master integrals are in general not independent but coupled among each other, i.e. in general for a topology with $n$ master integrals we will obtain a coupled system system of $n$ differential equations.

For the triangle integral $\mathcal{M}_3 = I(1,1,1)$ we have then similarly,

$$\begin{aligned}\partial_{m^2} I(1,1,1) &= \frac{\partial \mathcal{D}_1}{\partial m^2}\frac{\partial I(1,1,1)}{\partial \mathcal{D}_1} + \frac{\partial \mathcal{D}_2}{\partial m^2}\frac{\partial I(1,1,1)}{\partial \mathcal{D}_2} + \frac{\partial \mathcal{D}_3}{\partial m^2}\frac{\partial I(1,1,1)}{\partial \mathcal{D}_3} \\ &= I(2,1,1) + I(1,2,1) + I(1,1,2).\end{aligned} \tag{3.51}$$

The integrals obtained need to be IBP-reduced,

$$\begin{aligned}I(2,1,1) &= \frac{(\epsilon-1)\left((4\epsilon-2)m^2-\epsilon s\right)}{m^4 s(4m^2-s)} I(1,0,0) + \frac{4\epsilon-2}{s(4m^2-s)} I(1,0,1), \\ I(1,2,1) &= \frac{(3-2\epsilon)\epsilon-1}{m^4 s} I(1,0,0) + \frac{1-2\epsilon}{m^2 s} I(1,0,1) - \frac{\epsilon}{m^2} I(1,1,1), \\ I(1,1,2) &= \frac{(\epsilon-1)\left((4\epsilon-2)m^2-\epsilon s\right)}{m^4 s(4m^2-s)} I(1,0,0) + \frac{4\epsilon-2}{s(4m^2-s)} I(1,0,1),\end{aligned} \tag{3.52}$$

and we find the differential equation,

$$\partial_{m^2}\mathcal{M}_3(m) = \frac{\epsilon-1}{m^4(s-4m^2)}\mathcal{M}_1(m) + \frac{1-2\epsilon}{m^2(s-4m^2)}\mathcal{M}_2(m) - \frac{\epsilon}{m^2}\mathcal{M}_3(m). \tag{3.53}$$

We observe that the differential equation for $\mathcal{M}_3$ is coupled to the other two master integrals. We can make a more specific observation, master integrals seem to be coupled only to master integrals with the same number or fewer propagators. In general there can be of course multiple integrals with the same number of propagators and such couplings can be very complicated, however at least conjecturally this structure seems to hold in general.

A useful sanity check for the differential equations is to simply consider their mass dimensions. The triangle integral has mass dimension,

$$[I(1,1,1)] = 4 - 2\epsilon - 6, \tag{3.54}$$

the derivative with respect to $m^2$ has consequently,

$$[\partial_{m^2} I(1,1,1)] = (4-2\epsilon-6) - 2. \tag{3.55}$$

Considering the right-hand-side of the differential equation we see that the mass dimensions do indeed match,

$$\begin{aligned} \left[\frac{I(1,0,0)}{m^4(s-4m^2)}\right] &= (4-2\epsilon-2)-6, \\ \left[\frac{I(1,0,1)}{m^2(s-4m^2)}\right] &= (4-2\epsilon-4)-4, \\ \left[\frac{I(1,1,1)}{m^2}\right] &= (4-2\epsilon-6)-2. \end{aligned} \tag{3.56}$$

Since the differential equations are coupled it makes sense to view them as a system of differential equations and write the system as

$$\partial_{m^2}\mathcal{M}_i = \mathcal{A}_{ij}(s,m,\epsilon)\mathcal{M}_j, \tag{3.57}$$

where summation over $j$ is implied. This is the general structure of the differential equations for a given set of master integrals. In this specific case we can specialize the structure some more and write

$$\partial_{m^2}\mathcal{M}_i = \left(\frac{\mathcal{A}^{(0)}_{ij}}{4m^2-s} + \frac{\mathcal{A}^{(1)}_{ij}}{m^2} + \frac{\mathcal{A}^{(2)}_{ij}}{m^4}\right)\mathcal{M}_j \tag{3.58}$$

with the coefficient matrices

$$\begin{aligned} \mathcal{A}^{(0)} &= \begin{pmatrix} 0 & 0 & 0 \\ \frac{8(\epsilon-1)}{s} & 2-4\epsilon & 0 \\ \frac{16(1-\epsilon)}{s^2} & \frac{4(2\epsilon-1)}{s} & 0 \end{pmatrix}, \\ \mathcal{A}^{(1)} &= \begin{pmatrix} 1-\epsilon & 0 & 0 \\ \frac{2(1-\epsilon)}{s} & 0 & 0 \\ -\frac{4(1-\epsilon)}{s^2} & \frac{1-2\epsilon}{s} & -\epsilon \end{pmatrix}, \\ \mathcal{A}^{(2)} &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{1-\epsilon}{s} & 0 & 0 \end{pmatrix}. \end{aligned} \tag{3.59}$$

### Differential equations with respect to external invariants

Next we can consider differential equations with respect to external kinematic data, i.e. Mandelstam invariants. Deriving such differential equations is less straightforward since the integrands do not depend directly on them but rather are functions of the external momenta. Note that while one could argue that a propagator like

$$(k+p_1+p_2)^2 = k^2 + 2k\cdot(p_1+p_2) + s_{12}, \tag{3.60}$$

does indeed depend on $s_{12}$ directly, this manifest dependence on $s_{12}$ is not the complete dependence of the integral on $s_{12}$. When integrating a loop integral over such a propagator, the result will develop additional dependence on $s_{12}$ through the scalar products $k \cdot p_1$ and $k \cdot p_2$. Therefore, it is not possible to derive differential equations by simply taking derivatives of the integrand with respect to Mandelstam invariants.

Instead, differential equations with respect to external kinematics need to be constructed from derivatives with respect to external momenta as the dependence on them is manifest at the integrand level. To build a differential operator that takes the derivative with respect to a certain kinematic invariant of an $n$-point integral, we therefore begin with the general ansatz,

$$\partial_{s_{ij}} = \sum_{k,l=1}^{n-1} \alpha_{kl} p_l^\mu \partial_{p_k^\mu}. \tag{3.61}$$

Note that we are implementing total momentum conservation from the beginning by taking derivatives only with respect to $n-1$ momenta, eliminating the last momentum. The coefficients $\alpha_{kl}$ then need to be determined by demanding that $\partial_{s_{ij}}$ commutes with all constraints on the external kinematics. For $s_{ij}$ with $i \neq j$ one type of constraints arises from the demand that $\partial_{s_{ij}}$ should commute with all on-shell constraints of the external momenta

$$\partial_{s_{ij}} s_{kk} = 0 \ \ \forall\, k, \tag{3.62}$$

this yields $n$ equations that can be solved to determine $n$ of the $\alpha_{kl}$. Additionally, we demand that $\partial_{s_{ij}}$ be compatible with the definition of the Mandelstam invariants,

$$\partial_{s_{ij}} s_{kl} = 0 \ \text{ for } (i,j) \neq (k,l) \text{ and } (k,l) \neq (n-1,n). \tag{3.63}$$

Finally we have two normalization constraints. The first one is simply the definition of the Mandelstam invariant with respect to which we are differentiating,

$$\partial_{s_{ij}} s_{ij} = 1. \tag{3.64}$$

The last constraint arises from the fact that we can of course eliminate one of the Mandelstam invariants using momentum conservation. In this case we choose,

$$s_{n-1,n} = \sum_i s_{ii} - \sum_{i<j \text{ and } (i,j)\neq(n-1,n)} s_{ij}. \tag{3.65}$$

We can easily see that from this we get the additional constraint,

$$\partial_{s_{ij}} s_{n-1,n} = -1. \tag{3.66}$$

Analogously, we can also derive differential operators with respect to non-vanishing squares of external momenta,

$$\partial_{s_{ii}} = \sum_{k,l=1}^{n-1} \alpha_{kl} p_l^\mu \partial_{p_k^\mu}. \tag{3.67}$$

Here we find the constraints

$$\partial_{s_{ii}} s_{kk} = \delta_{ik}, \tag{3.68}$$

$$\partial_{s_{ii}} s_{kl} = 0 \quad \text{for } (k,l) \neq (n-1,n), \tag{3.69}$$

as well as

$$\partial_{s_{ii}} s_{n-1,n} = 1. \tag{3.70}$$

We can solve these constraints to determine the remaining $\alpha_{kl}$. Note that these constraints are not necessarily independent, depending on $n$ it is therefore possible that some of the $\alpha_{kl}$ remain undetermined after all constraints have been fulfilled. This is however not a problem as the undetermined coefficients will drop out of the differential equations after reduction to master integrals. Therefore, the differential equations obtained using this method are unique even though the differential operators are not.

In order to verify the differential operators as well as the differential equations obtained with them, one considers the so called *dilatation operator* $D$. The operator is defined as a weighted sum of all differential operators with respect to kinematic invariants and masses,

$$D = \sum_i m_i^2 \partial_{m_i^2} + \sum_{i<j} s_{ij} \partial_{s_{ij}} + \sum_i s_{ii} \partial_{s_{ii}}, \tag{3.71}$$

where the sums run over all internal masses $m_i$, all Mandelstam invariants $s_{ij}$ as well as all off-shell external momentum squares $s_{ii}$ respectively. Applying this operator to an integral yields the mass dimension of that integral by construction. Since the mass dimension of a given integral is known from dimensional analysis, this can be used as an important sanity check of the derivation of the differential operators.

*Example.*
Let us return now to our previous example of the triangle integral family that we defined in eq. (3.42). The master integrals of this topology are functions of $m$ as well as $s$. So far we have determined the differential equations with respect to $m^2$, c.f. eq. (3.58) and eq. (3.59). Now we are in a position to also determine the differential equations with respect to $s$.

For that we first need to derive a differential operator $\partial_s$. In three-point kinematics we can begin with the general ansatz,

$$\partial_s = \alpha_{11} p_1^\mu \partial_{p_1^\mu} + \alpha_{12} p_2^\mu \partial_{p_1^\mu} + \alpha_{21} p_1^\mu \partial_{p_2^\mu} + \alpha_{22} p_2^\mu \partial_{p_2^\mu}. \tag{3.72}$$

Next we need to determine the coefficients $\alpha$. We start by demanding that

$p_1$ and $p_2$ be on-shell. This yields the equations,

$$\begin{aligned} \partial_s p_1^2 &= \alpha_{12} s = 0, \\ \partial_s p_2^2 &= \alpha_{21} s = 0. \end{aligned} \tag{3.73}$$

Furthermore, we use the definition of $s$,

$$\partial_s s = \partial_s (p_1 + p_2)^2 = s(\alpha_{11} + \alpha_{12} + \alpha_{21} + \alpha_{22}) = 1. \tag{3.74}$$

Solving these three constraints for e.g. $\alpha_{11}, \alpha_{12}$ and $\alpha_{21}$, we find,

$$\alpha_{11} = \frac{1 - \alpha_{22} s}{s}, \quad \alpha_{12} = 0, \quad \alpha_{21} = 0, \tag{3.75}$$

which yields the differential operator,

$$\partial_s = \frac{1 - \alpha_{22} s}{s} p_1^\mu \partial_{p_1^\mu} + \alpha_{22} p_2^\mu \partial_{p_2^\mu}. \tag{3.76}$$

As we can see this differential operator still depends on $\alpha_{22}$, which we left undetermined since the external kinematics did not yield enough constraints to fix all coefficients. As such this differential operator is not unique. However, as we will see $\alpha_{22}$ will drop out from the differential equations that we obtain with this operator, so they are unique.

Now we can apply our differential operator to the master integrals in the triangle topology, eq. (3.44). We start with the tadpole integral $I(1, 0, 0)$,

$$\partial_s \mathcal{M}_1 = 0, \tag{3.77}$$

which is independent of $s$ as we would expect, as tadpole integrals are of course independent of the external kinematics due to the translation symmetry of the loop momentum. The bubble integral $I(1, 0, 1)$ is more interesting, applying the differential operator we find a variety of integrals with denominators raised to higher powers as well as numerator insertions,

$$\begin{aligned} \partial_s I(1, 0, 1) = &\left( \frac{1}{s} - \alpha_{22} \right) I(2, 0, 0) + \left( 2\alpha_{22} - \frac{1}{s} \right) I(1, -1, 2) \\ &+ (s\alpha_{22} - 1)\, I(1, 0, 2) - \alpha_{22} I(1, 0, 1). \end{aligned} \tag{3.78}$$

Not all integrals produced by the differentiation are elements of our basis of master integrals, consequently we need to find reduction identities for them,

$$
\begin{aligned}
I(2,0,0) &= \frac{1-\epsilon}{m^2} I(1,0,0) \\
I(1,-1,2) &= \left(\frac{s(2\epsilon-1)}{2(4m^2-s)} + \frac{1}{2}\right) I(1,0,1) + \frac{2(\epsilon-1)}{4m^2-s} I(1,0,0) \\
I(1,0,2) &= \frac{1-2\epsilon}{4m^2-s} I(1,0,1) + \left(\frac{1-\epsilon}{m^2 s} + \frac{4(\epsilon-1)}{s(4m^2-s)}\right) I(1,0,0).
\end{aligned}
\tag{3.79}
$$

Using these relations we obtain the differential equation with respect to $s$ for the bubble integral,

$$
\partial_s \mathcal{M}_2 = -\frac{2(\epsilon-1)}{s(4m^2-s)} \mathcal{M}_1 + \left(\frac{2\epsilon-1}{2(4m^2-s)} - \frac{1}{2s}\right) \mathcal{M}_2. \tag{3.80}
$$

Analogously, we can also differentiate the triangle integral $I(1,1,1)$,

$$
\begin{aligned}
\partial_s I(1,1,1) = &\left(\frac{1}{s} - \alpha_{22}\right) I(0,1,2) + \left(\frac{1}{s} - \alpha_{22}\right) I(0,2,1) \\
&+ \left(2\alpha_{22} - \frac{1}{s}\right) I(1,0,2) + (s\alpha_{22} - 1)\, I(1,1,2) - \frac{1}{s} I(1,1,1).
\end{aligned}
\tag{3.81}
$$

After IBP reduction this yields the differential equation for the triangle integral,

$$
\partial_s \mathcal{M}_3 = \left(\frac{1-\epsilon}{m^2 s^2} + \frac{4(\epsilon-1)}{s^2(4m^2-s)}\right) \mathcal{M}_1 + \frac{1-2\epsilon}{s(4m^2-s)} \mathcal{M}_2 - \frac{1}{s} \mathcal{M}_3. \tag{3.82}
$$

We can observe that the differential equations are independent of the undetermined parameter $\alpha_{22}$. As such we have obtained a unique system of differential equations for the master integrals of the triangle topology.

*Example.*
Moving to a slightly more interesting example, we can consider the integral family of one-loop 4-point integrals, which we defined in eq. (3.8). Recall that,

$$
\mathcal{T}_{\text{box}} = \{\mathcal{D}_i\}_{i=1\ldots 4} = \{k^2, (k+p_1)^2, (k+p_1+p_2)^2, (k+p_1+p_2+p_3)^2\}, \tag{3.83}
$$

with $p_i^2 = 0$ and the usual Mandelstam invariants,

$$s = (p_1 + p_2)^2, \quad t = (p_2 + p_3)^2 \quad \text{and} \quad u = (p_1 + p_3)^2. \tag{3.84}$$

The Mandelstam invariants are not independent because of momentum conservation and we have,

$$s + t + u = 0. \tag{3.85}$$

We can therefore consider for example $s$ and $t$ as the two independent variables and derive systems of differential equations with respect to them. One choice of master integrals for the system is

$$\begin{aligned} \mathcal{M}_1 &= I(1,0,1,0), \\ \mathcal{M}_2 &= I(0,1,0,1), \\ \mathcal{M}_3 &= I(1,1,1,1). \end{aligned} \tag{3.86}$$

To build the differential operator $\partial_s$ we start from the general ansatz,

$$\partial_s = \sum_{i,j=1}^{3} \alpha_{ij} p_j^\mu \partial_{p_i^\mu}. \tag{3.87}$$

After we demand that it respects $p_i^2 = 0$ we find,

$$\begin{aligned} \partial_s = &\left(2\alpha_{13} + \alpha_{22} + \frac{t\,(\alpha_{13}+\alpha_{23})}{s} + \frac{s\,(\alpha_{22}-\alpha_{23}+\alpha_{32}-\alpha_{33})}{t} + \frac{s\alpha_{32}}{s+t}\right) p_1^\mu \partial_{p_1^\mu} \\ &+ \left(\frac{t}{s}+1\right)\alpha_{13} p_2^\mu \partial_{p_1^\mu} + \alpha_{13} p_3^\mu \partial_{p_1^\mu} - \frac{t}{s}\alpha_{23} p_1^\mu \partial_{p_2^\mu} + \alpha_{22} p_2^\mu \partial_{p_2^\mu} + \alpha_{23} p_3^\mu \partial_{p_2^\mu} \\ &+ \frac{t}{s+t}\alpha_{32} p_1^\mu \partial_{p_3^\mu} + \alpha_{32} p_2^\mu \partial_{p_3^\mu} + \alpha_{33} p_3^\mu \partial_{p_3^\mu}. \end{aligned} \tag{3.88}$$

Using the remaining constraints $\partial_s s = 1$ and $\partial_s t = 0$ we have exhausted all independent constraints coming from the external kinematics and find the differential operator,

$$\begin{aligned}
\partial_s = & \frac{2\left(s^2\left(\alpha_{23}+\alpha_{32}\right)+2st\alpha_{23}+t^2\alpha_{23}+s\right)+t}{2s(s+t)} p_1^\mu \partial_{p_1^\mu} \\
& + \left(2\alpha_{23}+\alpha_{33}+\frac{t\alpha_{23}+\frac{1}{2}}{s}+\frac{s\left(\alpha_{23}+\alpha_{33}\right)}{t}\right) p_2^\mu \partial_{p_1^\mu} \\
& + \frac{2s^2\alpha_{23}+2s\alpha_{33}(s+t)+2t\alpha_{23}(2s+t)+t}{2t(s+t)} p_3^\mu \partial_{p_1^\mu} - \frac{t}{s}\alpha_{23} p_1^\mu \partial_{p_2^\mu} \\
& - \frac{s^2\left(\alpha_{23}+\alpha_{3,2}+\alpha_{33}\right)+st\left(2\alpha_{23}+\alpha_{33}\right)+t^2\alpha_{23}}{s(s+t)} p_2^\mu \partial_{p_2^\mu} + \alpha_{23} p_3^\mu \partial_{p_2^\mu} \\
& + \frac{t}{s+t}\alpha_{32} p_1^\mu \partial_{p_3^\mu} + \alpha 32 p_2^\mu \partial_{p_3^\mu} + \alpha_{33} p_3^\mu \partial_{p_3^\mu}.
\end{aligned} \tag{3.89}$$

While this differential operator may seem a bit unwieldy, we can easily apply it to the three master integrals in the topology and find the differential equations with respect to $s$,

$$\partial_s \mathcal{M}_i = \mathcal{A}^s_{ij} \mathcal{M}_j, \tag{3.90}$$

with the system matrix $\mathcal{A}^s$,

$$\mathcal{A}^s = \begin{pmatrix} -\frac{\epsilon}{s} & 0 & 0 \\ 0 & 0 & 0 \\ \frac{2-4\epsilon}{s^2(s+t)} & \frac{4\epsilon-2}{st(s+t)} & -\frac{s+\epsilon t+t}{s(s+t)} \end{pmatrix}. \tag{3.91}$$

We observe that the differential equations are independent of the undetermined coefficients $\alpha_{23}$, $\alpha_{32}$ and $\alpha_{33}$. We could therefore also simply set the undetermined $\alpha$ to some values in order to simplify the form of the differential operator, which would leave the differential equations invariant. Setting $\alpha_{23} = \alpha_{32} = \alpha_{33} = 0$, we obtain a simpler form for the differential operator,

$$\partial_s = \frac{2s+t}{2s(s+t)} p_1^\mu \partial_{p_1^\mu} + \frac{1}{2s} p_2^\mu \partial_{p_1^\mu} + \frac{1}{2(s+t)} p_3^\mu \partial_{p_1^\mu}. \tag{3.92}$$

In order to find the differential equations with respect to $t$ we need to determine the operator $\partial_t$ analogously to the determination of $\partial_s$. $\partial_t$ should also respect the on-shellness of the external particles, so that we can start from eq. (3.88) and demand that $\partial_t s = 0$ and $\partial_t t = 1$. With that we find the differential operator

$$
\begin{aligned}
\partial_t =\ & \frac{s^2\left(2t\left(\alpha_{23}+\alpha_{32}\right)-1\right)+4st^2\alpha_{23}+2t^3\alpha_{23}}{2st(s+t)} p_1^\mu \partial_{p_1^\mu} \\
& + \left(2\alpha_{23}+\alpha_{33}+\frac{s\left(2t\left(\alpha_{23}+\alpha_{33}\right)-1\right)}{2t^2}+\frac{t\alpha_{23}}{s}-\frac{1}{t})\right) p_2^\mu \partial_{p_1^\mu} \\
& + \frac{s^2\left(2t\left(\alpha_{23}+\alpha_{33}\right)-1\right)+2st\left(t\left(2\alpha_{23}+\alpha_{33}\right)-1\right)+2t^3\alpha_{23}}{2t^2(s+t)} p_3^\mu \partial_{p_1^\mu} \\
& - \frac{s^2\left(t\left(\alpha_{23}+\alpha_{32}+\alpha_{33}\right)-1\right)+st\left(t\left(2\alpha_{23}+\alpha_{33}\right)-1\right)+t^3\alpha_{23}}{st(s+t)} p_2^\mu \partial_{p_2^\mu} \\
& - \frac{t}{s}\alpha_{23} p_1^\mu \partial_{p_2^\mu} + \alpha_{23} p_3^\mu \partial_{p_2^\mu} + \frac{t}{s+t}\alpha_{32} p_1^\mu \partial_{p_3^\mu} + \alpha_{32} p_2^\mu \partial_{p_3^\mu} + \alpha_{33} p_3^\mu \partial_{p_3^\mu} .
\end{aligned} \tag{3.93}
$$

If we set $\alpha_{23}=\alpha_{32}=\alpha_{33}=0$ we find a more compact form,

$$
\partial_t = -\frac{s}{2t(s+t)} p_1^\mu \partial_{p_1^\mu} - \frac{s+2t}{2t^2} p_2^\mu \partial_{p_1^\mu} - \frac{s(s+2t)}{2t^2(s+t)} p_3^\mu \partial_{p_1^\mu} + \frac{1}{t} p_2^\mu \partial_{p_2^\mu} . \tag{3.94}
$$

Using either form of the operator we obtain the system of differential equations with respect to $t$,

$$
\partial_t \mathcal{M}_i = \mathcal{A}^t_{ij} \mathcal{M}_j , \tag{3.95}
$$

with the system matrix $\mathcal{A}^t$ defined as,

$$
\mathcal{A}^t = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{ep}{t} & 0 \\ \frac{4\epsilon-2}{st(s+t)} & \frac{2-4\epsilon}{t^2(s+t)} & -\frac{\epsilon s+s+t}{t(s+t)} \end{pmatrix} . \tag{3.96}
$$

To verify the systems of differential equations, we consider the dilatation operator,

$$
D = \mathcal{A}^s s + \mathcal{A}^t t = \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & -\epsilon & 0 \\ 0 & 0 & -2-\epsilon \end{pmatrix} . \tag{3.97}
$$

As required the dilatation operator is diagonal and its eigenvalues correspond to the mass dimensions of the integrals. We can always simplify such systems of differential equations by making a variable transformation that rescales all invariants by one particular invariant. In our case for example we can go from the variables $s$ and $t$ to $s$ and $x = t/s$. The differential equations in $s$ will become trivial as $\partial_s$ is just proportional to the dilatation operator $D$ and we only need to solve the new differential equations for $x$ which can be obtained using the chain rule. We should also note that the system matrices that we encounter in the calculation of master integrals are rational functions of $\epsilon$ and the kinematic invariants, as we can see explicitly in this example.

Equipped with tools to obtain any needed differential operator, we can now turn to the process of actually solving differential equations.

## 3.3 Solving differential equations

Finding an analytic solution in terms of useful functions is the main problem of the method of differential equations. For a generic system of differential equations,

$$\partial_x f_i(x) = A_{ij} f_j(x), \tag{3.98}$$

the solution is formally simply

$$f_i(x) = \left(\mathcal{P} e^{\int \mathrm{d}x A(x)}\right)_{ij} f_j(x_0), \tag{3.99}$$

where $\mathcal{P}$ is the path ordering operator and $x_0$ is the point at which we fix the boundary conditions $f_j(x_0)$ to specialize the general solutions of the differential equations.

This formal solution displays the two main problems in calculating master integrals with differential equations. One component of the solution is the set of boundary conditions $f_i(x_0)$, which need to be determined. This translates to calculating the master integrals in a certain limit for the kinematic invariant under consideration. For the moment we will not concern ourselves with boundary conditions, but we will come back to this problem in chapter 4. Instead we will focus on solving the actual differential equation, this is connected to the path-ordered exponential that appears in the formal solution e.q. (3.99). For general system matrices $A$ it is not possible to calculate the path-ordered exponential. Solving the differential equations therefore boils down to bringing $A$ into a form such that we can actually calculate the path-ordered exponential as an expansion in the dimensional regular $\epsilon$. Finding such a transformation of $A$ is of course nothing else then finding a basis transformation,

$$f_i(x) \to g_i(x) = T_{ij}(x) f_j(x). \tag{3.100}$$

Under this transformation the system matrix $A$ transforms as,

$$A_{ij} \to \tilde{A}_{ij} = \left(T^{-1}_{ik} A_{kl} T_{lj} - T^{-1}_{ik} \partial_x T_{kj}\right). \tag{3.101}$$

The requirements for a transformed system matrix $\tilde{A}$ have been formalized by Henn [77] in his proposition for a so-called *canonical form.* In the canonical form the system takes the form,

$$\partial_x f_i(x) = \epsilon \sum_k \frac{A_{ij}^{(k)}}{x - x_k} f_j(x). \tag{3.102}$$

The first advantage of this form is that the dependence of the system matrix on the dimensional regulator $\epsilon$ is drastically simplified. While generic system matrices can be arbitrary functions of $\epsilon$, in the canonical form $\epsilon$ factorizes completely from the system matrix, i.e. the right hand side of the differential equations is proportional to $\epsilon$, and the coefficient matrices $A^{(k)}$ in eq. (3.102) are independent of $\epsilon$. The benefit of this is that the system completely decouples in the limit $\epsilon \to 0$. This means that the path-ordered exponential in eq. (3.99) can be trivially solved as an expansion in $\epsilon$,

$$\begin{aligned}\left(\mathcal{P} e^{\epsilon \int \mathrm{d}x \sum_k \frac{A^k}{x - x_k}}\right)_{ij} &= \delta_{ij} + \epsilon \int_{x_0}^{x} \mathrm{d}x' \sum_k \frac{A_{ij}^k}{x' - x_k} \\ &\quad + \frac{\epsilon^2}{2} \int_{x_0}^{x} \mathrm{d}x' \sum_k \frac{A_{il}^{(k)}}{x' - x_k} \int_{x_0}^{x'} \mathrm{d}x'' \sum_{k'} \frac{A_{lj}^{(k')}}{x'' - x_{k'}} + \ldots .\end{aligned} \tag{3.103}$$

The second advantage of the canonical form is the simplification of the dependence on $x$. A general system matrix can be an arbitrary rational function of $x$, while in canonical form, the dependence on $x$ is only in the form of simple poles at the singular points $x_k$ with residue matrices $A^{(k)}$ that are independent of $x$. The integrals that appear in the expansion of the path ordered exponential are therefore always integrals over dlog forms,

$$\frac{\mathrm{d}x}{x - x_k} = \mathrm{dlog}(x - x_k), \tag{3.104}$$

for constant $x_k$. This immediately connects to the definition of the multiple polylogarithms in eqs. (2.2), (2.12) and (2.14).

It is therefore clear that the solution of a system that has been brought into canonical form as in eq. (3.102) will be a linear combination of multiple polylogarithms of $x$ with alphabet $\{x_k\}$. Finding the solution of a system of differential equations therefore boils down to finding the canonical form, as finding the actual solution is trivial at this point. Finding the canonical form is less trivial however. It is clear that not every system can be brought to canonical form. Unfortunately, it is not necessarily clear a priori whether a given system can be brought to canonical form or not. Several partial algorithms [76, 77, 158] have been proposed that allow the transformation of certain systems into canonical form.

In particular in the calculation of multiloop amplitudes involving internal massive lines one finds systems that can not be brought into a canonical form. Often such systems can only be brought into a form

$$\partial_x f_i(x) = \left(A_{ij}(x) + \epsilon B_{ij}(x)\right) f_j(x). \tag{3.105}$$

These systems do not decouple in the limit $\epsilon \to 0$ for non-vanishing $A(x)$. Depending on the size of the coupled system the solution lies outside of the function space of the multiple polylogarithms. For coupled $2 \times 2$ systems one expects to find elliptic generalizations of the multiple polylogarithms, i.e. integrals over punctured surfaces of genus 1. For bigger coupled systems one expects generalizations on manifolds of higher genus.

## 3.4 Boundary decomposition

After the functional dependence of the master integrals on the kinematic invariants has been obtained by solving the corresponding differential equations one proceeds with the determination of the relevant boundary conditions. The kinematical solutions are general functions that solve the differential equations. The unknown constants $f_j(x_0)$ in eq. (3.99) need to be determined to specialize the general solutions to the concrete physics problem by specifying *boundary conditions.*

To analyze these boundary conditions in more detail we consider a system,

$$f_i(x) = \epsilon \sum_\sigma \frac{A_{ij}^\sigma}{x - x_\sigma} f_j(x), \tag{3.106}$$

with the solution,

$$f_i(x) = \mathcal{P} e^{\epsilon \sum_\sigma \int \mathrm{d}x \frac{A_{ij}^\sigma}{x - x_\sigma}} f_j(x_0). \tag{3.107}$$

We assume that the system has been brought to canonical form to simplify the discussion. It should be noted however that the analysis of the boundary conditions also applies to non-canonical systems.

We can freely choose one of the singular points $x_\sigma$ to fix the boundary conditions. Without loss of generality we choose $x_0 = 0$. We can then expand the differential equations in eq. (3.106) in a Laurent series around $x = 0$ and find,

$$\partial_x f_i(x) = \epsilon \frac{A_{ij}^0}{x} f_j(x) + \mathcal{O}(x). \tag{3.108}$$

In the limit $x \to 0$ the solution of the system is consequently,

$$f_i(x) = x^{\epsilon A_{ij}^0} f_j(0). \tag{3.109}$$

The matrix exponential appearing in this solution can be evaluated trivially if $A^0$ is diagonalizable. This will not be the case in general. It is however possible to compute the Jordan decomposition of $A^0$. The Jordan decomposition of any matrix $A$ yields two matrices $R$ and $J$, such that

$$A = RJR^{-1}. \tag{3.110}$$

The matrix $J$ is block diagonal with $m$ blocks. Each block corresponds to an eigenvalue of $A$. The $i^{th}$ Jordan block $J^{(i)}$ corresponding to an eigenvalue $\lambda_i$ has the dimension $n_i \times n_i$, so that the $n_i$ diagonal entries each contain the eigenvalue. The elements on the first superdiagonal in each Jordan block are equal to 1. The diagonal of $J$ contains the eigenvalues of $A$, as it is the case for a diagonalized matrix,

$$J = \begin{pmatrix} J^{(1)} & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & \dots & J^{(m)} \end{pmatrix}, \qquad J^{(i)} = \begin{pmatrix} \lambda_i & 1 & 0 & \dots & 0 \\ 0 & \lambda_i & 1 & \ddots & 0 \\ & & \vdots & & \\ 0 & & \dots & & \lambda_i \end{pmatrix}. \tag{3.111}$$

The transformation matrix $R$ consists of the generalized eigenvectors of $A$. In the case that $A$ is diagonalizable, all Jordan $J_i$ blocks have dimension $n_i = 1$ and $R$ consists of the eigenvectors of $A$, i.e. the Jordan decomposition diagonalizes the matrix.

To simplify the differential equations in the limit $x \to 0$ we therefore decompose $A^0$ into $R$ and $J$. This yields the system,

$$\partial_x f_i(x) = \epsilon \frac{R_{ik} J_{kl} R^{-1}_{lj}}{x} f_j(x). \tag{3.112}$$

We can now use $R$ to rotate the vector of master integrals $f_i$, defining,

$$g_i(x) = R_{ij} f_j(x), \tag{3.113}$$

to obtain the simplified differential equations,

$$\partial_x g_i(x) = \epsilon \frac{J_{ij}}{x} g_j(x). \tag{3.114}$$

These differential equations permit the simple solution,

$$\begin{aligned} \vec{g}(x) &= \exp\left[\epsilon \begin{pmatrix} J^{(1)} & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & \dots & J^{(m)} \end{pmatrix} \log(x\right] \vec{g}_0 \\ &= \begin{pmatrix} e^{\epsilon J^{(1)} \log(x)} & \dots & 0 \\ 0 & \ddots & 0 \\ 0 & \dots & e^{\epsilon J^{(m)} \log(x)} \end{pmatrix} \vec{g}_0, \end{aligned} \tag{3.115}$$

with

$$e^{\epsilon J^{(i)}\log(x)} = x^{\epsilon\lambda_i}\begin{pmatrix} 1 & \frac{\log(x)}{1!} & \dots & \frac{\log^{n_i-1}(x)}{(n_i-1)!} \\ 0 & 1 & \ddots & \frac{\log^{n_i-1}(x)}{(n_i-2)!} \\ & & \vdots & \\ 0 & \dots & & 1 \end{pmatrix}. \tag{3.116}$$

We find therefore that the factors of $x^{\epsilon\lambda_i}$, commonly referred to as integrating factors [81], appear together with $\log(x)$ raised to a power of maximally $n_i - 1$. Note that these logarithms appear even though the solution is exact in $\epsilon$. Every constant $g_{0,i}$ is associated with exactly one eigenvalue $\lambda_i$. Conversely, multiple $g_{0,i}$ can be associated with the same $\lambda_i$.

These constants $g_{0,i}$ can then be used to express the limiting solution of the original functions $f_i(x)$ as

$$f_i(x) = R^{-1}_{ij} g_j(x) = R^{-1}_{ik} e^{\epsilon J_{kj}\log(x)} g_{0,j}. \tag{3.117}$$

Compared to the starting point in eq. (3.107) we have gained, in that the limiting solution is now expressed in terms of constants $g_{0,i}$ that are associated to a single integrating factor $x^{\epsilon\lambda_i}$. Therefore the scaling of each unknown constant is manifest. This decomposition of the boundary conditions facilitates the explicit calculation of the unknown boundary constants.

One way of determining the boundary conditions to fix the unknown constants is to analyze the analytic structure dictated by the external kinematics of a given integral. In practice, the external kinematic configuration often prohibits the presence of certain branch cuts. One famous example is the absence of branch cuts in the $u$-channel of planar four-point integrals.

In particular in the presence of phase-space cuts however it becomes necessary to calculate boundary conditions explicitly by evaluating the integral for a particular kinematic configuration. We will therefore dedicate the next chapter to the explicit calculation of boundary conditions.

CHAPTER 4

# Computing boundary conditions for master integrals

Using the method of differential equations the kinematic dependence of a master integral can be determined without any explicit reference to the integral representation. However, for the determination of the boundary conditions which specialize the general solutions obtained from the differential equations an explicit evaluation of integrals is usually required.

## 4.1 Feynman integrals

The elementary constituents of multiloop cross sections are multiloop Feynman integrals. After IBP reduction to master integrals we can assume without loss of generality that all integrals that need to be computed are scalar integrals of the form

$$F = \int \prod_{\ell=1}^{L} \frac{\mathrm{d}^d k_\ell}{(2\pi)^d} \prod_{i=1}^{N} \frac{1}{P_i^{\nu_i}(\{k\},\{p\},m_i^2)}, \tag{4.1}$$

where $L$ is the number of loops and $N$ the number of propagators. We are employing conventional dimensional regularization computing in $d = 4 - 2\epsilon$ dimensions in order to regulate the singularities of the integral. Each propagator $P_i$ can be raised to a power $\nu_i$. We can see that this integral is over $\mathbb{R}^L_{d-1,1}$ punctured by the Landau singularities of the integrand. One way to map the integration region to a more manageable manifold is to employ the so-called

"Schwinger trick",

$$\frac{1}{A^\nu} = \frac{1}{\Gamma(\nu)} \int_0^\infty \mathrm{d}x x^{\nu-1} e^{-xA}, \tag{4.2}$$

which holds for $\Re(A) > 0$. Applying this replacement to every propagator in the integrand the integral can be expressed as

$$F = \prod_{n=1}^{N} \frac{1}{\Gamma(\nu_n)} \int \prod_{j=1}^{N} \mathrm{d}x_j x^{\nu_j - 1} \prod_{\ell=1}^{L} \mathrm{d}k_\ell \exp\left( - \sum_{i=1}^{N} x_i P_i(\{k\}, \{p\}, m_i^2) \right). \tag{4.3}$$

Wick rotating to Euclidian space by letting,

$$l_0 = ik_0, \quad l_i = k_i, \tag{4.4}$$

we obtain,

$$F = \prod_{n=1}^{N} \frac{1}{\Gamma(\nu_n)} i^L \int \prod_{j=1}^{N} \mathrm{d}x_j x^{\nu_j - 1} \prod_{\ell=1}^{L} \mathrm{d}l_\ell \exp\left( \sum_{i=1}^{N} x_i P_i(\{l\}, \{p\}, m_i^2) \right). \tag{4.5}$$

The exponential is in general of the form,

$$\exp\left( \sum_{i=1}^{N} x_i P_i(\{l\}, \{p\}, m_i^2) \right) = \exp\left( - \sum_{ij}^{L} l_i A_{ij} l_j + 2 \sum_{i}^{L} q_i l_i + \mathcal{J} \right), \tag{4.6}$$

where the $L \times L$ matrix $A$, $\mathcal{J}$ and the $q_i$ can be read off by rearranging the sum of the propagators in eq. (4.5). After completing the square in the exponential, we can use the $d$ dimensional generalization of the Gaussian integral,

$$\int \frac{\mathrm{d}^d k}{(2\pi)^d} e^{-\alpha k^2} = \left[ \int \frac{\mathrm{d}k}{2\pi} e^{-\alpha k^2} \right]^d = \alpha^{-\frac{d}{2}} (4\pi)^{-\frac{d}{2}}, \tag{4.7}$$

to perform the integral over the loop momenta and obtain the *Schwinger representation* of the Feynman integral,

$$F = (4\pi)^{-\frac{dL}{2}} i^L e^{i\pi(\nu+L)} \frac{1}{\prod_{i=1}^{N} \Gamma(\nu_i)} \int_0^\infty \prod_{i=1}^{N} \mathrm{d}x_i x_i^{\nu_i - 1} \mathcal{U}^{-\frac{d}{2}} e^{-\frac{\mathcal{F}}{\mathcal{U}}}, \tag{4.8}$$

with $\nu = \sum_{i=1}^{N} \nu_i$. The functions $\mathcal{U}$ and $\mathcal{F}$ are the well-known Symanzik polynomials [159] defined as,

$$\begin{aligned} \mathcal{U} &= \det(A), \\ \mathcal{F} &= \det(A) \left( \sum_{i,j=1}^{L} q_i A_{ij} q_j - \sum_{i=1}^{N} x_i m_i^2 \right). \end{aligned} \tag{4.9}$$

From here we can obtain the so called *Feynman parametrization* by selecting an arbitrary non-empty subset $\mathcal{X}$ of the $x_i$ and introducing unity as,

$$\int_0^\infty \mathrm{d}\eta \; \delta\left(\sum_{x\in\mathcal{X}} x - \eta\right). \tag{4.10}$$

After rescaling all $x_i$ by $\eta$ and performing the integral over $\eta$ we obtain the conventional Feynman parametrization,

$$F = (4\pi)^{-\frac{dL}{2}}(-1)^\nu i^L \frac{\Gamma\left(\nu - \frac{Ld}{2}\right)}{\prod_{i=1}^N \Gamma(\nu_i)} \int_0^\infty \prod_{i=1}^N \mathrm{d}x_i x_i^{\nu_i-1} \delta\left(1 - \sum_{x\in\mathcal{X}} x\right) \frac{\mathcal{U}^{\nu-\frac{1}{2}(L+1)d}}{\mathcal{F}^{\nu-\frac{1}{2}Ld}}. \tag{4.11}$$

The fact that the Feynman parameterizations that we obtain this way differ only in the argument of the $\delta$-function depending on which subset of the $x_i$ we select to introduce the unity is commonly referred to as the *Cheng-Wu theorem*.

We can of course also arrive at the Feynman parametrization using the Feynman trick,

$$\frac{1}{AB} = \int_0^1 \mathrm{d}x \frac{1}{(xA + (1-x)B)^2}, \tag{4.12}$$

which can be generalized to an arbitrary number of propagators,

$$\frac{1}{A_1^{\nu_1} \dots A_n^{\nu_n}} = \frac{\Gamma(\nu)}{\prod_{i=1}^n \Gamma(\nu_i)} \int_0^1 \prod_{i=1}^n \mathrm{d}x_i x_i^{\nu_i-1} \frac{\delta\left(1 - \sum_{i=1}^n x_i\right)^\nu}{\left(\sum_{i=1}^n x_i A_i\right)}, \tag{4.13}$$

with $\nu = \sum_{i=1}^n \nu_i$. The Cheng-Wu theorem states then that we can replace the sum over the Feynman parameters $x_i$ in the $\delta$-function by an arbitrary non-empty subset of the $x_i$, provided that we integrate all $x_i$ from 0 to $\infty$. In practice one almost always uses the Feynman representation to perform calculations and it is often very useful to place only a single Feynman parameter in the argument of the $\delta$-function, such that the corresponding integration becomes fully localized. The integrals over the remaining Feynman parameters become then unrestricted, yielding a projective parametrization of the Feynman integral.

The Symanzik polynomials $\mathcal{U}$ and $\mathcal{F}$ can be read off from the momentum representation of the Feynman integral or alternatively can be obtained by graph-theoretical methods [159–161].

*Example.*

The canonical example of a Feynman parametrization is the simple one-loop bubble integral,

$$F = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{(k^2)^{\nu_1}((k+p)^2)^{\nu_2}}. \tag{4.14}$$

Using the above procedure we arrive at the Feynman representation,

$$\begin{aligned} F = & \, i(-1)^{\nu_1+\nu_2}(4\pi)^{\epsilon-2}\left(-p^2\right)^{-\nu_1-\nu_2-\epsilon+2}\frac{\Gamma(\epsilon+\nu_1+\nu_2-2)}{\Gamma(\nu_1)\Gamma(\nu_2)} \\ & \times \int_0^\infty \mathrm{d}x_1 \mathrm{d}x_2 x_1^{\nu_1-1}x_2^{\nu_2-1}(x_1+x_2)^{\nu_1+\nu_2+2\epsilon-4}\delta(1-x_1-x_2). \end{aligned} \tag{4.15}$$

Using the Cheng-Wu theorem to replace the $\delta$-function with $\delta(1-x_2)$, the integration over $x_2$ localizes and we obtain,

$$\begin{aligned} F = & \, i(-1)^{\nu_1+\nu_2}(4\pi)^{\epsilon-2}\left(-p^2\right)^{-\nu_1-\nu_2-\epsilon+2}\frac{\Gamma(\epsilon+\nu_1+\nu_2-2)}{\Gamma(\nu_1)\Gamma(\nu_2)} \\ & \times \int_0^\infty \mathrm{d}x_1 x_1^{\nu_1-1}(1+x_1)^{\nu_1+\nu_2+2\epsilon-4}. \end{aligned} \tag{4.16}$$

The integral over $x_1$ is now just the integral representation of the beta function,

$$B(a,b) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(a+b)} = \int_0^\infty \mathrm{d}x x^{a-1}(1+x)^{-a-b}. \tag{4.17}$$

With that we obtain the result,

$$\begin{aligned} F = & \, I(-1)^{\nu_1+\nu_2}(4\pi)^{\epsilon-2}\left(-p^2\right)^{-\nu_1-\nu_2-\epsilon+2} \\ & \times \frac{\Gamma(-\epsilon-\nu_1+2)\Gamma(-\epsilon-\nu_2+2)\Gamma(\epsilon+\nu_1+\nu_2-2)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(-2\epsilon-\nu_1-\nu_2+4)}. \end{aligned} \tag{4.18}$$

This example illustrates the main principle of projective Feynman integrals, that one always tries to perform integrals over Feynman parameters in terms of beta functions. Of course, in practice bringing the integrand to a form that permits such an integration is not always trivial and we will dedicate a later chapter to a technique which allows us to always bring integrands into such forms at the price of introducing auxiliary integrations.

*Example.*
Another more interesting example is the case of the one-loop triangle with one off-shell leg and massive propagators,

$$F = \int \frac{\mathrm{d}^d k}{(2\pi)^d}\frac{1}{(k^2-m^2)((k+p_1)^2-m^2)((k+p_1+p_2)^2-m^2)}, \tag{4.19}$$

with $p_i^2 = 0$ and $(p_1+p_2)^2 = s$. The Feynman parametrization for this integral is,

$$
\begin{aligned}
F = & -i(4\pi)^{\epsilon-2}\Gamma(\epsilon+1) \\
& \times \int_0^\infty \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3\delta(1-x_1-x_2-x_3)\frac{(x_1+x_2+x_3)^{2\epsilon-1}}{(m^2(x_1+x_2+x_3)^2-sx_1x_3)^{1+\epsilon}}.
\end{aligned}
\tag{4.20}
$$

Here we should note that we are computing in the *Euclidian region*, where all scalar products of external momenta are negative. In particular $s$ is negative, consequently the $\mathcal{F}$ polynomial does not have zeroes in the integration region. Because of the massive propagators, this integral is finite in dimensional regularization and we can expand in $\epsilon$ before performing the integration. Expanding up to $\mathcal{O}(\epsilon^1)$ we obtain for example,

$$
\begin{aligned}
\mathcal{N}F = & \int_0^\infty \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3\frac{\delta(1-x_1-x_2-x_3)}{(x_1+x_2+x_3)(m^2(x_1+x_2+x_3)^2-sx_1x_3)} \\
& \times \left(1+\epsilon\log\left(\frac{(x_1+x_2+x_3)^2}{m^2(x_1+x_2+x_3)^2-sx_1x_3}\right)\right),
\end{aligned}
\tag{4.21}
$$

with

$$
\mathcal{N} = ie^{\gamma\epsilon}(4\pi)^{2-\epsilon}, \tag{4.22}
$$

where $\gamma = -\psi(1)$ is the Euler-Mascheroni constant. We can simplify this expression by integrating over the simplex given by $\delta(1-x_1-x_2-x_3)$ rather than integrating projectively. We can furthermore simplify the expressions by setting $m = ms$ and $s = 1$. Since we can always restore the mass dimension of the integral using dimensional analysis we do not lose any information. Integrating out $x_3$ using the $\delta$-function we find,

$$
\begin{aligned}
\mathcal{N}F = & \int_0^\infty \mathrm{d}x_1\mathrm{d}x_2\Theta(1-x_1-x_2)\frac{1}{m^2-x_1(1-x_1-x_2)} \\
& \times \left(1+\epsilon\log(m^2-x_1(1-x_1-x_2))\right).
\end{aligned}
\tag{4.23}
$$

Next we would like to integrate $x_2$ between 0 and $1-x_1$ to satisfy the constraint. We can perform this integral using our knowledge of the multiple polylogarithms. Writing

$$
\begin{aligned}
\log(m^2-x_1(1-x_1-x_2)) = & G(0;m-x_1(1-x_1)) \\
& + G\left(-\frac{m^2-x_1(1-x_1)}{x_1};x_2\right),
\end{aligned}
\tag{4.24}
$$

we can see that the integral over $x_2$ can be performed in terms of the definition of the multiple polylogarithms as iterated integrals over dlog forms, eq. (2.15). Indeed the primitive with respect to $x_2$ is,

$$\begin{aligned}\mathcal{P}_{x_2} &= \int \mathrm{d}x_2 \frac{1}{m^2 - x_1(1-x_1-x_2)} \left(1 + \epsilon \log(m^2 - x_1(1-x_1-x_2))\right) \\ &= G\left(-\frac{m^2 - x_1(1-x_1)}{x_1}; x_2\right) \frac{1}{x_1} \left(1 - \epsilon G\left(0, m^2 - x_1(1-x_1)\right)\right) \\ &- \frac{\epsilon}{x_1} G\left(-\frac{m^2 - x_1(1-x_1)}{x_1}, -\frac{m^2 - x_1(1-x_1)}{x_1}; x_2\right)\end{aligned} \tag{4.25}$$

Next we need to take the appropriate limits of the primitive $\mathcal{P}_{x_2}$. Since $\mathcal{P}$ does not contain any MPLs of the form $G(0,\ldots,0;x_2)$ the limit

$$\lim_{x_2 \to 0} \mathcal{P}_{x_2} = 0, \tag{4.26}$$

vanishes. The interesting limit is the upper bound of the integration, where we obtain

$$\begin{aligned}\lim_{x_2 \to 1-x_1} \mathcal{P}_{x_2} = &- \frac{G\left(\frac{1-t}{2}; x_1\right) + G\left(\frac{1+t}{2}; x_1\right)}{x_1} \\ &+ \epsilon \frac{1}{x_1} \Bigg[ \left(G(1;t) - 2G(0;2)\right) G\left(\frac{1-t}{2}; x_1\right) \\ &- 2G(0;2)\, G\left(\frac{t+1}{2}; x_1\right) + G(1;t)\, G\left(\frac{t+1}{2}; x_1\right) \\ &+ G(-1;t) \left(G\left(\frac{1-t}{2}; x_1\right) + G\left(\frac{1+t}{2}; x_1\right)\right) \\ &+ G\left(\frac{1-t}{2}, \frac{1-t}{2}; x_1\right) + G\left(\frac{1-t}{2}, \frac{1+t}{2}; x_1\right) \\ &+ G\left(\frac{1+t}{2}, \frac{1-t}{2}; x_1\right) + G\left(\frac{1+t}{2}, \frac{1+t}{2}; x_1\right) \Bigg].\end{aligned} \tag{4.27}$$

Here we have defined,

$$m^2 = \frac{1}{4}(1-t^2), \tag{4.28}$$

to factor the square root appearing, and used the coproduct calculus to bring all MPLs into canonical form with respect to $x_1$. This enables us to perform the remaining integration over $x_1$. Once again we first determine the primitive and find,

$$
\begin{aligned}
\mathcal{P}_{x_1} = \int \mathrm{d}x_1 \left( \lim_{x_2 \to 1-x_1} \mathcal{P}_{x_2} - \lim_{x_2 \to 0} \mathcal{P}_{x_2} \right) &= -G\left(0, \frac{1-t}{2}; x_1\right) \\
&- G\left(0, \frac{1+t}{2}; x_1\right) + \epsilon \Bigg[ \left(G\left(1;t\right) - 2G\left(0;2\right)\right) G\left(0, \frac{1-t}{2}; x_1\right) \\
&- 2G\left(0;2\right) G\left(0, \frac{1+t}{2}; x_1\right) + G\left(1;t\right) G\left(0, \frac{1+t}{2}; x_1\right) \\
&+ G\left(-1;t\right) \left( G\left(0, \frac{1-t}{2}; x_1\right) + G\left(0, \frac{1+t}{2}; x_1\right) \right) \\
&+ G\left(\frac{1-t}{2}, \frac{1-t}{2}; x_1\right) + G\left(\frac{1-t}{2}, \frac{1+t}{2}; x_1\right) \\
&+ G\left(\frac{1+t}{2}, \frac{1-t}{2}; x_1\right) + G\left(\frac{1+t}{2}, \frac{1+t}{2}; x_1\right) \Bigg].
\end{aligned}
\tag{4.29}
$$

The limit,

$$
\lim_{x_1 \to 0} \mathcal{P}_{x_1} = 0,
\tag{4.30}
$$

vanishes simply, so that the upper limit immediately yields the final result of our calculation,

$$
\begin{aligned}
\mathcal{N}F = \frac{1}{2}\left(iH_{-1} + iH_1 + \pi\right)^2 + \epsilon \Bigg[ &- H_1\Big(2H_{0,-1} + 2H_{1,-1} - 2H_{1,0} \\
&+ H_1\big(2H_0 - 2\log(2)\big) - 9\zeta_2\Big) - \frac{1}{3}H_1\Big(6H_{0,-1} + 6H_{1,-1} - 6H_{1,0} \\
&+ H_1\big(H_1 + 3\log(2)\big) + 9\zeta_2\Big) + \frac{1}{3}H_{-1}^3 - \log(2)H_{-1}^2 + 6\log(2)\zeta_2 + 7\zeta_3 \\
&- 4\Big(H_{0,-1,-1} + H_{1,-1,-1} - H_{1,0,-1} - H_{1,1,-1} + H_{1,1,0}\Big) \\
&+ \frac{1}{2}i\pi\Big(H_1^2 - H_{-1}^2 - 2\big(2H_0 + H_1\big)H_{-1} + 4\big(H_{0,-1} + H_{1,-1} - H_{1,0}\big)\Big)\Bigg].
\end{aligned}
\tag{4.31}
$$

The result can be written in terms of HPLs of $t$; we have suppressed the arguments of the HPLs, writing e.g. $H_{1,-1}$ for $H(1,-1;t)$.

## 4.2 Phase-space integrals

Apart from loop integrals, the determination of boundary conditions for the master integrals appearing in a cross section calculation also involves phase-space integrals.

Phase-space integrals are integrals over the unresolved degrees of freedom of the real physical particles in the final-state. As such they are inherently more complicated then loop integrals since the integrals need to preserve the fact that the particles in the final state are on-shell and physical. Ignoring total momentum conservation for the moment, the integral over the physical degrees of freedom of a single real particle in the final-state can be written as

$$\int \frac{\mathrm{d}^d p}{(2\pi)^{d-1}}\delta^+(p^2-m^2) = \int \frac{\mathrm{d}^d p}{(2\pi)^{d-1}}\delta(p^2-m^2)\Theta(p_0). \tag{4.32}$$

The $\delta$-function guarantees here that the particle is on-shell, while the $\Theta$-function selects the physical positive energy solution. In addition to the constraints for a single particle to be physical, the integral over the phase-space also needs to respect the conservation of total momentum.

We will focus here on a specific set of phase-space integrals, namely phase space integrals with one massive particle and $N-2$ massless particles in the final-state that are produced by 2 massless particles in the initial-state. We denote the momenta of the initial-state particles by $q_1$ and $q_2$ and the momenta of the massless final-state particles by $q_3, \ldots q_N$. The massive particle is suggestively denoted by $q_H$. Just as in the case of loop integrals, we use dimensional regularization to regulate any divergences. Consequently, all momenta $q_i$ are $d$-dimensional. The phase-space integration measure can then be written as,

$$\begin{aligned} &\mathrm{d}\Phi_{N-1}(q_H, q_3, \ldots, q_N, m^2, s, d) \\ &\quad = (2\pi)^d \delta^{(d)}(q_{12} - q_H - q_{3\ldots N}) \frac{\mathrm{d}^d q_H}{(2\pi)^{d-1}}\delta^+(q_H^2 - m^2)\prod_{j=3}^{N}\frac{\mathrm{d}^d q_j}{(2\pi)^{d-1}}\delta^+(q_j^2). \end{aligned} \tag{4.33}$$

Here $\delta^{(d)}$ is a $d$-component delta function, which implements total momentum conservation. We can see that after integration the phase integral only depends on $s$ and $m^2$. We can therefore define one ratio

$$z = \frac{m^2}{s} \qquad \bar{z} = 1 - z, \tag{4.34}$$

that parametrizes the kinematic dependence of the phase-space integrals. We also use the notation,

$$q_{i\ldots k} = q_i + \cdots + q_j. \tag{4.35}$$

The momenta $q_i$ are rescaled momenta, so that,

$$q_i = \begin{cases} \sqrt{s}p_i, & \text{if } i = 1,2, \\ \sqrt{s\bar{z}}p_i, & \text{if } i = 3,\ldots,N. \end{cases} \tag{4.36}$$

We can employ total momentum conservation to localize one of the integrations. We will use this to eliminate the integration over the massive momentum at this stage. This has the benefit that all remaining integrations, which will require a parametrization of the integration domain, are over massless momenta. Performing the integral over $q_H$ we obtain,

$$\begin{aligned} &\mathrm{d}\Phi_{N-1}(q_H, q_3, \dots, q_N, m^2, s, d) \\ &= (2\pi) \prod_{j=3}^{N} \frac{\mathrm{d}^d q_j}{(2\pi)^{d-1}} \delta^+(q_j^2) \delta^+\left((q_{3\dots N} - q_{12})^2 - m^2\right). \end{aligned} \tag{4.37}$$

Here we can see that the $N-2$ integrations over the massless momenta are not independent. Instead the phase-space integral is an integral over the algebraic variety given by,

$$\begin{aligned} q_j^2 &= 0 \ \ \forall j \in \{3, \dots, N\} \\ (q_{3\dots N}^2 - q_{12})^2 &= m^2. \end{aligned} \tag{4.38}$$

In order to perform this integral, we thus need to find some parametrization of these constraints. One way of parametrizing is to go from integrals over the components of the momenta to integrals over the Lorentz invariants,

$$s_{ij} = (q_i + q_j)^2. \tag{4.39}$$

To arrive at such a parametrization, we start by splitting the momenta into longitudinal and transverse components $q_i = (q_{i,0}, q_{i,z}, q_{i,\perp})$, so that $q_{i,\perp}$ is the $(d-2)$-dimensional transverse component of the momentum. This separation is defined by Lorentz-boosting to a frame in which the longitudinal axis is defined by the initial state momenta,

$$q_1 = \frac{1}{2}(1, 1, 0, \dots, 0) \quad \text{and} \quad q_2 = \frac{1}{2}(1, -1, 0, \dots, 0). \tag{4.40}$$

The integration measure for a single momentum then becomes

$$\mathrm{d}^d q_i \delta^+(q_i^2) = \mathrm{d}q_{i,0} \mathrm{d}q_{i,z} \mathrm{d}^{d-2} q_{i,\perp} \Theta(q_{i,0}) \delta(q_{i,0}^2 - q_{i,z}^2 - q_{i,\perp}^2). \tag{4.41}$$

In this frame the $t$-channel ($i \geq 3$) invariants take a particularly simple form

$$\begin{aligned} s_{1i} &= (q_1 - q_i)^2 = -2q_1 q_i = -(q_{i,0} - q_{i,z}), \\ s_{2i} &= (q_2 - q_i)^2 = -2q_1 q_i = -(q_{i,0} + q_{i,z}). \end{aligned} \tag{4.42}$$

We can invert this relation and express the components of the momentum in terms of the invariants as

$$\begin{aligned} q_{i,0} &= -\frac{1}{2}(s_{1i} + s_{2i}) \\ q_{i,z} &= -\frac{1}{2}(s_{1i} - s_{2i}). \end{aligned} \tag{4.43}$$

Because of $q_i^2 = 0$ we also have,

$$q_{i,\perp}^2 = s_{1i}s_{2i}. \tag{4.44}$$

The $s$-channel invariants $(i, j \geq 3)$ can be written as,

$$\begin{aligned} s_{ij} = q_{ij}^2 = 2q_i \cdot q_j &= 2\left(q_{i,0}q_{j,0} - q_{i,z}q_{j,z} - q_{i,\perp} \cdot q_{j,\perp}\right) \\ &= (s_{1i}s_{2j} + s_{1j}s_{2i}) - 2q_{i,\perp} \cdot q_{j,\perp}. \end{aligned} \tag{4.45}$$

In this parametrization we can write the measure for a single particle as,

$$\mathrm{d}^2 q_i \delta^+(q_i^2) = \frac{1}{2}\mathrm{d}^{d-2}q_{i,\perp}\mathrm{d}s_{1i}\mathrm{d}s_{2i}\Theta(-s_{1i})\Theta(-s_{2i})\delta(s_{1i}s_{2i} - q_{i,\perp}^2), \tag{4.46}$$

so that the phase-space measure becomes,

$$\begin{aligned} &\mathrm{d}\Phi_{N-1} = 2^{3-N}\pi \\ &\prod_{i=3}^{N} \frac{\mathrm{d}^{d-2}q_{i,\perp}}{(2\pi)^{d-1}}\mathrm{d}s_{1i}\mathrm{d}s_{2i}\Theta(-s_{1i})\Theta(-s_{2i})\delta(s_{1i}s_{2i} - q_{i,\perp}^2)\delta^+\left((q_{3\ldots N}^2 - q_{12})^2 - m^2\right). \end{aligned} \tag{4.47}$$

Next we would like to rewrite the integral over the transverse components of the momenta. Here, we note that any matrix element that will be integrated over the phase-space is only a function of the Lorentz invariants $s_{ij}$. As such, the integrand, as well as the measure above, are invariant under rotation in the $(d-2)$-dimensional transverse space. We can therefore exploit the fact that rotationally invariant integrals of the form,

$$I = \int \prod_{i}^{N} \mathrm{d}^d q_i f(q_i \cdot q_j), \tag{4.48}$$

can be rewritten, making the integration over the scalar products manifest,

$$I = 2^{-N} \int \prod_{i=1}^{N} \Omega_{d+1-i} \prod_{j=1}^{i} \mathrm{d}(q_i \cdot q_j) \mathfrak{G}(q_1, \ldots, q_N)^{\frac{d-N-1}{2}} \Theta(\mathfrak{G}(q_1, \ldots, q_N)) f(q_i \cdot q_j). \tag{4.49}$$

Here we have use the Gram determinant $\mathfrak{G}$ of the vectors $q_i$ which is defined as,

$$\mathfrak{G}(q_1, \ldots, q_N) = \det(q_i \cdot q_j)_{i \leq i,j \leq N}. \tag{4.50}$$

Furthermore, we have the $d$-dimensional volume,

$$\Omega_d = \frac{2\pi^{\frac{d}{2}}}{\Gamma\left(\frac{d}{2}\right)}. \tag{4.51}$$

We can use this relation to rewrite the integral over the $(d-2)$ transverse components of the momenta in terms of scalar products,

$$\prod_{i=3}^{N} \mathrm{d}^{d-2} q_{i,\perp} = 2^{2-N} \prod_{i=3}^{N} \Omega_{d+1-i} \times \prod_{j=3}^{i} \mathrm{d}(q_{i,\perp} \cdot q_{j,\perp}) \mathfrak{G}(q_{3,\perp}, \ldots, q_{N,\perp})^{\frac{d-N-1}{2}} \Theta(\mathfrak{G}(q_{3,\perp}, \ldots, q_{N,\perp})) \tag{4.52}$$

The integration over the scalar products $q_{i,\perp} \cdot q_{j,\perp}$ can be related to the $s$-channel invariants using eq. (4.45),

$$\prod_{i=3}^{N} \prod_{j=3}^{i} \mathrm{d}(q_{i,\perp} \cdot q_{j,\perp}) = (-2)^{\frac{(N-2)(N-3)}{2}} \left[\prod_{i=3}^{N} \mathrm{d}q_{i,\perp}^2\right] \left[\prod_{3 \leq i < j \leq N} \mathrm{d}s_{ij}.\right] \tag{4.53}$$

Here we can perform the integral over the modulus of the transverse components using the on-shell delta functions, eq. (4.46), to arrive at

$$\prod_{i=3}^{N} \mathrm{d}^d q_i \delta^+(q_i^2) = (-1)^{\frac{(N-2)(N-3)}{2}} 2^{6-3N-\frac{(N-2)(N-3)}{2}} \times \left[\prod_{i=3}^{N} \Omega_{d+1-i}\right] \left[\prod_{\substack{1<i,j,N \\ i \neq j, (i,j) \neq (1,2)}} \mathrm{d}s_{ij}\right] \mathfrak{G}(q_1, \ldots, q_N)^{\frac{d-N-1}{2}} \Theta(\mathfrak{G}(q_1, \ldots, q_N)). \tag{4.54}$$

By definition, as the gram determinant only depends on scalar products, we can make the parametrization manifestly a function of the Mandelstam invariants by writing,

$$\mathfrak{G}_N(\{s_{ij}\}) = \mathfrak{G}(q_1, \ldots, q_N) = \det(s_{1i}s_{2j} + s_{1j}s_{2i} - s_{ij})_{3 \leq i,j \leq N}. \tag{4.55}$$

With this we finally arrive at the phase-space measure,

$$\mathrm{d}\Phi_{N-1} = \mathcal{N}_{N-2} \left[\prod_{\substack{1<i,j,N \\ i \neq j, (i,j) \neq (1,2)}} \mathrm{d}s_{ij}\right] \delta(m^2 - \sum_{i=3}^{N}(s_{1i} + s_{2i}) + \sum_{i=3}^{N} \sum_{j=3}^{i} s_{ij}) \times \mathfrak{G}_N(\{s_{ij}\})^{\frac{d-N-1}{2}} \Theta(\mathfrak{G}_N(\{s_{ij}\})), \tag{4.56}$$

with

$$\mathcal{N}_{N-2} = (-1)^{\frac{(N-2)(N-3)}{2}} 2^{-(N-2)\frac{d}{2}} (2\pi)^{(N-1)-(N-2)d} \prod_{i=3}^{N} \Omega_{d-i+1}. \tag{4.57}$$

The goal is to use this expression for the phase-space measure to compute boundary conditions for the solutions obtained from solving from differential equations. This means that we actually only need to perform the phase-space integral in a certain kinematic limit. We want to fix the boundary conditions in the soft limit $\bar{z} \to 0$. In this limit all radiation is soft. We can adapt our phase-space parametrization to make this limit manifest by rescaling the momenta as

$$q_i \to q_i \bar{z} \quad \forall i \in \{3, \ldots, N\}. \tag{4.58}$$

This implements the fact that the massless particles in the final-state will be suppressed in the soft limit. In this parametrization the phase-space measure becomes,

$$\begin{aligned} \mathrm{d}\Phi_{N-1} = \mathcal{N}_{N-2} \bar{z}^{(N-2)(d-2)-1} & \left[ \prod_{\substack{1<i,j,N \\ i \neq j, (i,j) \neq (1,2)}} \mathrm{d}s_{ij} \right] \\ & \times \delta(1 - \sum_{i=3}^{N} (s_{1i} + s_{2i}) + \bar{z} \sum_{i=3}^{N} \sum_{j=3}^{i} s_{ij}) \mathfrak{G}_N(\{s_{ij}\})^{\frac{d-N-1}{2}} \Theta(\mathfrak{G}_N(\{s_{ij}\})). \end{aligned} \tag{4.59}$$

Note that we have not yet taken any limit at this point. However, we can see how the phase-space will be simplified if we do actually take the limit $\bar{z} \to 0$. The momentum conservation $\delta$-function which couples the $s$-channel and $t$-channel invariants to each other will be simplified in the limit $\bar{z} \to 0$.

## 4.3 Mellin-Barnes techniques

Using Feynman parametrization and the phase-space measure derived before, we can obtain integral representations for any required combination of loop and phase space integrals. However, we realize that it quickly becomes tedious if not impossible to actually perform the required integrals. We would therefore like to have a systematic way of simplifying the integrands so that we are able to perform the integrals.

The most powerful technique for achieving this are the so-called Mellin-Barnes (MB) integrals. Mellin-Barnes integral representations can be introduced using the basic identity,

$$(x+y)^\lambda = \int_{c-i\infty}^{c+i\infty} \frac{d\omega}{2\pi i} x^\omega y^{\lambda-\omega} \frac{\Gamma(-\omega)\Gamma(\omega-\lambda)}{\Gamma(-\lambda)}. \tag{4.60}$$

The integral over the Mellin-Barnes variable $\omega$ is defined as a contour integral along a contour parallel to the imaginary axis which separates the poles of $\Gamma(-\omega)$ from the poles of $\Gamma(\omega - \lambda)$. Using Cauchy's theorem the integral can be performed by taking either series of residues and summing them. $\Gamma(-\omega)$ has poles at $\omega = n \ \forall\, n \in \mathbb{N}^0$, while $\Gamma(\omega-\lambda)$ has poles at $\omega = -n+\lambda \ \forall\, n \in \mathbb{N}^0$. We can therefore take, for example, the residues of $\Gamma(-\omega)$ and obtain,

$$\int_{c-i\infty}^{c+i\infty} \frac{d\omega}{2\pi i} x^{\omega} y^{\lambda-\omega} \frac{\Gamma(-\omega)\Gamma(\omega-\lambda)}{\Gamma(-\lambda)} = \sum_{n=0}^{\infty} (-1)^n x^n y^{\lambda-n} \frac{\Gamma(n-\lambda)}{n!\Gamma(\lambda)}. \tag{4.61}$$

This sum over the residues is nothing but a generalization of the binomial sum. The power of the Mellin-Barnes representation lies in the fact that it enables us to split polynomials of integration variables into monomials at the cost of introducing additional integrations over the Mellin-Barnes variables.

One important identity that can be used to perform Mellin-Barnes integrals is called Barnes' first lemma. It states that

$$\begin{aligned}\int_{c-i\infty}^{c+i\infty} \frac{\mathrm{d}\omega}{2\pi i} &\Gamma(\alpha+\omega)\Gamma(\beta+\omega)\Gamma(\gamma-\omega)\Gamma(\delta-\omega) \\ &= \frac{\Gamma(\alpha+\gamma)\Gamma(\alpha+\delta)\Gamma(\beta+\gamma)\Gamma(\beta+\delta)}{\Gamma(\alpha+\beta+\gamma+\delta)},\end{aligned} \tag{4.62}$$

for a contour that separates the poles of the $\Gamma$-functions with argument $(\ldots-\omega)$ from the ones of the $\Gamma$-functions with argument $(\ldots+\omega)$. This can be used to perform Mellin-Barnes integrals without having to explicitly sum over residues. This lemma as well as corollaries thereof have been implemented in the `Mathematica` package `barnesroutines` [162], which enables their automatic detection and application.

Mellin-Barnes representations can also be used to obtain series expansions by only summing over finitely many residues.

*Example.*
Consider

$$(1+\xi)^{-2} = \int \frac{\mathrm{d}\omega}{2\pi i} \xi^{-\omega-2} \Gamma(-\omega)\Gamma(\omega+2). \tag{4.63}$$

$\Gamma(-\omega)$ has poles at $\omega = 0, 1, \ldots$, while $\Gamma(\omega+2)$ has poles at $\omega = -2, -3, \ldots$. We can obtain a series in $\xi$ by taking the residues of $\Gamma(\omega+2)$ and summing up to finite order, e.g.

$$(1+\xi)^{-2} = \sum_{n=0}^{2} (-1)^{-n} \xi^n \frac{\Gamma(n+2)}{n!} + \mathcal{O}(\xi^3) = 1 - 2\xi + 3\xi^2 + \mathcal{O}(\xi^3). \tag{4.64}$$

Alternatively, we can obtain a series in $\xi^{-1}$ by taking the residues of $\Gamma(-\omega)$

$$(1+\xi)^{-2} = \sum_{n=0}^{2}(-1)^{-n}\xi^{-2-n}\frac{\Gamma(n+2)}{n!} + \mathcal{O}\left(\xi^{-5}\right) = \frac{1}{\xi^2} - \frac{2}{\xi^3} + \frac{3}{\xi^4} + \mathcal{O}\left(\xi^{-5}\right). \tag{4.65}$$

*Example.*
As an example of the usefulness of the Mellin-Barnes integral, we can revisit the one-loop triangle with one off-shell leg and massive propagators, eq. (4.19). Recall that we had the Feynman parametrization,

$$\begin{aligned} F &= -i(4\pi)^{\epsilon-2}\Gamma(\epsilon+1) \\ &\times \int_0^\infty \mathrm{d}x_1\mathrm{d}x_2\mathrm{d}x_3\delta(1-x_1-x_2-x_3) \times \frac{(x_1+x_2+x_3)^{2\epsilon-1}}{\left(m^2(x_1+x_2+x_3)^2 - sx_1x_3\right)^{1+\epsilon}}. \end{aligned} \tag{4.66}$$

We can simplify this by introducing a Mellin-Barnes integral as,

$$\begin{aligned} \left(m^2(x_1+x_2+x_3)^2 - sx_1x_3\right)^{-1-\epsilon} &= \int_{c-i\infty}^{c+i\infty}\frac{\mathrm{d}\omega}{2\pi i}\frac{\Gamma(-\omega)\Gamma(\omega+1+\epsilon)}{\Gamma(1+\epsilon)} \\ \times (-s)^{-\omega-1-\epsilon}(m^2)^{\omega}x_1^{-\omega-1-\epsilon}x_3^{-\omega-1-\epsilon}(x_1+x_2+x_3)^{2\omega}. \end{aligned} \tag{4.67}$$

Using the Cheng-Wu theorem to localize the integration over $x_2$ we arrive at,

$$\begin{aligned} F = -i(4\pi)^{\epsilon-2}\int_{c-i\infty}^{c+i\infty}\frac{\mathrm{d}\omega}{2\pi i}\int_0^\infty \mathrm{d}x_1\mathrm{d}x_2\Gamma(-\omega)\Gamma(\omega+1+\epsilon) \\ \times (-s)^{-\omega-1-\epsilon}(m^2)^{\omega}x_1^{-\omega-1-\epsilon}x_3^{-\omega-1-\epsilon}(1+x_1+x_3)^{2\omega+2\epsilon-1}. \end{aligned} \tag{4.68}$$

As the integration over the remaining Feynman parameters is projective, we can rescale $x_1 \to x_1(1+x_3)$ and find,

$$\begin{aligned} F = -i(4\pi)^{\epsilon-2}\int_{c-i\infty}^{c+i\infty}\frac{\mathrm{d}\omega}{2\pi i}\int_0^\infty \mathrm{d}x_1\mathrm{d}x_2\frac{\Gamma(-\omega)\Gamma(\omega+1+\epsilon)}{\Gamma(1+\epsilon)} \\ \times (-s)^{-\omega-1-\epsilon}(m^2)^{\omega}x_1^{-\omega-1-\epsilon}x_3^{-\omega-1-\epsilon}(1+x_1)^{2\omega+2\epsilon-1}(1+x_3)^{\omega+\epsilon-1}. \end{aligned} \tag{4.69}$$

We recognize that the integrals over $x_1$ and $x_3$ are now just beta functions and obtain the Mellin-Barnes representation of the triangle integral,

$$
\begin{aligned}
F = -i(4\pi)^{\epsilon-2} \int_{c-i\infty}^{c+i\infty} \frac{\mathrm{d}\omega}{2\pi i} (-s)^{-\omega-1-\epsilon} (m^2)^{\omega} \\
\times \frac{\Gamma(-\omega)\Gamma(-\omega-\epsilon)^2\Gamma(\omega+1+\epsilon)}{\Gamma(-2\omega+1-2\epsilon)}.
\end{aligned}
\tag{4.70}
$$

What remains to be done is to perform the integral over the Mellin-Barnes variable $\omega$. We should therefore inspect the pole structure of the $\Gamma$ functions. $\Gamma(-\omega)$ has poles at $\omega = 0, 1, \ldots$, while $\Gamma(-\omega-\epsilon)$ has poles at $\omega = 0-\epsilon, 1-\epsilon \ldots$. On the other side we have the poles of $\Gamma(\omega+1+\epsilon)$ at $\omega = -1-\epsilon, -2-\epsilon, \ldots$. A contour somewhere in the interval $(-1, 0)$ will therefore separate the poles of the $\Gamma$-functions with $-\omega$ in the argument from the poles of the $\Gamma$-functions with $+\omega$ in the argument. The simplest way to evaluate the integral is therefore to take and sum the residues of $\Gamma(\omega+1+\epsilon)$,

$$
F = -i(4\pi)^{\epsilon-2} \sum_{n=0}^{\infty} (-1)^n (-s)^n (m^2)^{-n-1-\epsilon} \frac{\Gamma(n+1)^2\Gamma(n+1+\epsilon)}{n!\Gamma(2n+3)}.
\tag{4.71}
$$

We recognize this sum to be similar to the sum representation of the hypergeometric function ${}_3F_2$,

$$
{}_3F_2\left[\begin{matrix} a_1 & a_2 & a_3 \\ & b_1 & b_2 \end{matrix}; z\right] = \sum_{n=0}^{\infty} \frac{(a_1)_n (a_2)_n (a_3)_n}{(b_1)_n (b_2)_n} \frac{z^n}{n!},
\tag{4.72}
$$

with

$$
(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)}.
\tag{4.73}
$$

Using this representation we find,

$$
F = -\frac{i}{2}(4\pi)^{\epsilon-2}(m^2)^{-1-\epsilon}\Gamma(1+\epsilon)\,{}_3F_2\left[\begin{matrix} 1 & 1 & 1+\epsilon \\ & \frac{3}{2} & 2 \end{matrix}; \frac{s}{4m}\right].
\tag{4.74}
$$

While the calculation of the triangle with Mellin-Barnes techniques arrives at a very compact result, it also illustrates two problems with using Mellin-Barnes integrals in this way. For one, the sums appearing when taking the residues will quickly become very complicated so that bringing them into a form where one can recognize a generalized hypergeometric function can be very involved. Furthermore, after one has obtained such a hypergeometric function, the work is not really done yet. Ultimately, we are interested in solutions for $\epsilon \to 0$ and not in solutions for arbitrary $\epsilon$. We need to therefore expand the result into a Laurent series in $\epsilon$. Simple hypergeometric functions like ${}_2F_1$ or the ${}_3F_2$ in the example can be easily expanded and algorithms to obtain the series are implemented e.g. in the package `HypExp` [163]. However, for more complicated functions there is often no direct way of obtaining a series expansion.

It would therefore be very beneficial if we could immediately obtain a Laurent series in $\epsilon$ from the Mellin-Barnes integral without having to find hypergeometric function first. In this particular example, we could have just expanded the integrand in $\epsilon$ at any stage, since the integral is finite in $d = 4$, and we did so in our first calculation of the triangle. However, in general, we would also like to be able to obtain Laurent series in $\epsilon$ for integrals that are divergent in $d = 4$. Mellin-Barnes integrals provide a canonical way of finding the Laurent series of such integrals. This requires however that we take some care when trying to find the contour that defines the Mellin-Barnes integral.

The problem of finding a valid contour that allows us to expand the integral in $\epsilon$ can be illustrated when computing a divergent integral using Mellin-Barnes techniques.

*Example.*
Consider the one-loop massless scalar box integral,

$$F = \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{k^2(k+p_1)^2(k+p_1+p_2)^2(k+p_1+p_2+p_3)^2}, \tag{4.75}$$

with

$$p_i^2 = 0, \quad (p_1+p_2)^2 = s, \quad (p_1+p_3)^2 = u, \quad (p_2+p_3)^2 = t, \quad s+t+u = 0. \tag{4.76}$$

We can easily obtain the Feynman parametrization,

$$\begin{aligned} F = i(4\pi)^{\epsilon-2}\Gamma(2+\epsilon) \int_0^\infty & \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 (1+x_1+x_2+x_3)^{2\epsilon} \\ & \times ((-s)x_1x_3 + (-t)x_2)^{-2-\epsilon}, \end{aligned} \tag{4.77}$$

where we have already used the $\delta$-function to localize the integral over $x_4$. Rescaling $x_1 \to x_1 x_2$ and afterwards $x_2 \to x_2 \frac{1+x_3}{1+x_1}$, the integration over $x_2$ factorizes,

$$\begin{aligned} F &= i(4\pi)^{\epsilon-2}\Gamma(2+\epsilon) \\ &\times \int_0^\infty \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3 x_2^{-1-\epsilon}(1+x_1)^{\epsilon}(1+x_2)^{2\epsilon}(1+x_3)^{\epsilon}((-s)x_1x_3 - t)^{-2-\epsilon}, \end{aligned} \tag{4.78}$$

and can be performed in terms of a beta function,

$$\begin{aligned} F &= i(4\pi)^{\epsilon-2}\frac{\Gamma(-\epsilon)^2\Gamma(2+\epsilon)}{\Gamma(-2\epsilon)} \\ &\times \int_0^\infty \mathrm{d}x_1\mathrm{d}x_3(1+x_1)^\epsilon(1+x_3)^\epsilon((-s)x_1x_3-t)^{-2-\epsilon}. \end{aligned} \tag{4.79}$$

Here we can introduce a Mellin-Barnes integral,

$$\begin{aligned} ((-s)x_1x_3-t)^{-2-\epsilon} = &\int_{c-i\infty}^{c+i\infty}\frac{\mathrm{d}\omega}{2\pi i} \\ &\times \frac{\Gamma(-\omega)\Gamma(\omega+2+\epsilon)}{\Gamma(2+\epsilon)}(-s)^\omega(-t)^{-\omega-2-\epsilon}x_1^\omega x_3^\omega, \end{aligned} \tag{4.80}$$

which will allow us to perform the integrations over $x_1$ and $x_3$ in terms of beta functions,

$$\begin{aligned} F &= i(4\pi)^{\epsilon-2}\int_{c-i\infty}^{c+i\infty}\frac{\mathrm{d}\omega}{2\pi i}(-s)^\omega(-t)^{-\omega-2-\epsilon} \\ &\times \Gamma(-\omega)\frac{\Gamma(\omega+1)^2\Gamma(-\omega-1-\epsilon)^2\Gamma(\omega+2+\epsilon)}{\Gamma(-2\epsilon)}. \end{aligned} \tag{4.81}$$

When we try to find a straight line contour that will allow us to separate the poles of the $\Gamma$-functions with $-\omega$ in the argument from the poles of the ones with $+\omega$ in the argument we notice that the contour will now depend on $\epsilon$ because the arguments of the $\Gamma$-functions depend on $\epsilon$. What is more surprising at first sight is that we have to choose a contour where $\epsilon$ is finite. For $\epsilon = -1$ for example, we will be able to separate the poles by choosing $c = -\frac{1}{2}$. For $\epsilon = 0$ we will not be able to separate the poles, as the poles of $\Gamma(1+\omega)$ and $\Gamma(-1-\omega-\epsilon)$ will coincide for $\epsilon \to 0$. This is of course a slight problem since we would like to know the value of the integral for $\epsilon \to 0$ rather then $\epsilon = -1$. However, this is nothing but $\epsilon$ regulating divergences of the integral. All this means is that we have found a value of $\epsilon$ that makes the integral finite, and we can now analytically continue to $\epsilon \to 0$ which will yield the result we want.

We would therefore like to have a way to analytically continue Mellin-Barnes integrals. This problem has been studied extensively in the literature [164–166], and there are several algorithms to perform the analytic continuation that have been automated in the `Mathematica` packages `MB` [167] and `MBresolve` [168]. The goal of the procedure is to find a straight line contour parallel to the imaginary axis that separates the poles as required for $\epsilon \to 0$. The starting point is a contour that separates the poles for finite $\epsilon$. When we now gradually take $\epsilon \to 0$ some poles will move towards the contour and at some point a pole will cross the contour. Since we need the pole to be on the correct side of the contour we would have to deform the contour at this stage to prevent the pole from crossing. Alternatively, we can keep a straight line contour by taking the residue of the pole rather than deforming the contour. This way we will take the residues of several poles that are about to cross the contour when we take $\epsilon$ to zero. When all critical poles have been treated this way we obtain a Mellin-Barnes representation which is valid for $\epsilon \to 0$. At this stage we are allowed to expand in $\epsilon$ and obtain a Mellin-Barnes representation for the Laurent series in $\epsilon$ of the integral.

*Example.*
Returning to our previous example, the critical Γ-function in eq. (4.81) is

$$\Gamma(-\omega - 1 - \epsilon), \tag{4.82}$$

with our starting contour of $c = -\frac{1}{2}$ for $\epsilon = -1$ the pole of this Γ-function at $\omega = -\epsilon - 1$ will cross the contour when we take $\epsilon$ to zero. We therefore need to take the residue at this pole. No further poles will cross the contour, which means that we obtain the analytic continuation of the Mellin-Barnes integral which is valid for $\epsilon \to 0$,

$$F = -i(4\pi)^{\epsilon-2} \left(\mathcal{F}_1 + \mathcal{F}_2\right), \tag{4.83}$$

with

$$\begin{aligned}\mathcal{F}_1 = &\frac{2(-s)^{-1-\epsilon}\Gamma(1-\epsilon)^2\Gamma(1+\epsilon)}{t\Gamma(1-2\epsilon)\epsilon} \\ &\times \left(\log(-s) - \log(-t) + 2\psi_0(1-\epsilon) - \psi_0(1+\epsilon) + \gamma + \frac{2}{\epsilon}\right),\end{aligned} \tag{4.84}$$

with the digamma function $\psi_0(z) = \partial_z \log(\Gamma(z))$ and,

$$\begin{aligned}\mathcal{F}_2 = &-\frac{1}{\Gamma(-2\epsilon)} \int_{-1/2+i\infty}^{1/2+i\infty} \frac{\mathrm{d}\omega}{2\pi i} \\ &\times \Gamma(-\omega)\Gamma(1+\omega)^2\Gamma(-\omega-1-\epsilon)^2\Gamma(\omega+2+\epsilon)(-s)^{\omega}(-t)^{-\omega-2-\epsilon}.\end{aligned} \tag{4.85}$$

$\mathcal{F}_1$ is the residue at $\omega = -\epsilon - 1$ that fully localizes the integration over the Mellin-Barnes variable. Consequently, we can easily expand $\mathcal{F}_1$ into a Laurent series in $\epsilon$. $\mathcal{F}_2$ is the same integral as before, however, now we have chosen a definite contour for the $\omega$ integration. We can therefore now expand in $\epsilon$ under the integration. Expanding up to order $\epsilon$ we find,

$$\mathcal{F}_2 e^{\gamma\epsilon} = 2\epsilon \int_{-1/2-i\infty}^{1/2+i\infty} \frac{\mathrm{d}\omega}{2\pi i} \frac{\omega^3}{1+\omega} (-s)^{\omega} (-t)^{-\omega-2} \Gamma(-\omega)^3 \Gamma(\omega)^3. \tag{4.86}$$

Here we can easily take the residues of $\Gamma(-\omega)$ at $\omega = -n$ and sum them,

$$\begin{aligned}\mathcal{F}_2 e^{\gamma\epsilon} = \epsilon \sum_{n=0}^{\infty} & (-1)^{-n} \frac{(-s)^n (-t)^{-2-n}}{(n+1)^3} \\ & \times \left(-2(1+n)\log(-s)((1+n)\log(-t)+1)\right. \\ & +(1+n)^2 \log^2(-s) + (1+n)^2 \log^2(-t) \\ & \left.+2(1+n)\log(-t) + (1+n)^2\pi^2 + 2\right).\end{aligned} \tag{4.87}$$

Using the method outlined above we can expand Mellin-Barnes integrals into Laurent series in $\epsilon$ and obtain sum representations for the coefficients. The remaining task is then to perform the sums in terms of useful functions. The types of sums that appear when summing over residues of Mellin-Barnes integrals that have been expanded in $\epsilon$ are Euler-Zagier sums as well as generalizations thereof [169, 170]. Euler-Zagier sums can be defined as generalizations of harmonic sums

$$Z_{i_1,\ldots,i_k}(x_1,\ldots,x_k;n) = \sum_{n_1 > \cdots > n_k \geq 1} \frac{x_1^{n_1}}{n_1^{i_1}} \cdots \frac{x_k^{n_k}}{n_k^{i_k}}. \tag{4.88}$$

These sums have a rich mathematical structure, e.g. they carry a quasi-shuffle algebra structure. From the definition it is obvious that the $Z$ sums satisfy the recursion,

$$Z_{i\vec{j}}(x,\vec{y};n) = \sum_{k=1}^{n} \frac{x^k}{k^i} Z_{\vec{j}}(\vec{y};n-1), \tag{4.89}$$

where the vector notation abbreviates a (possibly empty) set of indices and arguments. As starting point of the recursion one defines,

$$Z(;n) = 1. \tag{4.90}$$

Using the recursive definition it is possible to iteratively sum over sets of residues obtained from Mellin-Barnes integrals.

If the upper limit of summation tends to infinity the $Z$ sums degenerate to the sum representation of the multiple polylogarithms, eq. (6.77), or for $x_i = \pm 1$ to the colored multiple zeta values, eq. (2.28). This can be used to express the result of summing over the residues of a Mellin-Barnes integral in terms of well-known functions and constants.

*Example.*
Returning to our example, we can now perform the sums appearing in eq. (4.87) and obtain the final result,

$$
\begin{aligned}
Fi(4\pi)^{2-\epsilon}e^{\gamma\epsilon}st = {}& \frac{4}{\epsilon^2} - \frac{2}{\epsilon}\left(\log(-s)+\log(-t)\right) - 2\log(-s)\log(-t) \\
& + \frac{\epsilon}{6}\Big[ -12H_{0,0,1} - 12\left(\log(-s)-\log(-t)\right)H_{0,1} \\
& - 2\log^2(-s)\left(\log(-s)-3\log(-t)\right) - 6\zeta_2(7\log(-s)+\log(-t)) \\
& - 6\left(\left(\log(-s)-\log(-t)\right)^2 + 6\zeta_2\right)H_1 + 68\zeta_3\Big],
\end{aligned} \tag{4.91}
$$

where the argument $\left(-\frac{-s}{-t}\right)$ of the HPLs $H$ has been suppressed, i.e. $H_{0,1} = H\left(0,1;-\frac{-s}{-t}\right)$.

## From Mellin-Barnes integrals to parametric integrals

Mellin-Barnes techniques in the form presented above transform the problem of calculating integrals to the problem of evaluating nested sums. While these sums can be easily performed in many simple cases, the effort required for more interesting integrals is impractical. It would therefore be preferable if the problem could be formulated in terms of the more familiar language of integrals. One way to achieve this is to map the Mellin-Barnes integrals back to certain parametric integrals, which is possible for *balanced* Mellin-Barnes integrals.

Roughly speaking, a MB integral is said to be balanced if for each Mellin-Barnes variable $z_i$ the number of $\Gamma$ functions of the form $\Gamma(\ldots - z_i)$ is equal to the number of $\Gamma$ functions of the form $\Gamma(\ldots + z_i)$. More precisely, the integral,

$$
\int_{-i\infty}^{+i\infty} \frac{\mathrm{d}z_i}{2\pi i} \prod_{k_1=1}^{n_+} \Gamma(a_{k_1}+z_i)^{\alpha_{k_1}} \prod_{k_2=1}^{n_-} \Gamma(b_{k_2}-z_i)^{\beta_{k_2}}, \quad \alpha_{k_i}, \beta_{k_i} \in \mathbb{Z}, \tag{4.92}
$$

is said to be balanced if $\sum_{k_1}^{n_+} \alpha_{k_1} = \sum_{k_2}^{n_-} \beta_{k_2}$, where $n_+$ ($n_-$) is the number $\Gamma$-functions with argument $\ldots + z_i$ ($\ldots - z_i$). We assume in the following that the contours are straight vertical lines such that the real parts of the arguments of all the $\Gamma$-functions are positive[1].

In that case we can always derive an Euler-type integral representation for the MB integral. We start by noting that if an integral is balanced, then we

[1]Note that in dimensional regularization we might need to require $\epsilon$ to be finite for such a contour to exist.

can always express its integrand as a product of Beta functions,

$$B(x,y) = \frac{\Gamma(x)\Gamma(y)}{\Gamma(x+y)} = \int_0^\infty dt t^{x-1}(1+t)^{-x-y}. \tag{4.93}$$

The integral (4.93) is convergent whenever $\mathrm{Re}(x), \mathrm{Re}(y) > 0$. It is easy to convince oneself that this condition is satisfied whenever the real parts of all arguments of the $\Gamma$-functions are positive in the original MB integral. We can therefore replace each Beta function by its integral representation (4.93) in the *integrand* of the MB integral and, because all the integrals are convergent, we can exchange the MB integrations and the integrations coming from the Beta functions. This leaves us with an integral of the form

$$\int_0^\infty \left(\prod_{n=1}^N dt_i\right) R_0(\vec{t})R_\epsilon(\vec{t})^\epsilon \int_{-i\infty}^{+i\infty} \prod_{m=1}^M \frac{\mathrm{d}z_i}{2\pi i} R_i(\vec{t})^{z_i}, \tag{4.94}$$

where $\vec{t} = (t_1, \dots, t_N)$ and the $R_k$ are ratios of products of the $t_i$ and $1+t_i$. Next, we would like to perform the MB integrations. This can be done using the formula,

$$\int_{z_0-i\infty}^{z_0+i\infty} \frac{\mathrm{d}z}{2\pi i} a^z = \delta(1-a), \qquad a > 0. \tag{4.95}$$

Indeed, parametrizing the contour as $z = z_0 + it$, we obtain,

$$\int_{z_0-i\infty}^{z_0+i\infty} \frac{\mathrm{d}z}{2\pi i} a^z = a^{z_0} \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{it\ln a} = a^{z_0}\delta(\ln a) = \delta(1-a). \tag{4.96}$$

Equation (4.94) can thus be written in the form,

$$\int_0^\infty \left(\prod_{n=1}^N dt_i\right) R_0(\vec{t})R_\epsilon(\vec{t})^\epsilon \prod_{m=1}^M \delta\left(1 - R_i(\vec{t})\right). \tag{4.97}$$

We can solve the $\delta$ constraints, and the result is the desired parametric integral.

*Example.*
Consider Barnes' first lemma, i.e., we consider the integral,

$$\mathcal{I} = \int_{-i\infty}^{+i\infty} \frac{\mathrm{d}z}{2\pi i} \Gamma(a+z)\Gamma(b+z)\Gamma(c-z)\Gamma(d-z). \tag{4.98}$$

We assume that the integration contour and $a$, $b$, $c$ and $d$ are such that the real parts of all $\Gamma$ functions are positive. We rewrite the integrand in terms of Beta functions,

$$\begin{aligned}\frac{\mathcal{I}}{\Gamma(a+c)\Gamma(b+d)} &= \int_{-i\infty}^{+i\infty}\frac{\mathrm{d}z}{2\pi i}B(a+z,c-z)B(b+z,d-z)\\ &= \int_{-i\infty}^{+i\infty}\frac{\mathrm{d}z}{2\pi i}\int_0^\infty dt_1 dt_2 t_1^{a+z-1}(1+t_1)^{-a-c}t_2^{b+z-1}(1+t_2)^{-b-d}\\ &= \int_0^\infty dt_1 dt_2 t_1^{a-1}(1+t_1)^{-a-c}t_2^{b-1}(1+t_2)^{-b-d}\delta(1-t_1t_2),\end{aligned} \tag{4.99}$$

where the last step follows from eq. (4.95). Solving the $\delta$-function constraint leads to a one-fold integral that can immediately be recognized as a Beta function, and we recover the usual form of Barnes' first lemma,

$$\begin{aligned}\mathcal{I} &= \Gamma(a+c)\Gamma(b+d)\int_0^\infty dt_1 t_1^{a+d-1}(1+t_1)^{-a-b-c-d}\\ &= \frac{\Gamma(a+c)\Gamma(a+d)\Gamma(b+c)\Gamma(b+d)}{\Gamma(a+b+c+d)}.\end{aligned} \tag{4.100}$$

*Example.*
As a second example we consider is Gauss' hypergeometric function ${}_2F_1$. We consider the integral

$$\mathcal{J} = \int_{-i\infty}^{+i\infty}\frac{\mathrm{d}z}{2\pi i}\Gamma(-z)\frac{\Gamma(a+z)\Gamma(b+z)}{\Gamma(c+z)}x^z. \tag{4.101}$$

We again assume that all conditions for convergence are satisfied. Rewriting the integrand in terms of Beta functions, we obtain

$$\begin{aligned}\mathcal{J} &= \frac{\Gamma(b)}{\Gamma(c-a)}\int_{-i\infty}^{+i\infty}\frac{\mathrm{d}z}{2\pi i}B(b+z,-z)B(a+z,c-a)x^z\\ &= \frac{\Gamma(b)}{\Gamma(c-a)}\int_0^\infty dt_1 dt_2 t_1^{a-1}(1+t_1)^{-c}t_2^{b-1}(1+t_2)^{-b}\delta\left(1-\frac{xt_1t_2}{1+t_1}\right).\end{aligned} \tag{4.102}$$

Solving the $\delta$-function constraint with respect to $t_2$ and performing the change of variables $t_1 \to \xi/(1-\xi)$, we immediately arrive at the usual integral representation for the ${}_2F_1$ function,

$$\begin{aligned}\mathcal{J} &= \frac{\Gamma(b)}{\Gamma(c-a)}\int_0^\infty dt_1 t_1^{a-1}(1+t_1)^{b-c}(1+t_1+xt_1)^{-b} \\ &= \frac{\Gamma(b)}{\Gamma(c-a)}\int_0^1 d\xi \xi^{a-1}(1-\xi)^{c-a-1}(1+x\xi)^{-b} \\ &= \frac{\Gamma(a)\Gamma(b)}{\Gamma(c)} {}_2F_1\left[\begin{matrix} a\ b \\ c \end{matrix}; -x\right].\end{aligned} \tag{4.103}$$

## Computing the phase-space volume with Mellin-Barnes integrals

We have previously parametrized the measure for the phase-space for $2 \to H + (N-2)$ processes, i.e. the production of one massive particle together with $(N-2)$ massless particles. If we integrate this measure we obtain the phase-space volume, which is the simplest master integral we can obtain for a given phase-space. It also serves as an important reference point and normalization for other phase-space integrals. We will therefore study the phase space volume in some detail, and derive a general expression for the $2 \to H + (N-2)$ phase-space volume. We start by recalling the general phase-space factorization:

$$\mathrm{d}\Phi_{k+1}(m^2, s) = \int_{m^2}^s \frac{d\mu^2}{2\pi} \mathrm{d}\Phi_{l+1}(\mu^2, s)\mathrm{d}\Phi_{k-l+1}(m^2, \mu^2) \tag{4.104}$$

If we assume that we know the phase-space volume at N$^k$LO, i.e. for $2 \to H + k$,

$$\Phi_{k+1}(m^2, s) = \int \mathrm{d}\Phi_{k+1}(m^2, s), \tag{4.105}$$

this relation allows us to rewrite the phase-space volume at N$^{k+l}$LO as,

$$\Phi_{k+l+1}(m^2, s) = \int\int_{m^2}^s \frac{\mathrm{d}\mu^2}{2\pi} d\Phi_{l+1}(\mu^2, s)\mathrm{d}\Phi_{k+1}(m^2, \mu^2). \tag{4.106}$$

We are specifically interested in rewriting the phase-space volume at N$^{k+1}$LO as a convolution of the N$^k$LO phase-space with a two-particle phase-space. Specializing to $l = 1$, we can use this formula to inductively derive the phase-space volume for arbitrary orders. We have,

$$\begin{aligned}\Phi_{k+2}(m^2, s) &= \int\int_{m^2}^s \frac{\mathrm{d}\mu^2}{2\pi} d\Phi_2(\mu^2, s)\mathrm{d}\Phi_{k+1}(m^2, \mu^2) \\ &= \int_{m^2}^s \frac{\mathrm{d}\mu^2}{2\pi} \mathrm{d}\Phi_2(\mu^2, s)\Phi_{k+1}(m^2, \mu^2).\end{aligned} \tag{4.107}$$

From eq. (4.59) we obtain an explicit parametrization of the two-article phase-space and we find,

$$\Phi_{k+2}(m^2,s) = \frac{1}{4}(2\pi)^{-2+2\epsilon}s^{-\epsilon}\Omega_{2-2\epsilon}\int_{m^2}^{s}\frac{\mathrm{d}\mu^2}{2\pi}\int_0^\infty \mathrm{d}x_{1,k+3}\mathrm{d}x_{2,k+3}\left(1-\frac{\mu^2}{s}\right)^{1-2\epsilon} \\ \times (x_{1,k+3}x_{2,k+3})^{-\epsilon}\delta(1-x_{1,k+3}-x_{2,k+3})\Phi_{k+1}(m^2,\mu^2). \tag{4.108}$$

We can perform the integral over $x_{1,k+3}$ and $x_{2,k+3}$ in terms of beta functions and make the transformation $\mu^2 = sx$, $m^2 = sz$ to obtain,

$$\Phi_{k+2}(z,s) = (4\pi)^{-2+\epsilon}s^{1-\epsilon}\frac{\Gamma(1-\epsilon)}{\Gamma(2-2\epsilon)}\int_z^1 \mathrm{d}x\,(1-x)^{1-2\epsilon}\Phi_{k+1}(zs,xs). \tag{4.109}$$

In the following we use eq. (4.109) to prove inductively the following result:

$$\Phi_{n+1}(m^2,s) = \frac{1}{2}(4\pi)^{1-2n+n\epsilon}\frac{\Gamma(1-\epsilon)^n}{\Gamma(2n(1-\epsilon))}s^{n-1-n\epsilon}(1-z)^{2n-1-2n\epsilon} \\ \times {}_2F_1\left[\begin{matrix}(n-1)(1-\epsilon)\ \ n(1-\epsilon)\\ 2n(1-\epsilon)\end{matrix};1-z\right], \tag{4.110}$$

First, eq. (4.110) correctly describes the phase-space volume for $n=1$ and $n=2$. In order to derive $\Phi_{n+2}$ iteratively from $\Phi_{n+1}$ we use eq. (4.110) and find,

$$\Phi_{n+2}(z,s) = \frac{1}{2}(4\pi)^{1-2(n+1)+(n+1)\epsilon}\frac{\Gamma(1-\epsilon)^{n+1}}{\Gamma(2n(1-\epsilon))\Gamma(2-2\epsilon)}s^{n-(n+1)\epsilon} \\ \times \int_z^1 \mathrm{d}x(1-x)^{1-2\epsilon}x^{n-1-n\epsilon}\left(1-\frac{z}{x}\right)^{2n-1-2n\epsilon} \\ \times {}_2F_1\left[\begin{matrix}(n-1)(1-\epsilon)\ \ n(1-\epsilon)\\ 2n(1-\epsilon)\end{matrix};1-\frac{z}{x}\right]. \tag{4.111}$$

To solve the integral, we make the transformation $x = 1-(1-z)y$ and find

$$\Phi_{n+2}(z,s) = \mathcal{C}\int_0^1 \mathrm{d}y\,y^{1-2\epsilon}(1-y)^{2n-1-2n\epsilon}(1-(1-z)y)^{-n+n\epsilon} \\ \times {}_2F_1\left[\begin{matrix}(n-1)(1-\epsilon)\ \ n(1-\epsilon)\\ 2n(1-\epsilon)\end{matrix};(1-z)\frac{1-y}{1-(1-z)y}\right], \tag{4.112}$$

where we have factored out

$$\mathcal{C} = \frac{1}{2}(4\pi)^{1-2(n+1)+(n+1)\epsilon}\frac{\Gamma(1-\epsilon)^{n+1}}{\Gamma(2n(1-\epsilon))\Gamma(2-2\epsilon)} \\ \times s^{n-(n+1)\epsilon}(1-z)^{2(n+1)-1-2(n+1)\epsilon}. \tag{4.113}$$

Next, we introduce a Mellin-Barnes representation for the ${}_2F_1$ and exchange the MB integration with the parametric integration. This allows us to perform the integration over $y$ in terms of another ${}_2F_1$. Then we find,

$$\begin{aligned}\Phi_{n+2}(z,s) &= \mathcal{C}\frac{\Gamma(2n(1-\epsilon))\Gamma(2-2\epsilon)}{\Gamma((n-1)(1-\epsilon))\Gamma(n(1-\epsilon))}\int_{-i\infty}^{+i\infty}\frac{\mathrm{d}\xi}{2\pi i}(z-1)^{\xi}\Gamma(-\xi)\\ &\times\frac{\Gamma((n-1)(1-\epsilon)+\xi)}{\Gamma(2(n+1)(1-\epsilon)+\xi)}\\ &\times\Gamma(n(1-\epsilon)+\xi)\,{}_2F_1\left[\begin{matrix}n(1-\epsilon)+\xi\;\;2-2\epsilon\\ 2(1+n)(1-\epsilon)+\xi\end{matrix};1-z\right].\end{aligned} \tag{4.114}$$

Introducing another MB integral for the ${}_2F_1$, we arrive at

$$\begin{aligned}&\Phi_{n+2}(z,s)\\ &=\mathcal{C}\frac{\Gamma(2n(1-\epsilon))}{\Gamma((n-1)(1-\epsilon))\Gamma(n(1-\epsilon))}\int_{-i\infty}^{+i\infty}\frac{\mathrm{d}\xi\mathrm{d}\chi}{(2\pi i)^2}(z-1)^{\xi+\chi}\Gamma(-\xi)\Gamma(-\chi)\\ &\times\frac{\Gamma((n-1)(1-\epsilon)+\xi)\Gamma(n(1-\epsilon)+\xi+\chi)\Gamma(2-2\epsilon+\chi)}{\Gamma(2(n+1)(1-\epsilon)+\xi+\chi)}.\end{aligned} \tag{4.115}$$

In the next step we perform the change of variables $\xi\to\xi+\chi$, so that

$$\begin{aligned}&\Phi_{n+2}(z,s)\\ &=\mathcal{C}\frac{\Gamma(2n(1-\epsilon))}{\Gamma((n-1)(1-\epsilon))\Gamma(n(1-\epsilon))}\int_{-i\infty}^{+i\infty}\frac{\mathrm{d}\xi\mathrm{d}\chi}{(2\pi i)^2}(z-1)^{\xi}\Gamma(\chi-\xi)\Gamma(-\chi)\\ &\times\frac{\Gamma((n-1)(1-\epsilon)+\xi-\chi)\Gamma(n(1-\epsilon)+\xi)\Gamma(2-2\epsilon+\chi)}{\Gamma(2(n+1)(1-\epsilon)+\xi)}.\end{aligned} \tag{4.116}$$

The integral over $\chi$ can now be performed using Barnes' first lemma, and we find

$$\begin{aligned}\Phi_{n+2}(z,s) &= \mathcal{C}\frac{\Gamma(2n(1-\epsilon))}{\Gamma((n-1)(1-\epsilon))\Gamma(n(1-\epsilon))}\int_{-i\infty}^{+i\infty}\frac{d\xi}{2\pi i}\Gamma(-\xi)(z-1)^{\xi}\\ &\times\frac{\Gamma(n(1-\epsilon)+\xi)\Gamma((n+1)(1-\epsilon)+\xi)}{\Gamma(2(n+1)(1-\epsilon)+\xi)}.\end{aligned} \tag{4.117}$$

The integral over $\xi$ is just the MB representation of a ${}_2F_1$ so that we finally find,

$$\begin{aligned}\Phi_{n+2}(z,s) &= \frac{1}{2}(4\pi)^{1-2(n+1)+(n+1)\epsilon}s^{n-(n+1)\epsilon}(1-z)^{2(n+1)-1-2(n+1)\epsilon}\\ &\times\frac{\Gamma(1-\epsilon)^{n+1}}{\Gamma(2(n+1)(1-\epsilon))}{}_2F_1\left[\begin{matrix}n(1-\epsilon)\;\;(n+1)(1-\epsilon)\\ 2(1+n)(1-\epsilon)\end{matrix};1-z\right].\end{aligned} \tag{4.118}$$

We have therefore inductively shown the validity of (4.110) for all $n$.

## 4.4 From soft phase-space integrals to Mellin-Barnes integrals

In this section we show that there is a canonical way to derive a Mellin-Barnes representation for the soft phase-space integrals that appear in the calculation of boundary conditions for combined loop and phase-space integrals. The soft integrals we need to consider have the form,

$$F(\epsilon) = \int d\Phi^S_{N-1}\, f(\{p_j\}; p_1, p_2)\,, \tag{4.119}$$

where $f(\{p_j\}; p_1, p_2)$ is a ratio of products of multi-particle invariants that is homogeneous under a simultaneous rescaling of the final-state momenta, i.e.,

$$f(\{\lambda\, p_j\}; p_1, p_2) = f(\{p_j\}; p_1, p_2)\, \lambda^a\,, \tag{4.120}$$

for some $a$. Note that $f$ can contain the result of a loop-integral computation. As such this is not automatically true. However, we can always introduce a suitable Mellin-Barnes representation that takes $f$ to this form.

Next, we note that there is a subclass of soft integrals that have an additional property: they are homogeneous with respect to *individual* rescalings of the final-state momenta, i.e.,

$$f(\{\lambda_j\, p_j\}; p_1, p_2) = f(\{p_j\}; p_1, p_2) \prod_{j=3}^{N} \lambda_j^{a_j}\,, \tag{4.121}$$

for some $a_j$. This subclass of soft integrals is precisely the one where the integrand consists of products of powers of *two*-particle invariants,

$$f(\{p_j\}; p_1, p_2) = \prod_{k=1}^{m} s_{i_k j_k}^{-\alpha_k} = \prod_{k=1}^{m} (2p_{i_k} \cdot p_{j_k})^{-\alpha_k}\,, \tag{4.122}$$

where the index $k$ runs over all the two-particle invariants appearing in $f$. Every soft integral can be converted into an integral of this type, at the price of introducing additional MB integrations. Indeed, if we write every multi-particle invariant as a sum of two-particle invariants, then we can convert sums into products by using the usual Mellin-Barnes identity eq. (4.60). Without loss of generality we can thus assume that our soft integral is homogeneous with respect to individual rescalings of the final-state momenta.

If we concentrate on soft integrals that satisfy eq. (4.121), it is natural to choose a parametrization of the soft phase-space that makes the homogeneity explicit. One possible parametrization with this property is the so-called 'energies and angles' parametrization, where the final-state momenta are parametrized as,

$$\begin{aligned} p_1 &= \frac{1}{2}(1,1,0,\ldots)\,, \\ p_2 &= \frac{1}{2}(1,-1,0,\ldots)\,, \\ p_i &= \frac{1}{2}\,E_i\,\beta_i\,, \qquad 3 \le i \le N\,. \end{aligned} \tag{4.123}$$

The $E_i$ parametrize the energies of the final-state partons and $\beta_i$ is the $d$-velocity in the direction $p_i$. In this parametrization the phase-space measure for each final-state parton takes the form,

$$\mathrm{d}^d p_i\,\delta_+(p_i^2) = 2^{-(d-1)}\,\Theta(E_i)\,E_i^{D-3}\,\mathrm{d}E_i\,\mathrm{d}\Omega_i^{(D-1)}\,, \tag{4.124}$$

where $\mathrm{d}\Omega_i^{(D-1)}$ is the measure on the unit sphere parametrizing the solid angle of particle $i$. Furthermore we have seen in eq. (4.59) that the on-shell $\delta$-function simplifies in the soft limit $\bar{z} \to 0$. Thus, we obtain the soft phase-space measure, i.e. the soft limit of eq. (4.59), as

$$\mathrm{d}\Phi_{N-1}^S = (2\pi)^{N-1-(N-2)d}\,2^{-(N-2)(d-1)}\,\delta\left(1 - \sum_{i=3}^N E_i\right)\prod_{i=3}^N E_i^{d-3}\,\mathrm{d}E_i\,\mathrm{d}\Omega_i^{(d-1)}\,. \tag{4.125}$$

Using this parametrization, we see that every soft integral with an integrand of the form (4.122) can be written as,

$$F(\epsilon) = \int \mathrm{d}\Phi_{N-1}^S \prod_{k=1}^m s_{i_k j_k}^{-\alpha_k} = 2^\alpha \int \mathrm{d}\Phi_{N-1}^S \prod_{k=1}^m (E_{i_k}E_{j_k})^{-\alpha_k}\,(\beta_{i_k}\cdot\beta_{j_k})^{\alpha_k}, \tag{4.126}$$

with $\alpha = \sum_{k=1}^m \alpha_k$. Both the measure and the integrand can be written in a factorized form, and so we can integrate out the energies in terms of a generalized Beta function,

$$\int_0^1 \left(\prod_{k=3}^N \mathrm{d}E_k\,E_k^{a_k-1}\right)\,\delta\left(1 - \sum_{k=3}^N E_k\right) = \frac{\Gamma(a_1)\ldots\Gamma(a_m)}{\Gamma(a_1+\ldots+a_m)}\,. \tag{4.127}$$

Hence, the only non-trivial integration is a multiple angular integration over the solid angles of the final-state partons. Angular integrals can be written in the general form,

$$\Omega_{d-1}^{(\alpha_1,\ldots,\alpha_m)}\left(\{\beta_{j_a}\cdot\beta_{j_b}\}\right) = \int \frac{\mathrm{d}\Omega_i^{(d-1)}}{(\beta_{j_1}\cdot\beta_i)^{\alpha_1}\ldots(\beta_{j_m}\cdot\beta_i)^{\alpha_m}}\,. \tag{4.128}$$

In ref. [171] it was shown that such integrals fall into a class of generalized hypergeometric functions known as **H** functions, and an MB representation for the most general angular integral of this type was derived. We have thus a general recipe to derive MB representations for generic soft integrals.

Although the previous technique allows us to derive a multifold MB representation for every soft integral we need to consider, it can sometimes be useful to insert, if available, explicit closed expressions for the angular integrals. Indeed, for small values of $m$ the integrals (4.128) are very simple and can be evaluated in closed form. In the following we briefly review some results for angular integrals which will be useful in our case.

The case $m = 0$ corresponds to the volume of the solid angle,

$$\Omega_{d-1} = \int \mathrm{d}\Omega_i^{(d-1)} = \frac{2\pi^{(d-1)/2}}{\Gamma\left(\frac{d-1}{2}\right)}\,. \tag{4.129}$$

Note that this integral is sufficient to compute the soft phase-space volume, which corresponds to putting $m = 0$ in eq. (4.126): we simply obtain a factor $\Omega_{d-1}$ for each final-state parton. Thus we obtain,

$$\Phi^S_{N-1}(\epsilon) = (2\pi)^{-2N+5+(N-2)\epsilon}\, 2^{-(N-2)(2-\epsilon)}\, \frac{\Gamma(1-\epsilon)^{N-2}}{\Gamma(2(N-2)(1-\epsilon))}\,, \tag{4.130}$$

in agreement with the results of section 4.3.

As we are only interested in massless momenta, $\beta_j^2 = 0$, Lorentz invariance implies that the angular integral with one propagator must evaluate to a constant. Indeed, we have,

$$\Omega^{(\alpha)}_{d-1} = \int \frac{\mathrm{d}\Omega_i^{(d-1)}}{(\beta_j\cdot\beta_i)^{\alpha}} = 2^{2-\alpha-2\epsilon}\,\pi^{1-\epsilon}\,\frac{\Gamma(1-\epsilon-\alpha)}{\Gamma(2-2\epsilon-\alpha)}\,. \tag{4.131}$$

For angular integrals with two massless propagators one obtains [172],

$$\begin{aligned}\Omega^{(\alpha_{j_1},\alpha_{j_2})}_{d-1}(\beta_{j_1}\cdot\beta_{j_2}) &= \int \frac{\mathrm{d}\Omega_i^{(d-1)}}{(\beta_{j_1}\cdot\beta_i)^{\alpha_1}\,(\beta_{j_2}\cdot\beta_i)^{\alpha_2}}\\ &= 2^{2-\alpha_1-\alpha_2-2\epsilon}\,\pi^{1-\epsilon}\,\frac{\Gamma(1-\epsilon-\alpha_1)\Gamma(1-\epsilon-\alpha_2)}{\Gamma(1-\epsilon)\Gamma(2-2\epsilon-\alpha_1-\alpha_2)}\\ &\times {}_2F_1\left[\begin{matrix}\alpha_1\ \alpha_2\\ 1-\epsilon\end{matrix};1-\frac{\beta_{j_1}\cdot\beta_{j_2}}{2}\right].\end{aligned} \tag{4.132}$$

To our knowledge, there are no closed formulas for angular integrals with three or more massless propagators. The boundary conditions for phase-space integrals with three massless particles in the final-state however require the angular integral with three massless propagators, which admits the MB representation [171],

$$
\begin{aligned}
&\Omega_{d-1}^{(\alpha_{j_1},\alpha_{j_2},\alpha_{j_3})}(\beta_{j_1}\cdot\beta_{j_2},\beta_{j_2}\cdot\beta_{j_3},\beta_{j_1}\cdot\beta_{j_3})\\
&\quad=\frac{2^{2-\alpha_1-\alpha_2-\alpha_3-2\epsilon}\,\pi^{1-\epsilon}}{\Gamma(\alpha_1)\Gamma(\alpha_2)\Gamma(\alpha_3)\Gamma(2-\alpha_1-\alpha_2-\alpha_3-2\epsilon)}\\
&\quad\times\int_{-i\infty}^{+i\infty}\frac{\mathrm{d}z_{12}\mathrm{d}z_{13}\mathrm{d}z_{23}}{(2\pi i)^3}\Gamma(-z_{12})\Gamma(-z_{13})\Gamma(-z_{23})\Gamma(\alpha_1+z_{12}+z_{13})\Gamma(\alpha_2+z_{12}+z_{23})\\
&\qquad\times\Gamma(\alpha_3+z_{13}+z_{23})\Gamma(1-\alpha_1-\alpha_2-\alpha_3-\epsilon-z_{12}-z_{13}-z_{23})\\
&\qquad\times\left(\frac{\beta_{j_1}\cdot\beta_{j_2}}{2}\right)^{z_{12}}\left(\frac{\beta_{j_1}\cdot\beta_{j_3}}{2}\right)^{z_{13}}\left(\frac{\beta_{j_2}\cdot\beta_{j_3}}{2}\right)^{z_{23}},
\end{aligned}
\tag{4.133}
$$

with $z_{ij}=z_i+z_j$, and where the contours separate the poles coming from $\Gamma$ functions of the form $\Gamma(\ldots-z_{ij})$ from those coming from $\Gamma(\ldots+z_{ij})$.

Using these relations we can obtain a Mellin-Barnes representation for any combination of loop and phase-space integrals that appears in the calculation of boundary conditions.

## 4.5 Dimensional recurrence relations

It is well known that loop integrals in different space-time dimensions are related by so-called dimensional shift identities [149]. After reduction to master integrals, the dimensional shift identities reduce to recurrence relations in the space-time dimension $d$ for the master integrals themselves [173–177].

Dimensional shift identities for loop integrals can be understood easily by considering the Schwinger parametrization of a generic loop integral as given in eq. (4.8),

$$
F(d)=(4\pi)^{-\frac{dL}{2}}i^Le^{i\pi(\nu+L)}\frac{1}{\prod_{i=1}^N\Gamma(\nu_i)}\int_0^\infty\prod_{i=1}^N\mathrm{d}x_ix_i^{\nu_i-1}\mathcal{U}^{-\frac{d}{2}}e^{-\frac{\mathcal{F}}{\mathcal{U}}}. \tag{4.134}
$$

We observe that the only term in the integrand that depends on the dimension is the exponent of the $\mathcal{U}$ polynomial. We can therefore express the loop integral in $d-2$ dimensions as

$$
F(d-2)=(4\pi)^{-\frac{(d-2)L}{2}}i^Le^{i\pi(\nu+L)}\frac{1}{\prod_{i=1}^N\Gamma(\nu_i)}\int_0^\infty\prod_{i=1}^N\mathrm{d}x_ix_i^{\nu_i-1}\mathcal{U}^{-\frac{d}{2}}\mathcal{U}e^{-\frac{\mathcal{F}}{\mathcal{U}}}. \tag{4.135}
$$

Shifting the dimension from $d$ to $(d-2)$ just yields an additional factor of the $\mathcal{U}$ polynomial in the integrand. The goal is now to express the integral in $(d-2)$ dimensions in terms of the integral in $d$ dimensions. Recall the definitions of the Symanzik polynomials, eq. (4.9). The $\mathcal{U}$ polynomial is a polynomial of rank $L$ that is linear in each integration variable $x_i$. The $\mathcal{F}$ polynomial contains terms of the form $\mathcal{U}x_i m_i^2$. If we therefore assume that the masses $m_i$ are independent we can write,

$$\partial_{m_i^2} e^{-\frac{\mathcal{F}}{\mathcal{U}}} = x_i e^{-\frac{\mathcal{F}}{\mathcal{U}}}. \tag{4.136}$$

We can now invert this relation and rewrite every $x_i$ that appears in the additional factor of $\mathcal{U}$ in eq. (4.135) as the corresponding derivative $\partial_{m_i^2}$,

$$\begin{aligned} F(d-2) &= (4\pi)^{-\frac{(d-2)L}{2}} i^L e^{i\pi(\nu+L)} \frac{1}{\prod_{i=1}^N \Gamma(\nu_i)} \\ &\times \int_0^\infty \prod_{i=1}^N \mathrm{d}x_i x_i^{\nu_i-1} \mathcal{U}^{-\frac{d}{2}} \mathcal{U}(\{x_i \to \partial_{m_i^2}\}) e^{-\frac{\mathcal{F}}{\mathcal{U}}}. \end{aligned} \tag{4.137}$$

Since the derivatives with respect to the masses commute with the loop integration we can take the factor $\mathcal{U}(\{x_i = \partial_{m_i^2}\})$ out of the integration. Recalling how the derivatives with respect to masses act on general loop integrals we can use the definition eq. (3.11) of the $\oplus_i$ operators in order to write the relation between the loop integrals in $(d-2)$ and $d$ dimensions as,

$$F(d-2) = (4\pi)^{-L} \mathcal{U}(\{x_i \to \oplus_i\}) F(d). \tag{4.138}$$

We have therefore a way to obtain a loop integral in $(d-2)$ dimensions by taking a certain linear combination of $d$ dimensional integrals with modified exponents. Of course we can use IBP reductions to reduce this relation to master integrals. We can also invert this relation to obtain the integral in $(d+2)$ dimensions.

Reverse unitarity rules show that similar dimensional shift identities should hold for dual phase-space integrals (see also ref. [178]).

In the following we present an easy way to derive the dimensional shift identities for phase-space integrals. To start, let us consider a phase-space integral in $d$ dimensions,

$$F(d; \nu_1, \dots, \nu_n) = \int \mathrm{d}\Phi_{N-1}(d) f(\nu_1, \dots, \nu_n), \tag{4.139}$$

where we explicitly indicate the dependence on the space-time dimension $d$. The integrand $f$ can be written as a product,

$$f(\nu_1, \dots, \nu_N) = \prod_{l=1}^N P_l^{-\nu_l}, \tag{4.140}$$

where the $P_l$ are polynomials in the rescaled kinematic invariants $s_{ij}$, raised to some power $\nu_l$. In section 4.2 we showed that the phase-space measure

$\mathrm{d}\Phi_{N-1}(d)$ for parton + parton $\to H + (N-2)$ partons can be parametrized solely in terms of kinematic invariants, see eq. (4.59).

Obviously, the $d$-dependent constants factor out of the integral, and so the actual integral depends on $d$ only through the exponent of the Gram determinant. It is then easy to see that the phase-space measures in shifted dimensions are related by,

$$\mathrm{d}\Phi_{N-1}(d+2) = \frac{\mathcal{N}_{N-2}(d+2)}{\mathcal{N}_{N-2}(d)} \bar{z}^{2(N-2)}\, \mathrm{d}\Phi_{N-1}(d)\, \mathfrak{G}_N(\{s_{ij}\})\,. \tag{4.141}$$

We can thus express a phase-space integral in $d+2$ dimensions as,

$$\begin{aligned} &F(d+2;\nu_1,\ldots,\nu_n) \\ &= \frac{\mathcal{N}_{N-2}(d+2)}{\mathcal{N}_{N-2}(d)} \bar{z}^{2(N-2)} \int \mathrm{d}\Phi_{N-1}(d)\, \mathfrak{G}_N(\{s_{ij}\})\, f(\nu_1,\ldots,\nu_n)\,. \end{aligned} \tag{4.142}$$

For a given set of polynomials $\{P_l\}$, the form of the integrand $f$ depends only on the exponents $\{\nu_i\}$. If we assume that the $\{P_l\}$ are linearly independent, we can express the invariants $s_{ij}$ as linear combinations of the $\oplus_i$ and $\ominus_i$ operators. This allows us to rewrite the extra power of the Gram determinant in eq. (4.141) as a polynomial of degree $N$ in the $\ominus_i$

$$\mathfrak{G}_N(\{s_{ij}\}) f(\nu_1,\ldots,\nu_n) = \mathfrak{G}_N(\{\ominus_i\})\, f(\nu_1,\ldots,\nu_n)\,. \tag{4.143}$$

We thus obtain the following compact formula relating phase-space integrals in different dimensions,

$$F(d+2;\nu_1,\ldots,\nu_n) = \frac{\mathcal{N}_{N-2}(d+2)}{\mathcal{N}_{N-2}(d)} \bar{z}^{2(N-2)} \mathfrak{G}_N(\{\ominus_i\})\, F(d;\nu_1,\ldots,\nu_n)\,. \tag{4.144}$$

Every term in the polynomial can be evaluated according to the action of the $\ominus_i$ operators, yielding a linear combination of modified integrals in $d$ dimensions. By applying this method to a master integral, we can express the master integral in $d+2$ dimensions as a linear combination of integrals in $d$ dimensions. Using IBP identities, we can reduce the integrals in $d$ dimensions to master integrals and thus we find a relation between the master integral in $d+2$ dimensions and in $d$ dimensions. This dimensional recurrence relation can formally be written as,

$$F_i(d+2) = \sum_j c_{ij}(d) F_j(d)\,, \tag{4.145}$$

with coefficients $c_{ij}(d)$ that are determined from the IBP reduction.

The dimensional shift identities for loop and phase-space integrals provide a very useful check for the boundary conditions computed using the methods described before. If one was able to obtain a result that is valid for all $d$ it is very straightforward to test that the result fulfills the dimensional recurrence relation. Often it is only possible to calculate a boundary condition as a Laurent series in $\epsilon$ around $d = 4$. In that case one cannot simply shift the result to $d + 2$ dimensions as the expansion is only valid around $d = 4$. However, it is usually possible to obtain a Mellin-Barnes representation that is valid around e.g. $d = 6$, by simply shifting $\epsilon \to \epsilon - 1$ before expanding. The Mellin-Barnes integral can then be performed e.g. numerically using the package `MB` [167], which is usually sufficient to check the result in $d = 4$ using dimensional shift identities.

Dimensional shift identities also play an important role in a the so-called dimensional recurrence and analyticity (DRA) method by Lee [177] providing a completely orthogonal method for calculating boundary conditions. The method is based on the fact that dimensional shifts like in eq. (4.145) can also be viewed as difference equations in $d$. Consequently, $F_i$ can be determined by solving these difference equations.

CHAPTER 5

# Soft triple real corrections

## 5.1 Reverse unitarity, threshold expansion and soft integrals

We consider the production of a Higgs boson in association with $j = 3 \dots N$ massless partons in the final state from two massless partons $i = 1, 2$ in the initial state,

$$1 + 2 \to H + 3 + \dots + N. \tag{5.1}$$

The inclusive cross section for this process in dimensional regularization is given by a phase-space integral over the momenta $q_j$ of the final-state partons,

$$\sigma = \int d\Phi_{N-1}(q_H, q_3, \dots, q_N; M^2; s; d)\, |\mathcal{A}|^2 (\{q_j\}, q_1, q_2; d). \tag{5.2}$$

We work in $d = 4 - 2\epsilon$ dimensions and denote by $q_1, q_2$ the momenta of the initial-state partons and we also use the shorthand notation

$$q_{12} = q_1 + q_2,\ q_{345} = q_3 + q_4 + q_5,\ \text{etc.}$$

In the following we will often drop the functional dependence on the dimension $d$ for clarity. The mass of the Higgs boson is denoted by $M$, and we denote the (squared) center-of-mass energy by $s = (q_1 + q_2)^2$. $|\mathcal{A}|^2$ represents the squared matrix-element multiplied with the appropriate flux and symmetry factors. The $d$-dimensional phase-space measure is given by,

$$\begin{aligned} &d\Phi_{N-1}(q_H, q_3, \dots, q_N; M^2; s; d) \\ &\quad = (2\pi)^d\, \delta^{(d)}(q_{12} - q_H - q_{3\dots N})\, \frac{d^D q_H}{(2\pi)^{d-1}} \delta_+(q_H^2 - M^2) \prod_{j=3}^{N} \frac{d^D q_j}{(2\pi)^{d-1}} \delta_+(q_j^2)\,, \end{aligned} \tag{5.3}$$

with $\delta_+(q^2 - m^2) = \delta(q^2 - m^2)\Theta(q^0)$. Integrating out the momentum of the Higgs boson, we can rewrite eq. (5.2) as

$$\sigma = \frac{1}{2\pi} \int \left[ \prod_{j=3}^{N} \frac{d^D q_j}{(2\pi)^{d-1}} \delta_+(q_j^2) \right] \delta_+ \left( [q_{3\ldots N} - q_{12}]^2 - M^2 \right) |\mathcal{A}|^2 (\{q_j\}, q_1, q_2). \tag{5.4}$$

In this, we restrict ourselves to the case of real-radiation matrix-elements without virtual corrections. We introduce the variables

$$z = \frac{M^2}{s} \quad \text{and} \quad \bar{z} = 1 - z\,. \tag{5.5}$$

We now rescale the momenta of all the partons,

$$q_i = \begin{cases} \sqrt{s}\, p_i\,, & \text{if } i = 1,2\,, \\ \sqrt{s}\, \bar{z}\, p_i\,, & \text{if } i = 3 \ldots N\,, \end{cases} \tag{5.6}$$

which captures the scaling of the partonic momenta in the final state. We emphasize that this is not, as yet, an approximation, but rather a convenient change of integration variables which captures the correct asymptotic behavior at threshold as $\bar{z} \to 0$. In the following we assume $s = 1$, and we find,

$$\sigma = \bar{z}^{(d-2)(N-2)-1} \frac{1}{2\pi} \int \left[ \prod_{j=3}^{N} \frac{d^D p_j}{(2\pi)^{d-1}} \delta_+(p_j^2) \right] \delta_+ \left( [p_{3\ldots N} - p_{12}]^2 - z\, p_{3\ldots N}^2 \right) \\ \times |\mathcal{A}|^2 (\{\bar{z}\, p_j\}, p_1, p_2). \tag{5.7}$$

Note that the full $s$-dependence can easily be recovered from dimensional analysis.

The squared matrix-element $|\mathcal{A}|^2$ consists of a rapidly growing number of terms with $N$, yielding a correspondingly large number of phase-space integrals. The method of reverse unitarity, developed in refs. [83, 84, 155–157], see section 3.1, allows the reduction of phase-space integrals to a basis of fewer master integrals by establishing a duality of phase-space and loop integrals, where the latter are amenable to algebraic methods [81, 146] based on integration by parts [147, 148], see section 3.1.

According to the reverse unitarity method, we find a dual forward scattering loop-amplitude with $N-1$ cut-propagators for the real radiation contribution of eq. (5.7), namely,

$$\sigma = \bar{z}^{(d-2)(N-2)-1} \frac{1}{2\pi} \int \left[ \prod_{j=3}^{N} \frac{d^D p_j}{(2\pi)^{d-1}} \left( \frac{1}{p_j^2} \right)_c \right] \left[ \frac{1}{[p_{3\ldots N} - p_{12}]^2 - z\, p_{3\ldots N}^2} \right]_c \\ \times |\mathcal{A}|^2 (\{\bar{z} p_j\}, p_1, p_2)\,. \tag{5.8}$$

In this chapter, we take one further step and expand cut-propagators and the squared matrix-elements around $z = 1$,

$$|\mathcal{A}|^2 \left(\{\bar{z}\, p_j\}, p_1, p_2\right) = \bar{z}^{-2(N-2)} \sum_{k=0}^{\infty} |\mathcal{A}|_k^2 \left(\{p_j\}, p_1, p_2\right) \bar{z}^k, \tag{5.9}$$

and

$$\frac{1}{\left[p_{3\ldots N} - p_{12}\right]^2 - z\, p_{3\ldots N}^2} = \sum_{k=0}^{\infty} \bar{z}^k \frac{\left(-p_{3\ldots N}^2\right)^k}{\left[p_{12} \cdot (p_{12} - 2p_{3\ldots N})\right]^{k+1}}\,. \tag{5.10}$$

In this approximation, the cross section can be expanded in a power series in $\bar{z}$,

$$\sigma = \bar{z}^{(d-4)(N-2)-1} \sum_{k=0}^{\infty} \bar{z}^k\, \sigma^{S(k)}\,. \tag{5.11}$$

The coefficients of the power series are given by,

$$\begin{aligned} \sigma^{S(k)} = \sum_{l=0}^{k} (-1)^l \int d\Phi_{N-1}^S \left[\frac{1}{p_{12} \cdot (p_{12} - 2p_{3\ldots N})}\right]_c^l \left(p_{3\ldots N}^2\right)^l \\ \times |\mathcal{A}|_{k-l}^2 \left(\{p_j\}, p_1, p_2\right), \end{aligned} \tag{5.12}$$

where $d\Phi_{N-1}^S$ denotes the "soft" phase-space measure,

$$\begin{aligned} d\Phi_{N-1}^S &\equiv \frac{1}{2\pi} \left[\frac{1}{p_{12} \cdot (p_{12} - 2p_{3\ldots N})}\right]_c \prod_{j=3}^{N} \frac{d^D p_j}{(2\pi)^{d-1}} \left(\frac{1}{p_j^2}\right)_c \\ &= \frac{1}{2\pi}\, \delta_+(p_{12}^2 - 2p_{12} \cdot p_{3\ldots N}) \prod_{j=3}^{N} \frac{d^D p_j}{(2\pi)^{d-1}} \delta_+(p_j^2)\,. \end{aligned} \tag{5.13}$$

The integrals which emerge after the $\bar{z}$ expansion depend trivially on one dimensionful parameter $p_{12}^2 = s$. If we put $s = 1$, the integrals are numerical integrals whose only functional dependence is through the space-time dimension $d = 4 - 2\epsilon$. We will refer to such integrals as *soft (phase-space) integrals*, and they are the main subject of this chapter. We note that, apart from the cut Higgs-boson propagator, the integrands of soft phase-space integrals are homogeneous functions under a simultaneous rescaling of the final-state momenta. In addition, a soft integral can be reduced to a set of "soft" master integrals using IBP identities by exploiting the duality to loop integrals via reverse unitarity. We will illustrate this property in the next section where we check our method on several examples.

## 5.2 Validation of the method and examples

In this section, we study the validity of the method described in the previous section at NLO and NNLO – two perturbative orders that are well studied in the literature, so we can compare our results readily with known results. In particular, we show that our method reproduces the correct results for the leading behavior of NLO and NNLO real-emission amplitudes in the soft limit, as well as for the subleading terms in the expansion of the phase-space volume up to $N^3LO$ and for a non-trivial double real emission master integral at NNLO.

At NLO, all phase-space integrals that contribute to the real emission amplitude in general kinematics can be reduced to the phase-space volume for $H+1$ parton,

$$\Phi_2(\bar{z};\epsilon) = \frac{1}{2(4\pi)^{1-\epsilon}} \frac{\Gamma(1-\epsilon)}{\Gamma(2-2\epsilon)}\, \bar{z}^{1-2\epsilon}\,. \tag{5.14}$$

As there is only one master integral which is a monomial in $\bar{z}$, our method trivially gives the correct answer at NLO.

At NNLO all double real-emission phase-space integral can be reduced in general kinematics to a linear combination of 18 master integrals [83]. The leading contribution of all master integrals in the soft limit to all orders in $\epsilon$ was computed in ref. [34], and it was observed that in this limit 17 master integrals are proportional to the soft limit of the phase-space volume for $H+2$ partons,

$$\begin{aligned} \Phi_3(\bar{z};\epsilon) &= \frac{1}{2(4\pi)^{3-2\epsilon}}\, \bar{z}^{3-4\epsilon} \frac{\Gamma(1-\epsilon)^2}{\Gamma(4-4\epsilon)}\, {}_2F_1(1-\epsilon, 2-2\epsilon; 4-4\epsilon; \bar{z}) \\ &= \bar{z}^{3-4\epsilon}\, \Phi_3^S(\epsilon) + \mathcal{O}(\bar{z}^4)\,, \end{aligned} \tag{5.15}$$

where we define

$$\Phi_3^S(\epsilon) = \frac{1}{2(4\pi)^{3-2\epsilon}} \frac{\Gamma(1-\epsilon)^2}{\Gamma(4-4\epsilon)}\,. \tag{5.16}$$

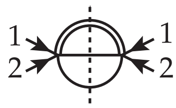
More precisely, it was shown in ref. [34] that if $\mathbf{X}_i^S(\bar{z};\epsilon)$ denotes the leading term in the soft limit of the double real-emission master integrals, then we can write[1],

$$\begin{aligned} \mathbf{X}_i^S(\bar{z};\epsilon) &= \mathbf{S}_i(\bar{z};\epsilon)\, \Phi_3^S(\epsilon)\,, \qquad 1 \le i \le 17\,, \\ \mathbf{X}_{18}^S(\bar{z};\epsilon) &= -4\, \bar{z}^{-1-4\epsilon}\, \frac{(1-2\epsilon)(3-4\epsilon)(1-4\epsilon)}{\epsilon^3} \\ &\quad \times {}_3F_2(1,1,-\epsilon; 1-\epsilon, 1-2\epsilon; 1)\, \Phi_3^S(\epsilon)\,, \end{aligned} \tag{5.17}$$

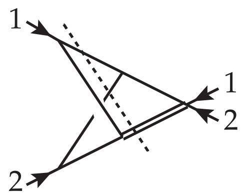
where $\mathbf{S}_i(\bar{z};\epsilon)$ are monomials in $\bar{z}$ and rational functions of $\epsilon$. Using the method described in the previous section, we can easily explain the structure

[1] Note that the normalization differs slightly from the normalization of ref. [34].

of eq. (5.17). Indeed, we observe that in the soft limit all the double real-emission phase-space integrals can be reduced to only two master integrals. In particular, the IBP identities in the soft limit allow us to express all but one of the $\mathbf{X}_i^S$ in terms of the phase-space volume, and the coefficients appearing in the reduction are precisely the functions $\mathbf{S}_i$. In other words, in the soft limit all double real emission phase-space integrals can be reduced to linear combinations of the following two soft master integrals



$$= \int d\Phi_3^S\,, \tag{5.18}$$



$$= \int \frac{d\Phi_3^S}{s_{14}s_{23}s_{34}}\,. \tag{5.19}$$

Our method thus provides the correct leading soft behavior of the double real-emission contribution at NNLO. We emphasize that all the diagrams in this chapter represent soft phase-space integrals, i.e., all the diagrams represent integrals with respect to the soft phase-space measure of eq. (5.13). In addition, the invariants appearing in the integrands of the soft integrals are defined with respect to the rescaled momenta defined in eq. (5.6),

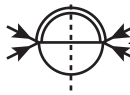
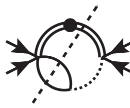
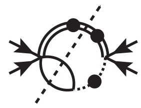
$$s_{ij} = (\tau_i p_i + \tau_j p_j)^2\,, \qquad \tau_i = \begin{cases} -1\,, & \text{if } i = 1,2\,, \\ +1\,, & \text{if } i = 3\ldots N\,. \end{cases} \tag{5.20}$$

Our method allow us to compute not only the leading soft behavior, but to consistently expand around the soft limit $\bar{z} = 0$. In the following we show that we can correctly reproduce the first few terms in the soft expansion of double- and triple-emission phase-space volumes, as well as of the NNLO master integral $\mathbf{X}_{18}$ of refs. [34, 83, 179].

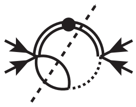
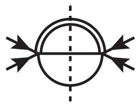
Let us start with the phase-space volume for $H + 2$ partons in the limit where the two partons are soft. On the one hand, from eq. (5.15) we immediately see that $\Phi_3$ admits the expansion,

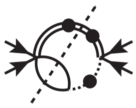
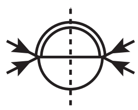
$$\begin{aligned} \Phi_3(\bar{z};\epsilon) &= \bar{z}^{3-4\epsilon}\,\Phi_3^S(\epsilon)\sum_{n=0}^{\infty}\frac{(1-\epsilon)_n(2-2\epsilon)_n}{(4-4\epsilon)_n}\,\bar{z}^n \\ &= \bar{z}^{3-4\epsilon}\,\Phi_3^S(\epsilon)\Big[1+\frac{1-\epsilon}{2}\,\bar{z}+\frac{(1-\epsilon)(2-\epsilon)(3-2\epsilon)}{4(5-4\epsilon)}\,\bar{z}^2+\mathcal{O}(\bar{z}^3)\Big]\,. \end{aligned} \tag{5.21}$$

On the other hand, using eq. (5.10) we obtain the diagrammatic expansion,

$$\Phi_3(\bar{z};\epsilon) = \bar{z}^{3-4\epsilon}\Bigg[$$  $- \bar{z}$  $+ \bar{z}^2$  $$+ \mathcal{O}(\bar{z}^3)\Bigg], \quad (5.22)$$

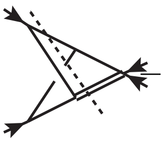
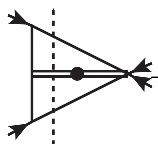
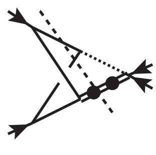
where the dashed lines indicate numerator factors and dots represent additional powers of the propagators or the numerators. The diagrams appearing in eq. (5.22) are in one-to-one correspondence with the terms in the expansion (5.21). Indeed, IBP reduction of the integrals in eq. (5.22) reveals that,

 $= -\dfrac{1-\epsilon}{2}$  , (5.23)

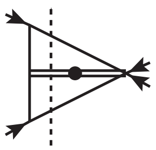
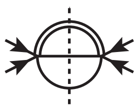
 $= \dfrac{(1-\epsilon)(2-\epsilon)(3-2\epsilon)}{4(5-4\epsilon)}$  , (5.24)

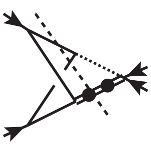
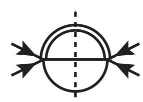
in perfect agreement with eq. (5.21). We checked explicitly that our method correctly reproduces the first ten terms of the soft expansion of the phase-space volume for $H+2$ partons.

As a second example we derive the subleading terms in the soft expansion of the double real-emission master integral $\mathbf{X}_{18}$. Unlike the phase-space volume, no result is known for $\mathbf{X}_{18}$ valid to all orders in $\epsilon$ in general kinematics, but the integral was evaluated explicitly up to $\mathcal{O}(\epsilon)$ in terms of harmonic polylogarithms [180] in ref. [34, 83, 179]. We can thus compare the result of our method order by order in $\epsilon$ to the expansion of the harmonic polylogarithms around $z=1$. Using eq. (5.10) we obtain,

$$\int \frac{d\Phi_3}{q_{14}^2 q_{23}^2 q_{34}^2} = \bar{z}^{-1-4\epsilon}\Bigg[$$  $- \bar{z}$  $+ \bar{z}^2$  $$+ \mathcal{O}(\bar{z}^3)\Bigg], \quad (5.25)$$

IBP reduction of the diagrams appearing in the subleading terms gives,

 $= -\dfrac{2(1-4\epsilon)(3-4\epsilon)(1-2\epsilon)}{\epsilon^2}$  , (5.26)

 $= \dfrac{(3-4\epsilon)(1-2\epsilon)\left(2\epsilon^2-2\epsilon+1\right)}{\epsilon^2}$  . (5.27)

We checked that using these identities we can correctly reproduce the first five terms in the soft expansion of $\mathbf{X}_{18}$.

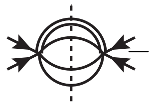
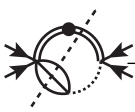
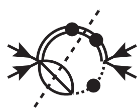
The aim of this chapter is to compute the leading terms in the soft expansion of the triple real-emission amplitude for inclusive Higgs production. In order to test our method at N$^3$LO, we verified that we can reproduce the correct soft expansion of the phase-space volume for $H+3$ partons. The phase-space volume for $H+3$ partons in general kinematics can be written in the form (see section 4.3),

$$\begin{aligned}\Phi_4(\bar{z};\epsilon) &= \frac{1}{2(4\pi)^{5-3\epsilon}}\,\bar{z}^{5-6\epsilon}\frac{\Gamma(1-\epsilon)^3}{\Gamma(6-6\epsilon)}{}_2F_1(2-2\epsilon,3-3\epsilon;6-6\epsilon;\bar{z})\\ &= \bar{z}^{5-6\epsilon}\,\Phi_4^S(\epsilon)\left[1+(1-\epsilon)\,\bar{z}+\frac{(1-\epsilon)(3-2\epsilon)(4-3\epsilon)}{2(7-6\epsilon)}\,\bar{z}^2+\mathcal{O}(\bar{z}^3)\right],\end{aligned} \tag{5.28}$$

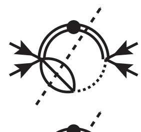
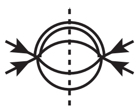
where we define,

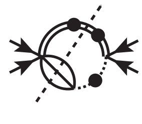
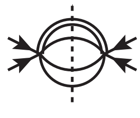
$$\Phi_4^S(\epsilon)=\frac{1}{2(4\pi)^{5-3\epsilon}}\,\frac{\Gamma(1-\epsilon)^3}{\Gamma(6-6\epsilon)}\,. \tag{5.29}$$

Using our method, we obtain the following diagrammatic expansion,

$\Phi_4(\bar{z};\epsilon)=\bar{z}^{5-6\epsilon}\Big[$  $-\,\bar{z}$  $+\,\bar{z}^2$  $+\,\mathcal{O}(\bar{z}^3)\Big]\,.$ (5.30)

All the diagrams in the expansion can be reduced to the soft phase-space volume, as expected,

 $=\;-(1-\epsilon)$  , (5.31)

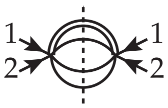
 $=\;\dfrac{(1-\epsilon)(3-2\epsilon)(4-3\epsilon)}{2(7-6\epsilon)}$  . (5.32)

To summarize, our method provides a systematic way to perform the threshold expansion of phase-space integrals for the production of a heavy colorless state. Every term in the expansion corresponds to a soft integral, as defined in Section 5.1, which can be reduced to a small set of soft master integrals using IBP reduction. In the next two sections we study some additional properties of soft integrals in general, before applying our method to compute the threshold expansion of the triple real-emission contribution to inclusive Higgs production.

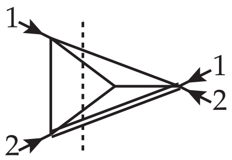
## 5.3 Triple real-emission phase-space integrals in the soft limit

### Triple-real soft master integrals for Higgs production

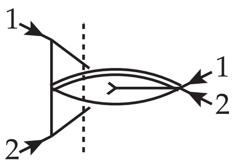
We will use the technology developed in the previous chapters to compute the threshold expansion of the leading-order cross sections for $H$ plus five partons. More details about the construction of the amplitude in this limit will be given in Section 5.4. Here it suffices to say that we have computed the squared amplitude and we have checked that in the limit where we only keep the first two terms in the threshold expansion, all the phase-space integrals can be reduced to linear combinations of the following ten soft master integrals,



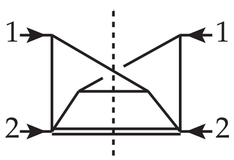
$$= \int d\Phi_4^S = \Phi_4^S(\epsilon)\,, \tag{5.33}$$



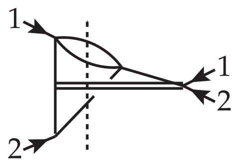
$$= \int \frac{d\Phi_4^S}{(s_{13}+s_{15})s_{34}} = \Phi_4^S(\epsilon)\,\mathcal{F}_2(\epsilon)\,, \tag{5.34}$$



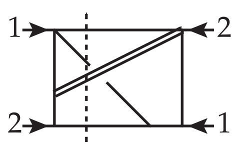
$$= \int \frac{d\Phi_4^S}{s_{14}s_{23}s_{34}} = \Phi_4^S(\epsilon)\,\mathcal{F}_3(\epsilon)\,, \tag{5.35}$$



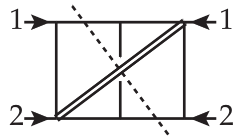
$$= \int \frac{d\Phi_4^S}{s_{13}s_{15}s_{34}s_{45}} = \Phi_4^S(\epsilon)\,\mathcal{F}_4(\epsilon)\,, \tag{5.36}$$



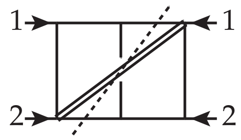
$$= \int \frac{d\Phi_4^S}{(s_{14}+s_{15})s_{23}s_{345}} = \Phi_4^S(\epsilon)\,\mathcal{F}_5(\epsilon)\,, \tag{5.37}$$



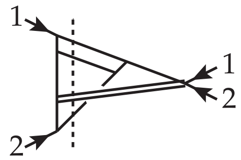
$$= \int \frac{d\Phi_4^S}{(s_{13}+s_{14})(s_{14}+s_{15})s_{23}s_{34}} = \Phi_4^S(\epsilon)\,\mathcal{F}_6(\epsilon)\,, \tag{5.38}$$



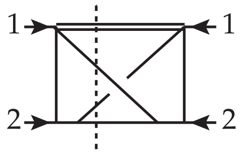

$$= \int \frac{d\Phi_4^S}{s_{15}s_{24}s_{34}s_{35}} = \Phi_4^S(\epsilon)\,\mathcal{F}_7(\epsilon)\,, \tag{5.39}$$




$$= \int \frac{d\Phi_4^S}{(s_{13}+s_{15})(s_{23}+s_{24})s_{34}s_{35}} = \Phi_4^S(\epsilon)\,\mathcal{F}_8(\epsilon)\,, \tag{5.40}$$




$$= \int \frac{d\Phi_4^S}{s_{15}(s_{14}+s_{15})s_{23}s_{34}s_{345}} = \Phi_4^S(\epsilon)\,\mathcal{F}_9(\epsilon)\,, \tag{5.41}$$




$$= \int \frac{d\Phi_4^S}{(s_{23}+s_{24})(s_{24}+s_{25})s_{34}s_{45}} = \Phi_4^S(\epsilon)\,\mathcal{F}_{10}(\epsilon) \tag{5.42}$$

We have normalized all the integrals to the soft phase-space volume for $H+3g$ defined in eq. (5.29). In the remainder of this section we give the dimensional recurrence relations satisfied by the master integrals and present the analytic results for each master integral as a Laurent expansion in the dimensional regulator $\epsilon$. Technical details about how to compute the master integrals analytically will be given in Section 5.5.

## Dimensional recurrence relations

Using the technique described in Section 4.5, we can derive dimensional recurrence relations for all the master integrals defined in the previous section. The knowledge of these recurrence relations provides us with a strong check on our results. In addition, it turns out that the master integral $\mathcal{F}_9(d)$ is easier to compute in $d = 6-2\epsilon$ dimensions, where it is finite, and the dimensional recurrence relations allow us to relate the six-dimensional and four-dimensional results in an easy way.

The recurrence relation for the soft phase-space volume is trivial to obtain from the recurrence relation for the $\Gamma$ function,

$$\Phi_4^S(d+2) = \frac{(d-4)(d-3)(d-2)^3}{72(d-1)(3d-5)(3d-4)(3d-2)(3d-1)}\frac{\Gamma(d-4)}{64\pi^3\Gamma(d-1)}\Phi_4^S(d)\,. \tag{5.43}$$

As we have defined all our master integrals relative to the phase-space volume $\Phi_4^S$, we can simplify their recurrence relations by factoring out the above result.

We therefore define the ratio

$$\mathcal{R} = \frac{\mathcal{N}_3^d}{\mathcal{N}_3^{d+2}} \frac{\Phi_4^S(d+2)}{\Phi_4^S(d)} = \frac{(d-4)(d-3)(d-2)^3}{72(d-1)(3d-5)(3d-4)(3d-2)(3d-1)}\,, \tag{5.44}$$

where $\mathcal{N}$ was defined in eq. (4.57). We give the results for the remaining master integrals relative to $\mathcal{R}$. The dimensional recurrence relations for the non-trivial master integrals are

$$\begin{aligned}
\mathcal{F}_2(d+2)\mathcal{R} &= -\frac{(d-4)(7d-18)}{3(3d-5)(3d-4)} \\
&\quad -\frac{(d-4)^2(3d-10)}{24(3d-7)(3d-5)(3d-4)}\mathcal{F}_2(d)\,,
\end{aligned} \tag{5.45}$$

$$\begin{aligned}
\mathcal{F}_3(d+2)\mathcal{R} &= \frac{\left(38-28d+5d^2\right)}{3(d-4)(3d-5)} \\
&\quad -\frac{(d-4)^3(d-3)}{18(3d-10)(3d-8)(3d-7)(3d-5)}\mathcal{F}_3(d)\,,
\end{aligned} \tag{5.46}$$

$$\begin{aligned}
\mathcal{F}_4(d+2)\mathcal{R} &= -\frac{4\left(386-387d+128d^2-14d^3\right)}{(d-4)^2(d-3)} \\
&\quad -\frac{(d-4)^2(3d-14)}{24(3d-11)(3d-8)(3d-7)}\mathcal{F}_4(d)\,,
\end{aligned} \tag{5.47}$$

$$\begin{aligned}
\mathcal{F}_5(d+2)\mathcal{R} &= -\frac{(d-4)\left(4752-9636d+6706d^2-1962d^3+207d^4\right)}{72(d-3)(d-1)(3d-10)(3d-8)(3d-5)} \\
&\quad +\frac{(d-4)^2(d-2)}{96(d-1)(3d-7)(3d-5)}\mathcal{F}_5(d)\,,
\end{aligned} \tag{5.48}$$

$$\begin{aligned}
\mathcal{F}_6(d+2)\mathcal{R} &= \frac{\left(4256-6684d+4224d^2-1345d^3+216d^4-14d^5\right)}{3(d-4)^2(d-3)(d-2)^2} \\
&\quad +\frac{(d-4)(3d-10)}{9(d-2)^2(3d-7)}\mathcal{F}_2(d) \\
&\quad -\frac{(d-4)^3}{24(d-2)(3d-11)(3d-7)}\mathcal{F}_6(d)\,,
\end{aligned} \tag{5.49}$$

$$\begin{aligned}
\mathcal{F}_7(d+2)\mathcal{R} &= -\frac{4(2d-7)}{(d-4)(d-3)} \\
&\quad +\frac{(d-4)^4}{72(3d-11)(3d-10)(3d-8)(3d-7)}\mathcal{F}_7(d)\,,
\end{aligned} \tag{5.50}$$

$$
\begin{aligned}
\mathcal{F}_8(d+2)\mathcal{R} &= \frac{2\left(231-114d+14d^2\right)}{3(d-4)(d-3)} + \frac{2(d-4)^2(7d-24)}{9(d-3)(3d-8)(3d-7)}\mathcal{F}_2(d) \\
&\quad + \frac{(d-4)^4}{72(3d-11)(3d-10)(3d-8)(3d-7)}\mathcal{F}_8(d)\,, \qquad (5.51)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{F}_9(d+2)\mathcal{R} &= \frac{2(3d-7)\left(6672-7824d+3460d^2-684d^3+51d^4\right)}{3(d-4)^2(d-3)^2(3d-10)} \\
&\quad + \frac{(d-4)(3d-10)(5d-17)}{12(d-3)^2(3d-8)}\mathcal{F}_2(d) + \frac{(d-4)}{6(d-3)(3d-8)}\mathcal{F}_5(d) \\
&\quad + \frac{(d-4)^3(3d-14)}{96(d-3)(3d-13)(3d-11)(3d-8)}\mathcal{F}_9(d)\,, \qquad (5.52)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{F}_{10}(d+2)\mathcal{R} &= -\frac{4\left(26-39d+16d^2-2d^3\right)}{(d-4)^2(d-3)} - \frac{(d-4)^2(3d-10)}{3(d-3)(3d-8)(3d-7)}\mathcal{F}_2(d) \\
&\quad - \frac{(d-4)^2(3d-14)}{24(3d-11)(3d-8)(3d-7)}\mathcal{F}_{10}(d)\,. \qquad (5.53)
\end{aligned}
$$

## Analytic results for the soft master integrals

In this section we present the analytical results for the master integrals contributing to hadronic Higgs production in the leading and next-to-leading soft approximation. As the explicit evaluation of the master integrals is rather long and technical, we defer all details about the computation to Section 5.5 and only summarize the results at this point. The first master integral, the soft phase-space volume, was already given in eq. (5.29) and will not be repeated here. All the remaining master integrals have been evaluated as a Laurent series in the dimensional regulator up to terms involving zeta values of weight at most six. We have checked that our results agree numerically with the MB integral representation for soft integrals derived in Section 4.4. In addition, the results satisfy the dimensional recurrence relations for the master integrals given in the previous section (integrals in the shifted dimension have been evaluated numerically using the MB representation). Finally, we make an intriguing observation in our results: if we express all the zeta values up to weight six in the basis $\{\zeta_2, \zeta_3, \zeta_4, \zeta_2\,\zeta_3, \zeta_5, \zeta_3^2, \zeta_6\}$, the coefficients in front of the values are integers in all cases. We note that this statement is only true in the specific basis of zeta values that we chose. The results for the master integrals are listed in the rest of this section.

$$
\begin{aligned}
\mathcal{F}_2(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{(s_{13}+s_{15})s_{34}} \\
&= \frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)^2}{\epsilon\,\Gamma(3-6\epsilon)\Gamma(2-2\epsilon)^2}\,{}_3F_2\left[\begin{matrix}1 & 1 & 1-\epsilon \\ 2-2\epsilon & 2-2\epsilon & \end{matrix};1\right] \\
&= \frac{60}{\epsilon}\,\zeta_2 + 420\,\zeta_3 - 282\,\zeta_2 + \epsilon\Big(1800\,\zeta_4 - 1974\,\zeta_3 + 432\,\zeta_2\Big) \\
&+ \epsilon^2\Big(5580\,\zeta_5 + 480\,\zeta_2\,\zeta_3 - 8460\,\zeta_4 + 3024\,\zeta_3 - 216\,\zeta_2\Big) \\
&+ \epsilon^3\Big(19260\,\zeta_6 + 1680\,\zeta_3^2 - 26226\,\zeta_5 - 2256\,\zeta_2\,\zeta_3 + 12960\,\zeta_4 - 1512\,\zeta_3\Big) \\
&+ \mathcal{O}(\epsilon^4)\,.
\end{aligned}
\tag{5.54}
$$

$$
\begin{aligned}
\mathcal{F}_3(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{s_{14}s_{23}s_{34}} \\
&= \frac{90}{\epsilon^4} - \frac{693}{\epsilon^3} + \frac{1}{\epsilon^2}\Big(-60\,\zeta_2 + 1917\Big) + \frac{1}{\epsilon}\Big(-300\,\zeta_3 + 462\,\zeta_2 - 2268\Big) \\
&- 930\,\zeta_4 + 2310\,\zeta_3 - 1278\,\zeta_2 + 972 + \epsilon\Big(-2220\,\zeta_5 - 120\,\zeta_2\,\zeta_3 + 7161\,\zeta_4 \\
&- 6390\,\zeta_3 + 1512\,\zeta_2\Big) + \epsilon^2\Big(-5555\,\zeta_6 - 300\,\zeta_3^2 + 17094\,\zeta_5 + 924\,\zeta_2\,\zeta_3 \\
&- 19809\,\zeta_4 + 7560\,\zeta_3 - 648\,\zeta_2\Big) + \mathcal{O}(\epsilon^3)\,.
\end{aligned}
\tag{5.55}
$$

$$
\begin{aligned}
\mathcal{F}_4(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{s_{13}s_{15}s_{34}s_{45}} \\
&= -\frac{3\,\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{2\epsilon^4\Gamma(1-6\epsilon)} \\
&\times\left[\frac{3\,\Gamma(1-2\epsilon)\Gamma(\epsilon+1)}{(1+3\epsilon)\Gamma(1-3\epsilon)}\,{}_3F_2\left[\begin{matrix}-3\epsilon-1 & -2\epsilon & -\epsilon \\ & -3\epsilon & -3\epsilon\end{matrix};1\right]\right. \\
&+\left.\frac{1}{(1+\epsilon)\Gamma(1-2\epsilon)}\,{}_4F_3\left[\begin{matrix}1 & 1 & 1-\epsilon & -2\epsilon \\ 1-2\epsilon & 1-2\epsilon & 2+\epsilon & \end{matrix};1\right]\right] \\
&= -\frac{600}{\epsilon^4} + \frac{10020}{\epsilon^3} - \frac{70560}{\epsilon^2} - \frac{1}{\epsilon}\Big(480\,\zeta_3 - 303480\Big) - 3600\,\zeta_4 + 8016\,\zeta_3 \\
&- 1007640 - \epsilon\Big(17280\,\zeta_5 - 60120\,\zeta_4 + 56448\,\zeta_3 - 3061800\Big) - \epsilon^2\Big(66000\,\zeta_6 \\
&+ 1920\,\zeta_3^2 - 288576\,\zeta_5 + 423360\,\zeta_4 - 242784\,\zeta_3 + 9185400\Big) + \mathcal{O}(\epsilon^3)\,.
\end{aligned}
\tag{5.56}
$$

$$
\begin{aligned}
\mathcal{F}_5(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{(s_{14}+s_{15})s_{23}s_{345}} \\
&= -\frac{120}{\epsilon}\,\zeta_2 - 960\,\zeta_3 + 684\,\zeta_2 + \epsilon\Big( - 4620\,\zeta_4 + 5472\,\zeta_3 - 1188\,\zeta_2\Big) \\
&+ \epsilon^2\Big( - 17160\,\zeta_5 - 720\,\zeta_2\,\zeta_3 + 26334\,\zeta_4 - 9504\,\zeta_3 + 648\,\zeta_2\Big) \\
&+ \epsilon^3\Big( - 64110\,\zeta_6 - 2880\,\zeta_3^2 + 97812\,\zeta_5 + 4104\,\zeta_2\,\zeta_3 - 45738\,\zeta_4 + 5184\,\zeta_3\Big) \\
&+ \mathcal{O}(\epsilon^4)\,.
\end{aligned}
\tag{5.57}
$$

$$
\begin{aligned}
\mathcal{F}_6(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{(s_{13}+s_{14})(s_{14}+s_{15})s_{23}s_{34}} \\
&= \frac{10}{\epsilon^5} - \frac{137}{\epsilon^4} + \frac{1}{\epsilon^3}\Big(40\,\zeta_2 + 675\Big) + \frac{1}{\epsilon^2}\Big(320\,\zeta_3 - 548\,\zeta_2 - 1530\Big) \\
&+ \frac{1}{\epsilon}\Big(1500\,\zeta_4 - 4384\,\zeta_3 + 2700\,\zeta_2 + 1620\Big) + 5160\,\zeta_5 + 320\,\zeta_2\,\zeta_3 - 20550\,\zeta_4 \\
&+ 21600\,\zeta_3 - 6120\,\zeta_2 - 648 + \epsilon\Big(18340\,\zeta_6 + 1280\,\zeta_3^2 - 70692\,\zeta_5 - 4384\,\zeta_2\,\zeta_3 \\
&+ 101250\,\zeta_4 - 48960\,\zeta_3 + 6480\,\zeta_2\Big) + \mathcal{O}(\epsilon^2)\,.
\end{aligned}
\tag{5.58}
$$

$$
\begin{aligned}
\mathcal{F}_7(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{s_{15}s_{24}s_{34}s_{35}} \\
&= -\frac{3}{2}\,\frac{\Gamma(6-6\epsilon)}{\epsilon^5\,\Gamma(1-6\epsilon)}\,{}_3F_2\left[\begin{matrix}1 \;\; 1 \;\; -2\epsilon \\ 1-2\epsilon \;\; 1-2\epsilon\end{matrix};1\right] \\
&= -\frac{360}{\epsilon^5} + \frac{4932}{\epsilon^4} + \frac{1}{\epsilon^3}\Big(720\,\zeta_2 - 24300\Big) + \frac{1}{\epsilon^2}\Big(4320\,\zeta_3 - 9864\,\zeta_2 + 55080\Big) \\
&+ \frac{1}{\epsilon}\Big(15120\,\zeta_4 - 59184\,\zeta_3 + 48600\,\zeta_2 - 58320\Big) + 43200\,\zeta_5 - 207144\,\zeta_4 \\
&+ 291600\,\zeta_3 - 110160\,\zeta_2 + 23328 + \epsilon\Big(111600\,\zeta_6 - 591840\,\zeta_5 + 1020600\,\zeta_4 \\
&- 660960\,\zeta_3 + 116640\,\zeta_2\Big) + \mathcal{O}(\epsilon^2)\,.
\end{aligned}
\tag{5.59}
$$

$$
\begin{aligned}
\mathcal{F}_8(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{(s_{13}+s_{15})(s_{23}+s_{24})s_{34}s_{35}} \\
&= -\frac{60}{\epsilon^5} + \frac{822}{\epsilon^4} + \frac{1}{\epsilon^3}\Big(240\,\zeta_2 - 4050\Big) + \frac{1}{\epsilon^2}\Big(2400\,\zeta_3 - 3288\,\zeta_2 + 9180\Big) \\
&+ \frac{1}{\epsilon}\Big(13320\,\zeta_4 - 32880\,\zeta_3 + 16200\,\zeta_2 - 9720\Big) + 51840\,\zeta_5 + 3360\,\zeta_2\,\zeta_3 \\
&- 182484\,\zeta_4 + 162000\,\zeta_3 - 36720\,\zeta_2 + 3888 + \epsilon\Big(207600\,\zeta_6 + 11760\,\zeta_3^2 \\
&- 710208\,\zeta_5 - 46032\,\zeta_2\,\zeta_3 + 899100\,\zeta_4 - 367200\,\zeta_3 + 38880\,\zeta_2\Big) + \mathcal{O}(\epsilon^2)\,.
\end{aligned}
\tag{5.60}
$$

$$
\begin{aligned}
\mathcal{F}_9(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{s_{15}(s_{14}+s_{15})s_{23}s_{34}s_{345}} \\
&= \frac{160}{\epsilon^5} - \frac{1712}{\epsilon^4} + \frac{1}{\epsilon^3}\Big(-120\,\zeta_2 + 2784\Big) + \frac{1}{\epsilon^2}\Big(-120\,\zeta_3 + 1284\,\zeta_2 + 31968\Big) \\
&+ \frac{1}{\epsilon}\Big(2520\,\zeta_4 + 1284\,\zeta_3 - 2088\,\zeta_2 - 216864\Big) + 15720\,\zeta_5 + 1920\,\zeta_2\,\zeta_3 \\
&- 26964\,\zeta_4 - 2088\,\zeta_3 - 23976\,\zeta_2 + 795744 + \epsilon\Big(82520\,\zeta_6 + 9600\,\zeta_3^2 \\
&- 168204\,\zeta_5 - 20544\,\zeta_2\,\zeta_3 + 43848\,\zeta_4 - 23976\,\zeta_3 + 162648\,\zeta_2 - 2449440\Big) \\
&+ \mathcal{O}(\epsilon^2)\,.
\end{aligned}
\tag{5.61}
$$

$$
\begin{aligned}
\mathcal{F}_{10}(\epsilon) &= \frac{1}{\Phi_4^S(\epsilon)} \int \frac{d\Phi_4^S}{(s_{23}+s_{24})(s_{24}+s_{25})s_{34}s_{45}} \\
&= -\frac{120}{\epsilon^4} + \frac{2004}{\epsilon^3} - \frac{14112}{\epsilon^2} + \frac{1}{\epsilon}\Big(240\,\zeta_3 + 60696\Big) + 1980\,\zeta_4 - 4008\,\zeta_3 \\
&- 201528 + \epsilon\Big(6960\,\zeta_5 + 1680\,\zeta_2\,\zeta_3 - 33066\,\zeta_4 + 28224\,\zeta_3 + 612360\Big) \\
&+ \epsilon^2\Big(32700\,\zeta_6 + 6840\,\zeta_3^2 - 116232\,\zeta_5 - 28056\,\zeta_2\,\zeta_3 + 232848\,\zeta_4 - 121392\,\zeta_3 \\
&- 1837080\Big) + \mathcal{O}(\epsilon^3)\,.
\end{aligned}
\tag{5.62}
$$

## 5.4 Setup of the calculation

The production of a Higgs boson in the collision of two hadrons $h_1, h_2$ is dominated by QCD processes. The hadronic cross section is related to the partonic cross section by the general factorization formula

$$
\sigma_{h_1+h_2\to H+X} = \sum_{i,j} \int_0^1 dx_1 dx_2 f_i^{h_1}(x_1) f_j^{h_2}(x_2) \sigma_{i+j\to H}(M^2, x_1 x_2 S). \tag{5.63}
$$

Here $f_i^h(x)$ are the parton-distribution functions for the parton $i$ inside of the hadron $h$, $\sigma_{i+j\to H}$ is the partonic cross section and $S$ is the square of the total centre-of-mass energy of the hadronic system. The centre-of-mass energy squared of the partonic system is consequently given by $s = x_i x_j S$. The partonic cross section is expanded perturbatively in the strong coupling constant $\alpha_S$. The leading QCD contribution arises in the SM via a top-quark loop at $\mathcal{O}(\alpha_S^2)$.

We consider the Higgs boson to be relatively light compared to the top quark. This justifies working in the limit of infinite top-quark mass and considering $N_f$ light quarks. We describe the interaction of the Higgs boson with gluons by introducing the effective Lagrangian,

$$\mathcal{L}_{eff} = -\frac{1}{4} c_H G^a_{\mu\nu} G^{a\mu\nu} H. \tag{5.64}$$

Here $G^a_{\mu\nu}$ denotes the gluon field strength tensor and $H$ is the Higgs field. The Wilson coefficient $c_H$ can be found, e.g. in ref. [100, 101, 181]. The next-to-next-to-leading (NNLO) order correction to the inclusive Higgs cross section was computed in the past by employing this effective theory. In this work we present a part of the next term in in the perturbative series ($\text{N}^3$LO) in the effective theory.

At every order in perturbative QCD, the cross section receives contributions from various real- and virtual-radiation processes. We consider only tree-level processes with three real-emission partons in the final state. A direct integration over the phase-space of the corresponding matrix elements is challenging. As we have discussed in the introduction, we pave the way towards the full computation by performing an expansion of the phase-space integrals around the kinematic limit where the Higgs boson is produced at threshold, $s \sim M^2$. In this limit, all partons emitted in the final state are soft and their momenta vanish as $\bar{z} \to 0$. We expand the cross section in the small parameter $\bar{z}$ defined in (5.5). In the following, we shall present the leading and subleading terms in the threshold expansion,

$$\sigma_{ij\to H+X}(s,\bar{z}) = \bar{z}^{-1-6\epsilon} s^{3\epsilon} \sum_{k=0}^{\infty} \bar{z}^k \sigma^{S(k)}_{ij\to H+X}. \tag{5.65}$$

Although we considered in our calculation the Higgs boson $H$ as a final state, we would like to stress the universality of our result for the leading term in the soft expansion for any other colorless final state produced by gluons in the initial state [182]. The subleading term in the soft expansion is no longer universal.

## Calculation

To obtain the real-emission cross section we generate Feynman diagrams using QGRAF [183] and compute squared matrix-elements using programs based on

GiNaC [137] or FORM [184] and our own C++ code for color and spin algebra. We perform our calculation in Feynman gauge with $d$ gluon polarizations in order to maintain a simple structure for the denominators of the squared amplitudes. To recover the result for physical gluon polarizations, we add matrix-elements with Faddeev-Popov ghosts as external states. We compare our results with a set of numeric cross sections for different phase-space points obtained with MadGraph [185] and find perfect agreement.

In a next step we use reverse unitarity, interpret the phase-space integrals as three-loop integrals as described in Section 5.1, and expand them in a Laurent series in $\bar{z}$. The leading and next-to-leading terms in this series are then referred to as the soft and next-to-soft limit of the real-emission cross section. We then derive integration-by-parts (IBP) identities for the scalar soft phase-space integrals. We reduce all integrals to a set of 10 master integrals by employing the Laporta algorithm [146]. We implemented this algorithm in a C++ code that was developed by us specifically for this project, as well as with the program AIR [150]. The calculation of the remaining 10 integrals is discussed in Section 5.5. The explicit expressions for the amplitude can be found in ref. [1].

## 5.5 Analytic computation of the master integrals

In this section we present some details on how to evaluate analytically all the master integrals $\mathcal{F}_i$ defined in Section 5.3. The analytic result for the soft phase-space volume can easily be obtained from the expression for the phase-space volume in general kinematics and will not be discussed here (see section 4.3 for the derivation).

In general, our strategy is to follow the steps outlined in Section 4.4: we use the 'energies and angles' parametrization to obtain a representation for the integral where the energies and angles appear in a factorized form. This may require the introduction of MB integrations in order to factorize sums of invariants in a denominator. We then integrate out the energies and angles to obtain a multifold MB representation for each master integral. Whenever we are able to do so, we evaluate the remaining MB integrals to all orders in $\epsilon$ in terms of hypergeometric functions that can easily be expanded into a Laurent series $\epsilon$ using the `HypExp` package [163]. In those cases where we did no manage to perform the MB integral in closed form for finite values of $\epsilon$, we only compute the Laurent expansion of the integral around $\epsilon = 0$, e.g., by resolving singularities in $\epsilon$ and summing up harmonic sums or by converting the MB integral to a parametric integral which can be computed more easily. Details on how to perform these steps for the different master integrals will be given in the rest of this section.

### The master integral $\mathcal{F}_3$

In this section we compute the master integral $\mathcal{F}_3$ defined by,

$$\Phi_4^S(\epsilon)\,\mathcal{F}_3(\epsilon) = \int \frac{d\Phi_4^S}{s_{14}s_{23}s_{34}}\,. \tag{5.66}$$

The integrand only involves two-particle invariants, so following the discussion in Section 4.4 we can immediately insert the energies and angles parametrization and integrate out the energies in terms of $\Gamma$ functions. The remaining angular integrations can easily be carried out using the formulas given in Section 4.4. Note that in the present case all the angular integrals can be performed in closed form, so there is no need to introduce MB representations for the angular integrals. We obtain,

$$\begin{aligned}
\mathcal{F}_3(\epsilon) &= 2^{6\epsilon-7}\pi^{3\epsilon-3}\frac{\Gamma(6-6\epsilon)\Gamma(2-2\epsilon)\Gamma(1-2\epsilon)^2}{\epsilon^2\,\Gamma(2-6\epsilon)\Gamma(1-\epsilon)^3}\int\frac{d\Omega_3^{(d-1)}\,d\Omega_4^{(d-1)}\,d\Omega_5^{(d-1)}}{(\beta_1\cdot\beta_4)\,(\beta_2\cdot\beta_3)\,(\beta_3\cdot\beta_4)}\\
&= 2^{6\epsilon-7}\pi^{3\epsilon-3}\frac{\Gamma(6-6\epsilon)\Gamma(2-2\epsilon)\Gamma(1-2\epsilon)^2}{\epsilon^2\,\Gamma(2-6\epsilon)\Gamma(1-\epsilon)^3}\,\Omega_{3-2\epsilon}\int\frac{d\Omega_3^{(d-1)}}{(\beta_2\cdot\beta_3)}\,\Omega_{d-1}^{(1,1)}(\beta_1\cdot\beta_3)\\
&= -2^{2\epsilon-1}\,\frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{\epsilon^3\,\Gamma(2-6\epsilon)\Gamma(1-\epsilon)^2}\int_{-1}^1\frac{d\cos\theta_3}{(1+\cos\theta_3)^{1+\epsilon}(1-\cos\theta_3)^\epsilon}\\
&\quad\times{}_2F_1\left(1,1;1-\epsilon;\frac{1+\cos\theta_3}{2}\right)\,.
\end{aligned} \tag{5.67}$$

The remaining integral can be brought into a more standard form by the change of variable $\cos\theta_3 = 2y-1$,

$$\begin{aligned}
\int_{-1}^1&\frac{d\cos\theta_3}{(1+\cos\theta_3)^{1+\epsilon}(1-\cos\theta_3)^\epsilon}\,{}_2F_1\left(1,1;1-\epsilon;\frac{1+\cos\theta_3}{2}\right)\\
&= 2^{-2\epsilon}\int_0^1 dy\,y^{-1-\epsilon}\,(1-y)^{-\epsilon}\,{}_2F_1(1,1;1-\epsilon;y)\,.
\end{aligned} \tag{5.68}$$

The integral over $y$ is now easily performed using the recursive definition of the hypergeometric function,

$$\begin{aligned}
{}_{p+1}F_p(a_1,\ldots,a_{p+1};b_1,\ldots,b_p;z) &= \frac{\Gamma(b_p)}{\Gamma(a_{p+1})\Gamma(b_p-a_{p+1})}\\
&\times\int_0^1 dt\,t^{a_{p+1}-1}\,(1-t)^{b_p-a_{p+1}-1}\,{}_pF_{p-1}(a_1,\ldots,a_p;b_1,\ldots,b_{p-1};zt)\,.
\end{aligned} \tag{5.69}$$

We immediately get,

$$\mathcal{F}_3(\epsilon) = \frac{\Gamma(6-6\epsilon)}{2\epsilon^4\Gamma(2-6\epsilon)}\,{}_3F_2(1,1,-\epsilon;1-2\epsilon,1-\epsilon;1)\,. \tag{5.70}$$

The ${}_3F_2$ function can be expanded to the desired order in $\epsilon$ using the `HypExp` package [163], and we arrive immediately at the Laurent series of eq. (5.55).

### The master integral $\mathcal{F}_2$

The integrand of the master integral $\mathcal{F}_2$ involves a sum of two-particle invariants in the denominator. We replace the sum by a product, at the price of introducing an MB integration via eq. (4.60),

$$\begin{aligned}\Phi_4^S(\epsilon)\,\mathcal{F}_2(\epsilon) &= \int \frac{d\Phi_4^S}{(s_{13}+s_{15})s_{34}} \\ &= \int_{-i\infty}^{+i\infty}\frac{dz_1}{2\pi i}\Gamma\left(-z_1\right)\Gamma\left(z_1+1\right)\int\frac{d\Phi_4^S}{s_{13}^{z_1+1}s_{15}^{-z_1}s_{34}}\,.\end{aligned} \tag{5.71}$$

The phase-space integral is now in the form (4.126), and so we can introduce the energies and angles parametrization and integrate out all the energy and the angular variables. This results in the following two-fold integral representation for $\mathcal{F}_2$, which is of mixed MB- and Euler-type,

$$\begin{aligned}\mathcal{F}_2(\epsilon) \;=\; &\frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{\epsilon\,\Gamma(3-6\epsilon)\Gamma(1-\epsilon)^4}\int_{-i\infty}^{+i\infty}\frac{dz_1}{2\pi i}\Gamma\left(-z_1\right)\Gamma\left(z_1+1\right)\Gamma\left(-\epsilon-z_1\right) \\ &\times\Gamma\left(1-\epsilon+z_1\right)\int_0^1 dy\,y^{-\epsilon}\left(1-y\right)^{-\epsilon}{}_2F_1\left(1,z_1+1;1-\epsilon;y\right)\,.\end{aligned} \tag{5.72}$$

The Euler integral over $y$ can be performed immediately in terms of a ${}_3F_2$ function, but after that we still need to integrate over the MB parameter $z_1$. We therefore prefer not to perform the integration over $y$, but rather insert the MB representation for the hypergeometric function in the integrand,

$$\begin{aligned}&{}_pF_q(a_1,\ldots,a_p;b_1,\ldots,b_q;x) \\ &\quad= \int_{-i\infty}^{+i\infty}\frac{dz}{2\pi i}(-x)^z\,\Gamma(-z)\left[\prod_{i=1}^{p}\frac{\Gamma(a_i+z)}{\Gamma(a_i)}\right]\left[\prod_{i=1}^{q}\frac{\Gamma(b_i)}{\Gamma(b_i+z)}\right]\,.\end{aligned} \tag{5.73}$$

The integral over $y$ evaluates to a Beta function, and we are left with the following two-dimensional MB integral,

$$\begin{aligned}\mathcal{F}_2(\epsilon) \;=\; &\frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{\epsilon\,\Gamma(3-6\epsilon)\Gamma(1-\epsilon)^2}\int_{-i\infty}^{+i\infty}\frac{dz_1dz_2}{(2\pi i)^2}\left(-1\right)^{z_2}\Gamma\left(-z_1\right)\Gamma\left(-z_2\right) \\ &\times\frac{\Gamma\left(z_2+1\right)\Gamma\left(z_1+z_2+1\right)\Gamma\left(-\epsilon-z_1\right)\Gamma\left(1-\epsilon+z_1\right)}{\Gamma\left(2-2\epsilon+z_2\right)}\,.\end{aligned} \tag{5.74}$$

The integral over $z_1$ is easily performed using Barnes' first lemma, and the remaining one-fold MB integral can immediately be recognized as a ${}_3F_2$ function (see eq. (5.73)). We finally obtain the following result for the master integral $\mathcal{F}_2$, in agreement with eq. (5.54),

$$\mathcal{F}_2(\epsilon) \;=\; \frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)^2}{\epsilon\,\Gamma(3-6\epsilon)\Gamma(2-2\epsilon)^2}\,{}_3F_2(1,1,1-\epsilon;2-2\epsilon,2-2\epsilon;1)\,. \tag{5.75}$$

### The master integral $\mathcal{F}_7$

The integrand of $\mathcal{F}_7$ only contains two-particle invariants,

$$\Phi_4^S(\epsilon)\,\mathcal{F}_7(\epsilon) = \int \frac{d\Phi_4^S}{s_{15}s_{24}s_{34}s_{35}}\,. \tag{5.76}$$

We can therefore immediately integrate out the energy and the angular variables. We obtain,

$$\begin{aligned}\mathcal{F}_7(\epsilon) &= 3\frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{\epsilon^4\,\Gamma(1-\epsilon)^2\Gamma(1-6\epsilon)}\int_0^1 dy\,y^{-\epsilon}\,(1-y)^{-\epsilon} \\ &\quad\times {}_2F_1(1,1;1-\epsilon;1-y)\,{}_2F_1(1,1;1-\epsilon;y)\,.\end{aligned} \tag{5.77}$$

In order to perform the integral over $y$, we introduce an MB representation for each ${}_2F_1$ function in the integrand and perform the $y$ integration. This leaves us with the following two-fold MB representation for $\mathcal{F}_7$,

$$\begin{aligned}\mathcal{F}_7(\epsilon) &= 3\frac{\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{\epsilon^4\,\Gamma(1-\epsilon)^2\Gamma(1-6\epsilon)} \\ &\quad\times\int_{-i\infty}^{+i\infty}\frac{dz_1dz_2}{(2\pi i)^2}\,(-1)^{z_1+z_2}\frac{\Gamma(-z_1)\,\Gamma(z_1+1)^2\,\Gamma(-z_2)\,\Gamma(z_2+1)^2}{\Gamma(-2\epsilon+z_1+z_2+2)}\,.\end{aligned} \tag{5.78}$$

To proceed, we notice that one of the two integrations evaluates to a ${}_2F_1$, which can be reduced to $\Gamma$ functions using Gauss's identity,

$$\begin{aligned}\int_{-i\infty}^{+i\infty}\frac{dz_1}{2\pi i}\,(-1)^{z_1}\frac{\Gamma(-z_1)\,\Gamma(z_1+1)^2}{\Gamma(-2\epsilon+z_1+z_2+2)} &= \frac{1}{\Gamma(2-2\epsilon+z_2)}\,{}_2F_1(1,1;2-2\epsilon+z_2;1) \\ &= \frac{\Gamma(-2\epsilon+z_2)}{\Gamma(1-2\epsilon+z_2)^2}\,.\end{aligned} \tag{5.79}$$

Inserting this result into the two-fold MB integral, we immediately see that the remaining MB integral evaluates to a ${}_3F_2$ function, and we get,

$$\mathcal{F}_7(\epsilon) = -\frac{3}{2}\,\frac{\Gamma(6-6\epsilon)}{\epsilon^5\,\Gamma(1-6\epsilon)}\,{}_3F_2(1,1,-2\epsilon;1-2\epsilon,1-2\epsilon;1)\,. \tag{5.80}$$

### The master integral $\mathcal{F}_4$

The integral $\mathcal{F}_4$ is defined by,

$$\Phi_4^S(\epsilon)\,\mathcal{F}_4(\epsilon) = \int \frac{d\Phi_4^S}{s_{13}s_{15}s_{34}s_{45}}\,. \tag{5.81}$$

The integrand contains only two-particle invariants, and we can immediately integrate out the energy and angular variables in the usual way. We obtain a one-fold MB representation,

$$\begin{aligned}\mathcal{F}_4(\epsilon) = &\frac{\Gamma(6-6\epsilon)\Gamma(-2\epsilon)}{\epsilon^4\Gamma(-6\epsilon)\Gamma(-\epsilon)^2}\int_{-i\infty}^{+i\infty}\frac{dz_1}{2\pi i}\Gamma\left(-z_1\right)\\ &\times\frac{\Gamma\left(z_1+1\right)^2\Gamma\left(z_1-2\epsilon\right)\Gamma\left(-z_1-\epsilon-1\right)\Gamma\left(z_1-\epsilon+1\right)}{\Gamma\left(z_1-2\epsilon+1\right)^2}.\end{aligned} \tag{5.82}$$

Closing the integration contour to the right and summing up residues at $z_1 = n$ and $z_1 = -1-\epsilon+n$, $n \in \mathbb{N}^\times$, we immediately see that $\mathcal{F}_4$ can be expressed as a combination of hypergeometric functions,

$$\begin{aligned}\mathcal{F}_4(\epsilon) \; = &-\frac{3\,\Gamma(6-6\epsilon)\Gamma(1-2\epsilon)}{2\epsilon^4\Gamma(1-6\epsilon)}\\ &\times\left[\frac{3\,\Gamma(1-2\epsilon)\Gamma(\epsilon+1)}{(1+3\epsilon)\Gamma(1-3\epsilon)}\,{}_3F_2(-3\epsilon-1,-2\epsilon,-\epsilon;-3\epsilon,-3\epsilon;1)\right.\\ &\left.+\frac{1}{(1+\epsilon)\Gamma(1-2\epsilon)}\,{}_4F_3(1,1,1-\epsilon,-2\epsilon;1-2\epsilon,1-2\epsilon,2+\epsilon;1)\right].\end{aligned} \tag{5.83}$$

### The master integral $\mathcal{F}_6$

The integral $\mathcal{F}_6$ contains two sums in the denominator, which we can replace by products to the price at introducing two MB integrations,

$$\begin{aligned}\Phi_4^S(\epsilon)\,\mathcal{F}_6(\epsilon) &= \int\frac{d\Phi_4^S}{(s_{13}+s_{14})(s_{14}+s_{15})s_{23}s_{34}}\\ &= \int_{-i\infty}^{+i\infty}\frac{dz_1dz_2}{(2\pi i)^2}\Gamma\left(-z_1\right)\Gamma\left(z_1+1\right)\Gamma\left(-z_2\right)\Gamma\left(z_2+1\right)\\ &\times\int\frac{d\Phi_4^S}{s_{13}^{-z_1}s_{14}^{z_1+z_2+2}s_{15}^{-z_2}s_{23}s_{34}}.\end{aligned} \tag{5.84}$$

We then proceed in the by-now familiar way, integrate out the energies and the angles, and arrive at the following two-fold MB representation for $\mathcal{F}_6$,

$$\begin{aligned}\mathcal{F}_6(\epsilon) = &\frac{\Gamma(6-6\epsilon)}{\epsilon\,\Gamma(1-6\epsilon)\Gamma(1-\epsilon)^2}\\ &\times\int_{-i\infty}^{+i\infty}\frac{dz_1dz_2}{(2\pi i)^2}\Gamma\left(-z_1\right)\Gamma\left(z_1+1\right)\Gamma\left(-z_2\right)\Gamma\left(z_2+1\right)\\ &\times\frac{\Gamma\left(-\epsilon+z_1-z_2\right)\Gamma\left(z_2-\epsilon\right)\Gamma\left(-2\epsilon-z_1+z_2\right)\Gamma\left(-\epsilon-z_1+z_2\right)}{\Gamma\left(-\epsilon+z_2+1\right)\Gamma\left(-2\epsilon-z_1+z_2+1\right)}.\end{aligned} \tag{5.85}$$

Unlike in the previous cases, we were not able to reduce this integral for generic $\epsilon$ to simple hypergeometric functions. We therefore only compute the Laurent expansion of the integral. We proceed in the standard way: we apply the packages `MB` [167], `MBresolve` [168] and `barnesroutines` [162] to resolve singularities in $\epsilon$ and to expand the resulting integrals under the integration sign and apply Barnes' lemmas in an automated way. The resulting MB integrals are at most two-fold, and all of them can easily be done by closing the contours to the right and summing up residues in terms of nested harmonic sums defined recursively by ref. [170],

$$S_i(n) = \sum_{k=1}^{n} \frac{1}{k^i} \quad \text{and} \quad S_{i\vec{\jmath}}(n) = \sum_{k=1}^{n} \frac{S_{\vec{\jmath}}(k)}{k^i} \,. \tag{5.86}$$

Note that in the limit $n \to \infty$ harmonic sums immediately reduce to combinations of multiple zeta values. The result for $\mathcal{F}_6$ reads,

$$\begin{aligned}\mathcal{F}_6(\epsilon) \; &= \frac{10}{\epsilon^5} - \frac{137}{\epsilon^4} + \frac{1}{\epsilon^3}\Big(40\,\zeta_2 + 675\Big) + \frac{1}{\epsilon^2}\Big(320\,\zeta_3 - 548\,\zeta_2 - 1530\Big) \\ &+ \frac{1}{\epsilon}\Big(1500\,\zeta_4 - 4384\,\zeta_3 + 2700\,\zeta_2 + 1620\Big) + 5160\,\zeta_5 + 320\,\zeta_2\,\zeta_3 \\ &- 20550\,\zeta_4 + 21600\,\zeta_3 - 6120\,\zeta_2 - 648 \\ &+ \epsilon\Big(18340\,\zeta_6 + 1280\,\zeta_3^2 - 70692\,\zeta_5 - 4384\,\zeta_2\,\zeta_3 \\ &+ 101250\,\zeta_4 - 48960\,\zeta_3 + 6480\,\zeta_2\Big) + \mathcal{O}(\epsilon^2)\,.\end{aligned} \tag{5.87}$$

## The master integral $\mathcal{F}_{10}$

The integrand of $\mathcal{F}_{10}$ involves two sums in the denominator, so we start by introducing two MB representations,

$$\begin{aligned}\Phi_4^S(\epsilon)\,\mathcal{F}_{10}(\epsilon) &= \int \frac{d\Phi_4^S}{(s_{23}+s_{24})(s_{24}+s_{25})s_{34}s_{45}} \\ &= \int_{-i\infty}^{+i\infty} \frac{dz_1 dz_2}{(2\pi i)^2} \Gamma\left(-z_1\right)\Gamma\left(z_1+1\right)\Gamma\left(-z_2\right)\Gamma\left(z_2+1\right) \\ &\times \int \frac{d\Phi_4^S}{s_{23}^{-z_1} s_{24}^{2+z_1+z_2} s_{25}^{-z_2} s_{34} s_{45}}\,.\end{aligned} \tag{5.88}$$

Integrating over the angles of particles 3 and 4 yields two hypergeometric functions, and we introduce an MB representation for each of them. Performing the integration over the last angle, we obtain a four-fold MB representation for $\mathcal{F}_{10}$. Two integrations can immediately be performed using Barnes' lemmas, and we obtain,

$$
\begin{aligned}
\mathcal{F}_{10}(\epsilon) = 6\frac{\Gamma(6-6\epsilon)}{\Gamma(1-\epsilon)^3\Gamma(1-6\epsilon)} \int_{-i\infty}^{+i\infty} \frac{dz_2 dz_3}{(2\pi i)^2}\Gamma\left(-z_2\right)\Gamma\left(-z_3\right)\Gamma\left(z_2+1\right) \\
\times \frac{\Gamma\left(-2\epsilon-z_2-1\right)\Gamma\left(-\epsilon+z_2+1\right)\Gamma\left(-2\epsilon-z_3-1\right)}{\Gamma\left(-2\epsilon-z_2\right)\Gamma\left(-2\epsilon-z_3\right)} \\
\times \Gamma\left(z_3+1\right)\Gamma\left(-\epsilon-z_2-z_3-1\right)\Gamma\left(z_3-\epsilon\right) .
\end{aligned}
\tag{5.89}
$$

After resolving the singularities in $\epsilon$ and expanding under the integration sign, all the twofold integrals can be reduced to one-fold integrals using Barnes' lemmas and their corollaries. The remaining one-fold integrals are trivial to compute by closing the contour and summing up residues. We find,

$$
\begin{aligned}
\mathcal{F}_{10}(\epsilon) \;&= -\frac{120}{\epsilon^4}+\frac{2004}{\epsilon^3}-\frac{14112}{\epsilon^2}+\frac{1}{\epsilon}\Big(240\,\zeta_3+60696\Big)+1980\,\zeta_4-4008\,\zeta_3 \\
&\quad -201528+\epsilon\Big(6960\,\zeta_5+1680\,\zeta_2\,\zeta_3-33066\,\zeta_4+28224\,\zeta_3+612360\Big) \\
&\quad +\epsilon^2\Big(32700\,\zeta_6+6840\,\zeta_3^2-116232\,\zeta_5-28056\,\zeta_2\,\zeta_3+232848\,\zeta_4 \\
&\quad -121392\,\zeta_3-1837080\Big)+\mathcal{O}(\epsilon^3)\,.
\end{aligned}
\tag{5.90}
$$

### The master integral $\mathcal{F}_5$

We start by replacing the sums in the denominator of the integrand of $\mathcal{F}_5$ by three MB integrals,

$$
\begin{aligned}
\Phi_4^S(\epsilon)\,\mathcal{F}_5(\epsilon) \;&= \int \frac{d\Phi_4^S}{(s_{14}+s_{15})s_{23}s_{345}} \\
&= \int_{-i\infty}^{+i\infty} \frac{dz_1 dz_2 dz_3}{(2\pi i)^3}\Gamma(-z_1)\Gamma(-z_2)\Gamma(-z_3)\Gamma(1+z_1+z_2)\Gamma(1+z_3) \\
&\quad \times \int \frac{d\Phi_4^S}{s_{14}^{1+z_1}s_{15}^{-z_1}s_{23}s_{34}^{1+z_1+z_2}s_{45}^{-z1}s_{35}^{-z2}}\,.
\end{aligned}
\tag{5.91}
$$

We insert the energies and angles parametrization for the final-state particles and introduce MB integrations for the angular integrals. Note that the first angular integral necessarily involves three massless propagators and can thus not be done in closed form as an ${}_2F_1$, so we insert the three-fold MB representation (4.133) for it. We then arrive at a representation for $\mathcal{F}_5$ as a six-fold MB integral convoluted with two angular integrations. It turns out that after performing the change of variables $z_3 \to z_3+z_5$ and $z_6 \to z_6+z_1+z_2$, the integrals over $z_1$, $z_2$ and $z_5$ can be done in closed form using Barnes' first lemma.

The remaining two angular integrations can easily be performed in terms of hypergeometric functions, and all but one MB integration can be performed using Barnes' lemmas. We thus arrive at a one-fold MB representation for $\mathcal{F}_5$,

$$\begin{aligned}\mathcal{F}_5(\epsilon) &= -\frac{\Gamma(6-6\epsilon)\Gamma(1-3\epsilon)}{\epsilon\,\Gamma(2-6\epsilon)\Gamma(2-2\epsilon)\Gamma(1-\epsilon)} \\ &\quad\times\int_{-i\infty}^{+i\infty}\frac{dz_1}{2\pi i}\frac{\Gamma(-z_1)\,\Gamma(z_1+1)^2\,\Gamma(-z_1-2\epsilon)\,\Gamma(z_1-\epsilon+1)}{\Gamma(z_1-3\epsilon+2)}\,.\end{aligned} \tag{5.92}$$

One might be tempted to sum up the residues at $z_1 = n$ and $z_1 = -2\epsilon + n$, $n \in \mathbb{N}^\times$, for finite values of $\epsilon$ to obtain an expression for $\mathcal{F}_5$ as a combination of two hypergeometric functions at 1 valid to all orders in $\epsilon$. The two hypergeometric functions are however separately divergent (even for finite values of $\epsilon$) and only their sum is finite. We therefore only compute a Laurent series for $\mathcal{F}_5$. Resolving singularities in $\epsilon$ and summing up residues in terms of harmonic sums we obtain,

$$\begin{aligned}\mathcal{F}_5(\epsilon) &= -\frac{120}{\epsilon}\,\zeta_2 - 960\,\zeta_3 + 684\,\zeta_2 + \epsilon\Big(-4620\,\zeta_4 + 5472\,\zeta_3 - 1188\,\zeta_2\Big) \\ &\quad+\epsilon^2\Big(-17160\,\zeta_5 - 720\,\zeta_2\,\zeta_3 + 26334\,\zeta_4 - 9504\,\zeta_3 + 648\,\zeta_2\Big) \\ &\quad+\epsilon^3\Big(-64110\,\zeta_6 - 2880\,\zeta_3^2 + 97812\,\zeta_5 + 4104\,\zeta_2\,\zeta_3 - 45738\,\zeta_4 \\ &\quad+5184\,\zeta_3\Big) + \mathcal{O}(\epsilon^4)\,.\end{aligned} \tag{5.93}$$

## The master integral $\mathcal{F}_8$

The master integral $\mathcal{F}_8$ is defined by,

$$\Phi_4^S(\epsilon)\,\mathcal{F}_8(\epsilon) = \int\frac{d\Phi_4^S}{(s_{13}+s_{15})(s_{23}+s_{24})s_{34}s_{35}}\,. \tag{5.94}$$

We start by introducing two MB integrations in order to remove the sums in the denominator of the integral $\mathcal{F}_8$. The energies are integrated out in terms of $\Gamma$ functions, and the angular integrations over particles 4 and 5 are performed using eq. (4.132). At this stage we have three integrations left to do: the two MB integrations and the integral over $\cos\theta_3 = 2y - 1$,

$$\begin{aligned}\mathcal{F}_8(\epsilon) &= -\frac{6\Gamma(6-6\epsilon)}{\epsilon\,\Gamma(1-\epsilon)^4\Gamma(1-6\epsilon)}\int_{-i\infty}^{+i\infty}\frac{dz_1dz_2}{(2\pi i)^2}\int_0^1 dy\,y^{z_2-\epsilon}\,(1-y)^{z_1-\epsilon} \\ &\quad\times\Gamma(z_1+1)\,\Gamma(-z_2)\,\Gamma(z_2+1)\,\Gamma(-\epsilon-z_1)\,\Gamma(-\epsilon-z_2) \\ &\quad\times{}_2F_1(1,z_1+1;1-\epsilon;y)\;{}_2F_1(1,z_2+1;1-\epsilon;1-y) \\ &\quad\times\Gamma(-z_1)\,\Gamma(-2\epsilon+z_1+z_2)\,.\end{aligned} \tag{5.95}$$

In order to proceed, we first apply the identity,

$$ {}_2F_1(a,b;c;x) = (1-x)^{-b}\, {}_2F_1\left(c-a,b;c;\frac{x}{x-1}\right) , \tag{5.96} $$

and then insert an MB representation for each hypergeometric function in the integrand of eq. (5.95). The reason to apply eq. (5.96) before inserting the MB integrations comes from the fact that in this way one of the four MB integrations can be performed using Barnes' first lemma. We then arrive at the following three-fold MB representation for $\mathcal{F}_8$,

$$ \begin{aligned} \mathcal{F}_8(\epsilon) \;=& -\frac{6\epsilon\,\Gamma(6-6\epsilon)}{\Gamma(1-\epsilon)^4\Gamma(1-6\epsilon)} \int_{-i\infty}^{+i\infty} \frac{dz_2 dz_3 dz_4}{(2\pi i)^3}\, \Gamma\left(-z_2\right)\Gamma\left(-z_3\right)\Gamma\left(-z_4\right) \\ & \times \Gamma\left(z_3+1\right)\Gamma\left(z_2-2\epsilon\right)\Gamma\left(-z_2-z_4\right)\Gamma\left(z_2+z_4+1\right)\Gamma\left(-\epsilon-z_3\right) \\ & \times \Gamma\left(z_3-\epsilon\right) \frac{\Gamma\left(-2\epsilon+z_2-z_3\right)\Gamma\left(-\epsilon-z_4\right)\Gamma\left(z_4-\epsilon\right)}{\Gamma\left(-2\epsilon+z_2+1\right)\Gamma\left(-2\epsilon-z_3-z_4\right)} . \end{aligned} \tag{5.97} $$

In the rest of this section we show how we can compute a Laurent expansion for this integral. We proceed in the standard way and resolve singularities in $\epsilon$. At the end of this procedure, we have a collection of MB integrals of dimensionality at most three with integration contours that are straight vertical lines. These integrals can then be safely expanded in $\epsilon$ under the integration sign. In the following we discuss the computation of the two and three-fold integrals.

**Three-fold MB integrals.** There is one three-fold integral contributing to $\mathcal{F}_8$,

$$ \begin{aligned} \mathcal{F}_{8,3} = & \int_{-i\infty}^{+i\infty} \frac{dz_2 dz_3 dz_4}{(2\pi i)^3} \Gamma\left(-z_2\right)\Gamma\left(z_2\right)\Gamma\left(-z_4\right)^2\Gamma\left(z_4\right) \\ & \times \frac{\Gamma\left(1-z_3-z_4\right)\Gamma\left(z_2+z_4+1\right)\Gamma\left(z_3+z_4\right)^2\Gamma\left(z_2+z_3+z_4\right)}{\Gamma\left(z_2+1\right)\Gamma\left(z_3\right)} \\ & \times \Gamma\left(-z_2-z_4\right)\Gamma\left(-z_3-z_4\right) . \end{aligned} \tag{5.98} $$

where we omit all $\Gamma$ function prefactors and where the integration contours are straight vertical lines defined by,

$$ \Re(z_3) = 0.28 \;\text{ and }\; \Re(z_4) = 0.97 \;\text{ and }\; \Re(z_5) = -0.36 . \tag{5.99} $$

We start by closing the $z_3$ contour to the right and take residues,

$$\int_{-i\infty}^{+i\infty} \frac{dz_2 dz_4}{(2\pi i)^2} \frac{\Gamma(-z_2)\Gamma(z_2)\Gamma(-z_2-z_4)\Gamma(-z_4)^2\Gamma(z_4)\Gamma(z_2+z_4+1)}{\Gamma(z_2+1)}$$
$$\times \sum_{n=1}^{\infty} \left\{ \frac{\Gamma(n+z_2)}{n\,\Gamma(n-z_4)} \psi(n+z_2) - \frac{\Gamma(n+z_2)}{n\,\Gamma(n-z_4)} \psi(n-z_4) \right.$$
$$\left. - \frac{\Gamma(n+z_2)}{n^2\,\Gamma(n-z_4)} \right\} . \tag{5.100}$$

The first two sums can be performed in terms of $\Gamma$ functions and their derivatives. We illustrate this on the first term (the second term is similar),

$$\begin{aligned} \sum_{n=1}^{\infty} \frac{\Gamma(n+z_2)}{n\,\Gamma(n-z_4)} \psi(n+z_2) &= \lim_{\eta\to 0} \frac{\partial}{\partial \eta} \sum_{n=1}^{\infty} \frac{\Gamma(n+z_2+\eta)}{n\,\Gamma(n-z_4)} \\ &= \lim_{\eta\to 0} \frac{\partial}{\partial \eta} \left\{ \frac{\Gamma(\eta+z_2)}{\Gamma(-z_4)} \left[\psi(-z_4) - \psi(-\eta-z_2-z_4)\right] \right\} \\ &= -\frac{\Gamma(z_2)}{\Gamma(-z_4)} \Big[ \psi(z_2+1)\,\psi(-z_2-z_4) - \frac{1}{z_2}\psi(-z_2-z_4) \\ &\quad - z_2\psi(z_2+1)\,\psi(-z_4) + \frac{1}{z_2}\psi(-z_4) - \psi'(-z_2-z_4) \Big] . \end{aligned} \tag{5.101}$$

In this way, the first two terms can effectively be reduced to the computation of two-fold integrals, and we will therefore not discuss them any further in this section.

The third term can also be summed up in closed form. However, unlike the first two terms, the sum cannot be expressed in terms of $\Gamma$ functions and their derivatives alone, but evaluates to a ${}_4F_3$ function. We therefore arrive at the following single three-fold MB integral,

$$\begin{aligned} \mathcal{F}_{8,3} = -\int_{-i\infty}^{+i\infty} &\frac{dz_2 dz_4}{(2\pi i)^2} \frac{\Gamma(-z_2)\Gamma(z_2)\Gamma(-z_2-z_4)\Gamma(-z_4)^2\Gamma(z_4)}{\Gamma(1-z_4)} \\ &\times \Gamma(z_2+z_4+1)\ {}_4F_3(1,1,1,z_2+1;2,2,1-z_4;1) . \end{aligned} \tag{5.102}$$

Although it looks as though we have managed to reduce the three-fold integral to a two-fold integral, it is still secretly three-fold, except that we have 'hidden' one integration inside the ${}_4F_3$ function. The advantage of this representation is that we can change the representation for the ${}_4F_3$ function in the integrand. More precisely, we perform the change of variables $z_4 \to -z_4 - z_2$ and chose the contours to be straight vertical lines given by,

$$\Re(z_2) = \frac{1}{3} \ \text{ and } \ \Re(z_4) = \frac{1}{5} . \tag{5.103}$$

We then insert an Euler integral representation for the ${}_4F_3$ function as an integral over a ${}_3F_2$. The ${}_3F_2$ function turns out to be reducible,

$$ {}_3F_2\left(1,1,1;2,2;t\right) = \frac{\mathrm{Li}_2(t)}{t}\,, \tag{5.104}$$

and so we finally arrive at,

$$\begin{aligned} \mathcal{F}_{8,3} = &-\int_{-i\infty}^{+i\infty} \frac{dz_2 dz_4}{(2\pi i)^2} \int_0^1 dt\, t^{z_2-1}\left(1-t\right)^{z_4-1}\mathrm{Li}_2(t) \\ &\times \frac{\Gamma\left(-z_2\right)\Gamma\left(z_2\right)\Gamma\left(1-z_4\right)\Gamma\left(-z_2-z_4\right)\Gamma\left(z_2+z_4\right)^2}{\Gamma\left(z_2+1\right)}\,, \end{aligned} \tag{5.105}$$

Next, we would like to exchange the MB and the Euler integration and sum up the residues of the poles of the $\Gamma$ functions in the integrand. However, we are only allowed to do so if the Euler integration does not produce any new poles whose residues need to be taken into account. It is easy to see that in our case the Euler integral converges whenever $\Re(z_2)$ and $\Re(z_4)$ are positive. We can thus close both contours to the right and exchange the Euler and MB integrations and then sum up the residues coming from the $\Gamma$ functions.

We start by taking residues in $z_2$ and then the residues in $z_4$. There are several cases to be considered separately:

1. The poles at $z_2 = n_2 \in \mathbb{N}^\times$ give rise to poles in $z_4$ at $n_4 \in \mathbb{N}^\times$. Hence, we obtain double sums of the form

$$\sum_{n_2,n_4=1}^{\infty} \binom{n_2+n_4}{n_2} \frac{S_{\vec{\imath}_1}(n_2)}{n_2^{j_1}} \frac{S_{\vec{\imath}_2}(n_4)}{n_4^{j_2}} \frac{S_{\vec{\imath}_3}(n_2+n_4)}{(n_2+n_4)^{j_3}}\, t^{n_2}\left(1-t\right)^{n_4}. \tag{5.106}$$

Sums of this type can be performed using XSummer [186, 187], and give rise to complicated multiple polylogarithms whose arguments are rational functions of $t$ and $(1-t)$. Using the coproduct calculus all these complicated multiple polylogarithms can be reduced to harmonic polylogarithms with indices 0 and 1 in $t$.

2. Taking the residues at the poles at $z_2 = -z_4 + n_2$, $n_2 \in \mathbb{N}^\times$ gives rise to the expression,

$$\begin{aligned} -\int_0^1 dt\,\mathrm{Li}_2(t) \sum_{n_2=1}^{\infty} \int_{-i\infty}^{+i\infty} \frac{dz_4}{2\pi i} \frac{z_4^2\, n_2!\,\Gamma\left(-z_4\right)^2\Gamma\left(z_4\right)}{n_2^2\left(n_2-z_4\right)^2\Gamma\left(n_2-z_4\right)} \\ \times\, t^{n_2-z_4-1}\left(1-t\right)^{z_4-1}. \end{aligned} \tag{5.107}$$

Next we want to close the $z_4$ contour and sum up the corresponding residues. From the previous discussion, we are forced to close the contour to the right, and the summand obviously only has poles at $z_4 = n_4 \in \mathbb{N}^\times$ inside the integration contour. There is however a subtlety, and we cannot just sum up the residues. Indeed, it is easy to see that

- for $n_4 < n_2$, there are double poles. Shifting the summation variable $n_2 \to n_2 + n_4$, these residues give rise to double sums similar to eq. (5.106) and can again be performed using `XSummer`. We obtain complicated multiple polylogarithms with rational functions of $t$ as argument. Using symbols, they can again be simplified to harmonic polylogarithms with indices 0 and 1 in $t$.
- for $n_4 = n_2$, there is a simple pole. This gives rise to a simple sum which is trivial to perform in terms of harmonic polylogarithms in $t$.
- for $n_4 > n_2$, there is a simple pole. Shifting the summation variable $n_4 \to n_2 + n_4$ this gives rise to a single double sum $S(1-t, 1-1/t)$, with

$$S(x,y) = -\sum_{n_2,n_4=0}^{\infty} \frac{n_2!\, n_4!}{(n_2+n_4+1)!} \frac{x^{n_2}}{n_2+1} \frac{y^{n_4}}{n_4+1} \,. \tag{5.108}$$

  This sum is not of the type (5.106), and we therefore need a different way to sum up the series. This procedure will be discussed in the rest of this section.

One way to sum the series $S(x,y)$ is to recognize that it is related to an integral over an Appell $F_3$ function. More precisely we can write,

$$\begin{aligned} S(x,y) &= -\frac{1}{xy} \sum_{n_2,n_4=0}^{\infty} \frac{n_2!\, n_4!}{(n_2+n_4+1)!} \frac{x^{n_2+1}}{n_2+1} \frac{y^{n_4+1}}{n_4+1} \\ &= -\frac{1}{xy} \int_0^x d\xi \int_0^y d\chi \sum_{n_2,n_4=0}^{\infty} \frac{(n_2!)^2\,(n_4!)^2}{(n_2+n_4+1)!} \frac{\xi^{n_2}}{n_2!} \frac{\chi^{n_4}}{n_4!} \\ &= -\frac{1}{xy} \int_0^x d\xi \int_0^y d\chi\, F_3(1,1,1,1;2;\xi,\chi) \,. \end{aligned} \tag{5.109}$$

The particular Appell $F_3$ function we obtain turns out to be reducible,

$$F_3(\alpha, \gamma-\alpha, \beta, \gamma-\beta; \gamma; \xi, \chi) = (1-\chi)^{\alpha+\beta-\gamma}\, {}_2F_1(\alpha, \beta; \gamma; \xi+\chi-\xi\chi) \,, \tag{5.110}$$

and so we obtain a simple two-fold integral representation for $S$,

$$\begin{aligned} S(x,y) &= -\frac{1}{xy} \int_0^x d\xi \int_0^y d\chi\, {}_2F_1(1,1;2;\xi+\chi-\xi\chi) \\ &= \frac{1}{xy} \int_0^x d\xi \int_0^y d\chi\, \frac{\log(1-\xi)+\log(1-\chi)}{\xi+\chi-\xi\chi} \,. \end{aligned} \tag{5.111}$$

This integral is trivial to perform in terms of multiple polylogarithms with rational functions in $x$ and $y$ as arguments using the algorithm described in section 2.6. It then follows that $S(1-t, 1-1/t)$ can be expressed in terms of multiple polylogarithms with rational functions in $t$ as arguments. Using symbols, we arrive at the following simple expression,

$$S\left(1-t,1-\frac{1}{t}\right)=\frac{t}{(1-t)^2}\Big[-4\mathrm{Li}_3(t)+2\mathrm{Li}_2(t)\log t + \frac{1}{6}\log^3 t+\frac{\pi^2}{3}\log t+4\zeta_3\Big]\,. \tag{5.112}$$

Putting everything together, we arrive at a representation for $\mathcal{F}_{8,3}$ as a one-fold integral over harmonic polylogarithms. This integral is trivial to perform, and we obtain,

$$\mathcal{F}_{8,3}=\frac{23\pi^6}{22680}-2\zeta_3^2\,. \tag{5.113}$$

**Two-fold MB integrals.** There is only one two-fold MB integral contributing to $\mathcal{F}_8$ that cannot be reduced to simpler integrals by Barnes' lemmas and their corollaries. This integral reads

$$\begin{aligned}\mathcal{F}_{8,2}(\epsilon) \;=&\int_{-i\infty}^{+i\infty}\frac{dz_3dz_4}{(2\pi i)^2}\frac{\Gamma(-z_3)^3\,\Gamma(z_3)\,\Gamma(z_3+1)\,\Gamma(-z_4)^3\,\Gamma(z_4)\,\Gamma(z_4+1)}{2\epsilon\Gamma(-z_3-z_4)}\\ &\times\Big[3\epsilon\psi(-z_3)+\epsilon\psi(z_3)-2\epsilon\psi(-z_3-z_4)\\ &\quad+\epsilon\psi(-z_4)+\epsilon\psi(z_4)-1\Big]\,,\end{aligned} \tag{5.114}$$

where the integration contours are straight vertical lines defined by,

$$\Re(z_3)=-0.64\ \text{ and }\ \Re(z_4)=-0.22\,. \tag{5.115}$$

The integral could in principle be done by closing contours to the left and summing up residues. This leads to double sums of the form (5.106) – thousands of them due to the presence of multiple poles – but without any parametric dependence. We therefore took a different route, which we present in the following.

We start by noting that the *integrand* of eq. (5.114) agrees, up to higher order terms of $\mathcal{O}(\epsilon)$, with the function

$$-\frac{\Gamma(z_3+1)\,\Gamma(-z_4)^2\,\Gamma(z_4+1)\,\Gamma(-\epsilon-z_3)^3\,\Gamma(z_3-\epsilon)\,\Gamma(-\epsilon-z_4)\,\Gamma(z_4-\epsilon)}{2\epsilon\Gamma(-2\epsilon-z_3-z_4)}\,. \tag{5.116}$$

It would however be wrong to conclude that then necessarily the *integrals*, seen as a Laurent expansion in $\epsilon$, are also equal to the same accuracy, because the Laurent expansion of eq. (5.116) around $\epsilon=0$ might require shifting the integration contours to avoid pinch singularities in the limit $\epsilon\to 0$. It is however easy to see that, for the contours given in eq. (5.115), no new pinch singularity is created for $\epsilon \to 0$ in eq. (5.116). We therefore consider from now on $\epsilon$ to be infinitesimal but finite: it is large enough to separate poles at, e.g., $z_2 = 0$ from $z_2 = \epsilon$, but small enough to ensure that no poles change their nature, i.e., poles that were left (right) of the contour (5.115) in eq. (5.114) remain left (right) of the contour in eq. (5.116). If we chose $\epsilon$ in this way, we conclude that

$$\mathcal{F}_{8,2}(\epsilon) = \widetilde{\mathcal{F}}_{8,2}(\epsilon) + \mathcal{O}(\epsilon)\,, \tag{5.117}$$

where $\widetilde{\mathcal{F}}_{8,2}$ is given by eq. (5.116) integrated over the straight vertical lines defined by eq. (5.115). Our aim will be to find an $\epsilon$ expansion for $\widetilde{\mathcal{F}}_{8,2}$.

We perform the change of variables $(z_3, z_4) \to (-1 - z_3, -z_4)$, and we close the $z_3$ contour to the right and take residues. There are two towers of poles we need to take into account:

$$z_3 = n_3 \in \mathbb{N} \ \text{ and } \ z_3 = -1 - \epsilon + n_3,\, n_3 \in \mathbb{N}^\times\,. \tag{5.118}$$

Two comments are in order:

1. At this stage our assumption that $\epsilon$ is infinitesimal but finite is vital, because otherwise the two towers of poles would merge and thus give rise to double poles.

2. The second tower of poles runs over the set $\{-\epsilon, -\epsilon + 1, \ldots\}$. For technical reasons that will become clear below, it is easier to explicitly take into account the residue at $z_3 = -1 - \epsilon$, and to compensate for this by adding it back,
$$\widetilde{\mathcal{F}}_{8,2}(\epsilon) = \mathcal{R}_{8,2}(\epsilon) + F_{8,2}(\epsilon)\,, \tag{5.119}$$
where $F_{8,2}$ is the integral obtained from $\widetilde{\mathcal{F}}_{8,2}$ by deforming the $z_3$ contour such that the pole at $z_3 = -1 - \epsilon$ is now to the right of the contour. The residue at $z_3 = -1 - \epsilon$ can be computed in closed form and gives rise to,

$$\begin{aligned}\mathcal{R}_{8,2}(\epsilon) \;=&\; -\frac{\Gamma(1-\epsilon)^2\Gamma(1+\epsilon)\Gamma(1-2\epsilon)^3}{16\epsilon^5\,(1+\epsilon)\,\Gamma(1-3\epsilon)}\,{}_3F_2(1,1,1-\epsilon;1-3\epsilon,\epsilon+2;1)\\ &+\frac{\Gamma(1-2\epsilon)^4\Gamma(1-\epsilon)^2\Gamma(1+\epsilon)^2}{8\epsilon^6\,\Gamma(1-4\epsilon)}\\ &-\frac{3\Gamma(1-2\epsilon)^3\Gamma(1-\epsilon)^3\Gamma(1+\epsilon)^2}{16\epsilon^6\,\Gamma(1-3\epsilon)}\,.\end{aligned} \tag{5.120}$$

Next we compute $F_{8,2}$ by closing the $z_3$ contour to the right and summing up residues. The resulting sums can easily be performed in terms of hypergeometric functions, and we get,

$$
\begin{aligned}
F_{8,2}(\epsilon) = & -\int_{-i\infty}^{+i\infty} \frac{dz_4}{2\pi i} \frac{\Gamma(1-z_4)\Gamma(z_4)^2\Gamma(-\epsilon-z_4)\Gamma(z_4-\epsilon)}{2\epsilon\Gamma(z_4-3\epsilon)\Gamma(-2\epsilon+z_4+1)} \\
& \times \Big[\Gamma(-\epsilon-1)\Gamma(1-\epsilon)^3\Gamma(z_4-3\epsilon) \\
& \times {}_3F_2(1-\epsilon,1-\epsilon,1-\epsilon;\epsilon+2,-2\epsilon+z_4+1;1) \\
& + \Gamma(-2\epsilon)^3\Gamma(\epsilon+1)\Gamma(-2\epsilon+z_4+1) \\
& \times {}_3F_2(-2\epsilon,-2\epsilon,-2\epsilon;-\epsilon,z_4-3\epsilon;1)\Big] .
\end{aligned}
\tag{5.121}
$$

In order to proceed, we insert an Euler integral representation for each of the ${}_3F_2$ functions. It is then easy to see that the Euler integrals are convergent for $\Re(z_4) > 0$ and $\epsilon$ infinitesimal but finite, and so we can exchange the Euler and MB integrations provided that we close the integration contour to the right. The important point is that the ${}_2F_1$ functions appearing inside the Euler integrals are independent of $z_4$, and so they can be pulled out of the MB integral. Summing up the residues in $z_4$, we then arrive at the following integral representation for $F_{8,2}$,

$$
\begin{aligned}
F_{8,2}(\epsilon) = & \frac{\Gamma(1-\epsilon)}{2\epsilon^3}\int_0^1 dt\, t^{-\epsilon}(1-t)^{-\epsilon} \\
\times & \Bigg\{(1-t)^{-\epsilon}\frac{\Gamma(1-\epsilon)^4\Gamma(1+\epsilon)}{\epsilon^2(1+\epsilon)(1-t)}\,{}_2F_1(1-\epsilon,1-\epsilon;\epsilon+2;t) \\
& + t^{-\epsilon-1}(1-t)^{-1-\epsilon}\frac{\Gamma(1-2\epsilon)^2\Gamma(1-\epsilon)\Gamma(1+\epsilon)^2}{4\epsilon^3}\,{}_2F_1(-2\epsilon,-2\epsilon;-\epsilon;t) \\
& - (1-t)^{-1-\epsilon}\frac{\Gamma(1-2\epsilon)^2\Gamma(1-\epsilon)\Gamma(1+\epsilon)^2}{4\epsilon^3\, t}\,{}_2F_1(-2\epsilon,-2\epsilon;-\epsilon;t) \\
& - \frac{\Gamma(1-2\epsilon)^2\Gamma(1+\epsilon)}{4\epsilon(1+\epsilon)\,t}\,{}_2F_1(-2\epsilon,-2\epsilon;-\epsilon;t)\,{}_2F_1(\epsilon+1,\epsilon+1;\epsilon+2;1-t) \\
& - t^{\epsilon}(1-t)^{-\epsilon}\frac{\Gamma(1-\epsilon)^4\Gamma(1+\epsilon)}{\epsilon^2(1+\epsilon)(1-t)}\,{}_2F_1(1-\epsilon,1-\epsilon;\epsilon+2;t) \\
& - t^{\epsilon}\frac{\Gamma(1-\epsilon)^3}{(1+\epsilon)^2}\,{}_2F_1(1-\epsilon,1-\epsilon;\epsilon+2;t)\,{}_2F_1(\epsilon+1,\epsilon+1;\epsilon+2;1-t)\Bigg\} .
\end{aligned}
\tag{5.122}
$$

The terms involving a single ${}_2F_1$ function in the integrand immediately evaluate to ${}_3F_2$ functions, which can be expanded in $\epsilon$ using `HypExp`. In addition, the fourth term can be done in closed form as follows: We insert an MB representation for each ${}_2F_1$ and perform the Euler integration as a Beta function.

One of the two remaining MB integrals evaluates to a ${}_2F_1$ evaluated at 1, which reduces to $\Gamma$ functions through Gauss's identity. The remaining one-fold MB integral then immediately evaluates to a ${}_4F_3$ function, which can be expanded in $\epsilon$ using HypExp. We were not able to find a closed form for the last remaining Euler integral. We therefore insert an Euler integration for each ${}_2F_1$, and we obtain the expression,

$$-\frac{\Gamma(1-\epsilon)^3\Gamma(1+\epsilon)}{2\epsilon^3\,\Gamma(1+2\epsilon)}\,\mathcal{I}(\epsilon)\,, \tag{5.123}$$

where $\mathcal{I}$ denotes the integral

$$\mathcal{I}(\epsilon) = \int_0^1 dt\,du\,dv\,(1-t)^{-\epsilon}(1-u)^{2\epsilon}u^{-\epsilon}v^{\epsilon}(1-tu)^{\epsilon-1}(1-(1-t)v)^{-\epsilon-1}\,. \tag{5.124}$$

It is easy to see that $\mathcal{I}$ is finite as $\epsilon \to 0$, and so we can expand in $\epsilon$ under the integration sign and perform the integration over $t$, $u$ and $v$ recursively using the algorithm described in section 2.6. This is a trivial exercise that leads to,

$$\mathcal{I}(\epsilon) = 2\zeta_3 - \frac{7\pi^4}{180}\epsilon + \left(25\zeta_5 - \frac{\pi^2}{2}\zeta_3\right)\epsilon^2 + \left(-6\zeta_3^2 - \frac{809\pi^6}{22680}\right)\epsilon^3 + \mathcal{O}(\epsilon^4)\,. \tag{5.125}$$

We have thus obtained the $\epsilon$ expansion of $F_{8,2}$, and thus of $\mathcal{F}_{8,2}$. We find,

$$\mathcal{F}_{8,2}(\epsilon) = \left(\frac{\pi^2}{6}\zeta_3 - \frac{9}{2}\zeta_5\right)\frac{1}{\epsilon} - 18\gamma_E\zeta_5 + 4\zeta_3^2 + \frac{2}{3}\gamma_E\pi^2\zeta_3 - \frac{817\pi^6}{45360} + \mathcal{O}(\epsilon)\,, \tag{5.126}$$

where $\gamma_E = \Gamma'(1)$ denotes the Euler-Mascheroni constant.

**The result for $\mathcal{F}_8$.** We have now computed all the two and three-fold integrals contributing to $\mathcal{F}_8$. The remaining one-fold integrals are trivial to compute and we obtain

$$\begin{aligned}\mathcal{F}_8(\epsilon) \;=&\; -\frac{60}{\epsilon^5} + \frac{822}{\epsilon^4} + \frac{1}{\epsilon^3}\Big(240\,\zeta_2 - 4050\Big) + \frac{1}{\epsilon^2}\Big(2400\,\zeta_3 - 3288\,\zeta_2 + 9180\Big)\\ &+ \frac{1}{\epsilon}\Big(13320\,\zeta_4 - 32880\,\zeta_3 + 16200\,\zeta_2 - 9720\Big) + 51840\,\zeta_5 + 3360\,\zeta_2\,\zeta_3\\ &- 182484\,\zeta_4 + 162000\,\zeta_3 - 36720\,\zeta_2 + 3888 + \epsilon\Big(207600\,\zeta_6 + 11760\,\zeta_3^2\\ &- 710208\,\zeta_5 - 46032\,\zeta_2\,\zeta_3 + 899100\,\zeta_4 - 367200\,\zeta_3 + 38880\,\zeta_2\Big) + \mathcal{O}(\epsilon^2)\,.\end{aligned} \tag{5.127}$$

## The master integral $\mathcal{F}_9$

In this section we describe the computation of the most complicated master integral,

$$\Phi_4^S(\epsilon)\,\mathcal{F}_9(\epsilon) = \int \frac{d\Phi_4^S}{s_{15}(s_{14}+s_{15})s_{23}s_{34}s_{345}}\,. \tag{5.128}$$

We start in the usual way and derive an MB representation for $\mathcal{F}_9$ by inserting the energies and angles parametrization and inserting MB integrations for the angular integrals. After applying Barnes' lemmas and their corollaries several times, we arrive at the following MB representation for $\mathcal{F}_9$,

$$\mathcal{F}_9(\epsilon) = \mathcal{F}_{9,1}(\epsilon) + \mathcal{F}_{9,2}(\epsilon)\,, \tag{5.129}$$

where,

$$\begin{aligned}\mathcal{F}_{9,1} =& \frac{3(1+6\epsilon)\Gamma(6-6\epsilon)\Gamma(1-4\epsilon)}{2\epsilon(1+4\epsilon)\Gamma(1-6\epsilon)\Gamma(1-\epsilon)^3}\int_{-i\infty}^{+i\infty}\frac{dz_1dz_2dz_3dz_4}{(2\pi i)^4}\Gamma\left(-z_2\right)\Gamma\left(-z_3\right)\\ &\times\Gamma\left(1-z_1-z_2\right)\Gamma\left(1-z_1-z_3\right)\Gamma\left(z_1+z_2+z_3\right)\Gamma\left(-z_1-z_2-z_3-z_4\right)\\ &\times\Gamma\left(z_1+z_2+z_4+1\right)\Gamma\left(z_1+z_3+z_4+1\right)\Gamma\left(-z_1-z_2-2\epsilon\right)\\ &\times\frac{\Gamma\left(z_1-\epsilon-1\right)\Gamma\left(-z_1-z_4-\epsilon-1\right)\Gamma\left(z_4-\epsilon+1\right)}{\Gamma\left(1-z_2\right)\Gamma\left(1-z_3\right)\Gamma\left(-z_1-z_2-4\epsilon\right)\Gamma\left(z_4-2\epsilon+1\right)}\,,\end{aligned} \tag{5.130}$$

$$\begin{aligned}\mathcal{F}_{9,2} =& -\frac{3(1+6\epsilon)\Gamma(6-6\epsilon)\Gamma(1-4\epsilon)}{2\epsilon(1+4\epsilon)\Gamma(1-6\epsilon)\Gamma(1-\epsilon)^3}\int_{-i\infty}^{+i\infty}\frac{dz_1dz_2dz_3dz_4}{(2\pi i)^4}\Gamma\left(1-z_1\right)\Gamma\left(-z_2\right)\\ &\times\Gamma\left(-z_3\right)\Gamma\left(-z_1-z_3+1\right)\Gamma\left(z_1+z_2+z_3\right)\Gamma\left(-z_1-z_2-z_3-z_4\right)\\ &\times\Gamma\left(z_1+z_2+z_4+1\right)\Gamma\left(z_1+z_3+z_4+1\right)\Gamma\left(-z_1-z_2-2\epsilon\right)\\ &\times\frac{\Gamma\left(z_1-\epsilon-1\right)\Gamma\left(-z_1-z_4-\epsilon-1\right)\Gamma\left(z_4-\epsilon+1\right)}{\Gamma\left(1-z_2\right)\Gamma\left(1-z_3\right)\Gamma\left(-z_1-4\epsilon\right)\Gamma\left(z_4-2\epsilon+1\right)}\,.\end{aligned} \tag{5.131}$$

We can resolve singularities for $\mathcal{F}_{9,1}$ and $\mathcal{F}_{9,2}$ and expand in $\epsilon$ up to and including $\mathcal{O}(\epsilon)$. The result is a collection of high-dimensional MB integrals which, after closing the contour and taking residues, result in multi-fold harmonic sums. While we were able to perform all the harmonic sums in terms of zeta values for all MB integrals up to $\mathcal{O}(\epsilon^0)$, at $\mathcal{O}(\epsilon)$ new polygamma functions appear in the integrand which make the combinatorics of the sums rather intricate. We therefore chose a different method to evaluate the integral $\mathcal{F}_9$, which we describe in the rest of this section.

We start by noting that the $\mathcal{F}_9$ is finite in $d = 6$ dimensions. This can easily be checked by replacing $\epsilon$ by $\epsilon - 1$ in the MB representations (5.130) and (5.131) and resolving singularities. Our goal is to find a parametric integral representation for $\mathcal{F}_9$ in $d = 6 - 2\epsilon$ dimensions and to expand under the integration and perform the parametric integrations recursively. The result in $d = 6 - 2\epsilon$ can then be related to the (divergent) result in $d = 4 - 2\epsilon$ using the dimensional recurrence relation for $\mathcal{F}_9$ of Section 5.3.

It is easy to derive a parametric representation for $\mathcal{F}_9$ using the technique described in section 4.3. We find,

$$\mathcal{F}_9(d=6-2\epsilon) = \frac{\Gamma(12-6\epsilon)\Gamma(3-3\epsilon)\Gamma(1-\epsilon)}{\Gamma(5-6\epsilon)\Gamma(2-\epsilon)^4}\Big[\mathcal{I}_{9,1}(\epsilon)+\mathcal{I}_{9,2}(\epsilon)\Big]\,, \tag{5.132}$$

with

$$\begin{aligned}
\mathcal{I}_{9,1}(\epsilon) &= -\int_0^\infty dt_1\, dt_2 \int_0^1 dx_1\, dx_2\, dx_3\, t_1^{2-4\epsilon}\,(1+t_1)^{\epsilon-1}\, t_2^{1-2\epsilon} \\
&\times\; x_1^{-\epsilon}\,(1-x_1)^{2-4\epsilon}\, x_2^{1-3\epsilon}\,(1-x_2)^{-\epsilon}\, x_3^{-\epsilon}\,(1+t_2x_3)^{1-3\epsilon}\,(1+t_2x_2x_3)^{\epsilon} \qquad (5.133)\\
&\times\; \Big(t_1t_2^2x_1x_2x_3 + t_2^2x_2x_3 + t_1t_2x_1x_2 + t_1t_2x_3 + t_2x_2x_3 + t_2 + t_1 + 1\Big)^{3\epsilon-3},
\end{aligned}$$

$$\begin{aligned}
\mathcal{I}_{9,2}(\epsilon) &= \int_0^\infty dt_1\, dt_2 \int_0^1 dx_1\, dx_2\, dx_3\, t_1^{2-4\epsilon}\,(1+t_1)^{\epsilon-1}\, t_2^{1-2\epsilon} \\
&\times\; x_1^{1-\epsilon}\,(1-x_1)^{2-4\epsilon}\, x_2^{1-3\epsilon}\,(1-x_2)^{-\epsilon}\, x_3^{-\epsilon}\,(1+t_2x_3)^{1-3\epsilon}\,(1+t_2x_2x_3)^{\epsilon} \qquad (5.134)\\
&\times\; \Big(t_1t_2^2x_1x_2x_3 + t_2^2x_1x_2x_3 + t_2x_1 + t_1t_2x_1x_2 + t_1t_2x_3 + t_2x_1x_2x_3 + t_1 + x_1\Big)^{3\epsilon-3},
\end{aligned}$$

Several comments are in order about the parametric integrals we just defined. First, one can easily check that both $\mathcal{I}_{9,1}$ and $\mathcal{I}_{9,2}$ are individually finite as $\epsilon \to 0$. Second, at first glance our goal to integrate out the integration variables one-by-one seems rather hopeless due to the appearance of the huge polynomial factor. However, the criterion of denominator reducibility, outlined in section 2.6, is satisfied for both $\mathcal{I}_{9,1}$ and $\mathcal{I}_{9,2}$. We have

$$\begin{aligned}
S^{(1)} &= \{1+t_1, 1-x_1, 1-x_2, 1+t_2x_3, 1+t_2x_2x_3, \qquad (5.135)\\
&\quad t_1t_2^2x_1x_2x_3 + t_2^2x_2x_3 + t_1t_2x_1x_2 + t_1t_2x_3 + t_2x_2x_3 + t_2 + t_1 + 1\},\\
S^{(2)} &= \{1+t_1, 1-x_1, 1-x_2, 1+t_2x_3, 1+t_2x_2x_3, \qquad (5.136)\\
&\quad t_1t_2^2x_1x_2x_3 + t_2^2x_1x_2x_3 + t_2x_1 + t_1t_2x_1x_2 + t_1t_2x_3 + t_2x_1x_2x_3 + t_1 + x_1\}\\
S^{(1)}_{(t_1)} &= \{1-x_1, 1-x_2, 1+t_2x_1x_2, 1+t_2x_3, 1+t_2x_2x_3, \qquad (5.137)\\
&\quad -t_2x_3x_2 + t_2x_1x_3x_2 + x_1x_2 - x_3x_2 + x_3 - 1\},\\
S^{(2)}_{(t_1)} &= \{1-x_1, 1-x_2, 1+t_2x_1x_2, 1+t_2x_3, 1+t_2x_2x_3, \qquad (5.138)\\
&\quad t_2x_1 - t_2x_2x_1 + t_2x_2x_3x_1 - t_2x_3 + x_1 - 1\},\\
S^{(1)}_{(t_1,x_1)} &= \{1-x_2, 1+t_2x_2, 1-x_3, 1+t_2x_3, 1+t_2x_2x_3, \qquad (5.139)\\
&\quad t_2x_2x_3 + x_2x_3 - x_3 + 1\},\\
S^{(2)}_{(t_1,x_1)} &= \{1-x_2, 1+t_2x_2, 1-x_3, 1+t_2x_3, 1+t_2x_2x_3, \qquad (5.140)\\
&\quad -t_2x_2 + t_2x_2x_3 + t_2 + 1\},\\
S^{(1)}_{(t_1,x_1,x_2)} &= \{1-x_3, 1+t_2x_3, 2t_2x_3 - t_2 + x_3\}, \qquad (5.141)\\
S^{(2)}_{(t_1,x_1,x_2)} &= \{2+t_2-x_3, 1-x_3, 1+t_2x_3\}, \qquad (5.142)\\
S^{(1)}_{(t_1,x_1,x_2,x_3)} &= \{1+t_2, 1+2t_2\}, \qquad (5.143)\\
S^{(2)}_{(t_1,x_1,x_2,x_3)} &= \{1+t_2, 2+t_2\}. \qquad (5.144)
\end{aligned}$$

We see that if we perform the integration in the order $(t_1, x_1, x_2, x_3, t_2)$ then at each step all the polynomials are linear in the next integration variable. The actual integration can be carried out in an algorithmic way as described in section 2.6. The result is,

$$
\begin{aligned}
&\mathcal{F}_9(d = 6 - 2\epsilon) = 1663200\zeta_3 - 554400\pi^2 + 3326400 \\
&\quad + 120\epsilon\left( + 1309\pi^4 - 244203\zeta_3 + 2861\pi^2 + 135294\right) \\
&\quad - 2\epsilon^2\left( - 25779600\zeta_5 - 970200\pi^2\zeta_3 + 838657\pi^4 - 8149392\zeta_3 - 201756\pi^2\right. \\
&\quad \left. - 31378284\right) + \frac{4}{15}\epsilon^3\left(960575\pi^6 + 180873000\zeta_3^2 - 1978358850\zeta_5\right. \\
&\quad \left. - 33612075\pi^2\zeta_3 + 56663280\zeta_3 + 3240501\pi^4 + 6836130\pi^2 + 810381510\right) \\
&\quad + \mathcal{O}(\epsilon^4)\,.
\end{aligned}
\tag{5.145}
$$

Using the dimensional recurrence relations for $\mathcal{F}_9$ derived in Section 5.3 we then finally find the value of $\mathcal{F}_9$ in $d = 4 - 2\epsilon$ dimensions,

$$
\begin{aligned}
\mathcal{F}_9(\epsilon) \;=\; & \frac{160}{\epsilon^5} - \frac{1712}{\epsilon^4} + \frac{1}{\epsilon^3}\Big( - 120\,\zeta_2 + 2784\Big) + \frac{1}{\epsilon^2}\Big( - 120\,\zeta_3 + 1284\,\zeta_2 + 31968\Big) \\
& + \frac{1}{\epsilon}\Big(2520\,\zeta_4 + 1284\,\zeta_3 - 2088\,\zeta_2 - 216864\Big) + 15720\,\zeta_5 + 1920\,\zeta_2\,\zeta_3 \\
& - 26964\,\zeta_4 - 2088\,\zeta_3 - 23976\,\zeta_2 + 795744 + \epsilon\Big(82520\,\zeta_6 + 9600\,\zeta_3^2 \\
& - 168204\,\zeta_5 - 20544\,\zeta_2\,\zeta_3 + 43848\,\zeta_4 - 23976\,\zeta_3 + 162648\,\zeta_2 - 2449440\Big) \\
& + \mathcal{O}(\epsilon^2)\,.
\end{aligned}
\tag{5.146}
$$

Chapter 6

# Real-virtual corrections

## 6.1 Setup of the calculation

We consider the partonic-processes for associated Higgs production,

$$\begin{aligned} g(p_1) + g(p_2) &\to g(p_3) + H(p_4) \\ q(p_1) + g(p_2) &\to q(p_3) + H(p_4) \\ q(p_1) + \bar{q}(p_2) &\to g(p_3) + H(p_4) \end{aligned} \tag{6.1}$$

where $g, q, \bar{q}$ are symbols for gluon, quark and anti-quark partons correspondingly and $H$ for the Higgs boson. The brackets refer to the momenta of the particles. We define the kinematic invariants,

$$\begin{aligned} s &\equiv 2p_1 \cdot p_2 + i0, \quad t \equiv 2p_2 \cdot p_3 - i0, \quad u \equiv 2p_1 \cdot p_3 - i0, \\ p_4^2 &= (p_1 + p_2 - p_3)^2 = s - t - u = M_h^2 + i0\,, \end{aligned} \tag{6.2}$$

where we indicated explicitly the small imaginary parts carried by them. The partonic cross sections for these processes are given by,

$$\sigma_X = \frac{\mathcal{N}_X}{2s} \int d\Phi_2 \sum |\mathcal{A}_X|^2\,, \tag{6.3}$$

where $X \in \{gg \to Hg, gq \to Hq, q\bar{q} \to Hg\}$ labels the different subprocesses[1] and the sum symbol denotes a summation over colors and polarizations of the initial- and final-state particles. We work in conventional regularization in $d =$

[1] In the following we will suppress the dependence on the final state as it can always be inferred from the initial state for the processes we consider.

$4 - 2\epsilon$ for both the phase space and the matrix element. The $d$-dimensional phase-space measure is given by,

$$d\Phi_2 = (2\pi)^d \, \delta^{(d)}\left(p_1 + p_2 - p_3 - p_4\right) \frac{d^d p_3}{(2\pi)^{d-1}} \, \delta_+(p_3^2) \, \frac{d^d p_4}{(2\pi)^{d-1}} \, \delta_+(p_4^2 - M_h^2) \, . \tag{6.4}$$

The $\mathcal{N}_X$ denote the averaging over initial-state spins and colors in $d$ dimensions,

$$\mathcal{N}_{gg} = \frac{1}{4V^2(1-\epsilon)^2} \, , \qquad \mathcal{N}_{gq} = \frac{1}{4VN(1-\epsilon)^2} \, , \qquad \mathcal{N}_{q\bar{q}} = \frac{1}{4N^2} \, , \tag{6.5}$$

with $N$ and $V \equiv N^2 - 1$ the number of quark and gluon colors respectively.

In the following it will be convenient to parametrize the invariants as,

$$s = \frac{M_h^2}{z}, \quad t = s\,\delta\,\lambda, \quad u = s\,\delta\,(1-\lambda) \, , \tag{6.6}$$

with $\delta = 1 - z$. Note that a physical scattering process corresponds to $s > 0$ and $0 < z, \lambda < 1$, and the limit $\delta \to 1$ corresponds to the threshold region where the additional final state parton is soft. Using the parametrization (6.6) we can specialize the previously derived phase-space measure to the case of one massless particle and eq. (4.59) becomes,

$$d\Phi_2 = \frac{(4\pi)^\epsilon \, s^{-\epsilon} \, \delta^{1-2\epsilon}}{8\pi \, \Gamma(1-\epsilon)} \, d\lambda \, [\lambda\,(1-\lambda)]^{-\epsilon} \, \Theta(\lambda) \, \Theta(1-\lambda) \, . \tag{6.7}$$

Equation (6.3) then reads

$$\sigma_X = s^{-1-\epsilon} \, \frac{\mathcal{N}_X \, (4\pi)^\epsilon}{16\pi \, \Gamma(1-\epsilon)} \, \delta^{1-2\epsilon} \int_0^1 d\lambda \, [\lambda\,(1-\lambda)]^{-\epsilon} \sum |\mathcal{A}_X|^2 \, . \tag{6.8}$$

In the rest of this chapter we compute in an effective theory of the Standard Model where the top quark is integrated out. The effective unrenormalized Lagrangian reads:

$$\mathcal{L} = \mathcal{L}^{\text{eff}}_{\text{QCD}} - \frac{1}{4} \, C \, H \, G^a_{\mu\nu} G^{a,\mu\nu}, \tag{6.9}$$

where the first term corresponds to an effective QCD Lagrangian with $N_f = 5$ flavors. The Wilson coefficient $C$ can be cast as a function of the QCD coupling, the bare heavy-quark masses and the Higgs field vacuum expectation value [181, 188–191].

Performing a loop-expansion of the amplitudes $\mathcal{A}_X = \sum_{j=0}^{\infty} \mathcal{A}_X^{(j)}$ in the effective theory with $j$ being the number of loops, we have:

$$|\mathcal{A}_X|^2 = \left|\mathcal{A}_X^{(0)}\right|^2 + 2\Re\left(\mathcal{A}_X^{(0)} \mathcal{A}_X^{(1)^*}\right) + \left[\left|\mathcal{A}_X^{(1)}\right|^2 + 2\Re\left(\mathcal{A}_X^{(0)} \mathcal{A}_X^{(2)^*}\right)\right] + \ldots \tag{6.10}$$

The first two terms of the above expansion enter the already-known inclusive Higgs boson cross section through NNLO [83, 98, 108, 109, 115, 116, 192]. The third term in square brackets contributes to the N$^3$LO coefficient. In this chapter, we compute the part of the partonic cross section due to the square of the one-loop amplitudes, namely,

$$\sigma_X^{1\otimes 1} = s^{-1-\epsilon}\,\frac{\mathcal{N}_X\,(4\pi)^{\epsilon}}{16\pi\,\Gamma(1-\epsilon)}\,\delta^{1-2\epsilon}\int_0^1 d\lambda\,[\lambda\,(1-\lambda)]^{-\epsilon}\sum\left|\mathcal{A}_X^{(1)}\right|^2. \quad (6.11)$$

## 6.2 Results

The computation of the cross sections (6.11) for the different subprocesses is the main subject of this chapter. We evaluated the phase-space and loop integrals in different ways that are detailed in Section 6.3. In this section, we summarize first our main findings.

We find for the partonic cross sections:

$$\sigma_X^{1\otimes 1} = \frac{\pi\,\omega_\Gamma\,|C|^2}{256\,s}\left(\frac{4\pi}{s}\right)^{3\epsilon}\left(\frac{\alpha_s}{\pi}\right)^3 \mathcal{C}_X\,\Sigma_X(z;\epsilon)\,, \quad (6.12)$$

where $g_s^2 \equiv 4\pi\alpha_s$, and we have,

$$\mathcal{C}_{gg} = \frac{N}{V\,(1-\epsilon)^2}\,, \qquad \mathcal{C}_{qg} = \frac{1}{N\,(1-\epsilon)}\,, \qquad \mathcal{C}_{q\bar{q}} = \frac{V}{N^2}\,. \quad (6.13)$$

In eq. (6.12) we have introduced the quantity,

$$\omega_\Gamma \equiv \frac{c_\Gamma^3}{\Gamma(1+\epsilon)\,\Gamma(1-\epsilon)} = \frac{\Gamma^2(1+\epsilon)\,\Gamma^5(1-\epsilon)}{\Gamma^3(1-2\epsilon)}\,, \qquad c_\Gamma = \frac{\Gamma(1+\epsilon)\,\Gamma^2(1-\epsilon)}{\Gamma(1-2\epsilon)}\,. \quad (6.14)$$

The function $\Sigma_{gg}(z;\epsilon)$ has a pole as $z \to 1$. This pole constitutes the soft singularity of the gluon initiated cross section; it will only be remedied by integrating the partonic cross section with parton distribution functions. We separate this singular part manifestly from the remainder and write:

$$\Sigma_{gg}(z;\epsilon) = \Sigma_{gg}^{\,\text{sing}}(z;\epsilon) + \Sigma_{gg}^{\,\text{reg}}(z;\epsilon) \quad (6.15)$$

where the $z \to 1$ singular part is given by

$$\begin{aligned}\Sigma_{gg}^{\,\text{sing}}(z;\epsilon) \;=\; & -(1-z)^{-1-2\epsilon}\frac{8N^2\left(\epsilon^3+2\epsilon^2-3\epsilon+1\right)^2}{(1-2\epsilon)^2(1-\epsilon)\epsilon^5} \\ & -(1-z)^{-1-4\epsilon}\frac{4N^2\left(\epsilon^3+2\epsilon^2-3\epsilon+1\right)\Gamma(\epsilon+1)\Gamma(2\epsilon+1)\Gamma(1-2\epsilon)^4}{(1-2\epsilon)\epsilon^5\Gamma(1-4\epsilon)^2\Gamma(1-\epsilon)\Gamma(4\epsilon+1)} \\ & -(1-z)^{-1-6\epsilon}\frac{2N^2(1-\epsilon)\Gamma(1-3\epsilon)^2\Gamma(\epsilon+1)^2\Gamma(1-2\epsilon)}{3\epsilon^5\Gamma(1-6\epsilon)}.\end{aligned} \quad (6.16)$$

The cross sections of the $q\bar{q}$ and $qg$ channels are regular in the limit $z \to 1$:

$$\begin{aligned} \Sigma_{qg}(z;\epsilon) &= \Sigma_{gq}^{\text{reg}}(z;\epsilon)\,, \\ \Sigma_{q\bar{q}}(z;\epsilon) &= \Sigma_{q\bar{q}}^{\text{reg}}(z;\epsilon)\,. \end{aligned} \tag{6.17}$$

We have calculated the regular functions $\Sigma_X^{\text{reg}}(x;\epsilon)$ as an expansion in the dimensional regulator $\epsilon$ through $\mathcal{O}(\epsilon^0)$. The expressions are composed of multiple polylogarithms up to weight five.

Due to the magnitude of the expressions obtained for the functions $\Sigma_X^{\text{reg}}(x;\epsilon)$ we refrain from stating them here explicitly but rather refer to ref. [2].

Given that the triple-real contributions to the inclusive Higgs boson cross section at N$^3$LO in chapter 5 have only been computed as an expansion around $z = 1-\delta \to 1$, we also provide the same expansion for the $(\text{RV})^2$ cross section functions $\Sigma_X(z,\epsilon)$. We have discovered a characteristic structure for $\Sigma_X(z,\epsilon)$ in the $\delta \to 0$ limit; all logarithmic contributions of the form $\log\delta$ exponentiate into factors of $\delta^{-a\epsilon}$, where $a$ is an integer in the interval $[2,6]$. Namely,

$$\Sigma_X(z,\epsilon) = \sum_{a=2}^{6} \delta^{-a\epsilon}\, \eta_X^{(a)}(\delta;\epsilon)\,, \tag{6.18}$$

where the functions $\eta_X^{(a)}(\delta;\epsilon)$ are meromorphic functions of $\delta$. We further decompose $\eta_X^{(a)}$,

$$\eta_X^{(a)}(\delta;\epsilon) = \phi_\Gamma^{(a;1)}(\epsilon)\, \hat{\eta}_X^{(a;1)}(\delta;\epsilon)\,, \tag{6.19}$$

for $a \neq 4$, while for $a = 4$ we write,

$$\eta_X^{(4)}(\delta;\epsilon) = \sum_{j=1}^{3} \phi_\Gamma^{(4;j)}(\epsilon)\, \hat{\eta}_X^{(4;j)}(\delta;\epsilon)\,, \tag{6.20}$$

with

$$\begin{aligned} \phi_\Gamma^{(2;1)}(\epsilon) &= 1\,, \\ \phi_\Gamma^{(3;1)}(\epsilon) &= \frac{\cos(\pi\epsilon)\Gamma(1-2\epsilon)^2}{\Gamma(1-3\epsilon)\Gamma(1-\epsilon)}\,, \\ \phi_\Gamma^{(4;1)}(\epsilon) &= \frac{\Gamma^3(1-2\epsilon)}{\Gamma(1-4\epsilon)\,\Gamma^2(1-\epsilon)}\,, \\ \phi_\Gamma^{(4;2)}(\epsilon) &= \frac{\cos(2\pi\epsilon)\Gamma(1-2\epsilon)^3\Gamma(\epsilon+1)}{\Gamma(1-4\epsilon)\Gamma(1-\epsilon)}\,, \\ \phi_\Gamma^{(4;3)}(\epsilon) &= \frac{\Gamma(1-2\epsilon)\,\Gamma(1-3\epsilon)}{\Gamma(1-4\epsilon)\,\Gamma(1-\epsilon)}\,, \\ \phi_\Gamma^{(5;1)}(\epsilon) &= \frac{\cos(\pi\epsilon)\Gamma(1-3\epsilon)\Gamma(1-2\epsilon)^2\Gamma(\epsilon+1)}{\Gamma(1-5\epsilon)\Gamma(1-\epsilon)}\,, \\ \phi_\Gamma^{(6;1)}(\epsilon) &= \frac{\Gamma(1-2\epsilon)\,\Gamma^2(1+\epsilon)\,\Gamma^2(1-3\epsilon)}{\Gamma(1-6\epsilon)}\,. \end{aligned} \tag{6.21}$$

The structure of Eqs. (6.18)–(6.20) originates from loop integrations over distinct kinematic configurations, where the loop momentum can be either soft ($s$), or collinear to the first incoming parton ($c_1$), or collinear to the second incoming parton ($c_2$), or, otherwise, hard ($h$). Every term in the squared amplitude may be thought of as associated to a product of two regions $r_1$ and $r_2$, $r_i \in \{s, c_1, c_2, h\}$, one from the amplitude itself and the other from its complex conjugate. In the following we denote the contribution from such a product of regions by $(r_1, r_2)$. The coefficients $\phi_\Gamma^{(i;j)}(\epsilon)\,\hat{\eta}_X^{(i;j)}(\delta;\epsilon)$ are in one-to-one correspondence with these regions. The correspondence is explicitly given by,

$$\begin{aligned}
\phi_\Gamma^{(2;1)}(\epsilon)\,\hat{\eta}_X^{(2;1)}(\delta;\epsilon) &\leftrightarrow (h,h)\,,\\
\phi_\Gamma^{(3;1)}(\epsilon)\,\hat{\eta}_X^{(3;1)}(\delta;\epsilon) &\leftrightarrow (c_1+c_2,h)+(h,c_1+c_2)\,,\\
\phi_\Gamma^{(4;1)}(\epsilon)\,\hat{\eta}_X^{(4;1)}(\delta;\epsilon) &\leftrightarrow (c_1,c_2)+(c_2,c_1)\,,\\
\phi_\Gamma^{(4;2)}(\epsilon)\,\hat{\eta}_X^{(4;2)}(\delta;\epsilon) &\leftrightarrow (s,h)+(h,s)\,,\\
\phi_\Gamma^{(4;3)}(\epsilon)\,\hat{\eta}_X^{(4;3)}(\delta;\epsilon) &\leftrightarrow (c_1,c_1)+(c_2,c_2)\,,\\
\phi_\Gamma^{(5;1)}(\epsilon)\,\hat{\eta}_X^{(5;1)}(\delta;\epsilon) &\leftrightarrow (c_1+c_2,s)+(s,c_1+c_2)\,,\\
\phi_\Gamma^{(6;1)}(\epsilon)\,\hat{\eta}_X^{(6;1)}(\delta;\epsilon) &\leftrightarrow (s,s)\,.
\end{aligned} \tag{6.22}$$

A derivation of the above decomposition will be given in Section 6.3. The analytic form of the double soft $(s,s)$ terms $\hat{\eta}_X^{(6;1)}(\delta;\epsilon)$ is rather simple. We find:

$$\begin{aligned}
\hat{\eta}_{q\bar{q}}^{(6;1)}(\delta;\epsilon) = \quad & \frac{1}{N^2}\Bigg[\frac{\delta}{24\epsilon^2-16\epsilon+2}+\frac{\delta^2\left(-2\epsilon^2-2\epsilon+1\right)}{24\epsilon^4-16\epsilon^3+2\epsilon^2}\\
&+\frac{\delta^3\left(3\epsilon^4+6\epsilon^3-3\epsilon+1\right)}{72\epsilon^6-48\epsilon^5+6\epsilon^4}\Bigg],
\end{aligned} \tag{6.23}$$

$$\begin{aligned}
\hat{\eta}_{qg}^{(6;1)}(\delta;\epsilon) = \quad & N^2\Bigg[\frac{\epsilon-1}{12\epsilon^5}+\frac{\delta}{6\epsilon^4(6\epsilon-1)}-\frac{\delta^2(\epsilon+1)\left(3\epsilon^3+12\epsilon^2-11\epsilon+2\right)}{24\epsilon^5\left(12\epsilon^2-8\epsilon+1\right)}\\
&+\frac{\delta^3(\epsilon-1)}{4\epsilon^2\left(12\epsilon^2-8\epsilon+1\right)}-\frac{\delta^4(\epsilon-1)}{8\epsilon^2\left(12\epsilon^2-8\epsilon+1\right)}\Bigg],
\end{aligned} \tag{6.24}$$

$$\begin{aligned}\hat{\eta}_{gg}^{(6;1)}(\delta;\epsilon) = \quad & N^2\Bigg[ + \frac{2(\epsilon-1)}{3\delta\epsilon^5} - \frac{4(\epsilon-1)}{3\epsilon^5} + \frac{2\delta\left(8\epsilon^2-7\epsilon+1\right)}{\epsilon^5(6\epsilon-1)} \\ & -\frac{4\delta^2\left(9\epsilon^2-7\epsilon+1\right)}{3\epsilon^5(6\epsilon-1)} - \frac{\delta^3(3\epsilon-1)\left(\epsilon^4-20\epsilon^3+35\epsilon^2-21\epsilon+4\right)}{6(1-2\epsilon)^2\epsilon^5(6\epsilon-1)} \\ & +\frac{\delta^4(\epsilon-2)(3\epsilon-1)}{3(1-2\epsilon)^2\epsilon^2(6\epsilon-1)} - \frac{\delta^5(\epsilon-2)(3\epsilon-1)}{6(1-2\epsilon)^2\epsilon^2(6\epsilon-1)}\Bigg]. \end{aligned} \tag{6.25}$$

The remaining $\hat{\eta}_X^{a;i}$ terms are more complicated combinations of generalized hypergeometric functions, which can be readily cast as a Laurent series in $\delta$,

$$\sum_{n=-1}^{\infty} c_n(\epsilon)\delta^n .$$

Due to the size and complexity of the expression in terms of hypergeometric functions we refer to ref. [189] for the terms in the $\delta$ expansion up to $\mathcal{O}\left(\delta^4\right)$. With our computer programs, we have explicitly generated the terms of the series up to order $\mathcal{O}\left(\delta^{10}\right)$. In addition, as explained earlier, we have computed the $\hat{\eta}_X^{(a;j)}$ functions for arbitrary values of $\delta$ as an expansion in $\epsilon$ through order $\mathcal{O}\left(\epsilon^0\right)$.

## 6.3 Methods

In this section, we discuss how we evaluated the loop and phase-space integrals that contribute to the real-virtual squared cross sections (6.12). We employed various methods that each have their own strengths and weaknesses. We checked that we obtain consistent results when comparing the different approaches. These methods are:

1. **Threshold expansion of the cross section**: In this approach, we derive a representation of the cross section as an expansion close to threshold where $\delta \to 0$. We first expand the loop amplitude in the limit where the final state parton is soft, and then perform the phase-space integration order-by-order in the expansion. The threshold expansion of the loop amplitude is obtained in two different ways: first by finding a suitable representation in terms of convergent hypergeometric functions within the entire phase-space, and, second, by expanding around the relevant soft, collinear and hard regions of the loop momentum.

2. **Differential equations for master integrals**: Using a duality of loop and phase-space integrals we reduce them simultaneously to a minimal set of master integrals. The master integrals satisfy differential equations that can be solved in two ways: either order-by-order in dimensional regularization in terms of harmonic polylogarithms, or in terms

of generalized hypergeometric functions. The boundary conditions for the differential equations are obtained by matching to the leading term of the threshold expansion, which we compute with one of our threshold expansion methods mentioned above.

3. **Direct integration using multiple polylogarithms**: It is possible to derive analytic results for the loop integrals entering our amplitudes in terms of polylogarithmic functions. These expressions are singular in soft and collinear limits of the phase-space and we render all integrals convergent by constructing appropriate counterterms. Then we perform the two-body phase-space integration by embedding the polylogarithmic functions into a larger class of multiple polylogarithms for which the integration is trivial. In the end, we recast the final result in terms of harmonic polylogarithms only.

## Expansion of the cross section around threshold

We start by computing the one-loop amplitudes $A_X^1$ with $X \in \{gg \to Hg, q\bar{q} \to Hg, qg \to Hq\}$ in dimensional regularization and for arbitrary values of the regulator $\epsilon$. We generate the Feynman diagrams with QGRAF [183] and perform the spin and color algebra using FORM [184]. Using the methods of refs. [174, 175] for tensor integrals and well established reduction techniques for scalar integrals [146, 150], the amplitudes are reduced to the one-loop scalar bubble and box master integrals,

$$\begin{aligned} \mathrm{Bub}(s_{12}) &= \int \frac{d^dk}{i\pi^{\frac{d}{2}}} \frac{1}{k^2\,(k+q_1+q_2)^2}, \\ \mathrm{Box}(s_{12}, s_{23}, s_{31}) &= \int \frac{d^dk}{i\pi^{\frac{d}{2}}} \frac{1}{k^2\,(k+q_1)^2\,(k+q_1+q_2)^2\,(k+q_1+q_2+q_3)^2}, \end{aligned} \tag{6.26}$$

where the $q_i$ are considered light-like and ingoing and $s_{ij} = (q_i + q_j)^2$.

In the next step, we construct the squared one-loop amplitudes and cast them in terms of three functions, in the form:

$$\begin{aligned} \sum \left|\mathcal{A}^{(1)}_{gg\to Hg}\right|^2 = \frac{N\,V\,|C|^2\,g_s^6}{(4\pi)^d\,s\,t\,u} \Big\{ & \left|A_{ggg}(s,-t,-u)\right|^2 \\ & + (1-\epsilon)\left[\left|B_{ggg}(s,-t,-u)\right|^2 + \left|B_{ggg}(-t,-u,s)\right|^2 + \left|B_{ggg}(-u,s,-t)\right|^2\right] \Big\}, \end{aligned} \tag{6.27}$$

$$\sum\left|\mathcal{A}^{(1)}_{qg\to Hq}\right|^2 = \frac{V\,|C|^2\,g_s^6\,u}{2\,(4\pi)^d}\Bigg\{(1-\epsilon)\,\left[\left|A_{q\bar{q}g}(-u,-t,s)\right|^2+\left|A_{q\bar{q}g}(-u,s,-t)\right|^2\right]$$
$$-2\epsilon\,\Re\left[A_{q\bar{q}g}(-u,-t,s)\,A^*_{q\bar{q}g}(-u,s,-t)\right]\Bigg\}, \tag{6.28}$$

$$\sum\left|\mathcal{A}^{(1)}_{q\bar{q}\to Hg}\right|^2 = \frac{V\,|C|^2\,g_s^6\,s}{2\,(4\pi)^d}\Bigg\{(1-\epsilon)\,\left[\left|A_{q\bar{q}g}(s,-t,-u)\right|^2+\left|A_{q\bar{q}g}(s,-u,-t)\right|^2\right]$$
$$-2\epsilon\,\Re\left[A_{q\bar{q}g}(s,-t,-u)\,A^*_{q\bar{q}g}(s,-u,-t)\right]\Bigg\}. \tag{6.29}$$

For explicit expressions for the functions $A_{q\bar{q}g}, A_{ggg}, B_{ggg}$ we refer to ref. [189].

**Threshold expansion using hypergeometric functions**. Loop integrals in dimensional regularization can be expressed, to all orders in the dimensional regulator, as (generalized) hypergeometric functions. For example, the box integral[2] defined in eq. (6.26) admits the representation (see, e.g., ref. [193]),

$$\mathrm{Box}(s_{12},s_{23},s_{31}) = \frac{2c_\Gamma}{\epsilon^2}\frac{1}{s_{12}s_{23}}\Bigg\{(-s_{23})^{-\epsilon}\,{}_2F_1\left(1,-\epsilon;1-\epsilon;-\frac{s_{31}}{s_{12}}\right)$$
$$+(-s_{12})^{-\epsilon}\,{}_2F_1\left(1,-\epsilon;1-\epsilon;-\frac{s_{31}}{s_{23}}\right)-\left(-M_h^2\right)^{-\epsilon}\,{}_2F_1\left(1,-\epsilon;1-\epsilon;-\frac{M_h^2 s_{31}}{s_{12}s_{23}}\right)\Bigg\}. \tag{6.30}$$

Our goal is to insert the parametrization (6.6) and then to perform the integration over $\lambda$ term-by-term in the series representation of the hypergeometric functions. The result is a power series in $\delta$, i.e., the desired expansion of the cross section close to threshold.

While all the hypergeometric series in eq. (6.30) are convergent in the Euclidean region where $s_{ij} < 0$, the one-loop amplitude in the physical region involves the functions $\mathrm{Box}(-t,-u,s)$, $\mathrm{Box}(s,-t,-u)$ and $\mathrm{Box}(s,-u,-t)$. It is easy to check that the corresponding hypergeometric series are no longer convergent in the physical scattering region. It is, however, always possible to analytically continue the ${}_2F_1$ function such that arguments lie inside the unit disc, yielding another representation in terms of ${}_2F_1$ functions. While this approach is adequate to find a meaningful expansion around $\epsilon$ in terms of polylogarithms, it does not allow one to find (convergent) hypergeometric series expansions around $\delta = 0$. Instead, one needs at least a double sum representation to achieve this task. It turns out that such a representation is

[2] The bubble integral is trivial, and will not be discussed any further.

known in the literature [193],

$$
\begin{aligned}
\mathrm{Box}(-t,-u,s) \;=\; & \frac{2c_\Gamma}{\epsilon^2}\Gamma(1+\epsilon)\Gamma(1-\epsilon)\, e^{-i\pi\epsilon}\,\frac{\left(\frac{tu}{s}\right)^{-\epsilon}}{tu} \\
& -\frac{2c_\Gamma}{\epsilon(1+\epsilon)}\frac{t^{-\epsilon-1}}{s}{}_2F_1\left(1,1+\epsilon;2+\epsilon;\frac{u}{s}\right) \\
& -\frac{2c_\Gamma}{\epsilon(1+\epsilon)}\frac{u^{-\epsilon-1}}{s}{}_2F_1\left(1,1+\epsilon;2+\epsilon;\frac{t}{s}\right) \\
& -\frac{2c_\Gamma}{\epsilon(1+\epsilon)}\, e^{i\pi\epsilon}\, s^{-2-\epsilon}\, F_2\left(2+\epsilon;1+\epsilon,1+\epsilon;2+\epsilon,2+\epsilon;\frac{u}{s},\frac{t}{s}\right) ,
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{Box}(s,-t,-u) \;=\; & \frac{2c_\Gamma}{\epsilon^2}\frac{t^{-\epsilon}}{s(-t)}{}_2F_1\left(1,-\epsilon;1-\epsilon;\frac{u}{s}\right) \\
& +\frac{2c_\Gamma}{\epsilon}s^{-2-\epsilon}\, e^{i\pi\epsilon}\, S_1\left(2+\epsilon;1,1+\epsilon;2,2+\epsilon,\frac{t}{s},\frac{u}{s}\right) .
\end{aligned}
\qquad (6.31)
$$

The corresponding result for $\mathrm{Box}(s,-u,-t)$ is obtained from $\mathrm{Box}(s,-t,-u)$ by exchanging $t$ and $u$. The generalized Kampé de Fériet function $S_1$ is defined as,

$$
S_1(a_1;a_2,b_1;a_3,b_2;x_1,x_2) = \sum_{n,m=0}^{\infty} \frac{(a_1)_{m+n}\,(a_2)_{m+n}\,(b_1)_m}{(a_3)_{m+n}\,(b_2)_m}\frac{x_1^m\, x_2^n}{m!\, n!}, \qquad (6.32)
$$

and the Appel function $F_2$ is defined as,

$$
F_2(a;b_1,b_2;c_1,c_2;x_1,x_2) = \sum_{n,m=0}^{\infty} \frac{(a)_{m+n}\,(b_1)_m\,(b_2)_n}{(c_1)_m\,(c_2)_n}\frac{x_1^m\, x_2^n}{m!\, n!}. \qquad (6.33)
$$

Using these expressions for the box functions, we can easily exchange the phase-space integration and the infinite summations, and all the integrals can be performed in terms of Euler's Beta function,

$$
B(\alpha,\beta) = \int_0^1 d\lambda\, \lambda^{\alpha-1}\,(1-\lambda)^{\beta-1} = \frac{\Gamma(\alpha)\,\Gamma(\beta)}{\Gamma(\alpha+\beta)} . \qquad (6.34)
$$

**Threshold expansion of hard, soft and collinear regions.** It is possible to derive representations such as the ones of eq. (6.31) with a more physical method, performing Taylor expansions around soft, collinear and hard regions of the integrand of loop integrals in momentum space. The method of expansions by regions [194] promises to hold in general, although its generality has only been stated as a conjecture and a verification of the validity of the approach is necessary in specific cases[3].

[3]Full proofs of the validity of asymptotic expansions by regions are hard to derive or unknown. For efforts in this direction we refer the reader to refs. [195, 196] and references therein.

For the production of the Higgs boson near threshold, the partonic center of mass energy is close in value to the Higgs boson mass, and thus we have a kinematic variable which is small, $\delta = 1 - z \sim 0$. From eq. (6.6) we infer that the external momenta scale as,

$$p_1 \sim p_2 \sim \sqrt{s}, \quad p_3 \sim \sqrt{s}\,\delta\,. \tag{6.35}$$

For a particle propagating in the loop, we find four types of non-trivial scalings of its momentum $k$:

- *Hard* $(h)$
$$k^\mu \sim \sqrt{s}\,,$$
where all propagators in the loop are off-shell,
- *Soft* $(s)$
$$k^\mu \sim \sqrt{s}\,\delta\,,$$
where the loop integrand is singular at the point $k^\mu = 0$,
- *Collinear to* $p_1$ $(c_1)$
$$\frac{2k\cdot p_1}{s} \sim \delta, \quad \frac{2k\cdot p_2}{s} \sim 1, \quad k_\perp \sim \sqrt{s\,\delta}\,,$$
where the integrand has a singular surface as $k^\mu \propto p_1^\mu$,
- *Collinear to* $p_2$ $(c_2)$
$$\frac{2k\cdot p_2}{s} \sim \delta, \quad \frac{2k\cdot p_1}{s} \sim 1, \quad k_\perp \sim \sqrt{s\,\delta}\,,$$
where the integrand has a singular surface as $k^\mu \propto p_2^\mu$.

In the above, the transverse momentum $k_\perp$ of the particle is defined via:

$$k = p_1\frac{2k\cdot p_2}{s} + p_2\frac{2k\cdot p_1}{s} + k_\perp\,. \tag{6.36}$$

A scaling of the loop momentum is called a *region*. In a given region, we can perform a systematic expansion of the integrand around $\delta = 0$. This yields multiple new integrals which are simpler than the unexpanded integral. For some regions, we are able to compute analytically all ( infinite number of) terms of the expansion. For the remaining regions, we limit ourselves to a finite number of terms in the expansion and perform an algebraic reduction [146, 150] (after expansion) to master integrals. The soft and collinear regions of our loop integrals correspond to the singular surfaces which solve the Landau equations [197] while the loop-momentum scalings can be identified with the scalings of the coordinates which are normal to the singular surfaces [198]. In the following we discuss how we can reproduce the hypergeometric function representations given in eq. (6.31).

We start by discussing the asymptotic expansion of $\text{Box}(s, -t, -u)$, which we find convenient to parametrize as,

$$\text{Box}(s,-t,-u) = \int \frac{d^d k}{i\pi^{\frac{d}{2}}} \frac{1}{A_1 A_2 A_3 A_4}\,, \tag{6.37}$$

with

$$\begin{aligned} A_1 &= (k-p_{12})^2\,, \\ A_2 &= (k-p_2)^2\,, \\ A_3 &= k^2\,, \\ A_4 &= (k-p_3)^2\,. \end{aligned} \tag{6.38}$$

We find that the full integral is reconstructed from two regions:

1. $(c_2)-$region, where $k$ is collinear to $p_2$.
2. $(h)-$region, where $k$ is hard.

After Taylor-expanding the loop integrand in every region in the small variable $\delta$, we can use integration-by-parts identities to reduce the coefficients of the Taylor expansion to a small set of master integrals. In the $(c_2)$-region we find that all the coefficients are proportional to the one-loop bubble integral $\text{Bub}\,(-t)$, and this region reconstructs, order by order in $\delta$, the first term of the hypergeometric representation for $\text{Box}(s,-t,-u)$ given eq. (6.31), and we have verified this statement explicitly up to $\mathcal{O}\left(\delta^{10}\right)$. The $(h)$-region yields the second and last term of eq. (6.31). In this region, we have been able to calculate all terms in the expansion around $\delta = 0$ via analytic integration. We see that the sum of the $(h)$ and $(c_2)$ regions is equal to the correct expression for the one-loop box. All other soft and collinear regions are zero, as we can readily verify.

Next, we turn to the asymptotic expansion of the $\text{Box}(-t,-u,s)$, given by,

$$\text{Box}(-t,-u,s) = \int \frac{d^d k}{i\pi^{\frac{d}{2}}} \frac{1}{A_1 A_2 A_3 A_4}\,, \tag{6.39}$$

with

$$\begin{aligned} A_1 &= (k-p_1)^2\,, \\ A_2 &= (k)^2\,, \\ A_3 &= (k-p_3)^2\,, \\ A_4 &= (k-p_3+p_2)^2\,. \end{aligned} \tag{6.40}$$

We find that the expression for $\text{Box}(-t,-u,s)$ given in eq. (6.31) is reconstructed entirely from the following regions:

1. $(s)-$region, where the $k \sim \delta$, yielding the first term of eq. (6.31). It is interesting that the $(s)-$region consists of a single term without any subleading terms in the expansion in $\delta$.

2. $(c_1)-$region where the momentum $k$ is collinear to $p_1$. This region reconstructs the second term of eq. (6.31) as we have verified explicitly up to $\mathcal{O}\left(\delta^{10}\right)$.

3. $(c_2)-$region where the momentum $k - p_3$ is collinear to $p_2$. This region reconstructs the third term of eq. (6.31) as we have verified explicitly up to $\mathcal{O}\left(\delta^{10}\right)$.

4. $(h)-$region, where $k$ is hard. This region reconstructs the last term of eq. (6.31) as we have verified explicitly up to $\mathcal{O}\left(\delta^{10}\right)$.

All other soft and collinear regions are zero.

We have seen that an expansion in hard, soft and collinear regions yields series representations for the one-loop master integrals of the required amplitudes which converge in the entire phase-space, and thus we can immediately perform the phase-space integration in terms of Beta functions order-by-order in the expansion. While in our case the strategy of expansion by regions is only an alternative method for deriving the threshold expansion, it can be the method of choice for the phase-space integration of more complicated one-loop amplitudes. Here we have presented expansions by regions at the level of master integrals. We would like to remark that such expansions can also be performed in the integrand of loop-amplitudes before any reduction to master integrals has taken place. Combined with the method of reverse unitarity [1] we have a powerful algebraic technique for the simultaneous threshold expansion of integrals over loop and external momenta.

## Reverse unitarity and differential equations

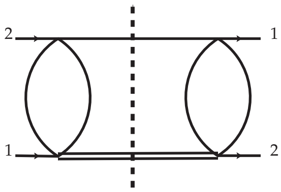
In this section we evaluate the real-virtual squared cross sections using the reverse-unitarity approach [83, 84, 155, 157]. Reverse unitarity establishes a duality between phase-space integrals and loop integrals. Specifically, on-shell and other phase-space constraints are dual to "cut" propagators,

$$\delta_+(q^2) \to \left[\frac{1}{q^2}\right]_c = \frac{1}{2\pi i}\,\mathrm{Disc}\,\frac{1}{q^2} = \frac{1}{2\pi i}\left[\frac{1}{q^2+i0} - \frac{1}{q^2-i0}\right]. \qquad (6.41)$$

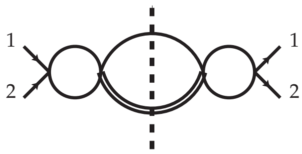
A cut propagator can be differentiated similarly to an ordinary propagator with respect to its momenta. It is therefore possible to derive integration-by-parts (IBP) identities [147, 148] for phase-space integrals in the same way as for loop integrals. The only difference is an additional simplifying constraint that a cut propagator raised to a negative power vanishes:

$$\left[\frac{1}{q^2}\right]_c^{-\nu} = 0, \qquad \nu \geq 0\,. \tag{6.42}$$

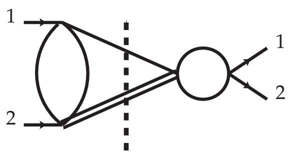
In this approach, we are not obliged to perform a strictly sequential evaluation of the loop integrals in the amplitude followed by the nested phase-space integrals. Rather, we combine the two types of integrals into a single multiloop-like type of integration by introducing cut propagators and then derive and solve IBP identities for the combined integrals. We solve the large system of IBP identities which are relevant for our calculation with the Gauss elimination algorithm of Laporta [146]. We have made an independent implementation of the algorithm in C++ using also the GiNaC library [137]. In comparison to AIR [150], which is a second reduction program used in this work, the C++ implementation is faster and more powerful, storing all identities in virtual memory rather than in the file system. All integrals that appear in the real-virtual squared cross section are reduced to linear combinations of 19 master integrals, which we choose as follows:

$\mathcal{M}_1 =$


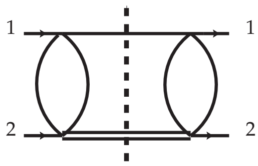

$$= \int d\Phi_2\, \mathrm{Bub}(s_{23})\, \mathrm{Bub}^*(s_{13}). \tag{6.43}$$

$\mathcal{M}_2 =$


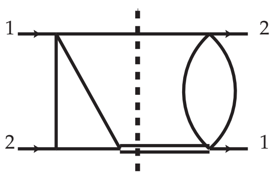

$$= \int d\Phi_2\, \mathrm{Bub}(s_{12})\, \mathrm{Bub}^*(s_{12}). \tag{6.44}$$

$\mathcal{M}_3 =$



$$= \int d\Phi_2\, \mathrm{Bub}(s_{13})\, \mathrm{Bub}^*(s_{12}). \tag{6.45}$$

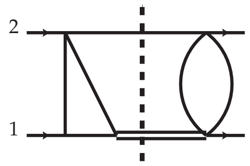
$\mathcal{M}_4 =$



$$= \int d\Phi_2\, \mathrm{Bub}(s_{13})\, \mathrm{Bub}^*(s_{13}). \tag{6.46}$$

$\mathcal{M}_5 =$


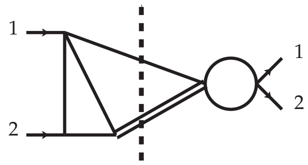

$$= \int d\Phi_2\, \mathrm{Tri}(s_{12} + s_{23})\, \mathrm{Bub}^*(s_{23}). \tag{6.47}$$

$\mathcal{M}_6 =$



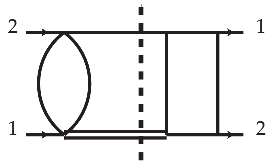

$$= \int d\Phi_2\, \mathrm{Tri}(s_{12} + s_{13})\, \mathrm{Bub}^*(s_{23}). \tag{6.48}$$

$\mathcal{M}_7 =$



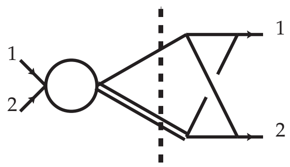

$$= \int d\Phi_2\, \mathrm{Tri}(s_{12} + s_{23})\, \mathrm{Bub}^*(s_{12}). \tag{6.49}$$

$\mathcal{M}_8 =$



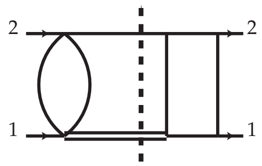

$$= \int d\Phi_2\, \mathrm{Bub}(s_{23})\, \mathrm{Box}^*(s_{12}, s_{23}, s_{13}). \tag{6.50}$$

$\mathcal{M}_9 =$



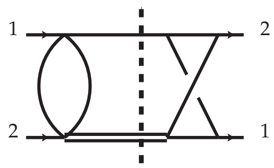

$$= \int d\Phi_2\, \mathrm{Bub}(s_{12})\, \mathrm{Box}^*(s_{13}, s_{23}, s_{12}). \tag{6.51}$$

$\mathcal{M}_{10} =$



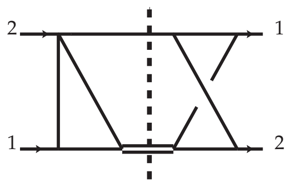

$$= \int d\Phi_2\, \mathrm{Bub}(s_{23})\, \mathrm{Box}^*(s_{12}, s_{13}, s_{23}). \tag{6.52}$$

$\mathcal{M}_{11} =$



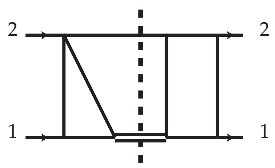

$$= \int d\Phi_2\, \mathrm{Bub}(s_{13})\, \mathrm{Box}^*(s_{13}, s_{23}, s_{12}). \tag{6.53}$$

$\mathcal{M}_{12} =$

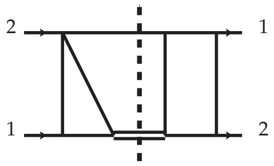



$$= \int d\Phi_2\, \mathrm{Tri}(s_{12} + s_{13})\, \mathrm{Box}^*(s_{13}, s_{23}, s_{12}). \tag{6.54}$$

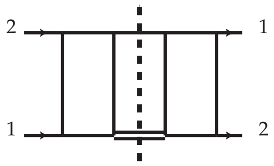
$\mathcal{M}_{13} =$



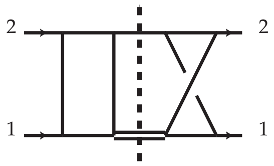

$$= \int d\Phi_2\, \mathrm{Tri}(s_{12} + s_{13})\, \mathrm{Box}^*(s_{12}, s_{13}, s_{23}). \tag{6.55}$$

$\mathcal{M}_{14} =$ 

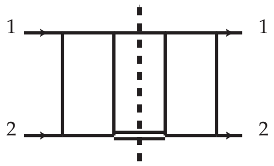
$$= \int d\Phi_2 \, \mathrm{Tri}(s_{12} + s_{13}) \, \mathrm{Box}^*(s_{12}, s_{23}, s_{13}). \tag{6.56}$$

$\mathcal{M}_{15} =$ 

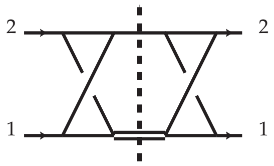
$$= \int d\Phi_2 \, \mathrm{Box}(s_{12}, s_{13}, s_{23}) \, \mathrm{Box}^*(s_{12}, s_{23}, s_{13}). \tag{6.57}$$

$\mathcal{M}_{16} =$ 

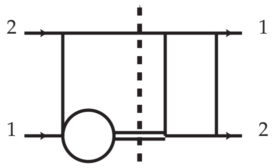
$$= \int d\Phi_2 \, \mathrm{Box}(s_{12}, s_{13}, s_{23}) \, \mathrm{Box}^*(s_{13}, s_{23}, s_{12}). \tag{6.58}$$

$\mathcal{M}_{17} =$ 

$$= \int d\Phi_2 \, \mathrm{Box}(s_{12}, s_{23}, s_{13}) \, \mathrm{Box}^*(s_{12}, s_{23}, s_{13}). \tag{6.59}$$

$\mathcal{M}_{18} =$ 

$$= \int d\Phi_2 \, \mathrm{Box}(s_{13}, s_{23}, s_{12}) \, \mathrm{Box}^*(s_{13}, s_{23}, s_{12}). \tag{6.60}$$

$\mathcal{M}_{19} =$ 

$$= \int d\Phi_2 \, \mathrm{Bub}(M_h^2) \, \mathrm{Box}^*(s_{12}, s_{23}, s_{13}) \frac{1}{s_{23}}. \tag{6.61}$$

Single solid lines represent scalar massless propagators. The phase-space integration is represented by the dashed line and the cut propagators are the lines cut by the dashed line. The cut propagator of the Higgs boson is depicted by the double line. Every master integral has a one-loop integral on the left- and a complex-conjugated one-loop integral on the right-hand side of the cut. In each side of the cut, we find scalar bubble, box or triangle integrals, where the latter is defined by

$$\begin{aligned}
\mathrm{Tri}(s_{12}) &= \int \frac{d^D k}{i(\pi)^{D/2}} \frac{1}{k^2(k+q_1)^2(k+q_1+q_2)^2}\,, \\
\mathrm{Tri}(p_1^2, p_2^2) &= \int \frac{d^D k}{i(\pi)^{D/2}} \frac{1}{k^2(k+p_1)^2(k+p_1+p_2)^2}\,,
\end{aligned} \tag{6.62}$$

with $q_i^2 = 0$, $p_i^2 \neq 0$ and $(p_1+p_2)^2 = 0$. The scalar bubble and box integrals have been defined in (6.26). A comment is in order about the appearance of the triangle integrals in this approach, which seems to be at odds with the fact that in the expression of the one-loop amplitude presented Section 6.3 only bubble and box integrals appeared. Indeed, it is well-known that eq. (6.62) can be expressed as a linear combination of bubble integrals,

$$\begin{aligned}
\mathrm{Tri}(s_{12}) &= \frac{1-2\epsilon}{\epsilon\, s_{12}} \mathrm{Bub}(s_{12})\,, \\
\mathrm{Tri}(p_1^2, p_2^2) &= \frac{1-2\epsilon}{\epsilon\,(p_1^2 - p_2^2)} \left[\mathrm{Bub}(p_1^2) - \mathrm{Bub}(p_1^2)\right].
\end{aligned} \tag{6.63}$$

These relations however introduce new denominators which need to be taken into account in the reduction of the phase-space integrals. We therefore prefer not to use eq. (6.63), but work directly with the triangle integrals instead.

To evaluate the master integrals we employ the method of differential equations [81, 83, 199] as described in sections 3.2 and 3.3. Differentiating the corresponding cut propagator with respect to the square of the Higgs mass,

$$\frac{\partial}{\partial M_h^2} \left(\frac{1}{p_h^2 - M_h^2}\right)_c = \left(\frac{1}{p_H^2 - M_h^2}\right)_c^2, \tag{6.64}$$

results in another phase-space integral. This new integral can again be reduced by IBP identities to our basis of master integrals. Proceeding in this way we obtain a system of linear first order differential equations for the master integrals,

$$\frac{\partial}{\partial \delta} \mathcal{M}_i(\delta) = A_{ij}(\delta)\, \mathcal{M}_j(\delta)\,. \tag{6.65}$$

The system is triangular

$$\frac{\partial}{\partial \delta} \mathcal{M}_i(\delta) = A_{ii}(\delta)\, \mathcal{M}_i(\delta) + y_i(\delta)\,, \tag{6.66}$$

where $y_i(\delta)$ depends only on master integrals that can be solved for independently of $\mathcal{M}_i(\delta)$. In other words, the system can be solved hierarchically, starting from the differential equations with vanishing or known functions $y$. Every time we solve such an equation, its solution serves to determine the $y$ function of a next equation. In this way, at any stage of this procedure the $y$ function is a linear combination of already evaluated master integrals

$$y_i(\delta) = \sum_{j \neq i} A_{ij}(\delta)\, \mathcal{M}_j(\delta)\,, \tag{6.67}$$

that can be integrated in order to determine the integral $\mathcal{M}_j(\delta)$. The coefficients $A_{ij}(\delta)$ are rational functions in $\delta$ and $\epsilon$ and have isolated singularities in $\delta$ only at $\delta = 0, 1, 2$. The first step to solving this type of differential equation is to find a solution for the homogeneous part. The general homogeneous solution associated to the differential equation (6.66) is given by

$$\mathcal{M}_i^h(\delta) = \mathcal{M}_i(0)\, \exp\left[\int_0^{\delta} d\delta' A_{ii}(\delta')\right]\,. \tag{6.68}$$

and is determined up to an integration constant $\mathcal{M}_i(0)$. We determine this integration constant by calculating the soft limit of the master integral explicitly following the methods discussed in Section 6.3. We find that only 7 of our 19 master integrals have non-trivial boundary conditions. Interestingly, with our choice of basis of master integrals, the non-trivial boundary conditions are in one-to-one correspondence to the leading terms of the 7 regions of the soft expansion of the squared amplitude of eqs. (6.19)-(6.20). The non-trivial boundary conditions are:

$$\begin{aligned}
\mathcal{M}_1^S &= (4\pi)^{-1+\epsilon}\, \omega_\Gamma\, \delta^{1-4\epsilon}\, \frac{\phi_\Gamma^{(4;1)}}{2\epsilon^2(1-2\epsilon)^2(1-4\epsilon)}\,,\\
\mathcal{M}_2^S &= (4\pi)^{-1+\epsilon}\, \omega_\Gamma\, \delta^{1-2\epsilon}\, \frac{\phi_\Gamma^{(2;1)}}{2\epsilon^2(1-2\epsilon)^3}\,,\\
\mathcal{M}_3^S &= (4\pi)^{-1+\epsilon}\, \omega_\Gamma\, \delta^{1-3\epsilon}\, \frac{\phi_\Gamma^{(3;1)}}{2\epsilon^2(1-2\epsilon)^2(1-3\epsilon)}\,,\\
\mathcal{M}_4^S &= (4\pi)^{-1+\epsilon}\, \omega_\Gamma \delta^{1-4\epsilon}\, \frac{\phi_\Gamma^{(4;3)}}{2\epsilon^2(1-2\epsilon)^2(1-4\epsilon)}\,,\\
\mathcal{M}_9^S &= -(4\pi)^{-1+\epsilon}\, \omega_\Gamma\, \delta^{-1-4\epsilon}\, \frac{\phi_\Gamma^{(4;2)}}{\epsilon^4(1-2\epsilon)}\,,\\
\mathcal{M}_{11}^S &= -(4\pi)^{-1+\epsilon}\, \omega_\Gamma\, \delta^{-1-5\epsilon}\, \frac{5\phi_\Gamma^{(5;1)}}{6\epsilon^4(1-2\epsilon)}\,,\\
\mathcal{M}_{18}^S &= -(4\pi)^{-1+\epsilon}\, \omega_\Gamma\, \delta^{-3-6\epsilon}\, \frac{8(1+6\epsilon)\phi_\Gamma^{(6;1)}}{3\epsilon^5(1+3\epsilon)}\,.
\end{aligned} \tag{6.69}$$

Only the real part of the boundary conditions is presented here, given that the imaginary part does not contribute to the cross section.

Once the homogeneous solution is found we can compute a particular solution to the inhomogeneous equation by

$$\mathcal{M}_i^p(\delta) = \mathcal{M}_i^h(\delta) \int_0^\delta d\delta' \frac{y(\delta')}{\mathcal{M}_i^h(\delta')}, \tag{6.70}$$

The full solution for the master integral is then given by

$$\mathcal{M}_i(\delta) = \mathcal{M}_i^h(\delta) + \mathcal{M}_i^p(\delta). \tag{6.71}$$

We perform the integration in the equation above with two different approaches.

**Solving differential equations in an expansion in $\epsilon$.** One well established strategy is to expand the differential equations in powers of the dimensional regulator [81, 199]. After expanding the integral of (6.70) a solution is naturally given by iterated integrals leading to multiple polylogarithms [46] of the form $G(a_1, \ldots, a_n; \delta)$, with $a_i \in \{0, 1, 2\}$. Expressing the functions in terms of the variable $z = 1 - \delta$ recasts the solutions in terms of more familiar harmonic polylogarithms [81].

**Solving differential equations in terms of hypergeometric functions.** The integrand of eq. (6.70) takes the form

$$\mathcal{M}_i^s(\delta) \sim \int_0^\delta d\delta' (\delta')^{c_1} (1-\delta')^{c_2} (2-\delta')^{c_3} \mathcal{M}_{j \neq i}(\delta'), \tag{6.72}$$

where $c_1, c_2$ and $c_3$ are linear polynomials in $\epsilon$. This structure is reminiscent of the Euler-type integral representation of hypergeometric functions. Inspired by the large variety of techniques available for the solution of iterated integrals in terms of multiple polylogarithms [46] we define an iterated integral with integration kernel $\delta^{a-1}(1 - x\delta)^{-b}$. The $n^{th}$ iterated integral is then recursively defined by,

$$\mathcal{F}_{\vec{a}_n, \ldots, \vec{a}_1}(x_n, \ldots, x_1; \delta) = \int_0^\delta d\delta' (\delta')^{a_n - 1} (1 - x_n \delta')^{-b_n} \mathcal{F}_{\vec{a}_{n-1}, \ldots, \vec{a}_1}(x_{n-1}, \ldots, x_1; \delta') . \tag{6.73}$$

where we have abbreviated $\vec{a}_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}$.

We find that these iterated integrals interpolate between multiple polylogarithms and hypergeometric functions. For example, in this framework the multiple polylogarithm is given by,

$$\begin{aligned} &\mathrm{Li}_{m_1, \ldots, m_k}(x_1, \ldots, x_k) \\ &\quad = \left( \prod_{i=1}^k x_i^{k-i+1} \right) \mathcal{F}_{\underbrace{\vec{0}, \ldots, \vec{0}}_{m_1 - 1}, \vec{1}, \ldots, \underbrace{\vec{0}, \ldots, \vec{0}}_{m_k - 1}, \vec{1}} (\underbrace{0, \ldots, 0}_{m_1 - 1}, x_1, \ldots, \underbrace{0, \ldots, 0}_{m_k - 1}, x_k \ldots x_1; 1) . \end{aligned} \tag{6.74}$$

where $\vec{0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $\vec{1} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. The Gauss hypergeometric function is given by,

$$ {}_2F_1(a_2, a_1; b_1; z) = a_1 \frac{\Gamma(b_1)}{\Gamma(a_2)\Gamma(b_1 - a_2)} \mathcal{F}_{\vec{v}\vec{u}}(1, z; 1), \tag{6.75} $$

with $\vec{v} = \begin{pmatrix} a_2 - a_1 \\ 1 - a_2 - b_1 \end{pmatrix}$ and $\vec{u} = \begin{pmatrix} a_1 \\ a_1 + 1 \end{pmatrix}$. A large variety of hypergeometric functions can be expressed in terms of these iterated integrals. With the definition

$$ A_n = \sum_{i=1}^{n} a_i, \qquad K_n = \sum_{i=1}^{n} k_i\,, \tag{6.76} $$

we find an explicit sum representation for this type of iterated integrals.

$$ \mathcal{F}_{\vec{a}_n,\dots,\vec{a}_1}(x_n, \dots, x_1; \delta) \;=\; \frac{\delta^{A_n}}{\prod\limits_{i=1}^{n} A_i} \sum_{k_1,\dots,k_n=0}^{\infty} \prod_{i=1}^{n} \left( \frac{(A_i)_{K_i}}{(A_i + 1)_{K_i}} (b_i)_{k_i} \frac{(x_i \delta)^{k_i}}{k_i!} \right) \tag{6.77} $$

Equation (6.77) is valid whenever the sums are convergent. Further properties and derivations are discussed in more detail in section 6.4. The solution of differential equations using iterated integrals is illustrated with an example in section 6.4.

The iterated integrals defined in this section are a powerful tool and enable us to solve all 19 master integrals in terms of hypergeometric functions. The results is valid to all orders in $\epsilon$. The iterated integrals can be written as multiple sums eq. (6.77) from which it is very convenient to extract a threshold expansion in $\delta$.

**Results for the master integrals**. The master integrals that we have computed in this section are useful for the evaluation of any cross section for a $2 \to 1$ process at N$^3$LO. For explicit expressions in terms of harmonic polylogarithms up to weight five we refer to ref. [189]. We have computed all 19 master integrals to all orders in $\epsilon$ in terms of hypergeometric functions and in an expansion in $\epsilon$ in terms of harmonic polylogarithms as described above.

## Direct integration using multiple polylogarithms

We present here an alternate method to compute the $(\mathrm{RV})^2$ Higgs boson cross section, based on subtraction terms. The phase-space integral over the squared amplitude can be written schematically as,

$$ \int d\Phi_2\, |\mathcal{A}|^2 = \int d\Phi_2 \sum_{i,j} M_i(s_{12}, s_{23}, s_{13})\, M_j(s_{12}, s_{23}, s_{13})\, N_{i,j}(s_{12}, s_{23}, s_{13}). \tag{6.78} $$

In this expression $M_i$ denote the one-loop master integrals and $N_{i,j}$ are rational functions, all of which depend on the invariants $s_{12}, s_{23}$ and $s_{13}$. As the results for the required one-loop master integrals are known to all orders in $\epsilon$ [193], the integrals are well defined in dimensional regularization. Our goal is to expand the integrals in $\epsilon$ under the integration sign and to perform the integration order by order in $\epsilon$. After expansion, however, the integrals may develop soft and collinear divergencies. The strategy is to subtract the singular limits of the integrand *before* expansion, and to perform the remaining (finite) integration in terms of multiple polylogarithms.

The construction of the counterterms that render the integration finite proceeds in two steps. First, we analytically continue all the hypergeometric functions that appear in the all order expressions of the one-loop master integrals such that they are convergent over the whole phase-space. This is achieved by using the well-known identities,

$$\begin{aligned}
{}_2F_1(a,b;c;z) &= (1-z)^{-b}\,{}_2F_1\left(b,c-a;c;\frac{z}{z-1}\right)\,,\\
{}_2F_1(a,b;c;z) &= \frac{\Gamma(b-a)\Gamma(c)}{\Gamma(b)\Gamma(c-a)}\,(-z)^{-a}\,{}_2F_1(a,a-c+1;a-b+1;z^{-1})\\
&\quad+\frac{\Gamma(a-b)\Gamma(c)}{\Gamma(a)\Gamma(c-b)}\,(-z)^{-b}\,{}_2F_1(b,b-c+1;b-a+1;z^{-1})\,.
\end{aligned} \tag{6.79}$$

Second, the soft and collinear counterterms are easily constructed by expanding the integrand around the collinear limits, i.e., $s_{13}\to 0$ or $s_{23}\to 0$. The counterterms can be trivially integrated to all orders in the dimensional regulator in terms of $\Gamma$ functions.

At the end of this procedure we are left with finite one-dimensional integrals. We expand the hypergeometric functions appearing in the integrand in $\epsilon$ using `HypExp` [200], resulting in a representation for the integrand in terms of classical polylogarithms up to weight four. More specifically, we are left with integrals of the form,

$$\int_0^1 d\lambda\,\sum_i\frac{P_i(\lambda,z)}{\lambda(1-\lambda)}\mathrm{Li}_n\left(R_{i,1}(\lambda,z)\right)\,\mathrm{Li}_m\left(R_{i,2}(\lambda,z)\right)\,, \tag{6.80}$$

with $n+m\leq 4$ and where $P_i$ is a polynomial and $R_{i,k}$ are rational functions. Note that, while individual terms in the sum are singular for $\lambda\to 0,1$, the sum is finite by construction, and so the integral is well defined. In order to perform the integration over $\lambda$, we rewrite the classical polylogarithms in terms of multiple polylogarithms of the form $G(a_1(z),\ldots,a_n(z);\lambda)$, where $a_i(z)$ are rational functions of $z$ using the coproduct calculus. All the integrals can then easily be performed using the algorithm described in section 2.6. Finally, we observe that the results of the integration can also be expressed in terms of harmonic polylogarithms of weight up to five, and we checked that the results are in agreement with the differential equation approach.

## 6.4 Hypergeometric functions through iterated integrals

In this section we define a class of iterated integrals as also introduced in Section 6.3. First let us define the integral,

$$\begin{aligned}
\mathcal{F}_{\vec{a}}(c;\delta) &= \int_0^\delta dt\, t^{a-1}\,(1-ct)^{-b} \\
&= \frac{\delta^a}{a}\, {}_2F_1(a,b;a+1;c\bar{z}) \\
&= \frac{\delta^a}{a}\sum_{n=0}^{\infty}\frac{(a)_n(b)_n}{(a+1)_n}\frac{(c\bar{z})^n}{n!}\,,
\end{aligned} \tag{6.81}$$

where we have abbreviated for later convenience $\vec{a} = \left(\begin{smallmatrix} a \\ b \end{smallmatrix}\right)$. We have made use of Gauss's hypergeometric function with the third argument being the first argument increased by one. Next, we define recursively the $n^{th}$ iterated integral,

$$\mathcal{F}_{\vec{a}_n,\ldots,\vec{a}_1}(x_n,\ldots,x_1;\delta) = \int_0^\delta dt\, t^{a_n-1}\,(1-x_n t)^{-b_n}\,\mathcal{F}_{\vec{a}_{n-1},\ldots,\vec{a}_1}(x_{n-1},\ldots,x_1;t)\,. \tag{6.82}$$

The integration kernel $t^{a-1}(1-ct)^{-b}$ has the same form for every iteration step with indices $a, b$ and argument $c$ changing. Next, we derive a hypergeometric series representation for these iterated integrals. To simplify the expressions we rewrite eq. (6.81) and introduce a function f that is implicitly given by,

$$\mathcal{F}_{\vec{a}}(c;\delta) = \sum_{n=0}^{\infty} f(a,b,c,n)\delta^{a+n}. \tag{6.83}$$

In the next step we integrate over the integration kernel and the $\mathcal{F}_{\vec{a}}(c;t)$,

$$\begin{aligned}
\mathcal{F}_{\vec{a}_2,\vec{a}_1}(c_2,c_1;\delta) &= \int_0^\delta dt\, t^{a_2-1}\,(1-c_2t)^{-b_2}\,\mathcal{F}_{\vec{a}}(c;t) \\
&= \sum_{n=0}^{\infty}\int_0^\delta dt\, t^{a_2+a_1+n-1}\,(1-c_2t)^{-b_2}\, f(a_1,b_1,c_1,n) \\
&= \sum_{n,m=0}^{\infty}\frac{\delta^{a_1+a_2+n+m}}{a_1+a_2+n}\frac{(a_1+a_2+n)_m(b_2)_m}{(a_1+a_2+n+1)_m}\frac{c_2^m}{m!} f(a_1,b_1,c_1,n)\,.
\end{aligned}$$

Using the identity,

$$(a+n)_m = (a)_{n+m}\frac{\Gamma(a)}{\Gamma(a+n)}\,, \tag{6.84}$$

we can write,

$$\begin{aligned}\mathcal{F}_{\vec{a}_2,\vec{a}_1}(c_2,c_1;\delta) = & \frac{\delta^{a_1+a_2}}{(a_1+a_2)a_1} \sum_{n,m=0}^{\infty} \frac{(a_1+a_2)_{m+n}}{(a_1+a_2+1)_{m+n}} \frac{(a_1)_n}{(a_1+1)_n} \\ & \times (b_2)_m (b_1)_n \frac{(c_2\delta)^m}{m!} \frac{(c_1\delta)^n}{n!}.\end{aligned} \tag{6.85}$$

We now proceed iteratively, and find the following series representation for the iterated integrals,

$$\mathcal{F}_{\vec{a}_n,\vec{a}_{n-1},\ldots,\vec{a}_1}(c_n,\ldots,c_1;\delta) = \frac{\delta^{A_n}}{\prod\limits_{i=1}^{n} A_i} \sum_{k_1,\ldots,k_n=0}^{\infty} \prod_{i=1}^{n} \frac{(A_i)_{K_i}}{(A_i+1)_{K_i}} (b_i)_{k_i} \frac{(c_i\delta)^{k_i}}{k_i!}, \tag{6.86}$$

with the abbreviations,

$$A_i = \sum_{n=1}^{i} a_n \quad \text{and} \quad K_i = \sum_{n=1}^{i} k_n\,. \tag{6.87}$$

Following the same procedure as for the sum representation we can derive a general Mellin-Barnes representation for our iterated integrals by utilizing the Mellin-Barnes representation of the Gauss Hypergeometric function

$${}_2F_1(a,b;c;\delta) = \frac{1}{2\pi i} \frac{\Gamma(c)}{\Gamma(a)\Gamma(b)} \int_{-i\infty}^{i\infty} ds \frac{\Gamma(a+s)\Gamma(b+s)}{\Gamma(c+s)} \Gamma(-s)(-\delta)^s. \tag{6.88}$$

This leads to

$$\begin{aligned}\mathcal{F}_{\vec{a}_n,\vec{a}_{n-1},\ldots,\vec{a}_1}(c_n,\ldots,c_1;\delta) = & \,\delta^{A_n} \int_{-i\infty}^{i\infty} \prod_{i=1}^{n} \frac{dk_i}{2\pi i} \\ & \times \frac{\Gamma(A_i+K_i)}{\Gamma(A_i+K_i+1)} \frac{\Gamma(b_i+k_i)}{\Gamma(b_i)} \Gamma(-k_i)(-c_i\delta)^{k_i}.\end{aligned} \tag{6.89}$$

These iterated integrals interpolate between multiple polylogarithms [46] and hypergeometric functions. In the framework of the above definitions the multiple polylogarithm is given by

$$\begin{aligned}& \mathrm{Li}_{m_1,\ldots,m_k}(x_1,\ldots,x_k) \\ & = \mathcal{F}_{\underbrace{\vec{0},\ldots,\vec{0}}_{m_1-1},\vec{1},\ldots,\underbrace{\vec{0},\ldots,\vec{0}}_{m_k-1},\vec{1}}(\underbrace{0,\ldots,0}_{m_1-1},x_1,\ldots,\underbrace{0,\ldots,0}_{m_k-1};x_k\ldots x_1) \prod_{i=1}^{k} x_i^{k-i+1}.\end{aligned} \tag{6.90}$$

Here the indices of the iterated integrals only take the form $\vec{0} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and $\vec{1} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. Even for general indices we discover further similarities of these iterated integrals to multiple polylogarithms. As in the case of polylogarithms, this class of hypergeometric functions may be written as multiple nested sums

$$\mathcal{F}_{\vec{a}_n,\vec{a}_{n-1},\ldots,\vec{a}_1}(c_n,\ldots,c_1;\delta) \;=\; \sum_{k_n\geq\cdots\geq k_1=0}^{\infty} \delta^{A_n+k_n} \prod_{i=1}^{n} \frac{1}{A_i+k_i} \frac{(b_i)_{k_i-k_{i-1}}(c_i)^{k_i-k_{i-1}}}{(k_i-k_{i-1})!}\,, \tag{6.91}$$

where $k_0 = 0$. The representation (6.91) may be useful for expanding the iterated integrals in terms of the dimensional regulator (see, e.g., ref. [186]).

The definition of these function as iterated integrals implies that they form a shuffle algebra,

$$\mathcal{F}_{\vec{a}_i,\ldots,\vec{a}_1}(c_i,\ldots,c_1;\delta)\,\mathcal{F}_{\vec{a}_n,\ldots,\vec{a}_{i+1}}(c_n,\ldots,c_{i+1};\delta) = \sum_{\sigma\in\Sigma(i,n-i)} \mathcal{F}_{\vec{a}_{\sigma(n)},\ldots,\vec{a}_{\sigma(1)}}(c_{\sigma(n)},\ldots,c_{\sigma(1)};\delta), \tag{6.92}$$

where $\Sigma(i,n-i)$ denotes the set of all shuffles of $n$ elements, i.e., the subset of the symmetric group $S_n$ defined in eq. (2.6). To illustrate an application of the shuffle-product for generalized iterated integrals, let us look at the following example. We would like to integrate an iterated integral over a non-standard integration kernel,

$$\mathcal{I} = \int_0^\delta dt\, t^{a_2-1}\,(1-c_2t)^{-b_2}\,(1-c_3t)^{-b_3}\,\mathcal{F}_{\vec{a}_1}(c_1;t). \tag{6.93}$$

To simplify the integral we make use of,

$$\mathcal{F}_{\left(\begin{smallmatrix} a \\ a+1 \end{smallmatrix}\right)}(1;\delta) = \frac{\delta^a}{a}(1-c\delta)^{-a} \tag{6.94}$$

and find,

$$\mathcal{I} = b_3 \int_0^\delta dt\, t^{a_2-b_3-1}\,(1-c_2t)^{-b_2}\,\mathcal{F}_{\left(\begin{smallmatrix} b_3 \\ b_3+1 \end{smallmatrix}\right)}(c_3;t)\mathcal{F}_{\left(\begin{smallmatrix} a_1 \\ b_1 \end{smallmatrix}\right)}(c_1;t). \tag{6.95}$$

Next, we apply the shuffle product and find,

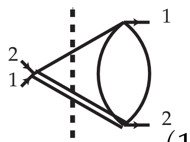
$$\begin{aligned}
\mathcal{I} &= b_3 \int_0^\delta dt\, t^{a_2-b_3-1}\,(1-c_2t)^{-b_2} \\
&\quad\times\left[\mathcal{F}_{\left(\begin{smallmatrix} b_3 \\ b_3+1 \end{smallmatrix}\middle|\begin{smallmatrix} a_1 \\ b_1 \end{smallmatrix}\right)}(c_3,c_1;t) + \mathcal{F}_{\left(\begin{smallmatrix} a_1 \\ b_1 \end{smallmatrix}\middle|\begin{smallmatrix} b_3 \\ b_3+1 \end{smallmatrix}\right)}(c_1,c_3;t)\right] \\
&= b_3\,\mathcal{F}_{\left(\begin{smallmatrix} a_2-b_3 \\ b_2 \end{smallmatrix}\middle|\begin{smallmatrix} b_3 \\ b_3+1 \end{smallmatrix}\middle|\begin{smallmatrix} a_1 \\ b_1 \end{smallmatrix}\right)}(c_2,c_3,c_1;\delta) \\
&\quad+ b_3\,\mathcal{F}_{\left(\begin{smallmatrix} a_2-b_3 \\ b_2 \end{smallmatrix}\middle|\begin{smallmatrix} a_1 \\ b_1 \end{smallmatrix}\middle|\begin{smallmatrix} b_3 \\ b_3+1 \end{smallmatrix}\right)}(c_2,c_1,c_3;\delta).
\end{aligned}$$

Further identities among iterated integrals can be derived using integration-by-parts or by partial fractioning products of integration kernels. Further properties and parallels of generalized iterated integrals and generalized polylogarithms are under investigation.

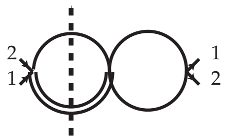
## NNLO RV Master Integrals as hypergeometric functions

In this section we demonstrate how certain differential equations for master integrals appearing in physical cross sections can be solved using iterated integrals introduced previously. We consider the example of the master integrals contributing to the $RV$ Higgs boson cross section at $NNLO$. The master integrals were introduced and evaluated as an expansion in the dimensional regulator $\epsilon$ in ref. [83] and evaluated to even higher order in ref. [34]. Here we solve them to all orders in $\epsilon$ in terms of hypergeometric functions.

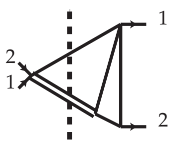
The master integrals and the corresponding differential equations are given by,

$\mathcal{Y}_1 =$  $$= \int d\Phi_2 \mathrm{Bub}^*(s_{13}), \tag{6.96}$$

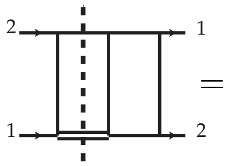
$$\partial_\delta \mathcal{Y}_1 = \frac{(1-3\epsilon)}{\delta}\mathcal{Y}_1, \tag{6.97}$$

$\mathcal{Y}_5 =$  $$= \int d\Phi_2 \mathrm{Bub}^*(s_{12}), \tag{6.98}$$

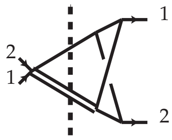
$$\partial_\delta \mathcal{Y}_5 = \frac{(1-2\epsilon)}{\delta}\mathcal{Y}_5, \tag{6.99}$$

$\mathcal{Y}_3 =$  $$= \int d\Phi_2 \mathrm{Tri}^*(s_{12}+s_{23}), \tag{6.100}$$

$$\partial_\delta \mathcal{Y}_3 = \frac{2\epsilon\delta}{1-\delta}\mathcal{Y}_3 - \frac{(1-3\epsilon)(1-2\epsilon)}{(1-\delta)\delta\epsilon}\mathcal{Y}_1 + \frac{(1-2\epsilon)^2(1-\delta)^{-1-\epsilon}}{\delta\epsilon}\mathcal{Y}_5, \tag{6.101}$$

$\mathcal{Y}_4 =$  $$= \int d\Phi_2 \mathrm{Box}^*(s_{12}, s_{23}, s_{13})\frac{1}{s_{23}}, \tag{6.102}$$

$$\partial_\delta \mathcal{Y}_4 = -\frac{(1+2\epsilon)}{\delta}\mathcal{Y}_4 - \frac{(2\delta-3)(1-3\epsilon)(1-2\epsilon)}{(1-\delta)\delta^3\epsilon}\mathcal{Y}_1 + \frac{2(1-2\epsilon)^2}{(1-\delta)^{1+\epsilon}\delta^2\epsilon}\mathcal{Y}_5 - \frac{2\epsilon}{(1-\delta)\delta}\mathcal{Y}_3. \tag{6.103}$$

$\mathcal{Y}_6 =$  $= \int d\Phi_2 \mathrm{Box}^*(s_{13}, s_{23}, s_{12}),$ (6.104)



$$\partial_\delta \mathcal{Y}_6 = -\frac{(1+4\epsilon)}{\delta}\mathcal{Y}_6 + \frac{2(1-3\epsilon)(1-2\epsilon)}{(1-\delta)\delta^2\epsilon}\mathcal{Y}_1 - \frac{4\epsilon}{(1-\delta)\delta}\mathcal{Y}_3. \tag{6.105}$$

We have abbreviated $\partial_\delta = \frac{\partial}{\partial\delta}$. Solid lines represent scalar propagators. The phase-space integral is represented by the dashed line and the cut propagators are the lines cut by the dashed line. The cut propagator of the Higgs boson is depicted by the double line. The complex conjugated one-loop integral is on the right-hand side of the phase-space cut. The differential equations were obtained using the methods described before.

The system of differential equations is decoupled and can be solved as described in Section 6.3. To solve the differential equations we require the following boundary conditions, which can be obtained from ref. [34],

$$\mathcal{Y}_1^S = \frac{(4\pi)^{\epsilon-1}s^{-2\epsilon}\Gamma(1-2\epsilon)\Gamma(1-\epsilon)^2\Gamma(\epsilon+1)}{\epsilon\Gamma(2-3\epsilon)\Gamma(2-2\epsilon)}, \tag{6.106}$$

$$\mathcal{Y}_5^S = \frac{(4\pi)^{\epsilon-1}(-s)^{-\epsilon}s^{-\epsilon}\Gamma(1-\epsilon)^3\Gamma(\epsilon+1)}{2\epsilon\Gamma(2-2\epsilon)^2}, \tag{6.107}$$

$$\mathcal{Y}_6^S = -\frac{(4\pi)^{\epsilon-1}(-s)^{-\epsilon}s^{-2-\epsilon}\Gamma(1-2\epsilon)\Gamma(1-\epsilon)^2\Gamma(\epsilon+1)^2}{\epsilon^3\Gamma(1-4\epsilon)}, \tag{6.108}$$

and all other cases vanish. These boundary conditions are given by the leading (soft) term of three master integrals in the limit of $\delta \to 0$. They are obtained using the methods described in Section 6.3. For convenience we will from now on set $s = 1$.

The first two differential equations are homogeneous and can be easily solved to give

$$\mathcal{Y}_1(\delta) = \delta^{1-3\epsilon}\mathcal{Y}_1^S. \tag{6.109}$$

$$\mathcal{Y}_5(\delta) = \delta^{1-2\epsilon}\mathcal{Y}_5^S. \tag{6.110}$$

We find that the homogeneous solution to the differential equation of master $\mathcal{Y}_3$ is vanishing and the inhomogeneous solution is according to eq. (6.70) given by,

$$
\begin{aligned}
\mathcal{Y}_3(\delta) &= (1-\delta)^{-2\epsilon}\frac{(1-2\epsilon)}{\epsilon} \\
&\times \int_0^\delta d\delta' \left((1-2\epsilon)(1-\delta')^{\epsilon-1}\delta'^{-2\epsilon}\mathcal{Y}_5^S - (1-3\epsilon)(1-\delta')^{2\epsilon-1}\delta'^{-3\epsilon}\mathcal{Y}_1^S\right) \\
&= \frac{(2\epsilon-1)^2(1-\delta)^{-2\epsilon}}{\epsilon}\mathcal{F}_{\left(\begin{smallmatrix}1-2\epsilon\\1-\epsilon\end{smallmatrix}\right)}(1;\delta)\,\mathcal{Y}_5^S \\
&- \frac{(2\epsilon-1)(3\epsilon-1)(1-\delta)^{-2\epsilon}}{\epsilon}\mathcal{F}_{\left(\begin{smallmatrix}1-3\epsilon\\1-2\epsilon\end{smallmatrix}\right)}(1;\delta)\,\mathcal{Y}_1^S\,,
\end{aligned}
\tag{6.111}
$$

with

$$
\mathcal{F}_{\left(\begin{smallmatrix}a\\b\end{smallmatrix}\right)}(1;\delta) = \frac{\delta^a}{a}\,{}_2F_1(a,b;a+1;\delta). \tag{6.112}
$$

To obtain this result we made use of eq. (6.81). As we proceed to solve the remaining two master integrals we find that the inhomogeneous solution to their differential equation is in turn dependent on $\mathcal{Y}_3$. We are able to find solutions to the inhomogeneous equation making use of the definition of our iterated integrals in eq. (6.82),

$$
\begin{aligned}
\mathcal{Y}_4(\delta) &= \delta^{-1-2\epsilon}\int_0^\delta d\delta' 2(1-3\epsilon)(1-2\epsilon)\delta'^{2\epsilon}(1-\delta')^{-2\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1-3\epsilon\\1-2\epsilon\end{smallmatrix}\right)}(1;\delta')\mathcal{Y}_1^S \\
&- \delta^{-1-2\epsilon}\int_0^\delta d\delta' 2(1-2\epsilon)^2\delta'^{2\epsilon}(1-\delta')^{-2\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1-2\epsilon\\1-\epsilon\end{smallmatrix}\right)}(1;\delta')\mathcal{Y}_5^S \\
&- \delta^{-1-2\epsilon}\int_0^\delta d\delta' \frac{(2\delta'-3)(1-3\epsilon)(1-2\epsilon)\delta'^{-\epsilon-1}}{(1-\delta')\epsilon}\mathcal{Y}_1^S \\
&+ \delta^{-1-2\epsilon}\int_0^\delta d\delta' \frac{2(1-2\epsilon)^2(1-\delta')^{-\epsilon-1}}{\epsilon}\mathcal{Y}_5^S\,.
\end{aligned}
\tag{6.113}
$$

Now we can use the definitions of the iterated integrals eqs. (6.81) and (6.82) to obtain,

$$\begin{aligned}
\mathcal{Y}_4(\delta) &= 2\left(6\epsilon^2-5\epsilon+1\right)\delta^{-2\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1+2\epsilon\\1+2\epsilon\end{smallmatrix}\middle|\begin{smallmatrix}1-3\epsilon\\1-2\epsilon\end{smallmatrix}\right)}(1,1;\delta)\mathcal{Y}_1^S \\
&- 2(1-2\epsilon)^2\delta^{-2\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1+2\epsilon\\1+2\epsilon\end{smallmatrix}\middle|\begin{smallmatrix}1-2\epsilon\\1-\epsilon\end{smallmatrix}\right)}(1,1;\delta)\mathcal{Y}_5^S \\
&+ \frac{\left(6\epsilon^2-5\epsilon+1\right)\delta^{-2\epsilon-1}}{\epsilon}\mathcal{F}_{\left(\begin{smallmatrix}1-\epsilon\\1\end{smallmatrix}\right)}(1;\delta)\mathcal{Y}_1^S \\
&- \frac{3\left(6\epsilon^2-5\epsilon+1\right)\delta^{-3\epsilon-1}}{\epsilon^2}\mathcal{Y}_1^S \\
&+ \frac{2(1-2\epsilon)^2\left((1-\delta)^{-\epsilon}-1\right)\delta^{-2\epsilon-1}}{\epsilon^2}\mathcal{Y}_5^S, \qquad (6.114)
\end{aligned}$$

$$\begin{aligned}
\mathcal{Y}_6(\delta) &= \delta^{-1-4\epsilon}4(1-3\epsilon)(1-2\epsilon)\int_0^\delta d\delta'\delta'^{4\epsilon}(1-\delta')^{-2\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1-3\epsilon\\1-2\epsilon\end{smallmatrix}\right)}(1;\delta')\mathcal{Y}_1^S \\
&- \delta^{-1-4\epsilon}4(1-2\epsilon)^2\int_0^\delta d\delta'\delta'^{4\epsilon}(1-\delta')^{-2\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1-2\epsilon\\1-\epsilon\end{smallmatrix}\right)}(1;\delta')\mathcal{Y}_5^S \\
&+ \delta^{-1-4\epsilon}\frac{2\left(6\epsilon^2-5\epsilon+1\right)}{\epsilon}\int_0^\delta d\delta'\frac{\delta'^{\epsilon}}{(1-\delta')}\mathcal{Y}_1^S \\
&+ \delta^{-1-4\epsilon}\mathcal{Y}_6^S \\
&= 4\left(6\epsilon^2-5\epsilon+1\right)\delta^{-4\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1+4\epsilon\\1+2\epsilon\end{smallmatrix}\middle|\begin{smallmatrix}1-3\epsilon\\1-2\epsilon\end{smallmatrix}\right)}(1,1;\delta)\mathcal{Y}_1^S \\
&- 4(1-2\epsilon)^2\delta^{-4\epsilon-1}\mathcal{F}_{\left(\begin{smallmatrix}1+4\epsilon\\1+2\epsilon\end{smallmatrix}\middle|\begin{smallmatrix}1-2\epsilon\\1-\epsilon\end{smallmatrix}\right)}(1,1;\delta)\mathcal{Y}_5^S \\
&+ \frac{2\left(6\epsilon^2-5\epsilon+1\right)\delta^{-4\epsilon-1}}{\epsilon}\mathcal{F}_{\left(\begin{smallmatrix}1+\epsilon\\1\end{smallmatrix}\right)}(1;\delta)\mathcal{Y}_1^S \\
&+ \delta^{-1-4\epsilon}\mathcal{Y}_6^S. \qquad (6.115)
\end{aligned}$$

The iterated integrals with two indices contributing to $\mathcal{Y}_4$ and $\mathcal{Y}_6$ can be written as,

$$\begin{aligned}
\mathcal{F}_{\left(\begin{smallmatrix}a_2\\b_2\end{smallmatrix}\middle|\begin{smallmatrix}a_1\\b_1\end{smallmatrix}\right)}(1,1,\delta) &= \frac{\delta^{a_1+a_2}}{(a_1+a_2)a_1}F^{1,2}_{1,1}\left(\begin{matrix}a_2+a_1\\a_2+a_1+1\end{matrix}\middle|\begin{matrix}a_1 & 1 & b_1 & b_2\\a_1+1 & 1 & - & -\end{matrix}\middle|\delta,\delta\right) \\
&= \frac{\delta^{a_1+a_2}}{(a_1+a_2)a_1}\sum_{n,m=0}^{\infty}\frac{(a_2+a_1)_{n+m}}{(a_2+a_1+1)_{n+m}}\frac{(a_1)_n(b_1)_n}{(a_1+1)_n}(b_2)_m\frac{\delta^n}{n!}\frac{\delta^m}{m!},
\end{aligned}$$

where we introduced the Kampé de Fériet function,

$$F^{p,q}_{p',q'}\left(\begin{array}{c|cc|c} \alpha_i & \beta_i & \gamma_i & \\ \alpha_i' & \beta_i' & \gamma_i' & x,y \end{array}\right) = \sum_{n,m=0}^{\infty} \frac{\prod_{i=1}^{p}(\alpha_i)_{n+m}\,\prod_{i=1}^{q}(\beta_i)_n\,(\gamma_i)_m}{\prod_{i=1}^{p'}(\alpha_i')_{n+m}\,\prod_{i=1}^{q'}(\beta_i')_n\,(\gamma_i')_m}\,\frac{x^n}{n!}\,\frac{y^m}{m!}\,. \tag{6.116}$$

Note that the generalized Kampé de Fériet function $S_1$ of Section 6.3 is a special case of eq. (6.116),

$$S_1(a_1;a_2,b_1;a_3,b_2;x_1,x_2) = F^{2,1}_{1,1}\left(\begin{array}{cc|cc|c} a_1 & a_2 & b_1 & 1 & \\ a_3 & - & b_2 & 1 & x,y \end{array}\right)\,. \tag{6.117}$$

CHAPTER 7

# DOUBLE-VIRTUAL REAL CORRECTIONS

## 7.1 The double-virtual real cross section

We consider the partonic QCD amplitudes for the production of a Higgs boson in association with one additional parton. We distinguish three different channels by their initial state,

$$\begin{aligned} g(p_1) + g(p_2) &\to g(p_3) + H(p_h) \\ q(p_1) + g(p_2) &\to q(p_3) + H(p_h) \\ q(p_1) + \bar{q}(p_2) &\to g(p_3) + H(p_h) \end{aligned} \tag{7.1}$$

where $q, \bar{q}, g$ and $H$ denote a quark, anti-quark, gluon or Higgs boson respectively with their associated momenta $p_1 \dots p_3$, $p_h$. This allows to define the following kinematic invariants,

$$\begin{aligned} s &= 2p_1 \cdot p_2, & p_h^2 &= M_h^2 \equiv sz, \\ s\bar{z}\lambda &= 2p_1 \cdot p_3, & s\bar{z}\bar{\lambda} &= 2p_2 \cdot p_3, \end{aligned} \tag{7.2}$$

where $z = \frac{M_h^2}{s}$, $\bar{z} = 1 - z$, $\bar{\lambda} = 1 - \lambda$. The partonic cross section for these processes is then given by,

$$\sigma_X = \frac{N_X}{2s} \int d\Phi_2 \sum_X |M_X|^2, \tag{7.3}$$

where $X \in \{g\,g \to H\,g, q\,\bar{q} \to H\,g, g\,q \to H\,q\}$. The summation sign indicates summation over final- and initial-state particle polarizations and colors. As before, we work in conventional dimensional regularization with $d = 4 - 2\epsilon$ space-time dimensions. The process dependent factors $N_X$ containing the averaging of initial state parton colors and polarizations are given by

$$\begin{aligned} N_{gg\to Hg} &= \frac{1}{4(N_c^2-1)^2(1-\epsilon)^2} \\ N_{g,q\to Hq} &= \frac{1}{4N_c(N_c^2-1)(1-\epsilon)} \\ N_{q\bar{q}\to Hg} &= \frac{1}{4N_c^2}. \end{aligned} \tag{7.4}$$

$N_c$ and $(N_c^2 - 1)$ are the number of quark and gluon colors respectively. The phase-space measure for the production of a massive Higgs boson in association with a massless parton is given by,

$$d\Phi_2 = \frac{d^d p_3}{(2\pi)^d}\delta_+(p_3^2)\frac{d^d p_h}{(2\pi)^d}\delta_+(p_h^2 - M_h^2)(2\pi)^d\delta^{(d)}(p_1 + p_2 - p_3 - p_h), \tag{7.5}$$

where $\delta_+(p^2) = (2\pi)\delta(p^2)\theta(p_0)$. Using the definitions of eq. (7.1) we can parametrize the phase-space measure and specialize eq. (4.59) to

$$\mathrm{d}\Phi_2 = \frac{(4\pi)^{-1+\epsilon}s^{-\epsilon}\bar{z}^{1-2\epsilon}}{2\Gamma(1-\epsilon)}\mathrm{d}\lambda(\lambda\bar{\lambda})^{-\epsilon}\theta(\lambda)\theta(\bar{\lambda}). \tag{7.6}$$

We consider the mass of the top quark to be large enough for the top quark to be integrated out. This description can be formulated using the effective Lagrangian

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_{QCD} - \frac{1}{4}CHG^a_{\mu\nu}G^{a,\mu\nu}. \tag{7.7}$$

$\mathcal{L}_{QCD}$ is the QCD Lagrangian with $N_f$ light quark flavors, $H$ the Higgs boson field and $G^a_{\mu\nu}$ the gluon field strength tensor. The Wilson coefficient $C$ can be explicitly calculated taking into account the interactions of the top quark [181, 188–191].

We perform an expansion of the partonic scattering matrix-elements in the number of loops

$$|M_X|^2 = \left|\sum_{i=1}^{\infty} M_X^{(i)}\right|^2, \tag{7.8}$$

where $i$ runs over the number of loops. The main result of this chapter is the partonic scattering cross section arising due to the interference of two-loop matrix-elements with the corresponding tree-level matrix elements and we refer to it as the double-virtual-real ($RVV$) cross section.

$$\sigma_X^{RVV} = \frac{N_X}{2s}\int d\Phi_2 \sum 2\Re\left(M_X^{(2)}M_X^{(0)*}\right) \tag{7.9}$$

The cross section can be separated into five different contributions.

$$\sigma_X^{RVV}(z) = \sum_{i=2}^{6} (1-z)^{-i\epsilon} \sigma_X^{(i)\,RVV}(z). \tag{7.10}$$

The individual terms $\sigma_X^{(i)\,RVV}(z)$ no longer contain logarithms with argument $(1-z)$, i.e. they are meromorphic functions of $z$ with at most a single pole at $z = 1$. They contain infrared and ultraviolet divergences that appear as poles in $\epsilon$. The $\sigma_X^{(i)\,RVV}(z)$ can be written as a Laurent series in the dimensional regulator. Each term in the series can be expressed as a linear combination of multiple polylogarithms with rational coefficients.

## 7.2 Results

We obtained the $RVV$ cross section for all partonic sub-channels completing the calculation of all two-loop contributions to the $\mathrm{N^3LO}$ Higgs boson cross section. Parts of the result of this chapter were essential ingredients of threshold expansion of the Higgs boson production cross section at $\mathrm{N^3LO}$ published in ref. [4]. In ref. [4] we also produced the coefficients of the leading three threshold logarithms of the $\mathrm{N^3LO}$ Higgs boson cross section. The result of this chapter and specifically the possibility of decomposing the $RVV$ cross section as in eq. (7.10) were key ingredients used in the derivation of the coefficients of these logarithms. The first threshold-expansion coefficient of the $RVV$ cross section was obtained in refs. [24, 201] and agrees with the corresponding expansion coefficient of our result.

Due to the length of the expressions we refrain from displaying the formulae for the $RVV$ cross section explicitly. Instead we refer to ref. [5] where we give the bare cross sections $\sigma_X^{RVV}$,

$$\sigma_X^{RVV} = \frac{N_X}{2s} \int d\Phi_2 \sum 2\mathcal{R}\left(M_X^{(2)} M_X^{(0)*}\right), \tag{7.11}$$

as a Laurent expansion in the dimensional regulator. $N_X$ is given in eq. (7.4). The cross section can furthermore be separated into contributions with a single pole at $z = 1$ and remaining contributions that are analytic as $z \to 1$,

$$\sigma_X^{RVV}(z) = \sum_{i\in\{2,4,6\}} (1-z)^{-1-i\epsilon} \sigma_X^{(i)\,\mathrm{sing}} + \sum_{i=2}^{6} (1-z)^{-i\epsilon} \sigma_X^{(i)\,\mathrm{reg}}(z). \tag{7.12}$$

For the singular terms we only expand the $\sigma_X^{(i)\,\mathrm{sing}}$ in the dimensional regulator up to order $\epsilon$, leaving the prefactor unexpanded, while for the regular pieces we expand the product $(1 - z)^{-i\epsilon} \sigma_X^{(i)\,\mathrm{reg}}(z)$ up to order $\epsilon^0$. We observe that the coefficients of the Laurent expansion of our cross section can be expressed as linear combinations of harmonic polylogarithms with indices $a_i \in \{0, 1\}$.

## 7.3 Calculation

To obtain all channels contributing to the $RVV$ cross section we compute the required two-loop and tree-level Feynman diagrams generated by `qgraf` [183]. We perform the contraction of spinor and color traces with custom C++ code based on the expression library GiNaC [202]. We work in Feynman gauge and restore gauge invariance by combining our matrix elements with the necessary Fadeev-Popov ghost matrix elements.

Having performed all algebraic manipulations of the Feynman diagrams we arrive at our matrix-elements in terms of scalar products of loop and external momenta. Rather than carrying out the integration over the loop and phase-space momenta in a sequential way, we treat all integrations on equal footing and combine them into a single integration measure,

$$d\Phi = \frac{d^d k_1}{(2\pi)^d} \frac{d^d k_2}{(2\pi)^d} d\Phi_2. \tag{7.13}$$

This combination allows us to apply the framework of reverse unitary [84, 155, 157] and to use IBP reductions. The large system of IBP identities for the integrals appearing in our calculation is solved using the Gauss elimination algorithm [146], which we implemented in a private C++ code using the GiNaC library [202] . All integrals appearing in the cross section can be related to linear combinations of 72 master integrals. We now discuss the methods used to solve our master integrals.

## 7.4 Calculating Master Integrals

In this section we describe the setup we used to solve our master integrals via first-order differential equations. We start by deriving the required differential equations. Their general solution has to be constrained by fixing one boundary condition per integral. We rely on our method of boundary decomposition, described in section 3.4, to facilitate the calculation of the required boundary conditions. Next, we discuss how the general solution of these differential equations can be computed. Finally, we illustrate the procedure using a simple example and demonstrate an explicit calculation of an actual $RVV$ boundary condition.

### Setup of the system of differential equations.

After integration over the final-state and loop momenta eq. (7.13), the integrals are functions of the Higgs mass $M_h$ and the partonic center of mass energy $s$. It is therefore convenient to define a single dimensionless ratio,

$$z = \frac{M_h^2}{s}, \qquad \bar{z} = 1 - z = \frac{s - M_h^2}{s}, \tag{7.14}$$

and write all master integrals as functions of this ratio,

$$f_i = f_i(\bar{z}). \tag{7.15}$$

For brevity, we set $s = 1$ as the exact $s$ dependence can be reconstructed using dimensional analysis.

In order to evaluate the master integrals we use the method of differential equations [81, 118]. Because the master integrals are functions of a single ratio $\bar{z}$, we can differentiate with respect to the square of the Higgs mass, which only appears in the cut propagator corresponding to the Higgs on shell condition. As outlined in section 7.3 using the framework of reverse unitarity we find,

$$\frac{\partial}{\partial \bar{z}}\left[\frac{1}{p_h^2 - M_h^2}\right]_c = -\frac{\partial}{\partial M_h^2}\left[\frac{1}{p_h^2 - M_h^2}\right]_c = \left[\frac{1}{p_h^2 - M_h^2}\right]_c^2. \tag{7.16}$$

By applying this differential to our master integrals, we obtain a set of new phase space integrals. Using IBP identities these integrals can again be expressed through our basis of master integrals. This way we are able to express the differential of each master integral through the master integral itself as well as other integrals, obtaining a coupled system of linear first order differential equations for the master integrals,

$$\partial_{\bar{z}} f_i(\bar{z}) = A_{ij}(\bar{z}, \epsilon) f_j(\bar{z}). \tag{7.17}$$

The Einstein summation convention is implied. The entries of the system matrix $A$ are in general rational functions in $\bar{z}$ as well as in $\epsilon$. The choice of basis is of course not unique and may be related to another one via a $\bar{z}$- and $\epsilon$-dependent transformation. We observe that the system matrix for the $RVV$ master integrals can be written as,

$$A_{ij}(\bar{z}, \epsilon) = \frac{A_{ij}^{(0)}(\bar{z}, \epsilon)}{\bar{z}} + \frac{A_{ij}^{(1)}(\bar{z}, \epsilon)}{\bar{z} - 1}, \tag{7.18}$$

i.e. only poles at $\bar{z} = 0$ and $\bar{z} = 1$ appear and $A_{ij}^{(0)}(\bar{z}, \epsilon)$ and $A_{ij}^{(1)}(\bar{z}, \epsilon)$ are holomorphic functions of $\bar{z}$.

## Boundary conditions

The solution to the above system of differential equations will require the specification of one boundary condition per integral. As was pointed out in ref. [74] a connection to the eigenvalues of the system of differential equations can be used to facilitate this step. Using the boundary decomposition discussed in section 3.4 we can make this connection manifest as in eq. (3.117),

$$f_i(x) = R_{ij}^{-1} g_j(x) = R_{ik}^{-1} e^{\epsilon J_{kj} \log(x)} g_{0,j}. \tag{7.19}$$

It is possible to arrive at the $g_{0,i}$ from a completely orthogonal point of view. Using the method of expansion by regions, the limiting solution of a master integral as $\bar{z} \to 0$ can be computed. Specifically, expansion by regions separates the limiting solution into different *regions* each associated with a specific integrating factor $\bar{z}^{\lambda}$. Having identified the constants $g_{0,i}$ contributing to a specific integral from the boundary decomposition, we can therefore match the constants $g_{0,i}$ to the regions. Any boundary condition $g_{0,i}$ associated with an integrating factor that does not correspond to a region vanishes and therefore does not even require the explicit calculation of a Feynman integral.

For example, analyzing the $RVV$ cross section using expansion by regions, we find only regions with integrating factors $\bar{z}^{a_i - b_i \epsilon}$, with $a_i \in \mathbb{Z}$ and $b_i \in \{2, 3, 4, 5, 6\}$. Therefore, only boundary conditions $f_{0,i}$ corresponding to $\lambda_i = a_i - b_i\epsilon$ can be non-vanishing. All other boundary constants appearing in the system are zero. Applying this boundary decomposition dramatically reduces the number of boundary conditions that we needed to compute for the $RVV$ master integrals from 72 to a mere 19.

The remaining boundary conditions can be computed explicitly using expansion by regions. This step is also facilitated by the boundary decomposition, as one constant $g_{0,i}$ may appear in the limiting solution of more than one master integral. It is therefore reasonable to pick the simplest integrals to calculate the remaining constants.

The actual computation is performed by deriving the integral representations of regions associated to the remaining boundary constants. This step is made especially viable by an algorithm exploiting a geometric interpretation of the parametric representation of Feynman integrals as implemented in the code asy [195, 203]. For a given integral and limit, asy provides a parametrization for each region, which allows the direct expansion of the Feynman integral to obtain integral representation of the regions.

In the case of the N$^3$LO Higgs production cross section a threshold expansion was performed and the “soft” master integrals appearing in these calculations may serve as boundary conditions for full kinematic integrals. Specifically the first term of the $RVV$ cross section was obtained in refs. [24, 201]; in order to complete the full kinematic calculation we could compare and confirm three of the boundary conditions given explicitly. However, we calculated 16 additional boundary conditions as described above. We observe that all explicit logarithms arising from eigenvalues with non-trivial Jordan blocks vanish in the final result. We provide an explicit example of how we calculate our boundary conditions later in this chapter.

We want to stress that our algorithm of boundary decomposition can be based around any singular point in the differential equation. For example, we could have also calculated the limiting solutions for $\bar{z} \to 1$. Repeating the procedure with further singular points may also lead to additional constraints on the boundary conditions and therefore further reduce the number of integrals that actually have to be calculated. Furthermore, we would like to point out that constraints on allowed eigenvalues, leading to non-vanishing $g_{0,i}$ can also be obtained from analyticity requirements and physical considerations [81, 118].

## Solving the differential equations

In this section we discuss the method for solving differential equations of the type given in eq.(7.17). In general a system of differential equations can be written as,

$$\partial_{\bar{z}} M_i(\bar{z}) = A^h_{ij}(\bar{z},\epsilon) M_j(\bar{z},\epsilon) + y_i(\bar{z}), \tag{7.20}$$

where $A^h_{ij}(\bar{z},\epsilon)M_j(\bar{z},\epsilon)$ is the homogeneous part and $y_i(\bar{z})$ is the inhomogeneity that is zero unless a subset of master integrals has already been computed. In general, the homogeneous solution is given by,

$$M^h_i(\bar{z}) = \left(e^{\int d\bar{z} A^h(\bar{z},\epsilon)}\right)_{ij} M_{j,0} = H_{ij}(\bar{z},\epsilon) M_{j,0}, \tag{7.21}$$

where $M_{i,0}$ is the boundary condition for master $M_i$. Next, we need to find a particular solution, which can depend on other master integrals. As $y_i(\bar{z})$ is known we find simply,

$$M^p_i(\bar{z}) = H_{ij}(\bar{z},\epsilon) \int d\bar{z} H^{-1}_{jk}(\bar{z},\epsilon) y_k(\bar{z}), \tag{7.22}$$

such that the full solution can be written as,

$$M_i(\bar{z}) = M^h_i(\bar{z}) + M^p_i(\bar{z}). \tag{7.23}$$

However, in general the differential equations are coupled and it is impossible to compute the matrix exponential in eq. (7.21). The desired result for our master integrals is a Laurent expansion in the dimensional regulator. A commonly used strategy to calculate the above matrix exponential is therefore to expand the differential equations in $\epsilon$ and decouple them order by order.

One particularly interesting version of this strategy has been proposed in ref. [77], which suggests that it is possible for Feynman integrals to find a transformation to a canonical basis such that the system takes the form,

$$\partial_{\bar{z}} M^c_i(\bar{z}) = \epsilon A^c_{ij}(\bar{z}) M^c_j(\bar{z}). \tag{7.24}$$

In this basis the $\epsilon$ dependence factorizes completely from the system matrix. In this scenario the inhomogeneity is zero. Furthermore, the system matrix takes the simple form,

$$A^c_{ij}(\bar{z}) = \sum_k \frac{A^{c\,(k)}_{ij}}{\bar{z} - \bar{z}_k}, \tag{7.25}$$

where the matrices $A^{c\,(k)}$ have constant entries. The canonical form of the system matrix (eq. (7.25)) makes the connection to multiple polylogarithms as defined in eq. (2.15) manifest. The formal solution of the canonical differential equations (eq. (7.24)) can be written as,

$$M_i^c(\bar{z}) = \left(\mathcal{P}e^{\epsilon \int d\bar{z} A^c(\bar{z})}\right)_{ij} M^c{}_{j,0}, \tag{7.26}$$

where $\mathcal{P}$ symbolizes the path-ordered exponential and $M_0^c$ is a vector of boundary conditions. Expanding the exponential in $\epsilon$ we obtain,

$$M_i^c(\bar{z}) = \left(1 + \epsilon \int d\bar{z} A^c{}_{ij}(\bar{z}) + \epsilon^2 \int d\bar{z} \left(A_{ik}^c(\bar{z}) \int d\bar{z} A^c{}_{kj}(\bar{z})\right) + \ldots\right) M^c{}_{j,0}. \tag{7.27}$$

At the time of our computation, no general algorithmic way to construct the transformation that takes the master integrals to the canonical basis, was available[1]. Obtaining the canonical form is therefore a non trivial task. A method, based on analyzing the leading singularities of the Feynman integrals was outlined in ref. [77], further insights are e.g. discussed in refs. [74, 76, 81, 86, 118, 204, 205].

To find a solution for differential equations the only necessary requirement is that the system can be sufficiently decoupled order by order in $\epsilon$ such that the matrix exponential in eq. (7.21) can be computed. While obtaining a canonical basis ensures this decoupling, this is not the only basis that decouples the system. We choose to transform only a subsystem of 56 integrals of the complete system of 72 master integrals to the canonical basis. The remaining 16 integrals can be easily computed using the general method.

In this manner we obtain a solution for the full system depending on 72 constants of integration. By imposing the boundary decomposition of the limiting solution obtained in the previous section, i.e. demanding that the full solution has the correct limit, we are able to uniquely fix all constants. We thereby calculated all 72 master integrals required for the $RVV$ Higgs boson cross section at N$^3$LO.

## A pedagogical example

We discuss a short pedagogical example. While this integral can also easily be calculated using various other techniques, it serves well to illustrate how the methods described above proceed. Recall the triangle topology defined in eq. (3.42),

$$T(a_1, a_2, a_3) = \int \frac{d^dk}{(2\pi)^d} \frac{1}{(k^2 - m^2)^{a_1}((k+p_1)^2 - m^2)^{a_2}((k+p_1+p_2)^2 - m^2)^{a_3}}, \tag{7.28}$$

[1]After our computation was finished, an algorithm for finding a transformation to the canonical basis for certain systems was published in ref. [158]. This algorithm would have been applicable to our situation.

with $p_1^2 = p_2^2 = 0$ and $p_1 \cdot p_2 = s/2$. We choose as a basis of master integrals

$$M_1 = T(2,0,0), \qquad M_2 = xT(2,0,1), \qquad M_3 = \epsilon T(1,1,1), \tag{7.29}$$

with $x = \sqrt{1 - 4\frac{m^2}{s}}$ and setting $s = 1$ for simplicity. With this we find the system of differential equations,

$$\frac{\partial}{\partial x}\vec{M}(x) = \epsilon \\ \times \left[ \begin{pmatrix} 0 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{x} + \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \frac{1}{1-x} + \begin{pmatrix} -1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & -1 \end{pmatrix} \frac{1}{1+x} \right] \vec{M}(x). \tag{7.30}$$

Next we analyze the system in the limit $x \to 1$. This limit corresponds to the situation when the internal mass $m$ is small compared to $s$,

$$\frac{\partial}{\partial x}\vec{\tilde{M}}(x) = \epsilon \left[ \begin{pmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 1 \end{pmatrix} \frac{1}{1-x} \right] \vec{\tilde{M}}(x). \tag{7.31}$$

Calculating the Jordan form $J$ and the associated transformation matrix $R$ of the system matrix yields,

$$J = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\epsilon & 1 \\ 0 & 0 & -\epsilon \end{pmatrix}, \qquad R = \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 1 \\ -\epsilon & 0 & 0 \end{pmatrix}. \tag{7.32}$$

The limiting solution in the Jordan basis and the original master integral basis is thus,

$$\vec{f}(x) = e^{J\log(1-x)}\vec{f}_0 = \begin{pmatrix} f_0^{(1)} \\ (1-x)^{-\epsilon} f_0^{(2)} + (1-x)^{-\epsilon}\log(1-x) f_0^{(3)} \\ (1-x)^{-\epsilon} f_0^{(3)} \end{pmatrix}, \tag{7.33}$$

$$\vec{\tilde{M}}(x) = \begin{pmatrix} -\frac{f_0^{(3)}(1-x)^{-\epsilon}}{\epsilon} \\ -\frac{f_0^{(3)}(1-x)^{-\epsilon}}{\epsilon} - f_0^{(1)} \\ f_0^{(2)}(1-x)^{-\epsilon} + f_0^{(3)}(1-x)^{-\epsilon}\log(1-x) + f_0^{(1)} \end{pmatrix}. \tag{7.34}$$

The next step is to determine the $f_0^{(i)}$ from expansion by regions. We start by determining $f_0^{(3)}$. The easiest integral to compute for $f_0^{(3)}$ is $M_1$. This integral, being a simple tadpole, is a one scale integral and as such has only one region. Fortunately, it is trivial to obtain the full solution from the integral representation,

$$M_1 = \int \frac{d^d k}{(2\pi)^d} \frac{1}{k^2 - m^2}, \tag{7.35}$$

and we obtain,

$$M_1 = i(4\pi)^{-2+\epsilon}\Gamma(\epsilon)(1-x)^{-\epsilon}(1+x)^{-\epsilon}. \tag{7.36}$$

The boundary condition is then obtained by comparing the leading term in the expansion around $x = 1$ to eq. (7.34) and we have,

$$f_0^{(3)} = -i(4\pi)^{-2+\epsilon}\epsilon\Gamma(\epsilon). \tag{7.37}$$

The next constant to be determined is $f_0^{(1)}$. Here we choose the integral $M_2$. This integral is a massive bubble and contains the scales $s$ and $m$. Analyzing this integral using the method of expansion by regions explicitly or using the code asy [195, 203] for guidance, one finds three regions $R_2^{(1)}$, $R_2^{(3)}$ and $R_2^{(3)}$ with the following scalings,

$$R_2^{(1)} \propto (1-x)^0, \quad R_2^{(2)} \propto (1-x)^{-\epsilon} \text{ and } R_2^{(3)} \propto (1-x)^{1-\epsilon}. \tag{7.38}$$

We see immediately that we do not need to compute $R_2^{(3)}$ as it is suppressed by one power of $(1-x)$ in comparison to the boundary conditions required. Furthermore, we know from the boundary decomposition, eq. (7.34), that the region $R_2^{(2)}$, proportional to $(1-x)^{-\epsilon}$ corresponds to the boundary condition $f_0^{(3)}$ that we determined before. We therefore only need to compute $R_2^{(1)}$ in order to obtain $g_0^{(1)}$. The parametric representation of this region is,

$$R_2^{(1)} = -i(4\pi)^{-2+\epsilon}\Gamma(1+\epsilon)\int_0^\infty dx_1 dx_2 \delta(1-x_1-x_2) x_1^{-\epsilon} x_2^{-1-\epsilon}(x_1+x_2)^{-1+2\epsilon}. \tag{7.39}$$

This integral can easily be solved in terms of beta functions and we obtain the boundary condition $f_0^{(1)}$ from comparison with eq. (7.34),

$$f_0^{(1)} = -i(4\pi)^{-2+\epsilon}\frac{\Gamma(1-\epsilon)^2\Gamma(1+\epsilon)}{\epsilon\Gamma(1-2\epsilon)}. \tag{7.40}$$

The final boundary condition $f_0^{(2)}$ is obtained from integral $M_3$, which has three regions $R_3^{(1)}$, $R_3^{(3)}$ and $R_3^{(3)}$ with the scalings,

$$R_3^{(1)} \propto (1-x)^0, \quad R_3^{(2)} \propto (1-x)^{-\epsilon} \text{ and } R_3^{(3)} \propto (1-x)^{-\epsilon}. \tag{7.41}$$

Here we observe a small subtlety in the computation. This integral has two regions with the same scaling that are not suppressed relative to one another. It will therefore be necessary to compute both of them. Furthermore, the logarithm that appears in the boundary decomposition eq. (7.34), suggests that these regions will have a divergence that is not regulated by dimensional regularization when they are computed separately. This is immediately confirmed when we derive the integral representation for $R_3^{(2)}$ or $R_3^{(3)}$. We therefore introduce an analytic regulator $\nu$ so that the Feynman integral for $M_3$ becomes

$$M_3' = \int \frac{d^dk}{(2\pi)^d} \frac{1}{(k^2-m^2)((k+p_1)^2-m^2)((k+p_1+p_2)^2-m^2)^{1+\nu}}. \quad (7.42)$$

Starting from this regulated integral we can perform expansion by regions as before and we obtain the parametric representation for $R_3^{(2)}$ as function of $\nu$,

$$\begin{aligned} R_3^{(2)}(\nu) = {} & (-1)^{1+\nu} i(4\pi)^{-2+\epsilon} 2^{-1-\epsilon+\nu} \epsilon (1-x)^{-\epsilon-\nu} \frac{\Gamma(1+\epsilon+\nu)}{\Gamma(1+\nu)} \int_0^\infty dx_1 dx_2 dx_3 \\ & \times \delta(1-x_1-x_2-x_3) x_3^\nu (x_2+x_3)^{-1+2\epsilon+\nu} \left(2x_1x_3 + (x_2+x_3)^2\right)^{-1-\epsilon-\nu}. \end{aligned} \quad (7.43)$$

Performing the integrals over the parameters $x_i$ as beta functions we find,

$$R_3^{(2)}(\nu) = (-1)^{1+\nu} i(4\pi)^{-2+\epsilon} 2^{-\epsilon+\nu} \epsilon (1-x)^{-\epsilon-\nu} \frac{\Gamma(\epsilon+\nu)}{\nu\Gamma(1+\nu)}. \quad (7.44)$$

Here we see how the $\nu$ regulates the divergence, and we cannot take the limit $\nu \to 0$ for this region separately. However we also need to compute $R_3^{(3)}$ with the regulator. This region has the parametric representation,

$$\begin{aligned} R_3^{(3)}(\nu) = {} & (-1)^{1+\nu} i(4\pi)^{-2+\epsilon} 2^{-1-\epsilon+\nu} \epsilon (1-x)^{-\epsilon} \frac{\Gamma(1+\epsilon+\nu)}{\Gamma(1+\nu)} \int_0^\infty dx_1 dx_2 dx_3 \\ & \times \delta(1-x_1-x_2-x_3) (x_1+x_2)^{-1+2\epsilon+\nu} x_3^\nu \left((x_1+x_2)^2 + 2x_1x_3\right)^{-1-\epsilon-\nu}. \end{aligned} \quad (7.45)$$

Once again we can perform the parametric integrals in terms of beta functions and find,

$$R_3^{(3)}(\nu) = (-1)^\nu i(4\pi)^{-2+\epsilon} 2^{-\epsilon} \epsilon (1-x)^{-\epsilon} \frac{\Gamma(\epsilon)}{\nu}. \quad (7.46)$$

Also here we can see the singularity being regulated by $\nu$. We can however combine both regions and take the limit $\nu \to 0$, obtaining the finite result,

$$\begin{aligned} \lim_{\nu\to 0}\left(R_3^{(2)} + R_3^{(3)}\right) = {} & -i(4\pi)^{-2+\epsilon} 2^{-\epsilon} \epsilon (1-x)^{-\epsilon} \Gamma(\epsilon) \\ & \times \left(\gamma_E + \log(2) + \psi(\epsilon) - \log(1-x)\right), \end{aligned} \quad (7.47)$$

with $\psi(x) = \frac{d\log(\Gamma(x))}{dx}$ and $\gamma_E = -\psi(1)$. Here we can see the explicit $\log(1-x)$ that was predicted by the boundary decomposition. If we compare the term proportional to $\log(1-x)$ with eq. (7.34) we can confirm that it in fact corresponds to $f_0^{(3)}$ as predicted. The remaining boundary condition $f_0^{(2)}$ is then obtained as,

$$f_0^{(2)} = \lim_{\nu\to 0}\left(R_3^{(2)} + R_3^{(3)}\right)\Bigg|_{\log(1-x)^0} = -i(4\pi)^{-2+\epsilon}2^{-\epsilon}\epsilon\Gamma(\epsilon)\left(\gamma_E + \log(2) + \psi(\epsilon)\right). \tag{7.48}$$

With this we have determined the last remaining boundary condition. The complete system can now be obtained trivially by solving eq. (7.30) and demanding consistency with the above boundary conditions.

## Exemplary calculation of an actual boundary condition

To outline our method of calculating the actual boundary conditions, we show the example of the double cut of the tennis court diagram, depicted in figure 7.1, which serves as a boundary condition to our system of differential equations. This integral was first calculated in refs. [24, 201]. The momentum

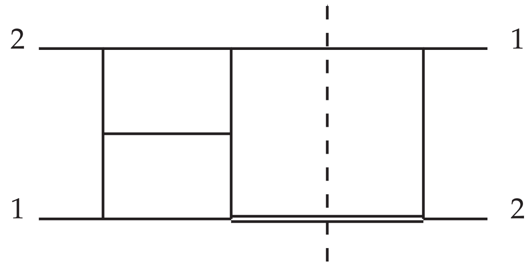



Figure 7.1: The two particle cut of the three-loop tennis court diagram which serves as a boundary condition.

space representation of the integral is,

$$\int d\Phi \frac{1}{k^2 l^2 (k+p_1)^2 (l-p_3)^2 (l+p_{23})^2 (k+p_{123})^2 (k+l+p_{123})^2} \frac{1}{-s_{13}}, \tag{7.49}$$

with $p_{23} = p_2 - p_3$ and $p_{123} = p_1 + p_2 - p_3$, where $p_3$ is the momentum of the massless cut propagator. The invariants are defined as $s_{12} = (p_1 + p_2)^2$, $s_{13} = (p_1 - p_3)^2$ and $s_{23} = (p_2 - p_3)^2$. For the purpose of calculating the loop integral we work in the so-called euclidean region where all invariants are negative. The analytic continuation to the physical region is then obtained by taking,

$$-s_{ij} - i0 \to e^{-i\pi} s_{ij}, \tag{7.50}$$

By using our method for decomposing the boundary conditions as outlined before, we obtain the different boundary conditions contributing to this integral,

$$
\begin{aligned}
&-\frac{12(4\epsilon+1)(5\epsilon+2)B_1\bar{z}^{-2-4\epsilon}}{\epsilon^2(2\epsilon+1)^2(3\epsilon+1)}+\frac{4(4\epsilon+1)B_2\bar{z}^{-2-4\epsilon}}{3\epsilon^2(2\epsilon+1)(3\epsilon+1)}+\frac{8(6\epsilon+1)B_3\bar{z}^{-2-6\epsilon}}{9\epsilon^2(3\epsilon+1)}\\
&+\frac{12B_4\bar{z}^{-2-3\epsilon}}{\epsilon^2(3\epsilon+1)}+\frac{9B_5\bar{z}^{-2-3\epsilon}}{\epsilon^2(3\epsilon+1)}+\frac{4(6\epsilon+1)B_6\bar{z}^{-2-6\epsilon}}{3\epsilon^2}+\frac{(5\epsilon+1)B_7\bar{z}^{-2-5\epsilon}}{\epsilon^2(\epsilon+1)(3\epsilon+1)}\\
&-\frac{4(4\epsilon+1)B_8\bar{z}^{-2-4\epsilon}}{\epsilon^2(2\epsilon+1)(3\epsilon+1)}-\frac{24(4\epsilon+1)B_9\bar{z}^{-2-4\epsilon}}{\epsilon^2(2\epsilon+1)^2}+\frac{B_{10}\bar{z}^{-2-3\epsilon}}{8\epsilon^2(3\epsilon+1)}\\
&+B_{11}\bar{z}^{-3-6\epsilon}\left(\frac{6\epsilon+1}{4\epsilon^3(3\epsilon+1)}-\bar{z}\frac{6\epsilon+1}{12\epsilon^2(3\epsilon+1)}\right).
\end{aligned}
\tag{7.51}
$$

The boundary condition that we want to determine here is $B_{11}$, all other boundary conditions can be determined independently from other integrals. To leading power in $\bar{z}$, $B_{11}$ is the only boundary condition contributing. Therefore, we need to compute the region proportional to $\bar{z}^{-3-6\epsilon}$ of this integral. Using expansion by regions we can derive a momentum space representation or use the code asy [195, 203] to obtain a parametric representation of the required region:

$$
\begin{aligned}
\mathcal{I} &\equiv (4\pi)^{4-2\epsilon}\frac{((1+6\epsilon)B_{11}}{(4\epsilon^3(1+3\epsilon))}\\
&=(4\pi)^{4-2\epsilon}\int d\Phi_2\frac{d^dk}{(2\pi)^d}\frac{d^dl}{(2\pi)^d}\\
&\times\frac{1}{k^2l^2(k-l)^2(2kp_2-2p_2p_3)(2lp_2-2p_2p_3)(2lp_2)(k-p_3)^2}\frac{1}{s_{13}}.
\end{aligned}
$$

Introducing Feynman parameters and transforming to projective space we obtain,

$$
\begin{aligned}
\mathcal{I}=&\int d\Phi_2\int_0^\infty dx_1dx_2dx_3dx_4dx_5dx_6\Gamma(3+2\epsilon)\left(x_4+x_6+x_2\left(1+x_4+x_6\right)\right)^{1+3\epsilon}\\
&\times\Big(s_{23}\left(\left(x_3+x_5\right)x_6+x_2\left(x_3+x_3x_4+x_5+x_3x_6+x_5x_6\right)\right)\\
&+x_1\left(s_{13}x_4+s_{12}\left(x_5+x_3\left(1+x_4+x_6\right)\right)\right)\Big)^{-3-2\epsilon}\frac{1}{s_{13}}.
\end{aligned}
\tag{7.52}
$$

The integration over $x_1$ can be performed immediately. Using the projective transformation $x_5\to x_5x_3$, the integral over $x_3$ can be computed as well and we obtain,

$$
\begin{aligned}
\mathcal{I} = & \int d\Phi_2 \int dx_2 dx_4 dx_5 dx_6 \Gamma(1-2\epsilon)\Gamma(2\epsilon)\Gamma(2+2\epsilon)\bar{z}^{-1-\epsilon} s_{12}^{2\epsilon} s_{13}^{-2-2\epsilon} s_{23}^{-2-2\epsilon} \\
& \times x_4^{-1-2\epsilon} \left(1+x_4+x_5+x_6\right)^{2\epsilon} \left(x_4+x_6+x_2(1+x_4+x_6)\right)^{1+3\epsilon} \\
& \times \left(x_2(1+x_4+x_5)+(1+x_2)(1+x_5)x_6\right)^{-2-2\epsilon} .
\end{aligned}
\tag{7.53}
$$

Next we split the second polynomial into,

$$
\frac{\Gamma(-z_1)\Gamma(-1+z_1-3\epsilon)}{\Gamma(-1-3\epsilon)} x_2^{1+3\epsilon-z_1} (x_4+x_6)^{z_1} (1+x_4+x_6)^{1-z_1+3\epsilon}, \tag{7.54}
$$

by introducing a Mellin-Barnes integral over $z_1$, such that we can perform the integral over $x_2$. After performing the projective transformations $x_6 \to x_6 x_4$ and $x_4 \to \frac{x_4}{1+x_6}$ we obtain,

$$
\begin{aligned}
\mathcal{I} = & \int_\gamma dz_1 \frac{\Gamma(-2\epsilon)\Gamma(1+2\epsilon)}{\Gamma(-1-3\epsilon)} \Gamma(2+3\epsilon-z_1)\Gamma(-z_1)\Gamma(-1-3\epsilon+z_1)\Gamma(-\epsilon+z_1) \\
& \times \int d\Phi_2 \int dx_4 dx_5 dx_6 s_{12}^{2\epsilon} s_{13}^{-2-2\epsilon} s_{23}^{-2-2\epsilon} x_4^{-\epsilon} (1+x_4)^{1+3\epsilon-z_1} (1+x_5)^{\epsilon-z_1} x_6^{\epsilon-z_1} \\
& \times (1+x_4+x_5)^{2\epsilon} (1+x_6)^{1+4\epsilon} \left(1+x_4+x_5+(1+x_4)(1+x_5)x_6\right)^{-2-3\epsilon+z_1} ,
\end{aligned}
\tag{7.55}
$$

where the contour $\gamma$ is such that the poles of gamma functions with $-z_i$ in the argument (left poles) and the poles of gamma functions with $+z_i$ in the argument (right poles) are separated. Next, we introduce a second Mellin-Barnes integration to split the last polynomial into,

$$
\begin{aligned}
& \frac{\Gamma(-z_2)\Gamma(2+z_2+3\epsilon-z_1)}{\Gamma(2+3\epsilon-z_1)} x_6^{-2-z_2-3\epsilon+z_1} (1+x_4)^{-2-z_2-3\epsilon+z_1} \\
& \quad \times (1+x_5)^{-2-z_2-3\epsilon+z_1} (1+x_4+x_5)^{z_2}.
\end{aligned}
\tag{7.56}
$$

Now we can perform the integral over $x_6$, $x_5$ and $x_4$ in that order and obtain

$$
\begin{aligned}
\mathcal{I} = & \int d\Phi_2 s_{12}^{2\epsilon} s_{13}^{-2-2\epsilon} s_{23}^{-2-2\epsilon} \frac{\Gamma(-\epsilon)\Gamma(1+2\epsilon)}{\Gamma(-1-4\epsilon)\Gamma(-1-3\epsilon)} \int_\gamma \frac{dz_1}{2\pi i}\frac{dz_2}{2\pi i} \Gamma(-z_1)\Gamma(-z_2) \\
& \times \frac{\Gamma(-1-3\epsilon+z_1)\Gamma(-\epsilon+z_1)\Gamma(-1-2\epsilon-z_2)\Gamma(-2\epsilon+z_2)}{(1+2\epsilon+z_2)\Gamma(1+z_2)} \\
& \times \Gamma(2+3\epsilon-z_1+z_2)\Big(\Gamma(-\epsilon)\Gamma(1+z_2)-\Gamma(-2\epsilon)\Gamma(1+\epsilon+z_2)\Big),
\end{aligned}
\tag{7.57}
$$

as the final Mellin-Barnes representation. Next, we need to perform the phase space integral. At this stage we perform the analytic continuation into the physical region, using the prescription indicated above. Next, we insert the appropriate parametrization,

$$s_{12} = 1, \quad s_{13} = \lambda, \quad s_{23} = 1 - \lambda, \tag{7.58}$$

with $\lambda \in [0, 1]$. Afterwards, we can perform the phase space integral as a simple beta function.

The contour of the Mellin-Barnes integration is defined by the requirement that it should separate the left and right poles of the integrand. At this point, this is only satisfied for the integral if $\epsilon$ is finite. Therefore, in order to be able to expand the integral in $\epsilon$, before the Mellin-Barnes integration is performed, we need to analytically continue the integral to infinitesimal $\epsilon$. This is achieved using the residue theorem, by taking the residues of poles that end up on the wrong side of the contour when $\epsilon$ is gradually taken to zero. This is automated in codes like `MB` [167] and `MBresolve` [168]. After the analytic continuation, the integral can be expanded in $\epsilon$. We refrain from printing the unwieldy expansion that is obtained in this step. Afterwards, we can apply Barnes' lemma and corollaries thereof to eliminate one of the two integrations and we are left with a one-dimensional Mellin-Barnes integral. This one-dimensional integral can be easily computed by taking the residues of, e.g. the left poles of the integrand, which yields a sum representation. These sums can be performed in terms of harmonic sums [170, 206], which yield multiple zeta-values when evaluated at infinity. This way we find the final result,

$$\begin{aligned} \Re(\mathcal{I}) e^{3\epsilon\gamma_E} &= \frac{1}{3\epsilon^5} - \frac{19}{3\epsilon^3}\zeta_2 - \frac{39}{2\epsilon^2}\zeta_3 + \frac{257}{16\epsilon}\zeta_4 \\ &+ \left(\frac{1481}{4}\zeta_2\zeta_3 - \frac{4967}{10}\zeta_5\right) + \epsilon\left(560\zeta_3^2 - \frac{8719}{48}\zeta_6\right) + \mathcal{O}(\epsilon^2) \end{aligned} \tag{7.59}$$

Our method of solving the integrals in the Mellin-Barnes representation also provides a way to cross-check the result as the Mellin-Barnes integrals can also be evaluated numerically. A large fraction of the required boundary conditions for the $RVV$ cross section can be obtained in a simpler fashion. For other integrals we proceed similarly to the above example.

CHAPTER 8

# THE HIGGS CROSS SECTION AT N$^3$LO

## 8.1 The fixed order cross section at N$^3$LO

Having at our disposal the complete set of master integrals as expansions around the threshold limit, we can easily obtain the cross sections at N$^3$LO for all partonic channels contributing to Higgs production via gluon fusion. The partonic cross sections are related to the hadronic cross section at the LHC through the integral

$$\sigma = \sum_{i,j} \int \mathrm{d}x_1 \mathrm{d}x_2 f_i(x_1, \mu_f) f_j(x_2, \mu_f) \hat{\sigma}_{ij}(z, \mu_r, \mu_f)\,, \tag{8.1}$$

where the summation indices $i, j$ run over the parton flavors in the proton, $f_i$ are parton densities and $\hat{\sigma}_{ij}$ are partonic cross sections. Furthermore, we define $z = \frac{m_H^2}{s}$ and $\tau = \frac{m_H^2}{S}$ as usual, where $m_H$ is the mass of the Higgs boson and $\sqrt{s}$ is the partonic center-of-mass energy, related to the hadronic center-of-mass energy $\sqrt{S}$ through $s = x_1\, x_2\, S$. The renormalization and factorization scales are denoted by $\mu_r$ and $\mu_f$ respectively.

We expand the partonic cross sections into a perturbative series in the strong coupling constant evaluated at the scale $\mu_r$,

$$\frac{\hat{\sigma}_{ij}}{z} = \frac{\pi C^2}{8(N_c^2 - 1)} \sum_{k=0} \infty \left( \frac{\alpha_s(\mu_r)}{\pi} \right)^k \eta_{ij}^{(k)}(z). \tag{8.2}$$

In this expression $C$ denotes the Wilson coefficient and the terms through NNLO in the above expansion have been computed in refs. [83, 98, 108–113, 115, 116, 192, 207]. The main result of this dissertation is the result for the N$^3$LO coefficient, corresponding to $\ell = 3$ in eq. (8.2), for all possible parton flavors in the initial state. The contributions to the cross section at N$^3$LO can formally be written as,

$$\begin{aligned}\eta_{ij}^{(3)} &= \langle \mathcal{M}_{3,0} | \mathcal{M}_{3,0} \rangle + 2\Re \langle \mathcal{M}_{2,1} | \mathcal{M}_{2,0} \rangle \\ &\quad + \langle \mathcal{M}_{1,1} | \mathcal{M}_{1,1} \rangle + 2\Re \langle \mathcal{M}_{1,2} | \mathcal{M}_{1,0} \rangle + 2\Re \langle \mathcal{M}_{0,3} | \mathcal{M}_{0,0} \rangle,\end{aligned} \tag{8.3}$$

where $\mathcal{M}_{n,m}$ is the $n$-loop matrix element with $m$ real partons in the final state.

The N$^3$LO coefficient therefore receives contributions from the three loop-corrections to inclusive Higgs production that are related to the QCD form factor computed in [20, 21]. Additionally, the two-loop corrections to Higgs production in association with an additional gluon in the final state need to be taken into account. These corrections can be divided into two categories. On one hand the corrections due to the square of one-loop corrections, discussed in chapter 6, published in ref. [2] and confirmed by ref. [22], and on the other hand the corrections due to genuine two-loop amplitudes interfered with the corresponding tree-level amplitudes discussed in chapter 7, which were published first in the soft limit in refs. [23, 24, 201] and later in general kinematics in refs. [5, 25]. Additionally, we need to take into account the one-loop corrections to the emission of two gluons, which were computed in refs. [7, 36] and the tree-level emission of three gluons in the final state that was discussed in chapter 5 and published in ref. [1].

Each of these contributions is ultraviolet (UV) and infrared (IR) divergent. The divergences manifest themselves as poles of up to sixth order in the dimensional regulator $\epsilon$. While the three leading poles cancel when summing over all contributions, the coefficients of the lower poles starting with $1/\epsilon^3$ are non-vanishing. The remaining divergences can only be cancelled when suitable UV and IR counterterms are included. These counterterms can be completely determined from the lower order cross cross sections [32–34], the QCD $\beta$-function [26–29] as well as the three-loop splitting functions [30, 31].

The contributions to the partonic cross section at N$^3$LO can be decomposed as,

$$\hat{\sigma}_{ij}^{(3)} = \sigma_{ij}^{(3,0)} \delta(1-z) + \sum_{m=2}^{6} (1-z)^{-m\epsilon} \sigma_{ij}^{(3,m)}(z,\epsilon). \tag{8.4}$$

The $\sigma_{ij}^{(3,m)}$ are meromorphic functions with at most a single pole at $z = 1$. When the partonic cross sections are convoluted with the pdfs, c.f. eq. (8.1), the pole at $z = 1$ introduces a divergence into this integral as $z \to 1$. In dimensional regularization this divergences can be regulated by expanding the factors $(1-z)^{-1-m\epsilon}$ in terms of delta functions and plus distributions,

$$(1-z)^{-1-m\epsilon} = -\frac{1}{m\epsilon}\delta(1-z) + \sum_{n=0}^{\infty} \frac{(-m\epsilon)^n}{n!} \left[\frac{\log^n(1-z)}{1-z}\right]_+, \tag{8.5}$$

where the plus distribution is defined by its action on a test function $\phi(z)$,

$$\int_0^1 \mathrm{d}z \left[\frac{\log^n(1-z)}{1-z}\right]_+ \phi(z) = \int_0^1 \mathrm{d}z \frac{\log^n(1-z)}{1-z}(\phi(z)-\phi(1)). \tag{8.6}$$

After this expansion, we can cast the N$^3$LO coefficients in the form,

$$\eta_{ij}^{(3)} = \delta_{ig}\,\delta_{jg}\,\eta_{\mathrm{SV}}^{(3)} + \eta_{ij}^{(3,\mathrm{reg})} \tag{8.7}$$

Here, $\hat{\sigma}_{\mathrm{SV}}^{(3)}$ denotes the soft-virtual cross section at N$^3$LO of refs. [3, 39] that contains all terms proportional to delta functions and plus distributions. For $\mu_r = \mu_f = m_H$ it can be explicitly given as,

$$\begin{aligned}
\hat{\sigma}_{\mathrm{SV}}^{(3)}(z) = \delta(1-z) \Bigg\{ & C_A^3 \left(-\frac{2003}{48}\,\zeta_6 + \frac{413}{6}\,\zeta_3^2 - \frac{7579}{144}\,\zeta_5 + \frac{979}{24}\,\zeta_2\,\zeta_3 - \frac{15257}{864}\,\zeta_4\right. \\
& \left. -\frac{819}{16}\,\zeta_3 + \frac{16151}{1296}\,\zeta_2 + \frac{215131}{5184}\right) + N_F \Bigg[ C_A^2 \left(\frac{869}{72}\,\zeta_5 - \frac{125}{12}\,\zeta_3\,\zeta_2 + \frac{2629}{432}\,\zeta_4\right. \\
& \left. +\frac{1231}{216}\,\zeta_3 - \frac{70}{81}\,\zeta_2 - \frac{98059}{5184}\right) + C_A\,C_F \left(\frac{5}{2}\,\zeta_5 + 3\zeta_3\zeta_2 + \frac{11}{72}\,\zeta_4 + \frac{13}{2}\,\zeta_3\right. \\
& \left. -\frac{71}{36}\,\zeta_2 - \frac{63991}{5184}\right) + C_F^2 \left(-5\zeta_5 + \frac{37}{12}\,\zeta_3 + \frac{19}{18}\right) \Bigg] + N_F^2 \Bigg[ C_A \left(-\frac{19}{36}\,\zeta_4 + \frac{43}{108}\,\zeta_3\right. \\
& \left. -\frac{133}{324}\,\zeta_2 + \frac{2515}{1728}\right) + C_F \left(-\frac{1}{36}\,\zeta_4 - \frac{7}{6}\,\zeta_3 - \frac{23}{72}\,\zeta_2 + \frac{4481}{2592}\right) \Bigg] \Bigg\} \qquad (8.8) \\
+ \left[\frac{1}{1-z}\right]_+ \Bigg\{ & C_A^3 \left(186\,\zeta_5 - \frac{725}{6}\,\zeta_3\,\zeta_2 + \frac{253}{24}\,\zeta_4 + \frac{8941}{108}\,\zeta_3 + \frac{8563}{324}\,\zeta_2 - \frac{297029}{23328}\right) \\
& + N_F^2\,C_A \left(\frac{5}{27}\,\zeta_3 + \frac{10}{27}\,\zeta_2 - \frac{58}{729}\right) + N_F \Bigg[ C_A^2 \left(-\frac{17}{12}\,\zeta_4 - \frac{475}{36}\,\zeta_3\right. \\
& \left. -\frac{2173}{324}\,\zeta_2 + \frac{31313}{11664}\right) + C_A\,C_F \left(-\frac{1}{2}\,\zeta_4 - \frac{19}{18}\,\zeta_3 - \frac{1}{2}\,\zeta_2 + \frac{1711}{864}\right) \Bigg] \Bigg\} \\
+ \left[\frac{\log(1-z)}{1-z}\right]_+ \Bigg\{ & C_A^3 \left(-77\zeta_4 - \frac{352}{3}\,\zeta_3 - \frac{152}{3}\,\zeta_2 + \frac{30569}{648}\right) + N_F^2\,C_A \left(-\frac{4}{9}\,\zeta_2\right. \\
& \left. +\frac{25}{81}\right) + N_F \Bigg[ C_A^2 \left(\frac{46}{3}\,\zeta_3 + \frac{94}{9}\,\zeta_2 - \frac{4211}{324}\right) + C_A\,C_F \left(6\,\zeta_3 - \frac{63}{8}\right) \Bigg] \Bigg\} \\
+ \left[\frac{\log^2(1-z)}{1-z}\right]_+ \Bigg\{ & C_A^3 \left(181\,\zeta_3 + \frac{187}{3}\,\zeta_2 - \frac{1051}{27}\right) + N_F \Bigg[ C_A^2 \left(-\frac{34}{3}\,\zeta_2 + \frac{457}{54}\right)
\end{aligned}$$

$$
\begin{aligned}
&+\frac{1}{2}\,C_A\,C_F\Bigg]-\frac{10}{27}\,N_F^2\,C_A\Bigg\}\\
&+\left[\frac{\log^3(1-z)}{1-z}\right]_+\left\{C_A^3\left(-56\,\zeta_2+\frac{925}{27}\right)-\frac{164}{27}\,N_F\,C_A^2+\frac{4}{27}\,N_F^2\,C_A\right\}\\
&+\left[\frac{\log^4(1-z)}{1-z}\right]_+\left(\frac{20}{9}\,N_F\,C_A^2-\frac{110}{9}\,C_A^3\right)+\left[\frac{\log^5(1-z)}{1-z}\right]_+\,8\,C_A^3\,.
\end{aligned}
$$

Here $N_F$ is the number of light fermions and $C_A$ and $C_F$ are the Casimirs of $SU(N_C)$. The terms proportional to plus distributions were determined previously from lower orders in ref. [37] and are confirmed by our result.

The regular contributions $\eta_{ij}^{(3,\text{reg})}(z)$ take the form of a polynomial in $\log(1-z)$,

$$
\eta_{ij}^{(3,\text{reg})}=\sum_{m=0}^{5}\log^m(1-z)\eta_{ij}^{(3,m)}(z), \tag{8.9}
$$

where the $\eta_{ij}^{(3,m)}$ are holomorphic around $z=1$. The functions $\eta_{ij}^{(3,m)}$ for $m=5,4,3$ have been given in a closed analytic from in [4]. The functions $\eta_{ij}^{(3,m)}$ for $m=2,1,0$ have been computed as a series expansion in $\bar{z}=(1-z)$ so that we can introduce the series representation

$$
\eta_{ij}^{(3,m)}=\lim_{N\to\infty}\eta_{ij}^{(3,m,N)}, \tag{8.10}
$$

with

$$
\eta_{ij}^{(3,m,N)}=\sum_{n=0}^{N}c_{ij}^{(m,n)}\bar{z}^n. \tag{8.11}
$$

If we truncate the sum in eq. (8.11) at $N=0$, we obtain the next-to-soft approximation of ref. [4].

Using our method for the threshold expansion of the master integrals, we were able to determine the $c_{ij}^{(m,n)}$ of eq. (8.11) analytically up to at least $n=30$. The analytic expressions for the coefficients of the threshold expansion are rather unwieldy. However, the $c_{ij}^{(m,n)}$ only consist of powers of $N_c$ and $n_f$ as well as $\zeta$-values. By setting $N_c=$ and $n_f=5$ we can give the $\eta_{ij}^{(3,m)}$ numerically in section 8.3. While this approach does not put the partonic cross sections in a closed analytic form, we argue that it yields the complete result for the value of the hadronic cross section. In Fig. 8.1 we show the contribution of the partonic cross section coefficients N$^3$LO to the hadronic cross section for a proton-proton collider with 13 TeV center-of-mass energy as a function of the truncation order $N$. We use the NNLO MSTW2008 [208] parton densities and a value for the strong coupling at the mass of the $Z$-boson of $\alpha_s(m_Z)=0.117$ as initial value for the evolution, and we set the factorization scale to $\mu_f = m_H = 125$GeV. We observe that the threshold expansion stabilizes starting from $N = 4$, leaving a negligible truncation uncertainty for the hadronic cross section thereafter. We note, though, that we observe a very small, but systematic, increase of the expansion in the range $N \in [15, 37]$, as illustrated in Fig. 8.1. We have observed similar behavior for the threshold expansion at NNLO which we illustrate in figure 8.2.

The systematic increase originates from values of the partonic cross section at very small $z$. Indeed, this increase appears only in the contributions to the hadronic cross section integral for values $z < 0.1$. It is natural that the terms of the threshold expansion computed here do not furnish a good approximation of the hadronic integral in the small $z$ region due to the divergent high-energy behavior of the partonic cross sections [209]. However, it is observed that this region is suppressed in the total hadronic integral and for $z < 0.1$ contributes less than 0.4% of the total N$^3$LO correction. The same region at NLO and NNLO, where analytic expressions valid for all regions are known, is similarly suppressed. We therefore believe that the uncertainty of our computation for the hadronic cross section due to the truncation of the threshold expansion is negligible (less than 0.2%).

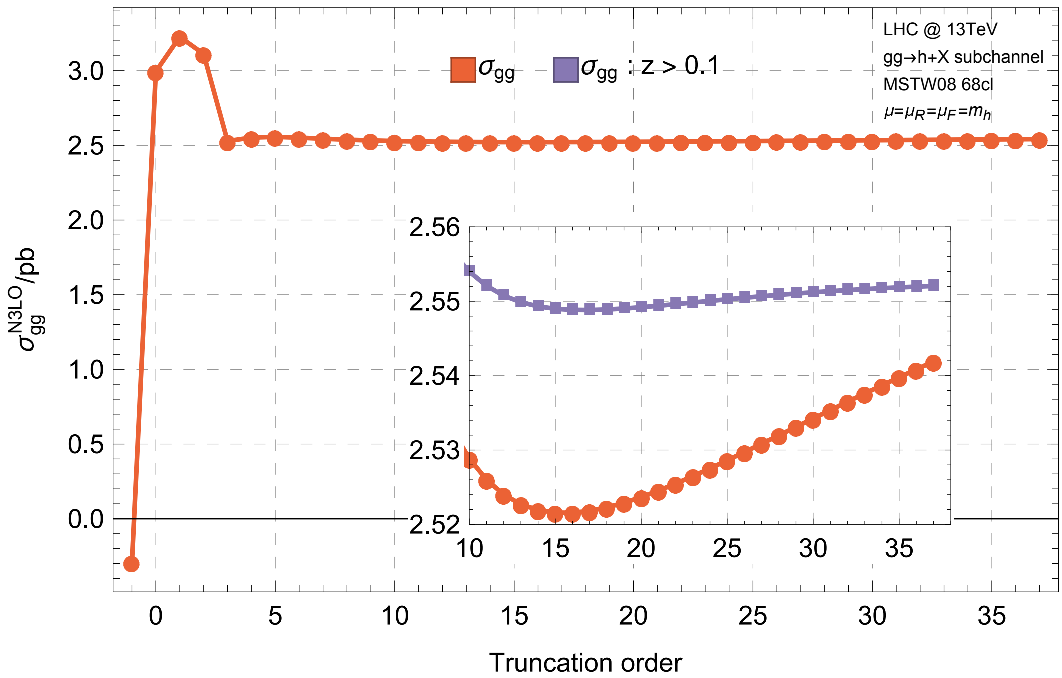



Figure 8.1: The N$^3$LO correction from the $gg$ channel to the hadronic cross section as a function of the truncation order $N$ in the threshold expansion for the scale choice $\mu = m_H$. The inlay shows that the convergence improves when the high-energy tail ($z < 0.1$) of the hadronic integral in eq. (8.1) is removed.

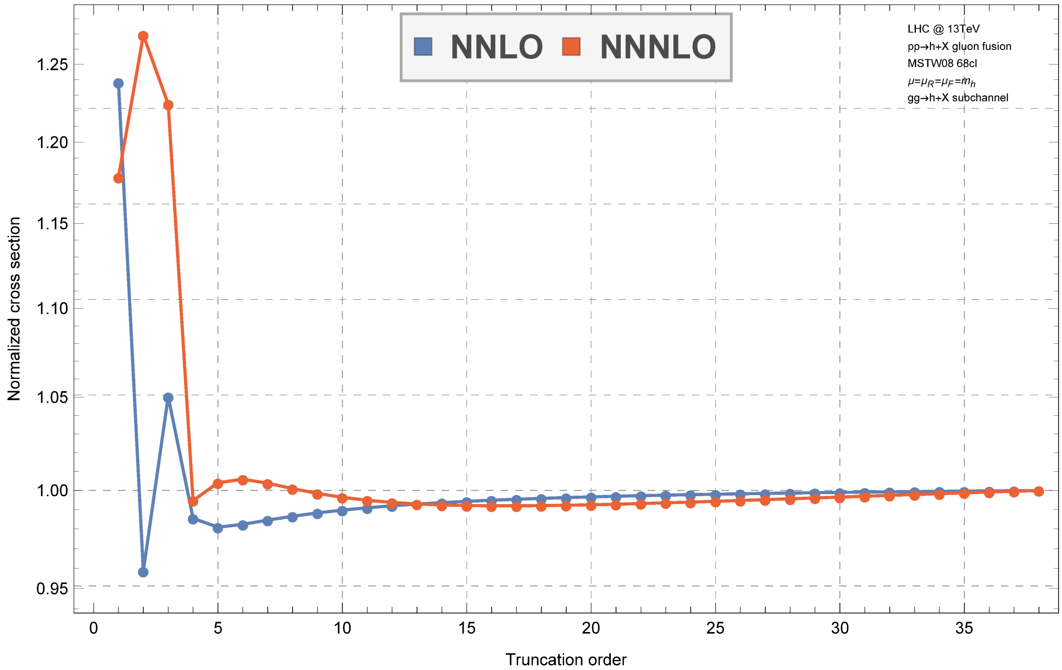



Figure 8.2: Comparison of the threshold expansion of the NNLO correction and the $N^3LO$ correction in the $gg$ channel to the hadronic cross section as a function of the truncation order $N$ for the scale choice $\mu = m_H$.

In Fig. 8.3 we present the hadronic gluon-fusion Higgs production cross section at $N^3LO$ as a function of a common renormalisation and factorization scale $\mu = \mu_r = \mu_f$. We use NNLO parton densities and N3LO evolution of the strong coupling not only in the N3LO predictions, but also in the LO, NLO and NNLO predictions. We observe a significant reduction of the sensitivity of the cross section to the scale $\mu$. Inside a range $\mu \in \left[\frac{m_H}{4}, m_H\right]$ the cross section at $N^3LO$ varies in the interval $[-2.7\%, +0.3\%]$ with respect to the cross section value at the central scale $\mu = \frac{m_H}{2}$. For comparison, we note that the corresponding scale variation at NNLO is about $\pm 9\%$ [16, 17]. This improvement in the precision of the Higgs cross section is a major accomplishment due to our calculation and will have a strong impact on future measurements of Higgs-boson properties. Furthermore, even though for the scale choice $\mu = \frac{m_H}{2}$ the $N^3LO$ corrections change the cross section by about $+2.2\%$, this correction is captured by the scale variation estimate for the missing higher order effects of the NNLO result at that scale. We illustrate this point in Fig. 8.5, where we present the hadronic cross section as a function of the hadronic center-of-mass energy $\sqrt{S}$ at the scale $\mu = \frac{m_H}{2}$. We observe that the $N^3LO$ scale uncertainty band is included within the NNLO band, indicating that the perturbative expansion of the hadronic cross section is convergent. However, we note that for a larger scale choice, e.g., $\mu = m_H$, the convergence of the perturbative series

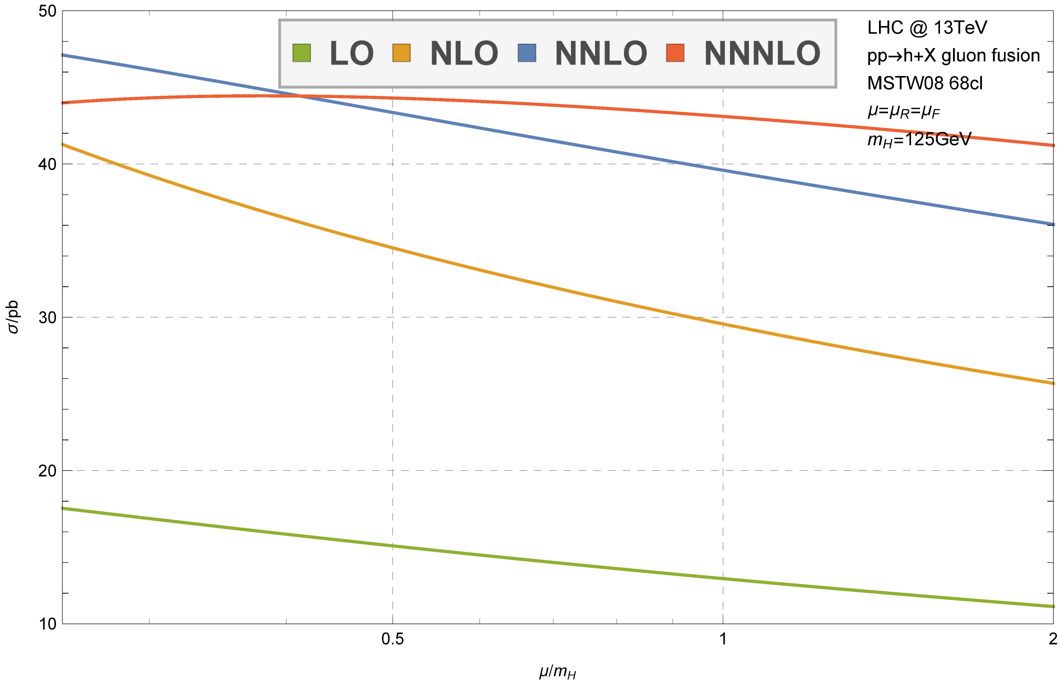



Figure 8.3: Scale $\mu = \mu_r = \mu_f$ variation of the gluon fusion cross section at all perturbative orders through N$^3$LO for $m_H = 125$GeV. We use NNLO MSTW2008 [208] parton densities and $\alpha_s(m_Z) = 0.117$ with N3LO evolution for these predictions.

is slower than for $\mu = \frac{m_H}{2}$.

In figure 8.4 we present the scale dependence of the hadronic gluon fusion cross section in the gluon-gluon initiated channel in comparison with the quark-gluon initiated channel. We observe that the quark-gluon channel becomes important at very low scales at every order. Near the preferred scale choice of $\mu = \frac{m_H}{2}$ the cross section is almost completely determined by the gluon-gluon initiated channel.

In table 8.1 we quote the gluon-fusion cross section in effective theory at N$^3$LO for different LHC energies. The perturbative uncertainty is determined by varying the common renormalisation and factorization scale in the interval $\left[\frac{m_H}{4}, m_H\right]$ around $\frac{m_H}{2}$ and in the interval $\left[\frac{m_H}{2}, 2m_H\right]$ around $m_H$.

Given the substantial reduction of the scale uncertainty at N$^3$LO, the question naturally arises whether other sources of theoretical uncertainty may contribute at a similar level.

First, we note that given the small size of the N$^3$LO corrections compared to NNLO, we expect that an estimate for the higher-order corrections at N$^4$LO and beyond can be obtained from the scale variation uncertainty. Alternatively, partial N$^4$LO results can be obtained by means of factorization theorems for

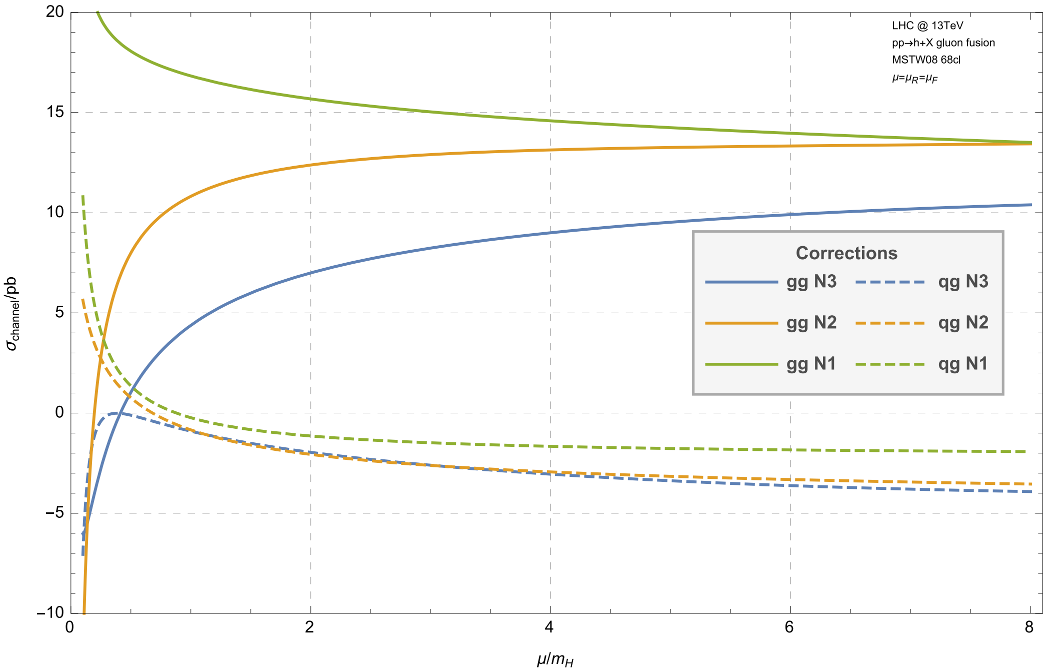



Figure 8.4: Scale $\mu = \mu_r = \mu_f$ variation of the gluon-gluon initiated channel compared to the quark-gluon initiated channel at all perturbative orders through N$^3$LO for $m_H = 125$GeV. We use NNLO MSTW2008 [208] parton densities and $\alpha_s(m_Z) = 0.117$ with N3LO evolution at all perturbative orders.

| $\sigma/$pb | 2 TeV | 7 TeV | 8 TeV | 13 TeV | 14 TeV |
|---|---|---|---|---|---|
| $\mu = \frac{m_H}{2}$ | $0.99^{+0.43\%}_{-4.65\%}$ | $15.31^{+0.31\%}_{-3.08\%}$ | $19.47^{+0.32\%}_{-2.99\%}$ | $44.31^{+0.31\%}_{-2.64\%}$ | $49.87^{+0.32\%}_{-2.61\%}$ |
| $\mu = m_H$ | $0.94^{+4.87\%}_{-7.35\%}$ | $14.84^{+3.18\%}_{-5.27\%}$ | $18.90^{+3.08\%}_{-5.02\%}$ | $43.14^{+2.71\%}_{-4.45\%}$ | $48.57^{+2.68\%}_{-4.24\%}$ |

Table 8.1: The gluon fusion cross section in the effective theory as a function of the (proton-proton) collider energy. Uncertainties are determined by varying in the interval $[\frac{m_H}{4}, m_H]$ around $\mu = \frac{m_H}{2}$ and in the interval $[\frac{m_H}{2}, 2m_H]$ around $\mu = m_H$.

threshold resummation. However, we expect that the insight from resummation on the N$^4$LO soft contributions is only qualitative given the importance of next-to-soft, next-to-next-to-soft and purely virtual contributions observed at N$^3$LO, as seen in Fig. 8.1.

Electroweak corrections to Higgs production have been calculated through two loops in ref. [102–104], and estimated at three loops in ref. [105]. They furnish a correction of less than $+5\%$ to the inclusive cross section. Thus,

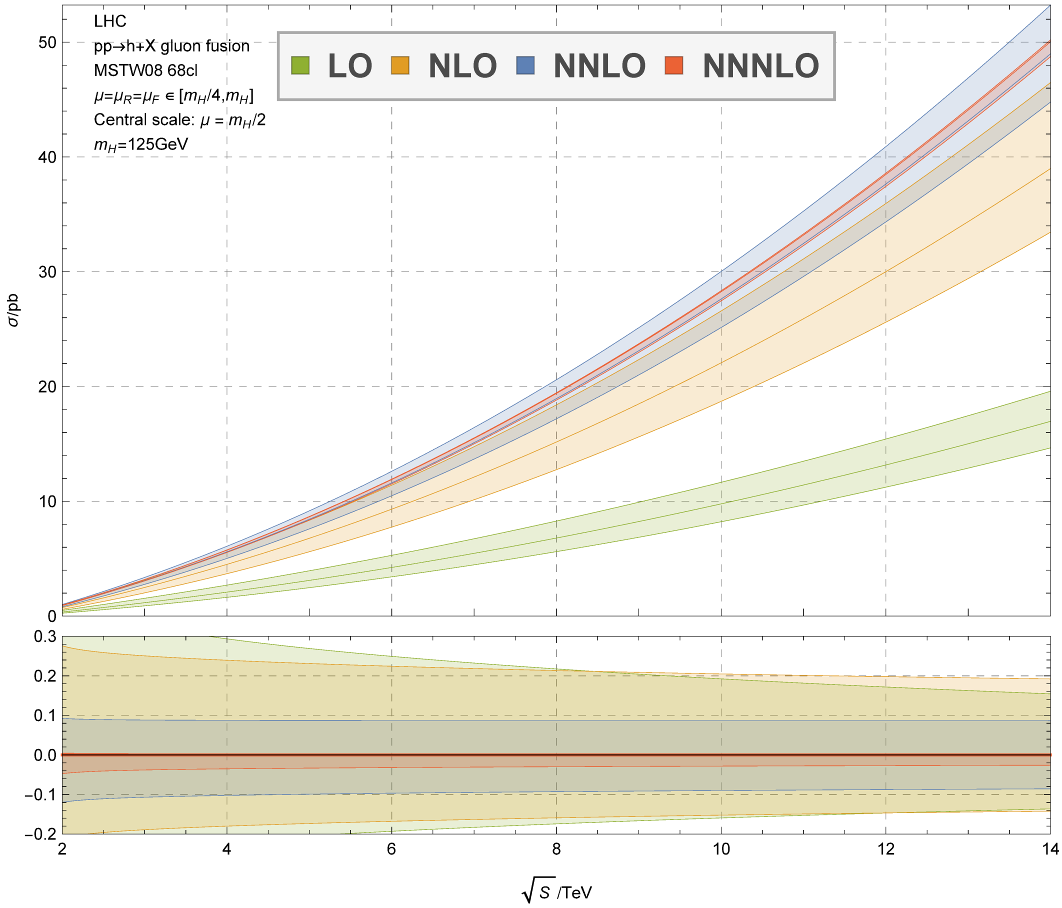



Figure 8.5: The LHC gluon fusion cross section through N$^3$LO for a common scale $\mu \in [\frac{m_H}{4}, m_H]$ as a function of the center-of-mass energy $\sqrt{S}$. In the lower panel the cross section is normalized to its value at $\mu = \frac{m_H}{2}$.

they are not negligible at the level of accuracy indicated by the scale variation at N$^3$LO and need to be combined with our result in the future. Mixed QCD-electroweak or purely electroweak corrections of even-higher order are expected to contribute at the sub-percent level and should be negligible.

Next, we have to comment on our assumption that the top-quark is infinitely heavy and can be integrated out, see eq. (1.1). Moreover, we assumed that all other quarks have a zero Yukawa coupling. Finite quark mass effects are important, but it is sufficient to include them through NLO or NNLO. Indeed, finite quark-mass effects have been computed fully through NLO in QCD [98, 108–113, 192, 207], while subleading top-quark mass corrections have been computed at NNLO systematically as an expansion in the inverse top-quark mass [106, 107]. In these references it was observed that through NLO finite quark mass effects amount to about 8% of the K-factor. At NNLO, the known $1/m_{\text{top}}$ corrections affect the cross section at the $\sim$ 1% level. A potentially significant contribution at NNLO which has not yet been computed in the literature originates from diagrams with both top- and bottom-quark Yukawa couplings. Assuming a similar perturbative pattern as for top-quark only diagrams in the effective theory, eq. (1.1), higher-order effects could be of the order of 2%. We thus conclude that the computation of the top-bottom interference through NNLO is highly desired in the near future.

Finally, the computation of the hadronic cross section relies crucially on the knowledge of the strong coupling constant and the parton densities. After our calculation, the uncertainty coming from these quantities has become dominant. Further progress in the determination of parton densities must be anticipated in the next few years due to the inclusion of LHC data in the global fits and the impressive advances in NNLO computations, improving the theoretical accuracy of many standard-candle processes.

## 8.2 Threshold resummation

The partonic cross section contains terms proportional to powers of threshold logarithms $\log(1-z)$. As $z$ approaches the threshold limit $z \to 1$, these logarithms diverge and thus lead to potentially large contributions to the cross section at every order in the perturbative expansion in $\alpha_s$. One can therefore argue that these contributions should be resummed in order to obtain partial results that are valid at any order in $\alpha_s$, which are better behaved in the threshold limit than the fixed-order result.

Threshold resummation is based on factorizing the Mellin transform of the hadronic cross section,

$$\sigma(N, m_H^2) = \int_0^1 \mathrm{d}\tau \tau^{N-1} \sigma(S, m_H^2). \tag{8.12}$$

In Mellin-space eq. (8.1) takes the simple form,

$$\sigma(N-1, m_H^2) = \sum_{ij} f_i(N, \mu_f) f_j(N, \mu_f) \hat{\sigma}_{ij}(N, \mu_r, \mu_f), \tag{8.13}$$

with the Mellin moments,

$$f_i(N, \mu_f) = \int_0^1 \mathrm{d}x\, x^{N-1} f_i(x, \mu_f) \tag{8.14}$$

$$\hat{\sigma}_{ij}(N, \mu_r, \mu_f) = \int_0^1 \mathrm{d}z\, z^{N-1} \hat{\sigma}_{ij}(z, \mu_r, \mu_f). \tag{8.15}$$

The Mellin transformation can be inverted as,

$$\sigma(S, m_H^2) = \sum_{ij} \int_{c-i\infty}^{c+i\infty} \frac{\mathrm{d}N}{2\pi i} \tau^{1-N} f_i(N, \mu_f) f_j(N, \mu_f) \sigma_{ij}(N, \mu_r, \mu_f), \tag{8.16}$$

where the contour of integration is chosen such that it lies to the right of all possible singularities of the Mellin moments in the complex $N$ plane. From the definition of the Mellin transformation we can convince ourselves that the limit $z \to 1$ of the partonic cross section corresponds to the limit $N \to \infty$ of $\sigma(N, \mu_r, \mu_f)$. In the limit $N \to \infty$ the partonic cross section in Mellin space can be written as [210],

$$\begin{aligned} \sigma(N, \mu_r, \mu_f) &= \sigma_{res}(N, \mu_r, \mu_f) + \mathcal{O}\left(\frac{1}{N}\right) \\ &= \alpha_s^2 \left[1 + \sum_{n=1}^{\infty} \alpha_s^n \sum_{m=0}^{2n} \sigma_{n,m} \log^m(N)\right] + \mathcal{O}\left(\frac{1}{N}\right). \end{aligned} \tag{8.17}$$

The constant and logarithmically divergent contributions in the $N \to \infty$ limit can be expressed in terms of the all-order resummation formula [210–213],

$$\sigma_{res}(N, \mu_r, \mu_f) = \alpha_s(\mu_r)^2 C_{gg}(\alpha_s(\mu_r^2), \mu_r, \mu_f) \exp\left[\mathcal{G}_H(\alpha_s(\mu_r^2), \log(N), \mu_r, \mu_f)\right]. \tag{8.18}$$

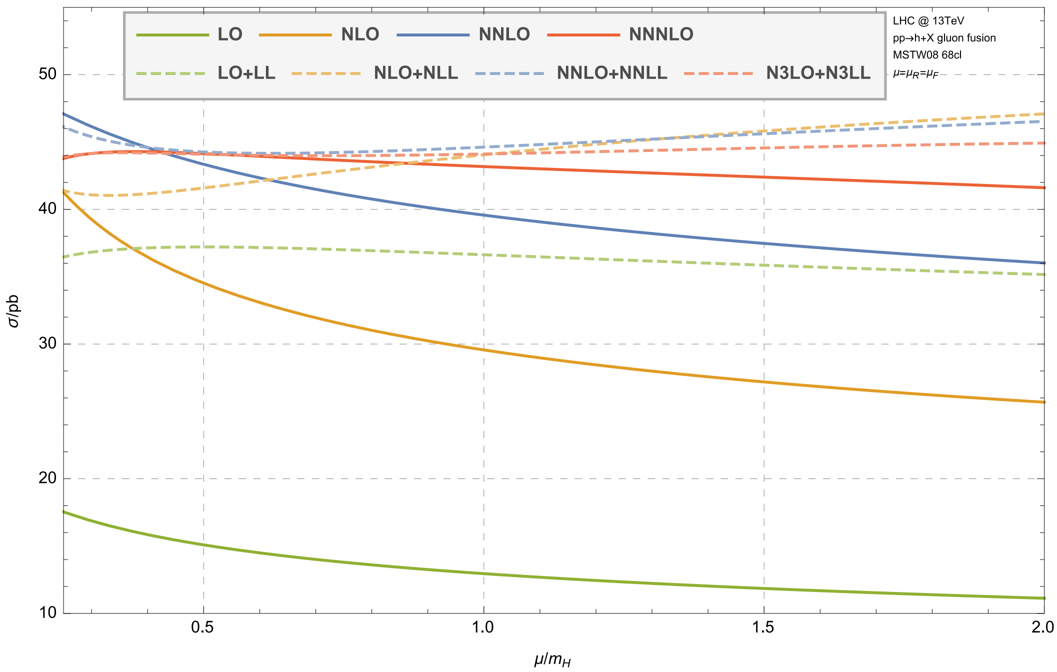



Figure 8.6: Scale variation ( $\mu = \mu_r = \mu_f$) of the gluon-fusion cross section at all perturbative orders through N$^3$LO for $m_H = 125$GeV resummed at the corresponding logarithmic accuracy compared to the fixed-order cross section through N$^3$LO. We use the NNLO MSTW2008 [208] parton densities and $\alpha_s(m_Z) = 0.117$ with N3LO evolution for these prediction.

Here the function $C_{gg}$ contains all contributions that are constant for $N \to \infty$. These contributions are due to the hard virtual and singular soft contributions in $\sigma^{(\ell)}_{\mathrm{SV}}$. The function $\mathcal{G}_H$ exponentiates the large logarithmic contributions $\log(N)$ to all orders. It is written as,

$$\begin{aligned}\mathcal{G}_H(\alpha_s(\mu_r^2), \log(N), \mu_r, \mu_f) = \log(N) g_H^{(1)}(b_0\alpha_s(\mu_r^2)\log(N)) \\ + g_H^{(2)}(b_0\alpha_s(\mu_r^2)\log(N), \mu_r, \mu_f) \\ + \sum_{n=3}^{\infty} \alpha_s^{n-2}(\mu_r^2) g_H^{(n)}(b_0\alpha_s(\mu_r^2), \mu_r, \mu_f).\end{aligned} \tag{8.19}$$

The coefficient functions $g_H^{(n)}$ can be determined from the cusp anomalous dimension of QCD [37, 210]. They are known exactly up to next-to-next-to-leading logarithmic accuracy $g_H^{(3)}$, which requires knowledge of the cusp anomalous dimension up to three loops. In order to perform resummation at next-to-next-to-next-to-leading logarithmic (N$^3$LL) accuracy, the function $g_H^{(4)}$ is needed. This function depends on the four loop cusp anomalous dimension which is not yet known in QCD. Consequently, $g_H^{(4)}$ is only known as an approximation.

From our fixed-order calculation we can determine the hard coefficient $C_{gg}$ up to order $\alpha_s^3$. For $\mu = \mu_r = \mu_f$ it can be written as,

$$C_{gg} = \sum_{n=1}^{3}\sum_{\ell=0}^{n} c_{n,\ell} \log^{\ell}\left(\frac{\mu^2}{m_H^2}\right)\left(\frac{\alpha_s}{\pi}\right)^n. \tag{8.20}$$

Setting $N_c = 3$ and $n_f = 5$, the coefficients $c_{n,\ell}$ up to $n = 3$ are,

$$\begin{aligned}
c_{1,1} &= 6\gamma, \\
c_{1,0} &= \frac{11}{2} + 6\gamma^2 + 2\pi^2, \\
c_{2,2} &= \frac{1}{4}\gamma(23 + 72\gamma), \\
c_{2,1} &= \frac{1}{6}\left(-81\zeta(3) + 26 + 69\gamma^2 + 216\gamma^3 + 23\pi^2 + \gamma\left(349 + 63\pi^2\right)\right), \\
c_{2,0} &= \frac{137}{24}\log\left(\frac{\mu^2}{m_t^2}\right) - \frac{87\zeta_3}{4} + \gamma\left(\frac{233}{9} - \frac{63\zeta_3}{2}\right) + \frac{1}{6}\gamma^2\left(349 + 63\pi^2\right) \\
&\quad + \frac{23\pi^4}{16} + \frac{349\pi^2}{18} + 18\gamma^4 + \frac{23\gamma^3}{3} + \frac{303}{8}, \\
c_{3,3} &= \frac{529\gamma}{72} + \frac{69\gamma^2}{2} + 36\gamma^3, \\
c_{3,2} &= \gamma\left(-81\zeta_3 + \frac{253\pi^2}{8} + \frac{1018}{9}\right) - \frac{207\zeta_3}{8} + \gamma^2\left(\frac{6529}{24} + 27\pi^2\right)
\end{aligned}$$

$$
\begin{aligned}
&+\frac{529\pi^2}{72}+108\gamma^4+\frac{207\gamma^3}{2}+\frac{299}{36}, \\
c_{3,1} =\ &\gamma^2\left(-270\zeta_3+\frac{161\pi^2}{4}+\frac{3200}{9}\right)-\frac{99\pi^2\zeta_3}{4}-\frac{2167\zeta_3}{8}+\frac{135\zeta_5}{2} \\
&+\frac{137}{4}\gamma\log\left(\frac{\mu^2}{m_t^2}\right)+\gamma^3\left(\frac{9529}{18}+54\pi^2\right)+\frac{345\pi^4}{64}+\frac{7235\pi^2}{108}+108\gamma^5 \\
&+115\gamma^4+\frac{7037}{72}+\gamma\left(-259\zeta_3+\frac{129\pi^4}{20}+\frac{875\pi^2}{6}+\frac{231065}{432}\right), \\
c_{3,0} =\ &\frac{81\zeta_3^2}{2}+\gamma^2\left(-259\zeta_3+\frac{129\pi^4}{20}+\frac{875\pi^2}{6}+\frac{231065}{432}\right)-\frac{929\pi^2\zeta_3}{16} \\
&+\gamma\left(-\frac{219}{4}\pi^2\zeta_3-\frac{17351\zeta_3}{36}+162\zeta_5-\frac{307\pi^4}{720}+\frac{4651\pi^2}{108}+\frac{2579507}{7776}\right) \\
&-\frac{7236713\zeta_3}{13824}+\frac{33353\zeta_5}{144}+\frac{3151}{288}\log^2\left(\frac{\mu^2}{m_t^2}\right)+\gamma^4\left(\frac{9529}{36}+27\pi^2\right) \\
&+\left(\frac{1927}{48}+\frac{137\gamma^2}{4}+\frac{137\pi^2}{12}\right)\log\left(\frac{\mu^2}{m_t^2}\right)+\frac{121\pi^6}{240}+\frac{1333921\pi^4}{77760}+36\gamma^6 \\
&+46\gamma^5+\frac{4154027}{20736}+\gamma^3\left(-189\zeta_3+\frac{23\pi^2}{2}+\frac{7330}{27}\right)+\frac{24221\pi^2}{144}. \qquad (8.21)
\end{aligned}
$$

The dependence on the top mass $m_t$ arises from the Wilson coefficient of the effective theory. With that we can use the resummation formula (8.18) to exponentiate the leading logarithms $\log^{3,\ldots,6}(N)$ of the inclusive Higgs cross section to all orders in $\alpha_s$. Expanding the resummation formula in $\alpha_s$ up to order $\alpha_s^5$ reproduces exactly the soft-virtual part of our calculation. We can therefore match the resummation to our fixed order calculation by subtracting the expansion up to $\alpha_s^5$ from the all-order resummation formula. This way we can guarantee that the resummation contributions only start at order $\alpha_s^6$ which is beyond the reach of our fixed-order calculation. We use this to calculate the $\mathrm{N^3LO} + \mathrm{N^3LL}$ threshold resummed inclusive Higgs cross section. In figure 8.6 we show the scale dependence of the resummed cross section in comparison to the fixed order cross section. As we can see, at lower orders in perturbation theory the resummation drastically improves the scale dependence of the cross section in comparison to the fixed order result. However, we can also see that at $\mathrm{N^3LO}$ the scale dependence of the fixed-order cross section is already so low that the resummation no longer improves upon it. We also note that at $\mu = \frac{m_H}{2}$ the effect of the resummation at on the $\mathrm{N^3LO}$ cross section is completely negligible.

## 8.3 Series coefficients of the threshold expansion

Here we give the threshold expansion of the regular part of the cross section in eq. 8.9 numerically for $N_c = 3$ and $n_f = 5$. We have obtain the expansion completely analytic as rational function of $N_c$ and $n_f$ in terms of $\zeta$-values, however due to the size of coefficients we choose to present them numerically.

$$\begin{aligned}
\eta_{gg}^{(3,2),\text{reg}} = \; & -11089.328 \\
& +1520.0814\,\bar{z} + 8805.7669\,\bar{z}^2 - 12506.932\,\bar{z}^3 - 440.32959\,\bar{z}^4 \\
& +1232.0873\,\bar{z}^5 + 1646.4249\,\bar{z}^6 + 1781.8637\,\bar{z}^7 + 1835.6555\,\bar{z}^8 \\
& +1861.3612\,\bar{z}^9 + 1876.6428\,\bar{z}^{10} + 1888.2649\,\bar{z}^{11} + 1899.1749\,\bar{z}^{12} \\
& +1910.7995\,\bar{z}^{13} + 1923.8791\,\bar{z}^{14} + 1938.8053\,\bar{z}^{15} + 1955.7742\,\bar{z}^{16} \\
& +1974.8643\,\bar{z}^{17} + 1996.0810\,\bar{z}^{18} + 2019.3836\,\bar{z}^{19} + 2044.7025\,\bar{z}^{20} \\
& +2071.9510\,\bar{z}^{21} + 2101.0331\,\bar{z}^{22} + 2131.8486\,\bar{z}^{23} + 2164.2968\,\bar{z}^{24} \\
& +2198.2785\,\bar{z}^{25} + 2233.6976\,\bar{z}^{26} + 2270.4621\,\bar{z}^{27} + 2308.4845\,\bar{z}^{28} \\
& +2347.6819\,\bar{z}^{29} + 2387.9764\,\bar{z}^{30} + 2429.2946\,\bar{z}^{31} + 2471.5678\,\bar{z}^{32} \\
& +2514.7317\,\bar{z}^{33} + 2558.7261\,\bar{z}^{34} + 2603.4947\,\bar{z}^{35} + 2648.9850\,\bar{z}^{36} \\
& +2695.1477\,\bar{z}^{37} + \mathcal{O}(\bar{z}^{38})
\end{aligned} \tag{8.22}$$

$$\begin{aligned}
\eta_{gg}^{(3,1),\text{reg}} = \; & 15738.441 \\
& -13580.184\,\bar{z} + 1757.5646\,\bar{z}^2 + 16078.884\,\bar{z}^3 + 82.947070\,\bar{z}^4 \\
& +222.78697\,\bar{z}^5 + 947.71319\,\bar{z}^6 + 1490.0998\,\bar{z}^7 + 1869.9658\,\bar{z}^8 \\
& +2145.3018\,\bar{z}^9 + 2354.6608\,\bar{z}^{10} + 2520.8158\,\bar{z}^{11} + 2657.1437\,\bar{z}^{12} \\
& +2771.7331\,\bar{z}^{13} + 2869.6991\,\bar{z}^{14} + 2954.4505\,\bar{z}^{15} + 3028.3834\,\bar{z}^{16} \\
& +3093.2654\,\bar{z}^{17} + 3150.4554\,\bar{z}^{18} + 3201.0314\,\bar{z}^{19} + 3245.8702\,\bar{z}^{20} \\
& +3285.6978\,\bar{z}^{21} + 3321.1237\,\bar{z}^{22} + 3352.6649\,\bar{z}^{23} + 3380.7639\,\bar{z}^{24} \\
& +3405.8019\,\bar{z}^{25} + 3428.1091\,\bar{z}^{26} + 3447.9734\,\bar{z}^{27} + 3465.6466\,\bar{z}^{28} \\
& +3481.3499\,\bar{z}^{29} + 3495.2787\,\bar{z}^{30} + 3507.6057\,\bar{z}^{31} + 3518.4844\,\bar{z}^{32} \\
& +3528.0516\,\bar{z}^{33} + 3536.4294\,\bar{z}^{34} + 3543.7272\,\bar{z}^{35} + 3550.0434\,\bar{z}^{36} \\
& +3555.4664\,\bar{z}^{37}
\end{aligned} \tag{8.23}$$

$$\begin{aligned}
\eta_{gg}^{(3,0),\text{reg}} = \; & -5872.5889 \\
& +12249.940\,\bar{z} - 9638.4528\,\bar{z}^2 - 4817.5592\,\bar{z}^3 + 1526.5421\,\bar{z}^4 \\
& +297.45929\,\bar{z}^5 - 328.25240\,\bar{z}^6 - 547.47104\,\bar{z}^7 - 581.33009\,\bar{z}^8 \\
& -530.54599\,\bar{z}^9 - 439.61074\,\bar{z}^{10} - 328.65590\,\bar{z}^{11} - 207.13607\,\bar{z}^{12} \\
& -79.706814\,\bar{z}^{13} + 51.184085\,\bar{z}^{14} + 184.13649\,\bar{z}^{15} + 318.27084\,\bar{z}^{16}
\end{aligned}$$

$$+452.98499\,\bar{z}^{17} + 587.83913\,\bar{z}^{18} + 722.49864\,\bar{z}^{19} + 856.70352\,\bar{z}^{20}$$
$$+990.25020\,\bar{z}^{21} + 1122.9794\,\bar{z}^{22} + 1254.7674\,\bar{z}^{23} + 1385.5192\,\bar{z}^{24}$$
$$+1515.1630\,\bar{z}^{25} + 1643.6461\,\bar{z}^{26} + 1770.9307\,\bar{z}^{27} + 1896.9918\,\bar{z}^{28}$$
$$+2021.8139\,\bar{z}^{29} + 2145.3897\,\bar{z}^{30} + 2267.7184\,\bar{z}^{31} + 2388.8041\,\bar{z}^{32}$$
$$+2508.6552\,\bar{z}^{33} + 2627.2831\,\bar{z}^{34} + 2744.7017\,\bar{z}^{35} + 2860.9272\,\bar{z}^{36}$$
$$+2975.9768\,\bar{z}^{37} \tag{8.24}$$

$$\begin{aligned}\eta_{qg}^{(3,2),\mathrm{reg}} = {} & 513.56298 \\ & -754.78793\,\bar{z} - 280.97494\,\bar{z}^{2} - 2.0101406\,\bar{z}^{3} + 503.52967\,\bar{z}^{4} \\ & +627.89991\,\bar{z}^{5} + 691.45552\,\bar{z}^{6} + 733.60753\,\bar{z}^{7} + 765.14788\,\bar{z}^{8} \\ & +790.66308\,\bar{z}^{9} + 812.57547\,\bar{z}^{10} + 832.30620\,\bar{z}^{11} + 850.73481\,\bar{z}^{12} \\ & +868.42184\,\bar{z}^{13} + 885.73010\,\bar{z}^{14} + 902.89588\,\bar{z}^{15} + 920.07262\,\bar{z}^{16} \\ & +937.35866\,\bar{z}^{17} + 954.81528\,\bar{z}^{18} + 972.47867\,\bar{z}^{19} + 990.36794\,\bar{z}^{20} \\ & +1008.4906\,\bar{z}^{21} + 1026.8464\,\bar{z}^{22} + 1045.4298\,\bar{z}^{23} + 1064.2318\,\bar{z}^{24} \\ & +1083.2414\,\bar{z}^{25} + 1102.4464\,\bar{z}^{26} + 1121.8338\,\bar{z}^{27} + 1141.3904\,\bar{z}^{28} \\ & +1161.1034\,\bar{z}^{29} + 1180.9600\,\bar{z}^{30} \end{aligned} \tag{8.25}$$

$$\begin{aligned}\eta_{qg}^{(3,1),\mathrm{reg}} = {} & -313.98523 \\ & +807.28021\,\bar{z} + 673.01632\,\bar{z}^{2} + 424.92437\,\bar{z}^{3} - 94.523260\,\bar{z}^{4} \\ & -16.197667\,\bar{z}^{5} + 53.689920\,\bar{z}^{6} + 107.82115\,\bar{z}^{7} + 152.20191\,\bar{z}^{8} \\ & +190.11227\,\bar{z}^{9} + 223.24799\,\bar{z}^{10} + 252.59416\,\bar{z}^{11} + 278.80517\,\bar{z}^{12} \\ & +302.36320\,\bar{z}^{13} + 323.64795\,\bar{z}^{14} + 342.97017\,\bar{z}^{15} + 360.58960\,\bar{z}^{16} \\ & +376.72599\,\bar{z}^{17} + 391.56667\,\bar{z}^{18} + 405.27209\,\bar{z}^{19} + 417.98023\,\bar{z}^{20} \\ & +429.81014\,\bar{z}^{21} + 440.86488\,\bar{z}^{22} + 451.23389\,\bar{z}^{23} + 460.99506\,\bar{z}^{24} \\ & +470.21638\,\bar{z}^{25} + 478.95737\,\bar{z}^{26} + 487.27030\,\bar{z}^{27} + 495.20115\,\bar{z}^{28} \\ & +502.79050\,\bar{z}^{29} + 510.07423\,\bar{z}^{30} \end{aligned} \tag{8.26}$$

$$\begin{aligned}\eta_{qg}^{(3,0),\mathrm{reg}} = {} & 204.62079 \\ & +94.711709\,\bar{z} - 516.31293\,\bar{z}^{2} - 86.222501\,\bar{z}^{3} + 112.69425\,\bar{z}^{4} \\ & +1.9010983\,\bar{z}^{5} - 27.130422\,\bar{z}^{6} - 21.392526\,\bar{z}^{7} + 0.27617630\,\bar{z}^{8} \\ & +30.304354\,\bar{z}^{9} + 65.175579\,\bar{z}^{10} + 103.01832\,\bar{z}^{11} + 142.72655\,\bar{z}^{12} \\ & +183.59437\,\bar{z}^{13} + 225.14662\,\bar{z}^{14} + 267.05174\,\bar{z}^{15} + 309.07290\,\bar{z}^{16} \\ & +351.03855\,\bar{z}^{17} + 392.82345\,\bar{z}^{18} + 434.33601\,\bar{z}^{19} + 475.50950\,\bar{z}^{20} \\ & +516.29577\,\bar{z}^{21} + 556.66066\,\bar{z}^{22} + 596.58065\,\bar{z}^{23} + 636.04035\,\bar{z}^{24} \\ & +675.03054\,\bar{z}^{25} + 713.54678\,\bar{z}^{26} + 751.58826\,\bar{z}^{27} + 789.15696\,\bar{z}^{28} \end{aligned}$$

$$+826.25696\,\bar{z}^{29} + 862.89396\,\bar{z}^{30} \tag{8.27}$$

$$\begin{aligned}
\eta_{q\bar{q}}^{(3,2),\text{reg}} = {} & 52.489897\,\bar{z} + 121.14225\,\bar{z}^2 + 546.26186\,\bar{z}^3 + 430.10665\,\bar{z}^4 \\
& +395.20262\,\bar{z}^5 + 377.03244\,\bar{z}^6 + 365.05682\,\bar{z}^7 + 356.30539\,\bar{z}^8 \\
& +349.64832\,\bar{z}^9 + 344.54422\,\bar{z}^{10} + 340.68027\,\bar{z}^{11} + 337.84848\,\bar{z}^{12} \\
& +335.89655\,\bar{z}^{13} + 334.70587\,\bar{z}^{14} + 334.18036\,\bar{z}^{15} + 334.24025\,\bar{z}^{16} \\
& +334.81815\,\bar{z}^{17} + 335.85649\,\bar{z}^{18} + 337.30562\,\bar{z}^{19} + 339.12245\,\bar{z}^{20} \\
& +341.26935\,\bar{z}^{21} + 343.71330\,\bar{z}^{22} + 346.42520\,\bar{z}^{23} + 349.37931\,\bar{z}^{24} \\
& +352.55277\,\bar{z}^{25} + 355.92522\,\bar{z}^{26} + 359.47847\,\bar{z}^{27} + 363.19620\,\bar{z}^{28} \\
& +367.06378\,\bar{z}^{29} + 371.06801\,\bar{z}^{30}
\end{aligned} \tag{8.28}$$

$$\begin{aligned}
\eta_{q\bar{q}}^{(3,1),\text{reg}} = {} & -13.561787\,\bar{z} - 122.83887\,\bar{z}^2 - 747.63122\,\bar{z}^3 - 396.29959\,\bar{z}^4 \\
& -305.88934\,\bar{z}^5 - 259.42707\,\bar{z}^6 - 228.03650\,\bar{z}^7 - 204.06989\,\bar{z}^8 \\
& -184.61437\,\bar{z}^9 - 168.25305\,\bar{z}^{10} - 154.17060\,\bar{z}^{11} - 141.84193\,\bar{z}^{12} \\
& -130.90258\,\bar{z}^{13} - 121.08653\,\bar{z}^{14} - 112.19267\,\bar{z}^{15} - 104.06504\,\bar{z}^{16} \\
& -96.580303\,\bar{z}^{17} - 89.639462\,\bar{z}^{18} - 83.162027\,\bar{z}^{19} - 77.081876\,\bar{z}^{20} \\
& -71.344195\,\bar{z}^{21} - 65.903187\,\bar{z}^{22} - 60.720315\,\bar{z}^{23} - 55.762951\,\bar{z}^{24} \\
& -51.003310\,\bar{z}^{25} - 46.417609\,\bar{z}^{26} - 41.985393\,\bar{z}^{27} - 37.688995\,\bar{z}^{28} \\
& -33.513090\,\bar{z}^{29} - 29.444339\,\bar{z}^{30}
\end{aligned} \tag{8.29}$$

$$\begin{aligned}
\eta_{q\bar{q}}^{(3,0),\text{reg}} = {} & -37.707516\,\bar{z} + 53.725755\,\bar{z}^2 + 144.18366\,\bar{z}^3 - 69.788040\,\bar{z}^4 \\
& -67.434087\,\bar{z}^5 - 50.987269\,\bar{z}^6 - 33.558429\,\bar{z}^7 - 16.662373\,\bar{z}^8 \\
& -0.44090329\,\bar{z}^9 + 15.148279\,\bar{z}^{10} + 30.159647\,\bar{z}^{11} + 44.637979\,\bar{z}^{12} \\
& +58.619322\,\bar{z}^{13} + 72.133997\,\bar{z}^{14} + 85.208698\,\bar{z}^{15} + 97.867667\,\bar{z}^{16} \\
& +110.13333\,\bar{z}^{17} + 122.02662\,\bar{z}^{18} + 133.56717\,\bar{z}^{19} + 144.77338\,\bar{z}^{20} \\
& +155.66254\,\bar{z}^{21} + 166.25087\,\bar{z}^{22} + 176.55354\,\bar{z}^{23} + 186.58480\,\bar{z}^{24} \\
& +196.35799\,\bar{z}^{25} + 205.88558\,\bar{z}^{26} + 215.17928\,\bar{z}^{27} + 224.25003\,\bar{z}^{28} \\
& +233.10811\,\bar{z}^{29} + 241.76313\,\bar{z}^{30}
\end{aligned} \tag{8.30}$$

$$\begin{aligned}
\eta_{qq}^{(3,2),\text{reg}} = {} & 52.489897\,\bar{z} + 115.88299\,\bar{z}^2 + 206.89141\,\bar{z}^3 + 237.16727\,\bar{z}^4 \\
& +253.85312\,\bar{z}^5 + 264.50690\,\bar{z}^6 + 271.88762\,\bar{z}^7 + 277.47724\,\bar{z}^8 \\
& +282.11036\,\bar{z}^9 + 286.26594\,\bar{z}^{10} + 290.22209\,\bar{z}^{11} + 294.14093\,\bar{z}^{12} \\
& +298.11608\,\bar{z}^{13} + 302.20004\,\bar{z}^{14} + 306.42029\,\bar{z}^{15} + 310.78904\,\bar{z}^{16} \\
& +315.30914\,\bar{z}^{17} + 319.97778\,\bar{z}^{18} + 324.78884\,\bar{z}^{19} + 329.73434\,\bar{z}^{20} \\
& +334.80540\,\bar{z}^{21} + 339.99280\,\bar{z}^{22} + 345.28737\,\bar{z}^{23} + 350.68023\,\bar{z}^{24}
\end{aligned}$$

$$+356.16287\,\bar{z}^{25} + 361.72729\,\bar{z}^{26} + 367.36598\,\bar{z}^{27} + 373.07194\,\bar{z}^{28} + 378.83869\,\bar{z}^{29} + 384.66021\,\bar{z}^{30} \tag{8.31}$$

$$\begin{aligned}\eta_{qq}^{(3,1),\mathrm{reg}} = {} & -13.561787\,\bar{z} - 100.44381\,\bar{z}^2 - 197.02897\,\bar{z}^3 - 201.49505\,\bar{z}^4 \\ & -196.70233\,\bar{z}^5 - 189.72948\,\bar{z}^6 - 181.90181\,\bar{z}^7 - 174.01305\,\bar{z}^8 \\ & -166.44104\,\bar{z}^9 - 159.32993\,\bar{z}^{10} - 152.70888\,\bar{z}^{11} - 146.55489\,\bar{z}^{12} \\ & -140.82408\,\bar{z}^{13} - 135.46673\,\bar{z}^{14} - 130.43420\,\bar{z}^{15} - 125.68188\,\bar{z}^{16} \\ & -121.17016\,\bar{z}^{17} - 116.86451\,\bar{z}^{18} - 112.73513\,\bar{z}^{19} - 108.75638\,\bar{z}^{20} \\ & -104.90636\,\bar{z}^{21} - 101.16628\,\bar{z}^{22} - 97.520078\,\bar{z}^{23} - 93.954009\,\bar{z}^{24} \\ & -90.456274\,\bar{z}^{25} - 87.016749\,\bar{z}^{26} - 83.626728\,\bar{z}^{27} - 80.278716\,\bar{z}^{28} \\ & -76.966251\,\bar{z}^{29} - 73.683754\,\bar{z}^{30} \end{aligned} \tag{8.32}$$

$$\begin{aligned}\eta_{qq}^{(3,0),\mathrm{reg}} = {} & -76.669104\,\bar{z} + 1.7118927\,\bar{z}^2 + 37.712253\,\bar{z}^3 + 25.200784\,\bar{z}^4 \\ & +23.595317\,\bar{z}^5 + 27.540180\,\bar{z}^6 + 34.067987\,\bar{z}^7 + 42.055171\,\bar{z}^8 \\ & +50.899550\,\bar{z}^9 + 60.227379\,\bar{z}^{10} + 69.795043\,\bar{z}^{11} + 79.441097\,\bar{z}^{12} \\ & +89.058095\,\bar{z}^{13} + 98.574786\,\bar{z}^{14} + 107.94449\,\bar{z}^{15} + 117.13733\,\bar{z}^{16} \\ & +126.13506\,\bar{z}^{17} + 134.92745\,\bar{z}^{18} + 143.50985\,\bar{z}^{19} + 151.88147\,\bar{z}^{20} \\ & +160.04416\,\bar{z}^{21} + 168.00161\,\bar{z}^{22} + 175.75867\,\bar{z}^{23} + 183.32099\,\bar{z}^{24} \\ & +190.69468\,\bar{z}^{25} + 197.88608\,\bar{z}^{26} + 204.90165\,\bar{z}^{27} + 211.74780\,\bar{z}^{28} \\ & +218.43084\,\bar{z}^{29} + 224.95696\,\bar{z}^{30} \end{aligned} \tag{8.33}$$

$$\begin{aligned}\eta_{qq'}^{(3,2),\mathrm{reg}} = {} & 52.489897\,\bar{z} + 115.95707\,\bar{z}^2 + 207.09717\,\bar{z}^3 + 237.47076\,\bar{z}^4 \\ & +254.23192\,\bar{z}^5 + 264.94538\,\bar{z}^6 + 272.37440\,\bar{z}^7 + 278.00388\,\bar{z}^8 \\ & +282.67045\,\bar{z}^9 + 286.85449\,\bar{z}^{10} + 290.83519\,\bar{z}^{11} + 294.77542\,\bar{z}^{12} \\ & +298.76938\,\bar{z}^{13} + 302.87003\,\bar{z}^{14} + 307.10519\,\bar{z}^{15} + 311.48736\,\bar{z}^{16} \\ & +316.01959\,\bar{z}^{17} + 320.69926\,\bar{z}^{18} + 325.52041\,\bar{z}^{19} + 330.47516\,\bar{z}^{20} \\ & +335.55474\,\bar{z}^{21} + 340.75002\,\bar{z}^{22} + 346.05189\,\bar{z}^{23} + 351.45154\,\bar{z}^{24} \\ & +356.94052\,\bar{z}^{25} + 362.51087\,\bar{z}^{26} + 368.15511\,\bar{z}^{27} + 373.86629\,\bar{z}^{28} \\ & +379.63795\,\bar{z}^{29} + 385.46411\,\bar{z}^{30} \end{aligned} \tag{8.34}$$

$$\begin{aligned}\eta_{qq'}^{(3,1),\mathrm{reg}} = {} & -13.561787\,\bar{z} - 101.23393\,\bar{z}^2 - 199.27314\,\bar{z}^3 - 204.58988\,\bar{z}^4 \\ & -200.32378\,\bar{z}^5 - 193.67683\,\bar{z}^6 - 186.04539\,\bar{z}^7 - 178.26735\,\bar{z}^8 \\ & -170.74845\,\bar{z}^9 - 163.65084\,\bar{z}^{10} - 157.01563\,\bar{z}^{11} - 150.82793\,\bar{z}^{12} \\ & -145.04949\,\bar{z}^{13} - 139.63457\,\bar{z}^{14} - 134.53740\,\bar{z}^{15} - 129.71545\,\bar{z}^{16} \\ & -125.13066\,\bar{z}^{17} - 120.74964\,\bar{z}^{18} - 116.54344\,\bar{z}^{19} - 112.48710\,\bar{z}^{20} \end{aligned}$$

$$
\begin{aligned}
&-108.55918\,\bar{z}^{21} - 104.74128\,\bar{z}^{22} - 101.01763\,\bar{z}^{23} - 97.374684\,\bar{z}^{24} \\
&-93.800809\,\bar{z}^{25} - 90.286003\,\bar{z}^{26} - 86.821649\,\bar{z}^{27} - 83.400317\,\bar{z}^{28} \\
&-80.015589\,\bar{z}^{29} - 76.661913\,\bar{z}^{30} \qquad (8.35)
\end{aligned}
$$

$$
\begin{aligned}
\eta_{qq'}^{(3,0),\mathrm{reg}} = &-38.124370\,\bar{z} + 21.925696\,\bar{z}^{2} + 62.593745\,\bar{z}^{3} + 62.740689\,\bar{z}^{4} \\
&+68.779415\,\bar{z}^{5} + 77.692571\,\bar{z}^{6} + 87.639674\,\bar{z}^{7} + 98.079383\,\bar{z}^{8} \\
&+108.73738\,\bar{z}^{9} + 119.43753\,\bar{z}^{10} + 130.06186\,\bar{z}^{11} + 140.53231\,\bar{z}^{12} \\
&+150.79875\,\bar{z}^{13} + 160.83049\,\bar{z}^{14} + 170.61028\,\bar{z}^{15} + 180.13007\,\bar{z}^{16} \\
&+189.38806\,\bar{z}^{17} + 198.38664\,\bar{z}^{18} + 207.13098\,\bar{z}^{19} + 215.62804\,\bar{z}^{20} \\
&+223.88584\,\bar{z}^{21} + 231.91300\,\bar{z}^{22} + 239.71843\,\bar{z}^{23} + 247.31108\,\bar{z}^{24} \\
&+254.69977\,\bar{z}^{25} + 261.89310\,\bar{z}^{26} + 268.89942\,\bar{z}^{27} + 275.72674\,\bar{z}^{28} \\
&+282.38271\,\bar{z}^{29} + 288.87465\,\bar{z}^{30} \qquad (8.36)
\end{aligned}
$$

CHAPTER 9

# CONCLUSION

Let us summarize the achievements of this thesis. In chapter 2 we have reviewed some of the progress of recent years in the study of multiple polylogarithms. Starting from the well known shuffle algebra, we have described the recent advances in the algebraic description of the multiple polylogarithms using Hopf algebras. Building upon this technology we have described several very powerful algorithms which were instrumental in the calculation of the integrals contributing to Higgs production at $N^3LO$. The methods for finding a canonical form and for building a basis for a given symbol alphabet are of prime importance for the treatment of the multiple polylogarithms allowing us to exploit the plethora of algebraic relations that exist between these functions. Finally, we described an algorithm for the iterative integration of certain parametric integrals in terms of multiple polylogarithms which has been a key ingredient in the computation in some of the most difficult integrals that were required.

In chapter 3 we briefly reviewed the methods that were used to decompose cross sections into a basis of integrals. We described the method of reverse unitary which enables the uniform treatment of loop as well as phase space integrals. Using integration-by-parts reductions, identities between different integrals can be exploited in order to express all integrals appearing in a cross section through a small set of master integrals. These master integrals can be calculated using the method of differential equations. This immediately connects to the multiple polylogarithms which are the natural functions to describe the master integrals appearing in the Higgs cross section. The solutions of master integrals obtained from differential equations need to be specialized by boundary conditions.

The determination of these boundary conditions has been one of the main themes of this dissertation. We discuss several technologies that we employed to calculate all boundary conditions required for the Higgs cross section at $N^3LO$ in chapter 4. We describe several ways of obtaining parametrizations for loop and phase space integrals and describe how we employ Mellin-Barnes techniques to extract the required boundary information from them.

This concluded the first part of our dissertation. In the second part we discussed the computation of several components of the Higgs cross section at $N^3LO$, which relied on the techniques that were discussed in the first part. In chapter 5 we described the contributions to Higgs production at $N^3LO$ due to the emission of three real partons in addition to the Higgs boson. We explicitly showed the computation of the boundary conditions required for these contributions.

In chapter 6 we discussed contributions arising from the square of the one loop corrections to the emission of a single parton. Here we showed several methods for calculating the master integrals, exploring the method of differential equations in more detail.

In chapter 7 we calculated the genuine two-loop corrections to the emission of a single parton in addition to the Higgs. Here we demonstrated the interplay between solving the differential equations and determining the boundary conditions.

In chapter 8 we combined the different contribution to obtain the finite inclusive Higgs production cross section at $N^3LO$. We showed phenomenological studies of the scale dependence of the cross section and determined the uncertainty of the new prediction for the Higgs cross section. We also briefly described the method of threshold resummation and used it to resum the potentially large threshold logarithms that appear in the Higgs cross section. By studying the scale depedence of the resummed cross section we showed the stability of the perturbative expansion of the cross section and determined that the fixed order results at $N^3LO$ provide a reliable prediction.

The calculation that was presented in this dissertation presents a major breakthrough in perturbative calculations. With the beginning of Run II of the LHC the measurements of properties of the Higgs boson are expected to improve rapidly, reducing the statistical uncertainty of the measurements to levels lower than the uncertainties due to NNLO predictions. The calculation of the inclusive Higgs cross section was therefore a long term goal of the particle physics community. With the completion of our calculation the uncertainty of the Higgs production cross section in gluon fusion is reduced to less than 3% rendering it competitive with future measurements.

The methods developed to compute the Higgs cross section can easily be applied to compute similar processes, like Drell-Yan, at $N^3LO$. Furthermore, an obvious way to extend our methods would be to allow for more exclusive observables in order to determine for example the rapidity distribution for Higgs production at $N^3LO$.

# Bibliography


[1] Charalampos Anastasiou, Claude Duhr, Falko Dulat, and Bernhard Mistlberger. "Soft triple-real radiation for Higgs production at N3LO". *JHEP* 1307 (2013). arXiv: 1302.4379 (cit. on pp. v, 2, 3, 32, 120, 150, 184, 223).

[2] Charalampos Anastasiou, Claude Duhr, Falko Dulat, Franz Herzog, and Bernhard Mistlberger. "Real-virtual contributions to the inclusive Higgs cross section at $N^3LO$". *JHEP* 12 (2013). arXiv: 1311.1425 (cit. on pp. v, 2, 3, 142, 184, 223).

[3] Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Thomas Gehrmann, Franz Herzog, and Bernhard Mistlberger. "Higgs boson gluon–fusion production at threshold in $\mathrm{N^3LO}$ QCD". *Phys. Lett.* B737 (2014). arXiv: 1403.4616 (cit. on pp. v, 2, 185, 223).

[4] Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Thomas Gehrmann, Franz Herzog, and Bernhard Mistlberger. "Higgs boson gluon-fusion production beyond threshold in $\mathrm{N^3LO}$ QCD". *JHEP* 03 (2015). arXiv: 1411.3584 (cit. on pp. v, 2, 169, 186, 223).

[5] Falko Dulat and Bernhard Mistlberger. "Real-Virtual-Virtual contributions to the inclusive Higgs cross section at N3LO" (2014). arXiv: 1411.3586 (cit. on pp. v, 3, 169, 184, 223).

[6] Charalampos Anastasiou, Claude Duhr, Falko Dulat, Franz Herzog, and Bernhard Mistlberger. "Higgs Boson Gluon-Fusion Production in QCD at Three Loops". *Phys. Rev. Lett.* 114.21 (2015). arXiv: 1503.06056 (cit. on pp. v, 2, 223).

[7] Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Franz Herzog, and Bernhard Mistlberger. "Soft Expansion of Double-Real-Virtual Corrections to Higgs Production at $\mathrm{N^3LO}$" (2015). arXiv: 1505.04110 (cit. on pp. v, 184, 223).

[8] Georges Aad et al. "Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC". *Phys. Lett.* B716 (2012). arXiv: 1207.7214 (cit. on p. 1).

[9] Serguei Chatrchyan et al. “Observation of a new boson at a mass of 125 GeV with the CMS experiment at the LHC”. *Phys. Lett.* B716 (2012). arXiv: 1207.7235 (cit. on p. 1).

[10] Z. Bern, L.J. Dixon, F. Febres Cordero, S. Höche, H. Ita, et al. “Next-to-Leading Order $W + 5$-Jet Production at the LHC”. *Phys.Rev.* D88.1 (2013). arXiv: 1304.1253 (cit. on p. 1).

[11] R. Keith Ellis, Zoltan Kunszt, Kirill Melnikov, and Giulia Zanderighi. “One-loop calculations in quantum field theory: from Feynman diagrams to unitarity cuts”. *Phys. Rept.* 518 (2012). arXiv: 1105.4319 (cit. on p. 1).

[12] J. Alwall, R. Frederix, S. Frixione, V. Hirschi, F. Maltoni, O. Mattelaer, H. -S. Shao, T. Stelzer, P. Torrielli, and M. Zaro. “The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations”. *JHEP* 07 (2014). arXiv: 1405.0301 (cit. on p. 1).

[13] T. Gehrmann, M. Grazzini, S. Kallweit, P. Maierhöfer, A. von Manteuffel, S. Pozzorini, D. Rathlev, and L. Tancredi. “$W^+W^-$ Production at Hadron Colliders in Next to Next to Leading Order QCD”. *Phys. Rev. Lett.* 113.21 (2014). arXiv: 1408.5243 (cit. on pp. 1, 3).

[14] Michal Czakon, Paul Fiedler, and Alexander Mitov. “Resolving the Tevatron top quark forward-backward asymmetry puzzle” (2014). arXiv: 1411.3007 (cit. on p. 1).

[15] Alexander Karlberg, Emanuele Re, and Giulia Zanderighi. “NNLOPS accurate Drell-Yan production”. *JHEP* 09 (2014). arXiv: 1407.2940 (cit. on p. 1).

[16] Charalampos Anastasiou, Stephan Buehler, Franz Herzog, and Achilleas Lazopoulos. “Inclusive Higgs boson cross section for the LHC at 8 TeV”. *JHEP* 04 (2012). arXiv: 1202.3638 (cit. on pp. 2, 188).

[17] Charalampos Anastasiou, Stephan Buehler, Franz Herzog, and Achilleas Lazopoulos. “Total cross section for Higgs boson hadroproduction with anomalous Standard Model interactions”. *JHEP* 12 (2011). arXiv: 1107.0683 (cit. on pp. 2, 188).

[18] Vardan Khachatryan et al. “Precise determination of the mass of the Higgs boson and tests of compatibility of its couplings with the standard model predictions using proton collisions at 7 and 8 TeV”. *Eur. Phys. J.* C75.5 (2015). arXiv: 1412.8662 (cit. on p. 2).

[19] Georges Aad et al. “Measurement of Higgs boson production in the diphoton decay channel in pp collisions at center-of-mass energies of 7 and 8 TeV with the ATLAS detector”. *Phys. Rev.* D90.11 (2014). arXiv: 1408.7084 (cit. on p. 2).

[20] P. A. Baikov, K. G. Chetyrkin, A. V. Smirnov, V. A. Smirnov, and M. Steinhauser. “Quark and gluon form factors to three loops”. *Phys. Rev. Lett.* 102 (2009). arXiv: 0902.3519 (cit. on pp. 2, 184).

[21] T. Gehrmann, E. W. N. Glover, T. Huber, N. Ikizlerli, and C. Studerus. “Calculation of the quark and gluon form factors to three loops in QCD”. *JHEP* 06 (2010). arXiv: 1004.3653 (cit. on pp. 2, 184).

[22] William B. Kilgore. “One-loop single-real-emission contributions to $pp \to H + X$ at next-to-next-to-next-to-leading order”. *Phys. Rev.* D89.7 (2014). arXiv: 1312.1296 (cit. on pp. 2, 184).

[23] T. Gehrmann, M. Jaquier, E. W. N. Glover, and A. Koukoutsakis. “Two-Loop QCD Corrections to the Helicity Amplitudes for $H \to 3$ partons”. *JHEP* 02 (2012). arXiv: 1112.3554 (cit. on pp. 2, 184).

[24] Claude Duhr and Thomas Gehrmann. “The two-loop soft current in dimensional regularization”. *Phys. Lett.* B727 (2013). arXiv: 1309.4393 (cit. on pp. 2, 169, 172, 178, 184).

[25] Claude Duhr, Thomas Gehrmann, and Matthieu Jaquier. “Two-loop splitting amplitudes and the single-real contribution to inclusive Higgs production at N$^3$LO”. *JHEP* 02 (2015). arXiv: 1411.3587 (cit. on pp. 2, 3, 184).

[26] O. V. Tarasov, A. A. Vladimirov, and A. Yu. Zharkov. “The Gell-Mann-Low Function of QCD in the Three Loop Approximation”. *Phys. Lett.* B93 (1980) (cit. on pp. 2, 184).

[27] S. A. Larin and J. A. M. Vermaseren. “The Three loop QCD Beta function and anomalous dimensions”. *Phys. Lett.* B303 (1993). arXiv: hep-ph/9302208 (cit. on pp. 2, 184).

[28] T. van Ritbergen, J. A. M. Vermaseren, and S. A. Larin. “The Four loop beta function in quantum chromodynamics”. *Phys. Lett.* B400 (1997). arXiv: hep-ph/9701390 (cit. on pp. 2, 184).

[29] M. Czakon. “The Four-loop QCD beta-function and anomalous dimensions”. *Nucl. Phys.* B710 (2005). arXiv: hep-ph/0411261 (cit. on pp. 2, 184).

[30] S. Moch, J. A. M. Vermaseren, and A. Vogt. “The Three loop splitting functions in QCD: The Nonsinglet case”. *Nucl. Phys.* B688 (2004). arXiv: hep-ph/0403192 (cit. on pp. 2, 184).

[31] A. Vogt, S. Moch, and J. A. M. Vermaseren. “The Three-loop splitting functions in QCD: The Singlet case”. *Nucl. Phys.* B691 (2004). arXiv: hep-ph/0404111 (cit. on pp. 2, 184).

[32] Stephan Buehler and Achilleas Lazopoulos. “Scale dependence and collinear subtraction terms for Higgs production in gluon fusion at N3LO”. *JHEP* 1310 (2013). arXiv: 1306.2223 (cit. on pp. 2, 184).

[33] Maik Höschele, Jens Hoff, Alexey Pak, Matthias Steinhauser, and Takahiro Ueda. "Higgs boson production at the LHC: NNLO partonic cross sections through order $\epsilon$ and convolutions with splitting functions to N$^3$LO". *Phys.Lett.* B721 (2013). arXiv: 1211.6559 (cit. on pp. 2, 184).

[34] Charalampos Anastasiou, Stephan Buehler, Claude Duhr, and Franz Herzog. "NNLO phase space master integrals for two-to-one inclusive cross sections in dimensional regularization". *JHEP* 11 (2012). arXiv: 1208.3130 (cit. on pp. 2, 108–110, 162, 163, 184).

[35] Hua Xing Zhu. "On the calculation of soft phase space integral". *JHEP* 02 (2015). arXiv: 1501.00236 (cit. on p. 2).

[36] Ye Li, Andreas von Manteuffel, Robert M. Schabinger, and Hua Xing Zhu. "N$^3$LO Higgs boson and Drell-Yan production at threshold: The one-loop two-emission contribution". *Phys. Rev.* D90.5 (2014). arXiv: 1404.5839 (cit. on pp. 2, 184).

[37] S. Moch and A. Vogt. "Higher-order soft corrections to lepton pair and Higgs boson production". *Phys. Lett.* B631 (2005). arXiv: hep-ph/0508265 (cit. on pp. 2, 186, 194).

[38] N. A. Lo Presti, A. A. Almasy, and A. Vogt. "Leading large-x logarithms of the quark–gluon contributions to inclusive Higgs-boson and lepton-pair production". *Phys. Lett.* B737 (2014). arXiv: 1407.1553 (cit. on p. 2).

[39] Ye Li, Andreas von Manteuffel, Robert M. Schabinger, and Hua Xing Zhu. "Soft-virtual corrections to Higgs production at N$^3$LO". *Phys. Rev.* D91.3 (2015). arXiv: 1412.2771 (cit. on pp. 2, 185).

[40] Taushif Ahmed, Maguni Mahakhud, Narayan Rana, and V. Ravindran. "Drell-Yan Production at Threshold to Third Order in QCD". *Phys. Rev. Lett.* 113.11 (2014). arXiv: 1404.0366 (cit. on p. 2).

[41] Taushif Ahmed, M. K. Mandal, Narayan Rana, and V. Ravindran. "Rapidity Distributions in Drell-Yan and Higgs Productions at Threshold to Third Order in QCD". *Phys. Rev. Lett.* 113 (2014). arXiv: 1404.6504 (cit. on p. 2).

[42] Taushif Ahmed, Narayan Rana, and V. Ravindran. "Higgs boson production through $b\bar{b}$ annihilation at threshold in N$^3$LO QCD". *JHEP* 10 (2014). arXiv: 1408.0787 (cit. on p. 2).

[43] Taushif Ahmed, M. K. Mandal, Narayan Rana, and V. Ravindran. "Higgs Rapidity Distribution in $b\bar{b}$ Annihilation at Threshold in N$^3$LO QCD". *JHEP* 02 (2015). arXiv: 1411.5301 (cit. on p. 2).

[44] M. C. Kumar, M. K. Mandal, and V. Ravindran. "Associated production of Higgs boson with vector boson at threshold N$^3$LO in QCD". *JHEP* 03 (2015). arXiv: 1412.3357 (cit. on p. 2).

[45] Stefano Catani, Leandro Cieri, Daniel de Florian, Giancarlo Ferrera, and Massimiliano Grazzini. "Threshold resummation at $N^3LL$ accuracy and soft-virtual cross sections at $N^3LO$". *Nucl. Phys.* B888 (2014). arXiv: 1405.4827 (cit. on p. 2).

[46] a. B. Goncharov. "Multiple polylogarithms, cyclotomy and modular complexes". *Mathematical Research Letters* 5.4 (2011). arXiv: 1105.2076 (cit. on pp. 2, 156, 160).

[47] Kuo-Tsai Chen. "Iterated path integrals". *Bulletin of the American Mathematical Society* 83.5 (Sept. 1977) (cit. on pp. 2, 7).

[48] a. B. Goncharov. "Galois symmetries of fundamental groupoids and noncommutative geometry" (Aug. 2002). arXiv: 0208144 (cit. on pp. 2, 20).

[49] a. B. Goncharov, M. Spradlin, C. Vergu, and a. Volovich. "Classical polylogarithms for amplitudes and wilson loops". *Physical Review Letters* 105.15 (Oct. 2010). arXiv: 1006.5703 (cit. on pp. 2, 7, 23).

[50] Francis Brown. "Iterated integrals in quantum field theory". 2009, pp. 1–40 (cit. on pp. 2, 7, 12, 15, 16).

[51] Francis Brown. "On the decomposition of motivic multiple zeta values" (Feb. 2011). arXiv: 1102.1310 (cit. on pp. 2, 26).

[52] Francis Brown. "Single-valued periods and multiple zeta values" (Sept. 2013). arXiv: 1309.5309 (cit. on pp. 2, 12).

[53] Erik Panzer. "On hyperlogarithms and Feynman integrals with divergences and many scales". *Journal of High Energy Physics* 2014.3 (Mar. 2014). arXiv: 1401.4361 (cit. on pp. 2, 27).

[54] Marcus Spradlin and Anastasia Volovich. "Symbols of One-Loop Integrals From Mixed Tate Motives". *Journal of High Energy Physics* 2011.11 (Nov. 2011). arXiv: 1105.2024 (cit. on pp. 2, 7).

[55] Claude Duhr, Herbert Gangl, and John R. Rhodes. "From polygons and symbols to polylogarithmic functions". *Journal of High Energy Physics* 2012.10 (Oct. 2012). arXiv: 1110.0458 (cit. on pp. 2, 7, 23, 38, 41).

[56] Claude Duhr. "Hopf algebras, coproducts and symbols: An application to Higgs boson amplitudes". *Journal of High Energy Physics* 2012.8 (Aug. 2012). arXiv: 1203.0454 (cit. on pp. 2, 7, 20, 26).

[57] Oliver Schnetz. "Graphical functions and single-valued multiple polylogarithms". *Communications in Number Theory and Physics* 8.4 (2013). arXiv: 1302.6445 (cit. on p. 2).

[58] Jens Vollinga and Stefan Weinzierl. "Numerical evaluation of multiple polylogarithms". *Computer Physics Communications* 167.3 (May 2005). arXiv: 0410259 (cit. on p. 2).

[59] Jakob Ablinger, Johannes Blümlein, and Carsten Schneider. "Harmonic sums and polylogarithms generated by cyclotomic polynomials". *Journal of Mathematical Physics* 52.10 (May 2011). arXiv: 1105.6063 (cit. on pp. 2, 7).

[60] J. Broedel, O. Schlotterer, and S. Stieberger. "Polylogarithms, multiple zeta values and superstring amplitudes". *Fortschritte der Physik* 61.9 (Sept. 2013). arXiv: 1205.1516 (cit. on pp. 2, 12).

[61] Henrik Johansson, David a. Kosower, Kasper J. Larsen, and Mads Søgaard. "Cross-order integral relations from maximal cuts". *Physical Review D* 92.2 (July 2015) (cit. on p. 2).

[62] J. K. Golden, a. B. Goncharov, M. Spradlin, C. Vergu, and a. Volovich. "Motivic amplitudes and cluster coordinates". *Journal of High Energy Physics* 2014.1 (Jan. 2014). arXiv: 1305.1617 (cit. on pp. 3, 7).

[63] John Golden, Mf Paulos, Marcus Spradlin, and Anastasia Volovich. "Cluster Polylogarithms for Scattering Amplitudes". *arXiv preprint arXiv: ...* 47.47 (Nov. 2014). arXiv: 1401.6446 (cit. on pp. 3, 7).

[64] Daniel Parker, Adam Scherlis, Marcus Spradlin, and Anastasia Volovich. "Hedgehog Bases for $A_n$ Cluster Polylogarithms and An Application to Six-Point Amplitudes" (2015) (cit. on pp. 3, 7).

[65] J. M. Drummond, G. Papathanasiou, and M. Spradlin. "A symbol of uniqueness: the cluster bootstrap for the 3-loop MHV heptagon". *Journal of High Energy Physics* 2015.3 (Mar. 2015) (cit. on pp. 3, 7, 24).

[66] Lance J. Dixon, James M. Drummond, Matt Von Hippel, and Jeffrey Pennington. "Hexagon functions and the three-loop remainder function". *Journal of High Energy Physics* 2013.12 (Dec. 2013). arXiv: 1308.2276 (cit. on pp. 3, 7, 24).

[67] Lance J. Dixon and Matt von Hippel. "Bootstrapping an NMHV amplitude through three loops". *Journal of High Energy Physics* 2014.10 (Oct. 2014) (cit. on pp. 3, 7, 24).

[68] Lance J. Dixon, Claude Duhr, and Jeffrey Pennington. "Single-valued harmonic polylogarithms and the multi-Regge limit". *Journal of High Energy Physics* 2012.10 (Oct. 2012). arXiv: 1207.0186 (cit. on pp. 3, 7).

[69] Federico Chavez and Claude Duhr. "Three-mass triangle integrals and single-valued polylogarithms". *Journal of High Energy Physics* 2012.11 (Nov. 2012). arXiv: 1209.2722 (cit. on pp. 3, 7, 43).

[70] Vittorio Del Duca, Lance J. Dixon, Claude Duhr, and Jeffrey Pennington. "The BFKL equation, mueller-navelet jets and single-valued harmonic polylogarithms". *Journal of High Energy Physics* 2014.2 (Feb. 2014). arXiv: 1309.6647 (cit. on pp. 3, 7).

[71] Samuel Abreu, Ruth Britto, Claude Duhr, and Einan Gardi. "From multiple unitarity cuts to the coproduct of Feynman integrals". *arXiv* 2014.10 (Oct. 2014). arXiv: 1401.3546 (cit. on pp. 3, 7).

[72] Lance J. Dixon, James M. Drummond, Claude Duhr, and Jeffrey Pennington. "The four-loop remainder function and multi-Regge behavior at NNLLA in planar N = 4 super-Yang-Mills theory". *Journal of High Energy Physics* 2014.6 (June 2014). arXiv: 1402.3300 (cit. on pp. 3, 7, 24).

[73] Lance J. Dixon, James M. Drummond, Claude Duhr, Matt von Hippel, and Jeffrey Pennington. "Bootstrapping six-gluon scattering in planar N=4 super-Yang-Mills theory". *Proceedings, 12th DESY Workshop on Elementary Particle Physics: Loops and Legs in Quantum Field Theory (LL2014)* LL2014 (2014) (cit. on pp. 3, 24).

[74] Johannes M. Henn, Alexander V. Smirnov, and Vladimir A. Smirnov. "Evaluating single-scale and/or non-planar diagrams by differential equations". *JHEP* 03 (2014). arXiv: 1312.2588 (cit. on pp. 3, 171, 174).

[75] Johannes M. Henn. "Lectures on differential equations for Feynman integrals". *J. Phys.* A48 (2015). arXiv: 1412.2296 (cit. on p. 3).

[76] Mario Argeri, Stefano Di Vita, Pierpaolo Mastrolia, Edoardo Mirabella, Johannes Schlenk, Ulrich Schubert, and Lorenzo Tancredi. "Magnus and Dyson Series for Master Integrals". *JHEP* 03 (2014). arXiv: 1401.2979 (cit. on pp. 3, 53, 69, 174).

[77] Johannes M. Henn. "Multiloop integrals in dimensional regularization made simple". *Phys. Rev. Lett.* 110 (2013). arXiv: 1304.1806 (cit. on pp. 3, 53, 68, 69, 173, 174).

[78] Ettore Remiddi and Lorenzo Tancredi. "Schouten identities for Feynman graph amplitudes; The Master Integrals for the two-loop massive sunrise graph". *Nucl. Phys.* B880 (2014). arXiv: 1311.3342 (cit. on pp. 3, 53).

[79] A.V. Kotikov. "Differential equation method. The calculation of N-point Feynman diagrams". *Physics Letters B* 267.1 (1991) (cit. on p. 3).

[80] Ettore Remiddi. "Differential equations for Feynman graph amplitudes". *Nuovo Cim.* A110 (1997). arXiv: hep-th/9711188 (cit. on p. 3).

[81] T. Gehrmann and E. Remiddi. "Differential equations for two loop four point functions". *Nucl. Phys.* B580 (2000). arXiv: hep-ph/9912329 (cit. on pp. 3, 72, 106, 154, 156, 171, 173, 174).

[82] T. Gehrmann and E. Remiddi. "Using differential equations to compute two loop box integrals". *Nucl. Phys. Proc. Suppl.* 89 (2000). arXiv: hep-ph/0005232 (cit. on p. 3).

[83] Charalampos Anastasiou and Kirill Melnikov. “Higgs boson production at hadron colliders in NNLO QCD”. *Nucl. Phys.* B646 (2002). arXiv: `hep-ph/0207004` (cit. on pp. 3, 5, 55, 56, 106, 108–110, 141, 150, 154, 162, 183).

[84] Charalampos Anastasiou, Lance J. Dixon, Kirill Melnikov, and Frank Petriello. “High precision QCD at hadron colliders: Electroweak gauge boson rapidity distributions at NNLO”. *Phys. Rev.* D69 (2004). arXiv: `hep-ph/0312266` (cit. on pp. 3, 56, 106, 150, 170).

[85] Thomas Gehrmann, Lorenzo Tancredi, and Erich Weihs. “Two-loop QCD helicity amplitudes for $gg \to Zg$ and $gg \to Z\gamma$”. *JHEP* 1304 (2013). arXiv: `1302.2630` (cit. on p. 3).

[86] Thomas Gehrmann, Lorenzo Tancredi, and Erich Weihs. “Two-loop master integrals for $q\bar{q} \to VV$: the planar topologies”. *JHEP* 1308 (2013). arXiv: `1306.6344` (cit. on pp. 3, 174).

[87] Thomas Gehrmann, Andreas von Manteuffel, Lorenzo Tancredi, and Erich Weihs. “The two-loop master integrals for $q\bar{q} \to VV$”. *JHEP* 06 (2014). arXiv: `1404.4853` (cit. on p. 3).

[88] F. Cascioli, T. Gehrmann, M. Grazzini, S. Kallweit, P. Maierhöfer, A. von Manteuffel, S. Pozzorini, D. Rathlev, L. Tancredi, and E. Weihs. “ZZ production at hadron colliders in NNLO QCD”. *Phys. Lett.* B735 (2014). arXiv: `1405.2219` (cit. on p. 3).

[89] Thomas Gehrmann, Andreas von Manteuffel, and Lorenzo Tancredi. “The two-loop helicity amplitudes for $q\bar{q}' \to V\_1V\_2 \to 4$ leptons” (2015). arXiv: `1503.04812` (cit. on p. 3).

[90] Andreas von Manteuffel and Lorenzo Tancredi. “The two-loop helicity amplitudes for $gg \to V\_1V\_2 \to 4$ leptons”. *JHEP* 06 (2015). arXiv: `1503.08835` (cit. on p. 3).

[91] Johannes M. Henn, Alexander V. Smirnov, and Vladimir A. Smirnov. “Analytic results for planar three-loop four-point integrals from a Knizhnik-Zamolodchikov equation”. *JHEP* 1307 (2013). arXiv: `1306.2799` (cit. on p. 3).

[92] Johannes M. Henn and Vladimir A. Smirnov. “Analytic results for two-loop master integrals for Bhabha scattering I”. *JHEP* 1311 (2013). arXiv: `1307.4083` (cit. on p. 3).

[93] Johannes M. Henn, Kirill Melnikov, and Vladimir A. Smirnov. “Two-loop planar master integrals for the production of off-shell vector bosons in hadron collisions”. *JHEP* 05 (2014). arXiv: `1402.7078` (cit. on p. 3).

[94] Fabrizio Caola, Johannes M. Henn, Kirill Melnikov, and Vladimir A. Smirnov. “Non-planar master integrals for the production of two off-shell vector bosons in collisions of massless partons”. *JHEP* 09 (2014). arXiv: `1404.5590` (cit. on p. 3).

[95] Fabrizio Caola, Johannes M. Henn, Kirill Melnikov, Alexander V. Smirnov, and Vladimir A. Smirnov. "Two-loop helicity amplitudes for the production of two off-shell electroweak bosons in quark-antiquark collisions". *JHEP* 11 (2014). arXiv: 1408.6409 (cit. on p. 3).

[96] Fabrizio Caola, Johannes M. Henn, Kirill Melnikov, Alexander V. Smirnov, and Vladimir A. Smirnov. "Two-loop helicity amplitudes for the production of two off-shell electroweak bosons in gluon fusion". *JHEP* 06 (2015). arXiv: 1503.08759 (cit. on p. 3).

[97] Mikhail A. Shifman, A. I. Vainshtein, M. B. Voloshin, and Valentin I. Zakharov. "Low-Energy Theorems for Higgs Boson Couplings to Photons". *Sov. J. Nucl. Phys.* 30 (1979). [Yad. Fiz.30,1368(1979)] (cit. on p. 4).

[98] S. Dawson. "Radiative corrections to Higgs boson production". *Nucl. Phys.* B359 (1991) (cit. on pp. 4, 5, 141, 183, 191).

[99] K. G. Chetyrkin, Bernd A. Kniehl, and M. Steinhauser. "Decoupling relations to O (alpha-s**3) and their connection to low-energy theorems". *Nucl. Phys.* B510 (1998). arXiv: hep-ph/9708255 (cit. on p. 4).

[100] Y. Schroder and M. Steinhauser. "Four-loop decoupling relations for the strong coupling". *JHEP* 01 (2006). arXiv: hep-ph/0512058 (cit. on pp. 4, 119).

[101] K. G. Chetyrkin, Johann H. Kuhn, and Christian Sturm. "QCD decoupling at four loops". *Nucl. Phys.* B744 (2006). arXiv: hep-ph/0512060 (cit. on pp. 4, 119).

[102] U. Aglietti, R. Bonciani, G. Degrassi, and A. Vicini. "Two loop light fermion contribution to Higgs production and decays". *Phys. Lett.* B595 (2004). arXiv: hep-ph/0404071 (cit. on pp. 4, 190).

[103] Stefano Actis, Giampiero Passarino, Christian Sturm, and Sandro Uccirati. "NLO Electroweak Corrections to Higgs Boson Production at Hadron Colliders". *Phys. Lett.* B670 (2008). arXiv: 0809.1301 (cit. on pp. 4, 190).

[104] Stefano Actis, Giampiero Passarino, Christian Sturm, and Sandro Uccirati. "NNLO Computational Techniques: The Cases H $\to$ gamma gamma and H $\to$ g g". *Nucl. Phys.* B811 (2009). arXiv: 0809.3667 (cit. on pp. 4, 190).

[105] Charalampos Anastasiou, Radja Boughezal, and Frank Petriello. "Mixed QCD-electroweak corrections to Higgs boson production in gluon fusion". *JHEP* 04 (2009). arXiv: 0811.3458 (cit. on pp. 4, 190).

[106] Robert V. Harlander and Kemal J. Ozeren. "Finite top mass effects for hadronic Higgs production at next-to-next-to-leading order". *JHEP* 11 (2009). arXiv: 0909.3420 (cit. on pp. 4, 191).

[107] Alexey Pak, Mikhail Rogal, and Matthias Steinhauser. "Finite top quark mass effects in NNLO Higgs boson production at LHC". *JHEP* 02 (2010). arXiv: 0911.4662 (cit. on pp. 4, 191).

[108] A. Djouadi, M. Spira, and P. M. Zerwas. "Production of Higgs bosons in proton colliders: QCD corrections". *Phys. Lett.* B264 (1991) (cit. on pp. 5, 141, 183, 191).

[109] M. Spira, A. Djouadi, D. Graudenz, and P. M. Zerwas. "Higgs boson production at the LHC". *Nucl. Phys.* B453 (1995). arXiv: hep-ph/9504378 (cit. on pp. 5, 141, 183, 191).

[110] Robert Harlander and Philipp Kant. "Higgs production and decay: Analytic results at next-to-leading order QCD". *JHEP* 12 (2005). arXiv: hep-ph/0509189 (cit. on pp. 5, 183, 191).

[111] U. Aglietti, R. Bonciani, G. Degrassi, and A. Vicini. "Analytic Results for Virtual QCD Corrections to Higgs Production and Decay". *JHEP* 01 (2007). arXiv: hep-ph/0611266 (cit. on pp. 5, 183, 191).

[112] R. Bonciani, Giuseppe Degrassi, and A. Vicini. "Scalar particle contribution to Higgs production via gluon fusion at NLO". *JHEP* 11 (2007). arXiv: 0709.4227 (cit. on pp. 5, 183, 191).

[113] Charalampos Anastasiou, Stefan Beerli, Stefan Bucherer, Alejandro Daleo, and Zoltan Kunszt. "Two-loop amplitudes and master integrals for the production of a Higgs boson via a massive quark and a scalar-quark loop". *JHEP* 01 (2007). arXiv: hep-ph/0611236 (cit. on pp. 5, 183, 191).

[114] Stefano Catani, Daniel de Florian, and Massimiliano Grazzini. "Higgs production in hadron collisions: Soft and virtual QCD corrections at NNLO". *JHEP* 05 (2001). arXiv: hep-ph/0102227 (cit. on p. 5).

[115] Robert V. Harlander and William B. Kilgore. "Next-to-next-to-leading order Higgs production at hadron colliders". *Phys. Rev. Lett.* 88 (2002). arXiv: hep-ph/0201206 (cit. on pp. 5, 141, 183).

[116] V. Ravindran, J. Smith, and W. L. van Neerven. "NNLO corrections to the total cross section for Higgs boson production in hadron hadron collisions". *Nucl. Phys.* B665 (2003). arXiv: hep-ph/0302135 (cit. on pp. 5, 141, 184).

[117] E. Remiddi and J. a. M. Vermaseren. "Harmonic Polylogarithms". *International Journal of Modern Physics A* 15.05 (Feb. 1999). arXiv: 9905237 (cit. on pp. 7, 12).

[118] T. Gehrmann and E. Remiddi. "Two loop master integrals for gamma* —> 3 jets: The Planar topologies". *Nucl. Phys.* B601 (2001). arXiv: hep-ph/0008287 (cit. on pp. 7, 171, 173, 174).

[119] Jianqiang Zhao. "Multiple Polylogarithms, Multiple Harmonic Sums and Multiple Zeta Values". 2013 (cit. on pp. 7, 12).

[120] Erik Panzer. "Feynman integrals and hyperlogarithms". PhD thesis. Humboldt-Universitaet zu Berlin, 2014 (cit. on pp. 7, 15, 16, 27).

[121] J. Broedel, O. Schlotterer, and S. Stieberger. "Polylogarithms, multiple zeta values and superstring amplitudes". *Fortschritte der Physik* 61.9 (Nov. 2013). arXiv: `1205.1516` (cit. on p. 12).

[122] S Stieberger. "Closed superstring amplitudes, single-valued multiple zeta values and the Deligne associator". *Journal of Physics A: Mathematical and Theoretical* 47.15 (Apr. 2014) (cit. on p. 12).

[123] R. Barbieri, J. a. Mignaco, and E. Remiddi. "Electron form factors up to fourth order. - II". *Il Nuovo Cimento A Series 11* 11.4 (Oct. 1972) (cit. on p. 12).

[124] R. Barbieri, J. a. Mignaco, and E. Remiddi. "Electron form factors up to fourth order. - I". *Il Nuovo Cimento A Series 11* 11.4 (Oct. 1972) (cit. on p. 12).

[125] J. M. Borwein, D. J. Broadhurst, and J. Kamnitzer. "Central Binomial Sums, Multiple Clausen Values and Zeta Values" (Apr. 2000). arXiv: `0004153` (cit. on p. 12).

[126] J. Blümlein, D. J. Broadhurst, and J. a M Vermaseren. "The Multiple Zeta Value data mine". *Computer Physics Communications* 181.3 (Mar. 2010). arXiv: `0907.2557` (cit. on p. 12).

[127] Jean Pierre Duval. "Factorizing words over an ordered alphabet". *Journal of Algorithms* 4.4 (1983) (cit. on p. 16).

[128] Wadim Valentinovich Zudilin. *Algebraic relations for multiple zeta values.* 2003 (cit. on p. 17).

[129] Michel Waldschmidt. "Multiple polylogarithms: An introduction". *Number theory and discrete mathematics* (2002) (cit. on p. 17).

[130] Michael E. Hoffman. "Quasi-shuffle products" (July 1999). arXiv: `9907173` (cit. on p. 17).

[131] David H Bailey and Helaman RP Ferguson. "Numerical results on relations between fundamental constants using a new algorithm". *Mathematics of Computation* 53.188 (1989) (cit. on pp. 28, 35).

[132] T. Gehrmann and E. Remiddi. "Numerical evaluation of harmonic polylogarithms". *Comput. Phys. Commun.* 141 (2001). arXiv: `hep-ph/0107173` (cit. on p. 35).

[133] T. Gehrmann and E. Remiddi. "Numerical evaluation of two-dimensional harmonic polylogarithms". *Comput. Phys. Commun.* 144 (2002). arXiv: `hep-ph/0111255` (cit. on p. 35).

[134] D Maitre. "HPL, a mathematica implementation of the harmonic polylogarithms". *Comput. Phys. Commun.* 174 (2006). arXiv: `hep-ph/0507152` (cit. on p. 35).

[135] Daniel Maitre. "Extension of HPL to complex arguments". *Comput. Phys. Commun.* 183 (2012). arXiv: hep-ph/0703052 (cit. on p. 35).

[136] Jens Vollinga and Stefan Weinzierl. "Numerical evaluation of multiple polylogarithms". *Comput. Phys. Commun.* 167 (2005). arXiv: hep-ph/0410259 (cit. on p. 35).

[137] Christian W. Bauer, Alexander Frink, and Richard Kreckel. "Introduction to the GiNaC framework for symbolic computation within the C++ programming language". *J. Symb. Comput.* 33 (2000). arXiv: cs/0004015 (cit. on pp. 35, 120, 151).

[138] Stephan Buehler and Claude Duhr. "CHAPLIN - Complex Harmonic Polylogarithms in Fortran". *Computer Physics Communication* 185 (2014). arXiv: 1106.5739 (cit. on p. 35).

[139] Francis Brown. "The Massless higher-loop two-point function". *Commun. Math. Phys.* 287 (2009). arXiv: 0804.1660 (cit. on pp. 43, 45).

[140] Vittorio Del Duca, Claude Duhr, E. W. Nigel Glover, and Vladimir A. Smirnov. "The One-loop pentagon to higher orders in epsilon". *JHEP* 01 (2010). arXiv: 0905.0097 (cit. on p. 43).

[141] Vittorio Del Duca, Claude Duhr, and Vladimir A. Smirnov. "The Two-Loop Hexagon Wilson Loop in N = 4 SYM". *JHEP* 05 (2010). arXiv: 1003.1702 (cit. on p. 43).

[142] Jakob Ablinger, Johannes Blumlein, Alexander Hasselhuhn, Sebastian Klein, Carsten Schneider, and Fabian Wissbrock. "Massive 3-loop Ladder Diagrams for Quarkonic Local Operator Matrix Elements". *Nucl. Phys.* B864 (2012). arXiv: 1206.2252 (cit. on p. 43).

[143] Christian Bogner and Francis Brown. "Symbolic integration and multiple polylogarithms" (2012). [PoSLL2012,053(2012)]. arXiv: 1209.6524 (cit. on p. 43).

[144] Erik Panzer. "Algorithms for the symbolic integration of hyperlogarithms with applications to Feynman integrals". *Computer Physics Communications* 188 (Mar. 2014). arXiv: 1403.3385 (cit. on p. 43).

[145] Claude Duhr, Herbert Gangl, and John R. Rhodes. "From polygons and symbols to polylogarithmic functions". *JHEP* 10 (2012). arXiv: 1110.0458 (cit. on p. 47).

[146] S. Laporta. "High precision calculation of multiloop Feynman integrals by difference equations". *Int. J. Mod. Phys.* A15 (2000). arXiv: hep-ph/0102033 (cit. on pp. 50, 53, 106, 120, 145, 148, 151, 170).

[147] F. V. Tkachov. "A Theorem on Analytical Calculability of Four Loop Renormalization Group Functions". *Phys. Lett.* B100 (1981) (cit. on pp. 50, 53, 106, 150).

[148] K. G. Chetyrkin and F. V. Tkachov. “Integration by Parts: The Algorithm to Calculate beta Functions in 4 Loops”. *Nucl. Phys.* B192 (1981) (cit. on pp. 50, 106, 150).

[149] O. V. Tarasov. “Connection between Feynman integrals having different values of the space-time dimension”. *Phys. Rev.* D54 (1996). arXiv: hep-th/9606018 (cit. on pp. 50, 101).

[150] Charalampos Anastasiou and Achilleas Lazopoulos. “Automatic integral reduction for higher order perturbative calculations”. *JHEP* 07 (2004). arXiv: hep-ph/0404258 (cit. on pp. 53, 120, 145, 148, 151).

[151] Alexander V. Smirnov. “FIRE5: a C++ implementation of Feynman Integral REduction”. *Comput. Phys. Commun.* 189 (2014). arXiv: 1408.2372 (cit. on p. 53).

[152] A. von Manteuffel and C. Studerus. “Reduze 2 - Distributed Feynman Integral Reduction” (2012). arXiv: 1201.4330 (cit. on p. 53).

[153] K.G. Chetyrkin and F.V. Tkachov. “Integration by parts: The algorithm to calculate $\beta$-functions in 4 loops”. *Nuclear Physics B* 192.1 (1981) (cit. on p. 53).

[154] R. E. Cutkosky. “Singularities and discontinuities of Feynman amplitudes”. *J. Math. Phys.* 1 (1960) (cit. on p. 55).

[155] Charalampos Anastasiou, Lance J. Dixon, Kirill Melnikov, and Frank Petriello. “Dilepton rapidity distribution in the Drell-Yan process at NNLO in QCD”. *Phys. Rev. Lett.* 91 (2003). arXiv: hep-ph/0306192 (cit. on pp. 56, 106, 150, 170).

[156] Charalampos Anastasiou and Kirill Melnikov. “Pseudoscalar Higgs boson production at hadron colliders in NNLO QCD”. *Phys. Rev.* D67 (2003). arXiv: hep-ph/0208115 (cit. on pp. 56, 106).

[157] Charalampos Anastasiou, Lance J. Dixon, and Kirill Melnikov. “NLO Higgs boson rapidity distributions at hadron colliders”. *Nucl. Phys. Proc. Suppl.* 116 (2003). [,193(2002)]. arXiv: hep-ph/0211141 (cit. on pp. 56, 106, 150, 170).

[158] Roman N. Lee. “Reducing differential equations for multiloop master integrals”. *JHEP* 04 (2015). arXiv: 1411.0911 (cit. on pp. 69, 174).

[159] Christian Bogner and Stefan Weinzierl. “Feynman graph polynomials”. *Int.J. Mod. Phys.* A25 (2010). arXiv: 1002.3458 (cit. on pp. 74, 75).

[160] Vladimir A. Smirnov. “Analytic tools for Feynman integrals”. *Springer Tracts Mod.Phys.* 250 (2012) (cit. on p. 75).

[161] Christian Bogner and Stefan Weinzierl. “Periods and Feynman integrals”. *J. Math. Phys.* 50 (2009). arXiv: 0711.4863 (cit. on p. 75).

[162] D. A. Kosower. *barnesroutines*. https://mbtools.hepforge.org/. 2007 (cit. on pp. 85, 125).

[163] T. Huber and Daniel Maitre. "HypExp: A Mathematica package for expanding hypergeometric functions around integer-valued parameters". *Comput. Phys. Commun.* 175 (2006). arXiv: hep-ph/0507094 (cit. on pp. 88, 120, 121).

[164] J. B. Tausk. "Nonplanar massless two loop Feynman diagrams with four on-shell legs". *Phys. Lett.* B469 (1999). arXiv: hep-ph/9909506 (cit. on p. 89).

[165] Vladimir A. Smirnov. "Evaluating Feynman integrals". *Springer Tracts Mod. Phys.* 211 (2004) (cit. on p. 89).

[166] Charalampos Anastasiou and Alejandro Daleo. "Numerical evaluation of loop integrals". *JHEP* 10 (2006). arXiv: hep-ph/0511176 (cit. on p. 89).

[167] M. Czakon. "Automatized analytic continuation of Mellin-Barnes integrals". *Comput. Phys. Commun.* 175 (2006). arXiv: hep-ph/0511200 (cit. on pp. 89, 104, 125, 181).

[168] A. V. Smirnov and V. A. Smirnov. "On the Resolution of Singularities of Multiple Mellin-Barnes Integrals". *Eur. Phys. J.* C62 (2009). arXiv: 0901.0386 (cit. on pp. 89, 125, 181).

[169] J. M. Borwein, D. M. Bradley, and David J. Broadhurst. "Evaluations of K fold Euler / Zagier sums: A Compendium of results for arbitrary k". *Submitted to: Electron. J. Combin.* (1996). arXiv: hep-th/9611004 (cit. on p. 91).

[170] J. A. M. Vermaseren. "Harmonic sums, Mellin transforms and integrals". *Int. J. Mod. Phys.* A14 (1999). arXiv: hep-ph/9806280 (cit. on pp. 91, 125, 181).

[171] Gabor Somogyi. "Angular integrals in d dimensions". *J. Math. Phys.* 52 (2011). arXiv: 1101.3557 (cit. on pp. 99, 101).

[172] W. L. van Neerven. "Dimensional Regularization of Mass and Infrared Singularities in Two Loop On-shell Vertex Functions". *Nucl. Phys.* B268 (1986) (cit. on p. 100).

[173] Vladimir A. Smirnov and O. L. Veretin. "Analytical results for dimensionally regularized massless on-shell double boxes with arbitrary indices and numerators". *Nucl. Phys.* B566 (2000). arXiv: hep-ph/9907385 (cit. on p. 101).

[174] C. Anastasiou, E. W. Nigel Glover, and C. Oleari. "The two loop scalar and tensor pentabox graph with lightlike legs". *Nucl. Phys.* B575 (2000). [Erratum: Nucl. Phys.B585,763(2000)]. arXiv: hep-ph/9912251 (cit. on pp. 101, 145).

[175] C. Anastasiou, T. Gehrmann, C. Oleari, E. Remiddi, and J. B. Tausk. "The Tensor reduction and master integrals of the two loop massless crossed box with lightlike legs". *Nucl. Phys.* B580 (2000). arXiv: hep-ph/0003261 (cit. on pp. 101, 145).

[176] C. Anastasiou, J. B. Tausk, and M. E. Tejeda-Yeomans. "The On-shell massless planar double box diagram with an irreducible numerator". *Nucl. Phys. Proc. Suppl.* 89 (2000). arXiv: hep-ph/0005328 (cit. on p. 101).

[177] R. N. Lee. "Space-time dimensionality D as complex variable: Calculating loop integrals using dimensional recurrence relation and analytical properties with respect to D". *Nucl. Phys.* B830 (2010). arXiv: 0911.0252 (cit. on pp. 101, 104).

[178] Roman N. Lee and Vladimir A. Smirnov. "The Dimensional Recurrence and Analyticity Method for Multicomponent Master Integrals: Using Unitarity Cuts to Construct Homogeneous Solutions". *JHEP* 12 (2012). arXiv: 1209.0339 (cit. on p. 102).

[179] Alexey Pak, Mikhail Rogal, and Matthias Steinhauser. "Production of scalar and pseudo-scalar Higgs bosons to next-to-next-to-leading order at hadron colliders". *JHEP* 09 (2011). arXiv: 1107.3391 (cit. on pp. 109, 110).

[180] E. Remiddi and J. A. M. Vermaseren. "Harmonic polylogarithms". *Int. J. Mod. Phys.* A15 (2000). arXiv: hep-ph/9905237 (cit. on p. 110).

[181] Elisabetta Furlan. "Gluon-fusion Higgs production at NNLO for a non-standard Higgs sector". *JHEP* 10 (2011). arXiv: 1106.4024 (cit. on pp. 119, 140, 168).

[182] Stefano Catani and Massimiliano Grazzini. "Infrared factorization of tree level QCD amplitudes at the next-to-next-to-leading order and beyond". *Nucl. Phys.* B570 (2000). arXiv: hep-ph/9908523 (cit. on p. 119).

[183] Paulo Nogueira. "Automatic Feynman graph generation". *J. Comput. Phys.* 105 (1993) (cit. on pp. 119, 145, 170).

[184] J. A. M. Vermaseren. "New features of FORM" (2000). arXiv: math-ph/0010025 (cit. on pp. 120, 145).

[185] Johan Alwall, Michel Herquet, Fabio Maltoni, Olivier Mattelaer, and Tim Stelzer. "MadGraph 5 : Going Beyond". *JHEP* 06 (2011). arXiv: 1106.0522 (cit. on p. 120).

[186] Sven Moch, Peter Uwer, and Stefan Weinzierl. "Nested sums, expansion of transcendental functions and multiscale multiloop integrals". *J. Math. Phys.* 43 (2002). arXiv: hep-ph/0110083 (cit. on pp. 130, 161).

[187] S. Moch and P. Uwer. "XSummer: Transcendental functions and symbolic summation in form". *Comput. Phys. Commun.* 174 (2006). arXiv: math-ph/0508008 (cit. on p. 130).

[188] P. A. Baikov and K. G. Chetyrkin. "Top Quark Mediated Higgs Boson Decay into Hadrons to Order $\alpha\_s^5$". *Phys. Rev. Lett.* 97 (2006). arXiv: hep-ph/0604194 (cit. on pp. 140, 168).

[189] Charalampos Anastasiou, Radja Boughezal, and Elisabetta Furlan. "The NNLO gluon fusion Higgs production cross section with many heavy quarks". *JHEP* 06 (2010). arXiv: 1003.4677 (cit. on pp. 140, 144, 146, 157, 168).

[190] K. G. Chetyrkin, Bernd A. Kniehl, and M. Steinhauser. "Hadronic Higgs decay to order alpha-s**4". *Phys. Rev. Lett.* 79 (1997). arXiv: hep-ph/9705240 (cit. on pp. 140, 168).

[191] Michael Kramer, Eric Laenen, and Michael Spira. "Soft gluon radiation in Higgs boson production at the LHC". *Nucl. Phys.* B511 (1998). arXiv: hep-ph/9611272 (cit. on pp. 140, 168).

[192] D. Graudenz, M. Spira, and P. M. Zerwas. "QCD corrections to Higgs boson production at proton proton colliders". *Phys. Rev. Lett.* 70 (1993) (cit. on pp. 141, 184, 191).

[193] C. Anastasiou, E. W. Nigel Glover, and C. Oleari. "Application of the negative dimension approach to massless scalar box integrals". *Nucl. Phys.* B565 (2000). arXiv: hep-ph/9907523 (cit. on pp. 146, 147, 158).

[194] M. Beneke and Vladimir A. Smirnov. "Asymptotic expansion of Feynman integrals near threshold". *Nucl. Phys.* B522 (1998). arXiv: hep-ph/9711391 (cit. on p. 147).

[195] A. Pak and A. Smirnov. "Geometric approach to asymptotic expansion of Feynman integrals". *Eur. Phys. J.* C71 (2011). arXiv: 1011.4863 (cit. on pp. 147, 172, 176, 179).

[196] Bernd Jantzen. "Foundation and generalization of the expansion by regions". *JHEP* 12 (2011). arXiv: 1111.2589 (cit. on p. 147).

[197] S. Coleman and R. E. Norton. "Singularities in the physical region". *Nuovo Cim.* 38 (1965) (cit. on p. 148).

[198] George F. Sterman. "Mass Divergences in Annihilation Processes. 1. Origin and Nature of Divergences in Cut Vacuum Polarization Diagrams". *Phys. Rev.* D17 (1978) (cit. on p. 148).

[199] A. V. Kotikov. "Differential equations method: New technique for massive Feynman diagrams calculation". *Phys. Lett.* B254 (1991) (cit. on pp. 154, 156).

[200] Tobias Huber and Daniel Maitre. "HypExp 2, Expanding Hypergeometric Functions about Half-Integer Parameters". *Comput. Phys. Commun.* 178 (2008). arXiv: 0708.2443 (cit. on p. 158).

[201] Ye Li and Hua Xing Zhu. "Single soft gluon emission at two loops". *JHEP* 11 (2013). arXiv: 1309.4391 (cit. on pp. 169, 172, 178, 184).

[202] Christian Bauer, Alexander Frink, and Richard Kreckel. "Introduction to the GiNaC Framework for Symbolic Computation within the C++ Programming Language". *Journal of Symbolic Computation* 33.1 (2002) (cit. on p. 170).

[203] Bernd Jantzen, Alexander V. Smirnov, and Vladimir A. Smirnov. "Expansion by regions: revealing potential and Glauber regions automatically". *Eur. Phys. J.* C72 (2012). arXiv: 1206.0546 (cit. on pp. 172, 176, 179).

[204] Maik Höschele, Jens Hoff, and Takahiro Ueda. "Adequate bases of phase space master integrals for gg $\rightarrow$ h at NNLO and beyond". *JHEP* 09 (2014). arXiv: 1407.4049 (cit. on p. 174).

[205] Simon Caron-Huot and Johannes M. Henn. "Iterative structure of finite loop integrals". *JHEP* 06 (2014). arXiv: 1404.2922 (cit. on p. 174).

[206] Johannes Blumlein and Stefan Kurth. "Harmonic sums and Mellin transforms up to two loop order". *Phys. Rev.* D60 (1999). arXiv: hep-ph/9810241 (cit. on p. 181).

[207] Charalampos Anastasiou, Stefan Bucherer, and Zoltan Kunszt. "HPro: A NLO Monte-Carlo for Higgs production via gluon fusion with finite heavy quark masses". *JHEP* 10 (2009). arXiv: 0907.2362 (cit. on pp. 184, 191).

[208] A. D. Martin, W. J. Stirling, R. S. Thorne, and G. Watt. "Parton distributions for the LHC". *Eur. Phys. J.* C63 (2009). arXiv: 0901.0002 (cit. on pp. 186, 189, 190, 193).

[209] F. Hautmann. "Heavy top limit and double logarithmic contributions to Higgs production at m(H)**2 / s much less than 1". *Phys. Lett.* B535 (2002). arXiv: hep-ph/0203140 (cit. on p. 187).

[210] Stefano Catani, Daniel de Florian, Massimiliano Grazzini, and Paolo Nason. "Soft gluon resummation for Higgs boson production at hadron colliders". *JHEP* 07 (2003). arXiv: hep-ph/0306211 (cit. on pp. 193, 194).

[211] George F. Sterman. "Summation of Large Corrections to Short Distance Hadronic cross sections". *Nucl. Phys.* B281 (1987) (cit. on p. 193).

[212] S. Catani and L. Trentadue. "Resummation of the QCD Perturbative Series for Hard Processes". *Nucl. Phys.* B327 (1989) (cit. on p. 193).

[213] S. Catani and L. Trentadue. "Comment on QCD exponentiation at large x". *Nucl. Phys.* B353 (1991) (cit. on p. 193).

[214] Bernhard Mistlberger and Falko Dulat. "Limit setting procedures and theoretical uncertainties in Higgs boson searches" (2012). arXiv: 1204.3851 (cit. on p. 223).

# Curriculum vitae

## Personals

| | |
|---|---|
| Name: | Falko Dulat |
| Date of birth: | June 13, 1987 |
| Nationality: | German |
| Email: | dulatf@itp.phys.ethz.ch |
| Office: | HIT K 21.2<br>Institut für theoretische Physik<br>Wolfgang-Pauli-Strasse 27<br>8093 Zürich<br>Switzerland |

## Education and employment

| | |
|---|---|
| 2016-2018 | **SLAC Stanford**<br>Postdoctoral researcher |
| 2015-2016 | **ETH Zürich**<br>Postdoctoral researcher |
| 2012-2015 | **ETH Zürich**<br>PhD in theoretical particle physics<br>Supervisor: Charalampos Anastasiou<br>The PhD was focused on the calculation and phenomenology of Higgs production at $N^3LO$ in gluon fusion |
| 2010-2012 | **ETH Zürich**<br>MSc in physics, with distinction |
| 2007-2010 | **RWTH Aachen**<br>BSc in physics |
| 1997-2006 | **Silverberg Gymnasium Bedburg**<br>German Abitur |

# Talks

| | |
|---|---|
| 2015 | Invited talk at Amplitudes 2015<br>*Higgs production at three loops in QCD* |
| 2015 | Seminar at DESY Zeuthen<br>*Calculating Higgs production at N3LO* |
| 2015 | Talk at Phenomenology Symposium 2015<br>*The Higgs cross section at N3LO* |
| 2015 | Invited talk at HiggsTools 2015<br>*The Higgs cross section at N3LO* |
| 2015 | Seminar at MPI München<br>*The Higgs cross section at N3LO* |
| 2014 | Seminar at UC Louvain<br>*Calculating the Higgs cross section at N3LO beyond threshold* |
| 2014 | Talk at HPL2 2014<br>*Calculating the double-virtual real corrections to Higgs production at N3LO* |
| 2014 | Loopfest 2014<br>*The Higgs cross section at N3LO* |
| 2014 | Seminar at Fermilab<br>*Higgs production at N3LO* |
| 2014 | Invited talk at Recontres de Blois 2014<br>*The Higgs cross section at N3LO* |
| 2013 | Talk at Loopfest 2013<br>*Soft triple-real radiation for Higgs production at N3LO* |

# Schools and workshops

| | |
|---|---|
| 2015 | Amplitudes, Motives and Beyond, MITP |
| 2014 | Prospects and Precision at the LHC, Galileo Galilei Institute |
| 2013 | School of analyic computing in theoretical high-energy physics, Atrani |
| 2013 | Prospects in theoretical physics: LHC physics, IAS |
| 2013 | LMS symposium: Polylogarithms as bridge between number theory and particle physics |
| 2012 | 69th scottish universities summer school: LHC physics |

# Publications

- Charalampos Anastasiou, Claude Duhr, Falko Dulat, and Bernhard Mistlberger. "Soft triple-real radiation for Higgs production at N3LO". *JHEP* 1307 (2013)
- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Franz Herzog, and Bernhard Mistlberger. "Real-virtual contributions to the inclusive Higgs cross section at $N^3LO$". *JHEP* 12 (2013)
- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Thomas Gehrmann, Franz Herzog, and Bernhard Mistlberger. "Higgs boson gluon–fusion production at threshold in $\mathrm{N}^3$LO QCD". *Phys. Lett.* B737 (2014)
- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Thomas Gehrmann, Franz Herzog, and Bernhard Mistlberger. "Higgs boson gluon-fusion production beyond threshold in $\mathrm{N}^3$LO QCD". *JHEP* 03 (2015)
- Falko Dulat and Bernhard Mistlberger. "Real-Virtual-Virtual contributions to the inclusive Higgs cross section at N3LO" (2014)
- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Franz Herzog, and Bernhard Mistlberger. "Higgs Boson Gluon-Fusion Production in QCD at Three Loops". *Phys. Rev. Lett.* 114.21 (2015)
- Charalampos Anastasiou, Claude Duhr, Falko Dulat, Elisabetta Furlan, Franz Herzog, and Bernhard Mistlberger. "Soft Expansion of Double-Real-Virtual Corrections to Higgs Production at $\mathrm{N}^3$LO" (2015)
- Bernhard Mistlberger and Falko Dulat. "Limit setting procedures and theoretical uncertainties in Higgs boson searches" (2012)