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Verallgemeinerungen von Polylogarithmen in der Berechnung von Feynman-Integralen

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Generalizations of polylogarithms in the computation of Feynman integrals

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CHAPTER 1

Introduction

This cumulative thesis is dedicated to the application of generalized polylogarithms in analytic computations of multi-loop Feynman integrals. The following chapters serve as an introduction to the publications [**6, 7, 8, 9, 11, 45, 47**], motivating and summarizing their main results. To provide the reader with all details, these articles are re-printed in the appendix of this thesis.

The main motivation to improve methods for the computation of Feynman integrals is given by the demand of increasingly complex theoretical predictions of observables for the phenomenology at modern particle colliders such as the LHC. In general the increase in the required precision of these predictions implies an increase in both the number of Feynman integrals to be considered as well as the intricacy of the individual integrals.

It is very common for such computations to include two steps: In a first step, the given set of Feynman integrals is expressed in terms of a smaller set of integrals, the so-called master integrals of the problem, by use of integration-by-parts (IBP) relations [**83**]. By use of Baikov's method [**24, 25**], Laporta's algorithm [**137**] or alternative approaches, implemented in efficient computer programs such as [**19, 141, 142, 153, 188, 189, 192, 194**], this step serves for a drastic reduction of the number of integrals to be computed. However, the number of master integrals still may be large in today's research projects. To give just one example, let us refer to the impressive computation of the gluon fusion Higgs boson cross-section at the LHC [**18**] where at N^3LO a set of 1028 master integrals remained after a reduction (see [**17**]). Clearly efficient methods and algorithms are also required for the second step: the computation of the master integrals. Such methods and the underlying mathematics are in the focus of this thesis.

The difficulty of an analytic Feynman integral computation varies strongly from case to case. The loop-number of the Feynman graph and the number of kinematic invariants and particle masses which the function depends on only give a very vague and biased guidance to determine the difficulty of the problem. Let us consider the graphs of fig. 1.0.1 (a) and (b) as examples. In fig. 1.0.1 (a) we indicated the family of mass-less ladder-graphs with four off-shell legs. At the dashed line we may insert further rungs of the ladder up to a desired loop-number. Results for these Feynman integrals are known to arbitrary loop-number [**91**]. The on-shell case is more difficult. Here first results for the two- and three-loop ladders were obtained later in [**190, 191**]. The graph in fig. 1.0.1 (b) is an example for a change in difficulty by assigning masses to the propagators. In the mass-less case, a result for the graph in fig. 1.0.1 (b), even to all orders in the parameter of

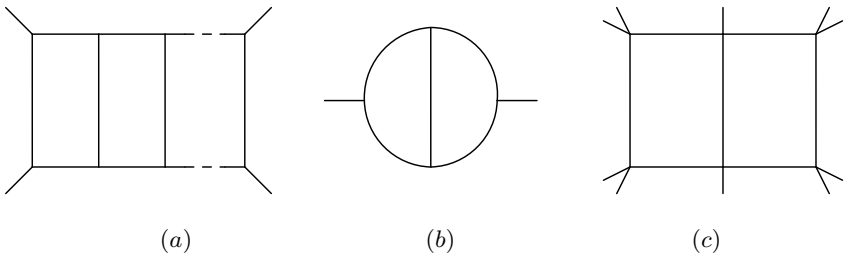


FIGURE 1.0.1. (a) The n-loop four-point ladder-graphs (b) The two-loop two-point 5-propagator-graph (c) A ten-point double-box

dimensional regularization, is given in **[36]**. However, if all five propagators are massive, a result is unknown so far.

These examples show that apart from the number of loops and legs, our ability to compute a Feynman integral may depend on other properties, sometimes in a quite subtle way. There are Feynman integrals which, even if we assume unlimited computational resources, can not be computed with today's most powerful techniques. We do not have a definite classification which would tell us which integral can be computed with today's methods. In general we have to try. However, there are some very useful criteria to be mentioned below which help to decide, whether certain methods succeed for a given integral.

Some of the most powerful computational approaches rely on the use of particular classes of functions. Obviously these methods will fail for a given Feynman integral if the latter simply can not be expressed in terms of these functions. This leads to the crucial question: *Which classes of functions should we use in our attempts to compute Feynman integrals?* Ideally we would work with a class of functions which is sufficient to express as many Feynman integrals as possible and which has well-understood properties, allowing for the automatization of the computations and the evaluation of the results.

A class of functions with an exceptional success-story in particle physics computations are polylogarithms and their generalizations. The classical polylogarithms (see e.g. **[148]**) are defined by

$$\mathrm{Li}_n(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^n}, \ |z| < 1$$

and their multivariate generalizations are the multiple polylogarithms

$$\mathrm{Li}_{n_1,...n_k}(z_1,...,z_k) = \sum_{0<j_1<...<j_k} \frac{z_1^{j_1}...z_k^{j_k}}{j_1^{n_1}...j_k^{n_k}} \text{ for } |z_i| < 1$$

introduced by Goncharov in **[111, 112]**. The use of these functions is by now standard in the particle physics literature and there are countless examples of Feynman integrals expressed in terms of these. The mentioned ladders in fig. 1.0.1 (a) belong to these examples. Also the result for the mass-less case of fig. 1.0.1 (b) which is expressed in terms of multiple zeta values, can be understood as given by special values of multiple

polylogarithms. However, in the case of the same graph where all propagators are massive, there are strong reasons to assume that the integral can not be expressed in terms of multiple polylogarithms only. We will provide more details on these reasons. Apparently this problem does not just arise in one or a few pathological cases. In fact there seems to be a large family of Feynman integrals, appearing in different physical contexts, which can not be expressed in terms of multiple polylogarithms. In [**29, 184**] this problem is exhibited for massive integrals arising in electroweak physics while also mass-less integrals arising in $\mathcal{N}$=4 super Yang-Mills theory, such as the ten-point on-shell double-box of fig. 1.0.1 (c), are known to admit this problem [**76, 165**].

In this thesis we focus on two methods for the computation of Feynman integrals which both make use of generalized polylogarithms. We will refer to these methods as the method of parametric integration and the method of differential equations. As we will see, both methods make use of the iterated integral structure of generalized polylogarithms. In the case of the classical polylogarithms, this property is reflected in the obvious relation

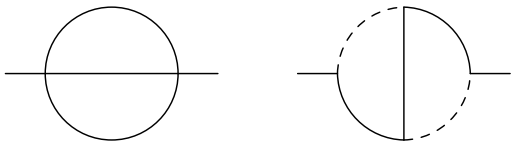
$$\mathrm{Li}_n(z) = \int_0^z \frac{dx}{x} \mathrm{Li}_{n-1}(x) \text{ for } n > 1.$$

The mentioned methods are both widely used in particle physics and their success may serve as a strong reason to rely on generalizations of polylogarithms in Feynman integral computations.

If a Feynman integral can be expressed in terms of multiple polylogarithms, these and other methods may be applied and our good understanding of multiple polylogarithms allows us to automatize computations. On the other hand, in the case of Feynman integrals which apparently can not be expressed in terms of multiple polylogarithms, computational techniques are much further behind. As a crucial step towards automated computations of these cases in the future, we have to find out at first, which classes of functions beyond multiple polylogarithms may be appropriate here. Because of this general situation, the present thesis proceeds in two directions. Both directions improve the use of generalized polylogarithms in Feynman integral computations, but in quite different ways.

The first direction is worked out in our joint work with Brown [**47**] and in [**45**]. Here we assume the case of Feynman integrals which can be expressed in terms of multiple polylogarithms. In [**47**] we present algorithms for certain computations with multiple polylogarithms. These are based on a representation of these functions in terms of an appropriate class of iterated integrals. The algorithms serve for an automatization of the method of parametric integration and may support other approaches as well. In [**45**] we present the program MPL which is an implementation of these algorithms for the computer algebra system Maple [**154**].

The second direction is followed in our joint work with Adams, Schweitzer and Weinzierl [**6, 7, 8, 9, 11**]. Here we focus on the two-loop sunrise graph with three massive propagators, shown in fig. 1.0.2 (a) and on the kite graph with three massive propagators (straight lines) and two mass-less propagators (dashed lines), shown in fig. 1.0.2 (b).



(a) (b)

FIGURE 1.0.2. (a) The two-loop sunrise graph (b) The kite graph

Both of these graphs have been considered in the literature for a long time and it is common knowledge that multiple polylogarithms are not sufficient to express their Feynman integrals. The massive sunrise integral turns out to be a very useful showcase of this general problem. In [**7**] we consider this integral for the case of arbitrary masses in $D = 2$ space-time dimensions and express the result with the help of integrals over elliptic integrals. In [**8**] we present a further result of this integral in terms of a new function, which can be understood as an elliptic generalization of the dilogarithm Li_2. Using the same type of elliptic generalizations of polylogarithms, we present a result for the case of four space-time dimensions in [**9**]. In [**11**] we focus on the case of three equal masses in two dimensions and provide an algorithm to obtain the result in all orders of the parameter ϵ of dimensional regularization. In [**6**] finally, we use the same framework of functions to provide a result for the kite graph to all orders in four dimensions.

The most important point in the latter series of projects is the introduction of a new class of elliptic generalizations of (multiple) polylogarithms. These functions admit an iterated integral structure, and therefore they are very well suited for the method of differential equations, as our computations show. The fact that not only the massive sunrise integral but also the kite integral can be expressed in terms of these functions give rise to the hope that in the future they may serve for a larger class of Feynman integrals which could not be computed so far - possibly including the graphs of fig. 1.0.1 (b) or even the graph of fig. 1.0.1 (c). If these functions continue to be useful in the future, we furthermore may hope that their use will eventually enable the automatization of computations to the level which is already reached for the cases where multiple polylogarithms are sufficient.

This thesis is structured as follows: In chapter 2 we give a brief introduction to well-known aspects of polylogarithms and some of their generalizations which will be required for the understanding of the further material. In chapter 3 we recall basic notions of Feynman integrals including the method of parametric integration and the method of differential equations. In chapter 4 we discuss the class of iterated integrals representing multiple polylogarithms which we use in our joint work with Brown. We review the most important algorithms of this work and of our resulting computer program MPL. In chapter 5 we review our class of elliptic generalizations of polylogarithms and their use in the computations of the sunrise and kite integrals from our work with Adams,

Schweitzer and Weinzierl. In chapter 6 we state our conclusions and point out some open questions to be addressed in future research. The appendix contains reprinted versions of the mentioned publications.

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CHAPTER 2

Classical and multiple polylogarithms

For the later discussion of methods for the computation of Feynman integrals, it is important to be aware of some properties of the functions they rely on. In this chapter we recall basic properties of polylogarithms and of some of their generalizations. In the case of classical and multiple polylogarithms, this material is presented more exhaustively in introductions and reviews such as [**62, 77, 119, 203, 210, 211**]. We also mention some additional developments in the physics literature.

2.1. Definitions and basic properties

Let us begin with a quick detour via two letters of Gottfried Wilhelm Leibniz which may be seen as the historical birthplace of polylogarithms. Near the end of the year 1696 Leibniz writes two letters to Johann Bernoulli including the following passages (see N. 46, p. 176 f. and N.47, p. 179 in [**146**]):

> [...] *Quaeritur summa horum numerorum* $\frac{1}{1}+\frac{1}{4}+\frac{1}{9}+\frac{1}{16}$ *etc. Fingo esse casum specialem hujus:* $\frac{x^2}{1}+\frac{x^3}{4}+\frac{x^4}{9}+\frac{x^5}{16}$ *etc.* $= y$ *cum scilicet fit* $x = 1$. *Quod si ergo semper haberi posset* y, *haberetur et summa quaesita. Ergo et* $\frac{x}{1}+\frac{x^2}{2}+\frac{x^3}{3}+\frac{x^4}{4}$ *etc.* $= \frac{dy}{dx}$ = *log,1-x, seu* $\frac{ddy}{dx} = x^0+x^1+x^2+x^3$ *etc.* $= \frac{1}{1-x}$ *seu* $y = \int\int \overline{\frac{1}{1-x}dxdx}$. [...]

> [...] *Literis ad Te dimissis, mox in mentem venit oportere ut error in illis admissus fuerit. Nam area illa quam aequalem feceram seriei de qua agitur in nita est. Re ergo resumta vidi sic procedendum:* $\frac{1}{1}+\frac{x}{2}+\frac{x^2}{3}+\frac{x^3}{4}$ *etc.* $= dy$. *Unde* $\frac{x}{1}+\frac{x^2}{4}+\frac{x^3}{9}+\frac{x^4}{16}$ *etc.* $= y$. *Ergo* $dy = \frac{\log.\overline{1-x}\,dx}{x}$, *seu* $y = \int \frac{\log.\overline{1-x}}{x}dx$. [...]

In the first sentence, Leibniz expresses his interest in the series today known as

$$\sum_{j=1}^{\infty}\frac{1}{j^2} = \frac{\pi^2}{6}$$

due to Euler [**103**]. Nowadays this series is usually considered as Riemann's zeta function

$$\zeta(n) = \sum_{j=1}^{\infty}\frac{1}{j^n} \tag{2.1.1}$$

evaluated at $n = 2$. Leibniz suggests to consider a function of x which evaluates to this series in the special case ("casum specialem") $x = 1$. In a first attempt, he considers

$\frac{x^2}{1} + \frac{x^3}{4} + \frac{x^4}{9} + \frac{x^5}{16} + ...$ and erroneously claims that the function[1]

$$-\ln(1-x) = \sum_{j=1}^{\infty} \frac{x^j}{j} \tag{2.1.2}$$

is obtained by differentiating this series with respect to x. He derives an integral representation from this false result. Despite this mistake, these are the lines of thought leading to the definition of polylogarithms.

The second excerpt above stems from his next letter to Bernoulli, written a few days later. Here Leibniz corrects his mistake and considers the function

$$y(x) = \sum_{j=1}^{\infty} \frac{x^j}{j^2}. \tag{2.1.3}$$

By differentiation he obtains

$$\frac{dy}{dx} = \frac{-\ln(1-x)}{x}$$

and hence he arrives at an integral which in modern notation reads

$$y(x) = -\int_0^x \frac{dx'}{x'} \ln(1-x').$$

Today the function $y(x)$ in eq. 2.1.3 is known as the dilogarithm denoted $\mathrm{Li}_2(x)$ and some of its properties already pointed out in the above letters will be shared by its generalizations: a definition in terms of a series, a representation as an integral over a closely related function and an interesting special value at $x = 1$.

As a generalization of the dilogarithm, *classical polylogarithms* are defined as

$$\mathrm{Li}_n(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^n} \tag{2.1.4}$$

for $n \in \mathbb{N}$ and a complex variable z with $|z| < 1$. Standard references such as **[148]** discuss these functions at length. Clearly the first two members of this class of functions, $\mathrm{Li}_1(z)$ and $\mathrm{Li}_2(z)$, are the series of eqs. 2.1.2 and 2.1.3 as mentioned in the above letters. Following Leibniz' main idea, one differentiates these series, obtaining the differential equations

$$\frac{d}{dz}\mathrm{Li}_n(z) = \frac{1}{z}\mathrm{Li}_{n-1}(z),\ n \geq 2. \tag{2.1.5}$$

These lead to the integral relations

$$\mathrm{Li}_n(z) = \int_\gamma \frac{dx}{x}\mathrm{Li}_{n-1}(x),\ n \geq 2, \tag{2.1.6}$$

where γ is a smooth path from 0 to z in $\mathbb{C}\setminus\{0,1\}$. As the end-point z of the path is allowed to be outside the unit-circle here, this integral serves for the analytic continuation of the polylogarithms to multivalued functions on $\mathbb{C}\setminus\{0,1\}$. Integrals like this are central to this thesis and will be discussed in more detail in section 2.2.

[1]Notice that Leibniz' notation log.1-x and log,1-x as printed in **[146]** can only mean our $-\ln(1-x)$.

As a further generalization the *multiple polylogarithms in one variable* are defined by

$$\mathrm{Li}_{n_1,...,n_r}(z) = \sum_{0<j_1<...<j_r} \frac{z^{j_r}}{j_1^{n_1}...j_r^{n_r}} \tag{2.1.7}$$

for $n_1, ..., n_r \in \mathbb{N}$ and a complex variable z with $|z| < 1$. They satisfy differential equations

$$\frac{d}{dz}\mathrm{Li}_{n_1,...,n_r}(z) = \begin{cases} \frac{1}{z}\mathrm{Li}_{n_1,...,n_r-1}(z) & \text{for } n_r > 1, \\ \frac{1}{1-z}\mathrm{Li}_{n_1,...,n_{(r-1)}}(z) & \text{for } n_r = 1. \end{cases} \tag{2.1.8}$$

Again, an analytic continuation to $\mathbb{C}\setminus\{0,1\}$ is given by integrals to be discussed below.

Multiple polylogarithms in several variables **[112, 111]** are defined by

$$\mathrm{Li}_{n_1,...,n_r}(z_1, ..., z_r) = \sum_{0<j_1<...<j_r} \frac{z_1^{j_1}...z_r^{j_r}}{j_1^{n_1}...j_r^{n_r}} \tag{2.1.9}$$

for $n_1, ..., n_r \in \mathbb{N}$ and converging where all the complex variables z_i admit $|z_i| < 1$. We will refer to these functions as *multiple polylogarithms* and state explicitly, if we only mean the one-variable case. One main subject of this thesis will be an implementation of the integrals representing the multiple polylogarithms as functions of several variables. As we will see below, these integrals provide an analytic continuation to a certain moduli space, which can be seen as a multi-dimensional generalization of $\mathbb{C}\setminus\{0,1\}$.

We have seen that Leibniz' consideration of the dilogarithm was motivated by interest in the special value $\zeta(2)$ obtained by evaluation at $z = 1$. The above generalizations have meaningful special values as well. The series in eq. 2.1.4 for the classical polylogarithms converges at $z = 1$ for $n > 1$. One obtains

$$\mathrm{Li}_n(z) = \zeta(n),$$

where $\zeta(n)$ is the Riemann zeta function of eq. 2.1.1. The series in eqs. 2.1.7 and 2.1.9 for the multiple polylogarithms converge as well at $z = 1$ and respectively at $z_1 = z_2 = ... = z_r = 1$ if $n_r > 1$. The values at these points are *multiple zeta values* **[209]** defined by

$$\zeta(n_1, ...n_r) = \sum_{0<j_1<...<j_r} \frac{1}{j_1^{n_1}...j_r^{n_r}} \in \mathbb{R}. \tag{2.1.10}$$

Let us consider the multiplication of polylogarithms and multiple polylogarithms using their above series representations. For the product of two classical polylogarithms with $n, m \in \mathbb{N}$ and with $|z| < 1$, $|y| < 1$ we obtain

$$\begin{aligned} \mathrm{Li}_n(z)\mathrm{Li}_m(y) &= \sum_{0<j,k} \frac{z^j y^k}{j^n k^m} \\ &= \sum_{0<j<k} \frac{z^j y^k}{j^n k^m} + \sum_{0<k<j} \frac{z^j y^k}{j^n k^m} + \sum_{0<j} \frac{(zy)^j}{j^{n+m}} \\ &= \mathrm{Li}_{n,m}(z, y) + \mathrm{Li}_{m,n}(y, z) + \mathrm{Li}_{n+m}(zy). \end{aligned}$$

$\underline{n'}$	$\underline{m'}$	$\underline{l}$	$\underline{x}$
(n_1, n_2)	$(m_1, 0)$	$(n_1 + m_1, n_2)$	$(z_1 y_1, z_2)$
(n_1, n_2)	$(0, m_1)$	$(n_1, n_2 + m_1)$	$(z_1, z_2 y_1)$
$(0, n_1, n_2)$	$(m_1, 0, 0)$	(m_1, n_1, n_2)	(y_1, z_1, z_2)
$(n_1, 0, n_2)$	$(0, m_1, 0)$	(n_1, m_1, n_2)	(z_1, y_1, z_2)
$(n_1, n_2, 0)$	$(0, 0, m_1)$	(n_1, n_2, m_1)	(z_1, z_2, y_1)

TABLE 1. Construction of a stuffle product

The concept generalizes to products of multiple polylogarithms as follows (see e.g. **[203]**): For this purpose, us write $\mathrm{Li}_{n_1,...,n_r}(z_1, ..., z_r) = \mathrm{Li}_{\underline{n}}(\underline{z})$ with ordered sets $\underline{n} = (n_1, ..., n_r)$ and $\underline{z} = (z_1, ..., z_r)$. For sets $\underline{n} = (n_1, ..., n_r)$, $\underline{z} = (z_1, ..., z_r)$, $\underline{m} = (m_1, ..., m_s)$, $\underline{y} = (y_1, ..., y_s)$ we have the product

$$\mathrm{Li}_{\underline{n}}(\underline{z})\,\mathrm{Li}_{\underline{m}}(\underline{y}) = \sum_{\underline{l}} \mathrm{Li}_{\underline{l}}(\underline{x}) \tag{2.1.11}$$

where the sum on the right-hand side runs over all possible ordered sets $\underline{l}$ with t elements, $\max(r, s) \leq t \leq r + s$, whose elements are $l_i = n'_i + m'_i$ for $i = 1, ..., t$, where the sets $\underline{n'} = (n'_1, ..., n'_t)$, $\underline{m'} = (m'_1, ..., m'_t)$ both of length t are obtained from $\underline{n}$ and $\underline{m}$ respectively by inserting zeroes, such that all $l_i \neq 0$. In the corresponding term $\mathrm{Li}_{\underline{l}}(\underline{x})$ the arguments $\underline{x}$ are obtained as

$$x_i = \begin{cases} z_j & \text{for } l_i = n_j, \\ y_j & \text{for } l_i = m_j, \\ z_j y_k & \text{for } l_i = n_j + m_k. \end{cases}$$

EXAMPLE. In the case of $\underline{n} = (n_1, n_2)$, $\underline{m} = (m_1)$, $\underline{z} = (z_1, z_2)$, $\underline{y} = (y_1)$ the sum runs through the cases shown in table 1 and we obtain

$$\begin{aligned} \mathrm{Li}_{n_1,n_2}(z_1, z_2)\mathrm{Li}_{m_1}(y_1) &= \mathrm{Li}_{n_1+m_1,n_2}(z_1 y_1, z_2) + \mathrm{Li}_{n_1,n_2+m_1}(z_1, z_2 y_1) \\ &\quad + \mathrm{Li}_{m_1,n_1,n_2}(y_1, z_1, z_2) + \mathrm{Li}_{n_1,m_1,n_2}(z_1, y_1, z_2) + \mathrm{Li}_{n_1,n_2,m_1}(z_1, z_2, y_1). \end{aligned}$$

Note that every $\underline{l}$ preserves the internal ordering of $\underline{n}$ and of $\underline{m}$. This way of multiplying multiple polylogarithms can be formulated with the help of a product of the sets $\underline{n}$ and $\underline{m}$ known as *stuffle* or *quasi-shuffle product*. A recursive definition and properties of the corresponding algebra are given in **[122]**. For our purposes, another product known as the *shuffle product* based on iterated integrals will be more important. Let us now turn to iterated integrals.

2.2. General aspects of iterated integrals

We have seen that Leibniz already knew

$$\mathrm{Li}_2(z) \;=\; -\int_0^z \frac{dx}{x}\ln(1-x).$$

He was also aware of the integral representation of the logarithm, and hence of the formula

$$\mathrm{Li}_2(z) = \int_0^z \frac{dx}{x}\int_0^x \frac{dx'}{1-x'}.$$

The right-hand side of the latter equation is called an iterated integral. Following work of Poincaré and Lappo-Danilevsky, Chen developed a general theory of such integrals. We discuss some aspects of the general theory and then focus on the cases of classical and multiple polylogarithms.

As a general set-up, let us consider a smooth manifold M over a field K and let

$$\gamma : [0,1] \to M$$

be a piecewise smooth path, meaning that this path is the union of finitely many smooth paths. We denote the set of piecewise smooth paths on M by PM. Let $\omega_1, ...\omega_r$ be smooth, K-valued differential 1-forms on M. With respect to the path γ, let the pull-back of these 1-forms to $[0,1]$ be denoted by $\gamma^\star(\omega_i)(t) = f_i(t)dt$.

The *iterated integral* of $\omega_1, ..., \omega_r$ along γ is defined by

$$\begin{aligned}\int_\gamma \omega_1...\omega_r \;&=\; \int_{0\le t_1\le ...\le t_r\le 1} \gamma^\star(\omega_r)(t_1)...\gamma^\star(\omega_1)(t_r) \\ &=\; \int_{0\le t_1\le ...\le t_r\le 1} f_r(t_1)\,dt_1...f_1(t_r)\,dt_r.\end{aligned} \tag{2.2.1}$$

We will use the term *iterated integral* as well for K-linear combinations of such integrals. The case $r = 0$ is the empty integral, defined to be 1. The case $r = 1$ is the ordinary line integral

$$\int_\gamma \omega_1 = \int_0^1 f_1(t_1)\,dt_1.$$

Iterated integrals satisfy the following properties (see **[79, 119, 62]**):

- The iterated integral $\int_\gamma \omega_1...\omega_r$ is independent of the parametrization of the path γ.
- For $\gamma^{-1}(t) = \gamma(1-t)$ being the reversal of the path γ, one has

$$\int_{\gamma^{-1}} \omega_1...\omega_r = (-1)^r \int_\gamma \omega_r...\omega_1. \tag{2.2.2}$$

- The product of two iterated integrals along the same path γ is computed as

$$\int_\gamma \omega_1...\omega_r \cdot \int_\gamma \omega_{r+1}...\omega_{r+s} = \sum_{\sigma\in\Sigma(r,s)} \int_\gamma \omega_{\sigma(1)}...\omega_{\sigma(r+s)} \tag{2.2.3}$$

where $\Sigma(r,s)$ is the set of (r,s)-*shuffles*, defined as

$$\Sigma(r,s) = \{\sigma \in \Sigma(r+s) : \sigma(1) < ... < \sigma(r) \text{ and } \sigma(r+1) < ... < \sigma(r+s)\} \tag{2.2.4}$$

with $\Sigma(n)$ being the symmetric group.

- Let α, $\beta : [0,1] \to M$ be two paths with $\alpha(1) = \beta(0)$, i.e. the end of α coincides with the beginning of β, and let $\alpha\beta$ denote the path composed of these two. Then

$$\int_{\alpha\beta} \omega_1 ... \omega_r = \sum_{i=0}^{r} \int_{\alpha} \omega_1 ... \omega_i \cdot \int_{\beta} \omega_{i+1} ... \omega_r. \tag{2.2.5}$$

It is useful to relate the latter properties to certain constructions on the corresponding sequences of 1-forms. For tensor products of differential 1-forms, let us introduce the bar notation

$$[\omega_1|...|\omega_r] = \omega_1 \otimes ... \otimes \omega_r. \tag{2.2.6}$$

We refer to such tensor products and their K-linear combinations

$$\xi = \sum_{k=0}^{r} \sum_{i_1 ... i_r} c_{i_1 ... i_r} [\omega_{i_1}|...|\omega_{i_k}] \text{ with } c_{i_1 ... i_r} \in K \tag{2.2.7}$$

as *words* up to length r. We will also consider tensor products of such words and the bar notation will help to steer clear of any possible confusion between different levels of tensor products. The concatenation of words $a = [a_1|...|a_k]$, $b = [b_1|...|b_m]$ is denoted by

$$a \sqcup b = [a_1|...|a_k|b_1|...|b_m].$$

The commutative *shuffle product* $a \text{ ш } b$ is recursively defined by

$$a \text{ ш } b = [a_1] \sqcup ([a_2|...|a_k] \text{ ш } b) + [b_1] \sqcup (a \text{ ш } [b_2|...|b_m]).$$

The sum on the right-hand side of eq. 2.2.3 runs through the terms of the shuffle product of $[\omega_1|...|\omega_r] \text{ ш } [\omega_{r+1}|...|\omega_{r+s}]$, so we may re-write eq. 2.2.3 as

$$\int_{\gamma} \omega_1 ... \omega_r \cdot \int_{\gamma} \omega_{r+1} ... \omega_{r+s} = \int_{\gamma} \omega_1 ... \omega_r \text{ ш } \omega_{r+1} ... \omega_{r+s}. \tag{2.2.8}$$

We furthermore define the *de-concatenation co-product* Δ by

$$\Delta[a_1|a_2|...|a_k] = 1 \otimes [a_1|a_2|...|a_k] + [a_1] \otimes [a_2|...|a_k] + ... + [a_1|...|a_k] \otimes 1. \tag{2.2.9}$$

Note that the terms on the right-hand side of eq. 2.2.5 correspond to the terms in $\Delta[\omega_1|...|\omega_r]$. We will make further use of these constructions in chapter 4.

The above properties are true for every iterated integral. In this thesis, we work with classes of iterated integrals which furthermore have the property of being *homotopy invariant* or in other words a *homotopy functional*. Two continuous paths γ_1, γ_2 on M are called *homotopic* (relative to their end-points) if their end-points coincide as $\gamma_1(0) = \gamma_2(0)$ and $\gamma_1(1) = \gamma_2(1)$ and if furthermore there exists a continuous map $\phi : [0,1] \times [0,1] \to M$

such that

$$\phi(0,t) = \gamma_1(t) \text{ and } \phi(1,t) = \gamma_2(t)$$

for all $0 \leq t \leq 1$ and $\phi(s,0) = \gamma_1(0)$, $\phi(s,1) = \gamma_1(1)$ for all $0 \leq s \leq 1$. This defines an equivalence relation on PM and we write $\gamma_1 \sim \gamma_2$ for homotopic paths. A map $F : PM \to K$ is called a homotopy functional or homotopy invariant, if

$$\gamma_1 \sim \gamma_2 \Rightarrow F(\gamma_1) = F(\gamma_2).$$

In other words, for a homotopy invariant iterated integral $\int_{\gamma_1} \omega_1 ... \omega_r$ we have

$$\int_{\gamma_1} \omega_1 ... \omega_r = \int_{\gamma_2} \omega_1 ... \omega_r$$

for every path γ_2 which begins and ends at the same points as γ_1 respectively, and which can be transformed continuously into γ_1.

Not every iterated integral is homotopy invariant. For the case of $r = 1$ one can show with the help of Stokes' theorem and Poincaré's lemma, that $\int_\gamma \omega_1$ is homotopy invariant if and only if ω_1 is closed. For the general case, Chen proved a criterion which can be formulated as follows. Assuming that all differentiations in the following relation exist, we define the operator D acting on words by

(2.2.10)

$$D([\omega_1|...|\omega_r]) = \sum_{j=1}^{r} [\omega_1|...|\omega_{j-1}|d\omega_j|\omega_{j+1}|...|\omega_r] - \sum_{j=1}^{r-1} [\omega_1|...|\omega_{j-1}|\omega_j \wedge \omega_{j+1}|\omega_{j+2}|...|\omega_r].$$

A word ξ as in eq. 2.2.7 is called *integrable* if

(2.2.11)
$$D(\xi) = 0.$$

Chen has proven in **[79]**, that there is an isomorphism between integrable words and homotopy invariant iterated integrals: Consider a word

$$\xi = \sum_{k=0}^{r} \sum_{i_1 ... i_r} c_{i_1 ... i_r} [\omega_{i_1}|...|\omega_{i_k}]$$

and the corresponding iterated integral

$$I = \sum_{k=0}^{r} \sum_{i_1 ... i_r} c_{i_1 ... i_r} \int_\gamma \omega_{i_1} ... \omega_{i_k}$$

along some path $\gamma \in PM$. Then I is homotopy invariant if and only if ξ is integrable. This statement has important implications for our work in **[47, 45]** to be discussed in chapter 4: We will construct a vector space of certain homotopy invariant iterated integrals by constructing their corresponding integrable words. After fixing certain boundary conditions, the isomorphism between integrable words and homotopy invariant iterated integrals will allow us to express all functions of our class by the corresponding word of 1-forms. As a consequence, all our main computations in chapter 4 are manipulations

on words and therefore they are very well suited for the implementation in a computer program as discussed there.

We furthermore note a simple consequence from Chen's work: If we consider words of closed 1-forms of the type $\omega = f(x)dx$ with some rational function f then due to $dx \wedge dx = 0$ every word in these 1-forms clearly satisfies 2.2.11 and therefore no ordering among such 1-forms will violate the homotopy invariance of the corresponding iterated integral. As we will see, this is the case for classical polylogarithms and multiple polylogarithms in one variable and for some related classes of functions to be mentioned in section 2.5. However, in chapter 4 we will work with words in 1-forms for which eq. 2.2.11 is a non-trivial condition and where not every ordering of 1-forms is admissible.

2.3. Tangential basepoints

Before we apply the language of iterated integrals to classical and multiple polylogarithms on $\mathbb{C}\setminus\{0,1\}$, let us discuss some preparative steps regarding this space. Let x denote the complex coordinate of the space $\mathbb{C}\setminus\{0,1\}$ and let us consider a smooth path $\gamma : [0,1] \to \mathbb{C}\setminus\{0,1\}$ which begins at $\gamma(0) = x_0$ and ends at $\gamma(1) = z$. We consider the parametrization $\gamma(t) = x_0 + (z - x_0)t$ and the 1-form $\frac{dx}{x}$ on $\mathbb{C}\setminus\{0,1\}$. We easily compute the integral

$$\int_\gamma \frac{dx}{x} = \int_{0\leq t\leq 1} \frac{(z-x_0)dt}{x_0 + (z-x_0)t} = \ln(z) - \ln(x_0).$$

As a direct consequence of the multiplication rule in eqs. 2.2.3 and 2.2.8 we have

$$\int_\gamma \frac{dx}{x} \cdot \int_\gamma \frac{dx}{x} = \int_\gamma \frac{dx}{x} \text{ш} \frac{dx}{x} = 2\int_\gamma \frac{dx}{x}\frac{dx}{x}$$

and more generally

$$\left(\int_\gamma \frac{dx}{x}\right)^n = n! \int_\gamma \underbrace{\frac{dx}{x}...\frac{dx}{x}}_{n \text{ times}}.$$

We therefore arrive at

$$\int_\gamma \underbrace{\frac{dx}{x}...\frac{dx}{x}}_{n \text{ times}} = \frac{1}{n!}(\ln(z) - \ln(x_0))^n. \tag{2.3.1}$$

So far, the endpoints x_0 and z of the path were treated equally, but it will be convenient to let them play different roles. We want to consider the iterated integrals as functions of endpoint z (consisting of several complex components in chapter 4) and fix x_0 at the same value for all of our paths. We adapt the convention to choose $x_0 = 0$ for all paths γ, by abuse of our original set-up where the point 0 is excluded. Clearly, this choice causes a divergence in eq. 2.3.1. However, we will consider classes of iterated integrals where such logarithmic divergences are the only ones caused by the choice $x_0 = 0$. As a regularization of these divergences we formally set the logarithm at $x_0 = 0$ equal to zero, replacing the

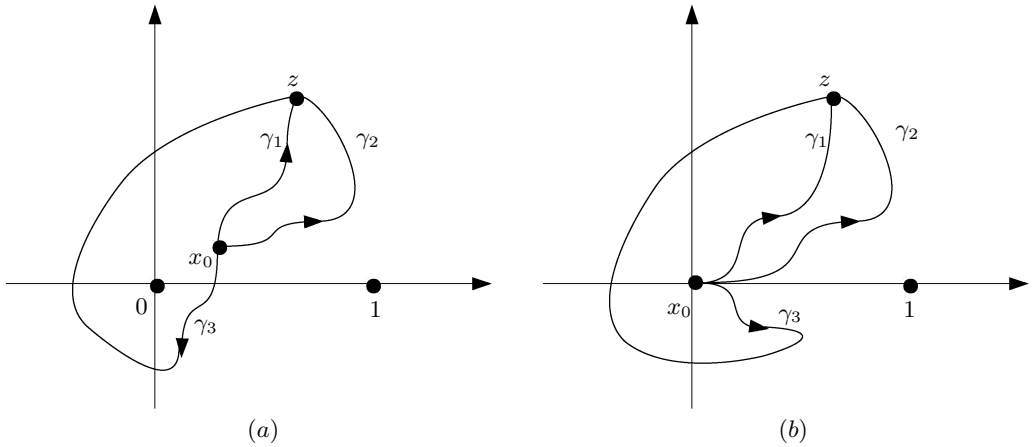


FIGURE 2.3.1. Three paths, initiating at $x_0 \neq 0$ in (a) and at the tangential basepoint $x_0 = 0$ in (b).

result eq. 2.3.1 by

$$\int_\gamma \underbrace{\frac{dx}{x} \ldots \frac{dx}{x}}_{n \text{ times}} = \frac{1}{n!} \ln^n (z) \,. \tag{2.3.2}$$

In the same sense we define the function in eq. 2.3.2 to vanish at $z = 0$.

In this re-definition we have to fix the branch of $\ln (x_0)$ which we eliminate at x_0 going to zero. This choice requires a further condition introduced on the path γ : In addition to the value $x_0 = 0$ of the initial point, we also fix the initial direction in which the path starts there. With this additional condition, x_0 is called a *tangential basepoint* of γ. Here we choose $\frac{d\gamma}{dt}|_{t=0} = 1$, meaning that γ starts in the direction of the positive real axis. Therefore there is a region sufficiently close to x_0 where the path does not intersect the branch cut $(-\infty, 0]$ of the logarithm. Hence we can unambiguously choose a Riemann sheet there. We fix $\ln (x_0)$ to be located on the principal sheet near $x_0 = 0$.

Figure 2.3.1 illustrates that the notion of the tangential basepoint is necessary to preserve the homotopy equivalence classes of paths when we send the basepoint to zero. In fig. 2.3.1 (a) we have three paths starting at some $x_0 \neq 0$ and ending at some other point z. Clearly, γ_1 and γ_2 are homotopic and γ_3 belongs to a different equivalence class. We can not continuously deform γ_3 into γ_1 or γ_2 in $\mathbb{C} \setminus \{0, 1\}$ because the point 0 lies in the region enclosed by γ_3 and γ_1 or γ_2 respectively. As we send x_0 to 0, the latter is not true anymore. However, due to the condition $\frac{d\gamma_i}{dt}|_{t=0} = 1$ for $i = 1, 2, 3$, we keep the same equivalence relations. As we see in fig. 2.3.1 (b) the path γ_3 still can not be transformed continuously into one of the two other paths.

In this thesis we consider classes of iterated integrals where re-definitions as in eq. 2.3.2 are sufficient for a regularization at the origin. If every iterated integral admits an expansion

$$I = \sum_i f_i(z) \ln (z)^i \tag{2.3.3}$$

where the f_i are finite at $z = 0$, the only possible divergences are cured by this regularization. In chapter 4 we will have a similar property for functions of several variables.

For practical computations it can be useful to make the reduction to the logarithmic divergences explicit. One considers an iterated integral $\int_\gamma ... \frac{dx}{x}$ which diverges at the origin due to its right-most 1-form $\frac{dx}{x}$ and relations from the shuffle product involving this integral. Using these relations one expresses the iterated integral in terms of the functions of eq. 2.3.2 and of iterated integrals whose right-most 1-form is different from $\frac{dx}{x}$.

EXAMPLE. From the shuffle-relations

$$\begin{aligned}\int_\gamma \frac{dx}{x}\frac{dx}{1-x} \cdot \int_\gamma \frac{dx}{x} &= 2\int_\gamma \frac{dx}{x}\frac{dx}{x}\frac{dx}{1-x} + \int_\gamma \frac{dx}{x}\frac{dx}{1-x}\frac{dx}{x},\\ \int_\gamma \frac{dx}{x}\frac{dx}{x} \cdot \int_\gamma \frac{dx}{1-x} &= \int_\gamma \frac{dx}{1-x}\frac{dx}{x}\frac{dx}{x} + \int_\gamma \frac{dx}{x}\frac{dx}{1-x}\frac{dx}{x} + \int_\gamma \frac{dx}{x}\frac{dx}{x}\frac{dx}{1-x},\end{aligned}$$

derived from eqs. 2.2.3 and 2.2.8, we obtain

$$\int_\gamma \frac{dx}{1-x}\frac{dx}{x}\frac{dx}{x} = \int_\gamma \frac{dx}{x}\frac{dx}{x} \cdot \int_\gamma \frac{dx}{1-x} + \int_\gamma \frac{dx}{x}\frac{dx}{x}\frac{dx}{1-x} + \int_\gamma \frac{dx}{x}\frac{dx}{1-x} \cdot \int_\gamma \frac{dx}{x}.$$

We see that in the last equation, the divergence on the right-hand side is cured by eq. 2.3.2.

2.4. Classical and multiple polylogarithms in terms of iterated integrals

Let γ be a piecewise smooth path starting at the tangential basepoint $x_0 = 0$ with $\frac{d\gamma}{dt}|_{t=0} = 1$ and ending at some point $z \in \mathbb{C}\backslash\{0,1\}$. We consider the set

$$\Omega_P = \{\omega_0, \omega_1\}$$

of the differential 1-forms

$$\omega_0 = \frac{dx}{x} \text{ and } \omega_1 = \frac{dx}{1-x}$$

on $\mathbb{C}\backslash\{0,1\}$. It is clear from section 2.2 that every word in these 1-forms is integrable.

As a solution to the differential equations in eq. 2.1.5 the classical polylogarithms can be written as

$$\mathrm{Li}_n(z) = \int_\gamma \underbrace{\omega_0 ... \omega_0}_{n-1 \text{ times}} \omega_1. \tag{2.4.1}$$

Recall that according to our conventions chosen in eq. 2.2.1, the iterated integration begins always with the right-most 1-form, here ω_1, and proceeds to the left. The differential equations eq. 2.1.5 for $n > 1$ can be expressed in terms of differential forms as

$$d\mathrm{Li}_n(z) = \omega_0 \mathrm{Li}_{n-1}(z) = \omega_0 \int_\gamma \underbrace{\omega_0 ... \omega_0}_{n-2 \text{ times}} \omega_1$$

by de-concatenation of the leftmost 1-form.

The functions in eq. 2.4.1 are multivalued on $\mathbb{C}\setminus\{0,1\}$ and their value depends on the homotopy class of γ. Let γ_a and γ_b be paths starting at the same tangential basepoint and ending at the same z in $\mathbb{C}\setminus\{0,1\}$. Furthermore let γ_i for $i=0,1$ be closed paths winding once around the point i respectively in anti-clockwise direction. We can always construct a piecewise smooth path homotopic to γ_2 by concatenating pieces of γ_a and the loops γ_i, possibly using several copies of these paths and inverting their direction. Therefore, the multiple values of $\mathrm{Li}_n(z)$ can be expressed with the help of the loops γ_0 and γ_1.

One defines the *monodromy* $\mathcal{M}_i$ around the point $i=0,1$ as the operator, which to a local branch of a multivalued function associates its analytic continuation along the path γ_i. One can show (see e.g. **[62]** and references therein) that on classical polylogarithms this operator acts as

$$\begin{aligned}\mathcal{M}_0\mathrm{Li}_n(z) &= \mathrm{Li}_n(z),\\ \mathcal{M}_1\mathrm{Li}_n(z) &= \mathrm{Li}_n(z)+\frac{2\pi i}{(n-1)!}\ln^{n-1}(z).\end{aligned}$$

This determines the analytic continuation of classical polylogarithms. We notice that with each walk around the point 0, the polylogarithm itself remains unchanged. With each walk around 1 the polylogarithms are changed by adding logarithms, and these in turn change with walks around 0 by adding powers of $2\pi i$.

Multiple polylogarithms in one variable can be expressed as

$$\mathrm{Li}_{n_1,\ldots,n_r}(z)=\int_\gamma \underbrace{\omega_0\ldots\omega_0}_{n_r-1\text{ times}}\ \omega_1\ldots\ \underbrace{\omega_0\ldots\omega_0}_{n_1-1\text{ times}}\ \omega_1. \tag{2.4.2}$$

In the special case of $z=1$ this provides an integral representation for multiple zeta values found by Kontsevich (see **[209]**). The differential equations of eq. 2.1.8 can be written as

$$d\mathrm{Li}_{n_1,\ldots,n_r}(z)=\begin{cases}\omega_0\mathrm{Li}_{n_1,\ldots,n_r-1}(z) & \text{for } n_r>1,\\ \omega_1\mathrm{Li}_{n_1,\ldots,n_{(r-1)}}(z) & \text{for } n_r=1.\end{cases}$$

As we have seen, iterated integrals with 1-forms in Ω_P are sufficient to express classical polylogarithms and multiple polylogarithms in one variable. For multiple polylogarithms of several variables, we require a more general set of 1-forms. For a set of numbers $\Sigma\subset\mathbb{C}$ including $0\in\Sigma$ let us define the set of 1-forms

$$\Omega_\Sigma=\left\{\omega(\sigma;x)=\frac{dx}{x-\sigma}\text{ for all }\sigma\in\Sigma\right\}.$$

The resulting iterated integrals are called *hyperlogarithms*. They were studied by Kummer **[136]**, Poincaré **[174]** and extensively by Lappo-Danilevsky **[139, 140]**. They are recursively defined by

$$L_{\sigma_1,\ldots,\sigma_r}(z)=\int_0^z\omega(\sigma_1;x)L_{\sigma_2,\ldots,\sigma_r}(x) \tag{2.4.3}$$

where $\sigma_i \in \Sigma$ for $i = 1, ..., r$. In the case of all 1-forms being $\omega(0) = \frac{dx}{x}$ one defines

$$L_{\underbrace{0, ..., 0}_{n \text{ times}}}(z) = \frac{1}{n!} \ln^n(z),$$

as we did in eq. 2.3.2. For a path γ in $\mathbb{C}\backslash\Sigma$ from tangential basepoint $x_0 = 0$ to z we can more elegantly write

$$L_{\sigma_1,...,\sigma_r}(z) = \int_\gamma \omega_1 ... \omega_r$$

with $\omega_i = \omega(\sigma_i; x) \in \Omega_\Sigma$ for $i = 1, ..., r$. We have the familiar type of differential equation

$$dL_{\sigma_1,...,\sigma_r} = \omega_1 L_{\sigma_2,...,\sigma_r}. \tag{2.4.4}$$

Goncharov found [**112, 111**] that hyperlogarithms can be used to express the multiple polylogarithms as

$$(-1)^r \operatorname{Li}_{n_1,...,n_r}\left(\frac{\sigma_2}{\sigma_1}, \frac{\sigma_3}{\sigma_2}, ..., \frac{z}{\sigma_r}\right) = L_{\underbrace{0, ..., 0}_{n_r - 1 \text{ times}}, \sigma_r, ..., \underbrace{0, ..., 0}_{n_1 - 1 \text{ times}}, \sigma_1}(z). \tag{2.4.5}$$

Hyperlogarithms will not be in the main focus of this thesis, but they will play an auxiliary role in chapter 4. Note that in eq. 2.4.5 the last argument of the multiple polylogarithm $\operatorname{Li}_{n_1,...,n_r}$ is somehow special. It depends on the *variable* z, while the other arguments are fractions of the fixed numbers σ_i. In chapter 4 we will apply a different set of iterated integrals for multiple polylogarithms whose 1-forms involve several variables instead.

Very briefly we mention some further properties of multiple polylogarithms:

- We have seen that a product of multiple polylogarithms can be computed in two ways: Based on the series representation using the quasi-shuffle product as in eq. 2.1.11 or based on hyperlogarithms using the shuffle product of eq. 2.2.8. For the same product of multiple polylogarithms, one usually obtains two different expressions in these ways. This gives rise to identities between multiple polylogarithms and therefore also between multiple zeta values. An important conjecture states, that this interplay of quasi-shuffle and shuffle multiplication is in a certain sense the only source of algebraic relations between multiple zeta values. We refer to [**203**] for an overview.
- The words of differential 1-forms form a commutative *algebra* with the above shuffle product. In eq. 2.2.9 we have furthermore introduced the co-product of de-concatenation, which can be used to express the path concatenation formula 2.2.5. These structures together define a *bi-algebra*, which due to the existence of an antipode

  $$S(\omega_1 ... \omega_r) = (-1)^r \omega_r ... \omega_1$$

  furthermore constitutes a *Hopf algebra*. In chapter 4 we will make extensive use of the product and co-product while the antipode will play a minor role in the

computation of certain limits. For recent explicit applications of the Hopf algebra structure in Feynman integral computations we refer to **[98, 99]**.

- Apart from relations given by shuffle and quasi-shuffle multiplication, classical and multiple polylogarithms satisfy *functional equations*, relating multiple polylogarithms with different arguments to each other. Some standard examples are (see e.g. **[210]**)

$$\mathrm{Li}_2\left(\frac{1}{z}\right) = -\mathrm{Li}_2(z) - \zeta(2) - \frac{1}{2}\ln^2(-z), \tag{2.4.6}$$

$$\mathrm{Li}_2(1-z) = -\mathrm{Li}_2(z) + \zeta(2) - \ln(z)\ln(1-z), \tag{2.4.7}$$

$$\mathrm{Li}_2(x) = n\sum_{z^n=x}\mathrm{Li}_2(z) \text{ for } n\in\mathbb{N}, \tag{2.4.8}$$

$$\begin{aligned}\mathrm{Li}_2(x)+\mathrm{Li}_2(y)+\mathrm{Li}_2(z) &= \frac{1}{2}\left(\mathrm{Li}_2\left(-\frac{xy}{z}\right)+\mathrm{Li}_2\left(-\frac{yz}{x}\right)+\mathrm{Li}_2\left(-\frac{xz}{y}\right)\right)\\ &\quad \text{for } \frac{1}{x}+\frac{1}{y}+\frac{1}{z}=1,\end{aligned} \tag{2.4.9}$$

$$\begin{aligned}\mathrm{Li}_2(x)+\mathrm{Li}_2(y) &= -\mathrm{Li}_2\left(\frac{1-x}{1-xy}\right)-\mathrm{Li}_2(1-xy)-\mathrm{Li}_2\left(\frac{1-y}{1-xy}\right)\\ &\quad +\zeta(2)-\ln(x)\ln(1-x)-\ln(y)\ln(1-y)\\ &\quad +\ln\left(\frac{1-x}{1-xy}\right)\ln\left(\frac{1-y}{1-xy}\right),\end{aligned} \tag{2.4.10}$$

  where the two latter equations are known as the six-term relation of Kummer and Newman and the five-term relation discovered by Spence and several other authors thereafter. From a physicist's point of view, such relations can be useful for the analytic continuation and the simplification of a result.

- We have seen that for every homotopy invariant iterated integral there is an integrable word of 1-forms and that a hyperlogarithm admits the same differential behavior as the multiple polylogarithm in one of the variables. It is furthermore possible to construct an integrable word which reflects the differential behavior of the multiple polylogarithm in all of its variables. Such words will be the backbone of our work to be discussed in chapter 4. In this discussion, we will fix certain boundary conditions such that the iterated word entirely determines the function (up to monodromy).

  In some computations, it is sufficient to know the differential behavior of the function and to compute with integrable words without fixing the boundary conditions. This is the idea behind the use of the so-called *symbol* **[113, 115, 100]** in particle physics (also see **[99]** for an introduction and further references). This strategy has been successful in two ways: Firstly, if a result is expressed in terms of hyperlogarithms, its simplicity may be obscured and the expression may be much longer than necessary as symmetries and functional relations may not be

manifest. Associating the corresponding integrable words can lead to drastic simplifications, as was shown in [**115**] and later references. Secondly, the assumption that a quantity can be expressed in terms of multiple polylogarithms and further known properties of the quantity may determine the result completely. In such cases, one constructs all integrable words of a desired weight and eliminates the ones contradicting the known physical properties. Recent results with such approaches include [**95, 96, 97**].

Hyperlogarithms are very well established in mathematics and in particle physics today and all of the mentioned aspects are extensively discussed in the literature. We recommend chapter 3 of Panzer's PhD thesis [**170**] for a recent and very thorough introduction to this important class of functions.

2.5. Related developments in particle physics

Some aspects of the above framework of functions have been known for a long time. However, the general attention on these functions has apparently grown just in the last few decades[2]. Therefore it is not a surprise that particle physicists have not always referred to these functions as discussed above. In some cases, different names were used for the same objects while in other cases, alternative functions have appeared more convenient to express certain results. Let us quickly go through some of these notions which play some role in the physics literature.

A first appearance of polylogarithms in quantum field theory may be[3] the article [**177**] in the context of quantum electrodynamics. Eq. 39 of this reference introduces the function

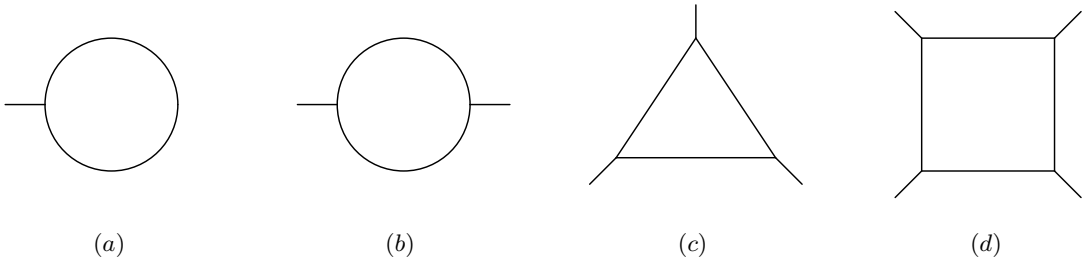
$$R(x) = \int_0^x \ln(1+y)\frac{dy}{y}$$

which is clearly equal to $-\mathrm{Li}_2(-x)$. The author does not use the term "dilogarithm" and does not refer to the mathematical literature at this point, but he mentions the series expansion and the functional equation we have seen in eq. 2.4.6.

An important early benchmark in the systematic computation of Feynman integrals are t'Hooft and Veltman's results for the four one-loop integrals given by the graphs in figure 2.5.1 to order ϵ^0 in dimensional regularization [**200**]. The results for the graphs in fig. 2.5.1 (a) and (b) involve the logarithm while the results for (c) and (d) furthermore involve the dilogarithm. The authors use the term *Spence function* and clarify that this is just another name for the dilogarithm. The term was used in some later references as well. The result for fig. 2.5.1 (d) was simplified in [**94**]. Together with the methods of [**173, 156**] these results show, that for one-loop integrals in general, no function more

[2]This development is documented in Zagier's article [**210**]: In the first version, published in 1988, he refers to the dilogarithm as a *"remarkable and too little-known function"*. In the extended second version, published fifteen years later, he adds: *The comment about "too little-known" is now no longer applicable, since the dilogarithm has become very popular in both mathematics and mathematical physics, due to its appearance in algebraic K-theory on the one hand and in conformal field theory on the other. [...]*

[3]We are referred to this article by a remark in [**182**].



(a) (b) (c) (d)

FIGURE 2.5.1. The first four one-loop Feynman graphs

complicated than the dilogarithm is required at order ϵ^0. For an overview of these results we refer to **[93]**.

Another important benchmark was the introduction of *harmonic polylogarithms* **[182]** to the particle physics literature. These functions are defined by

$$\begin{aligned} \mathrm{H}(\underbrace{0,...,0}_{n \text{ times}};z) &= \frac{1}{n!}\ln^n(z), \\ \mathrm{H}(m_1,m_2,...,m_n;z) &= \int_0^z \omega(m_1;z')\mathrm{H}(m_2,...,m_n;z') \end{aligned}$$

where in the latter equation $m_i \in \{0,1,-1\}$, not all of these numbers being zero, and $\omega(m_i;z) = (-1)^{\delta_{1m_i}}\frac{dx}{x-m_i}$ with $\delta_{1m_i} = 1$ for $m_i = 1$ and $\delta_{1m_i} = 0$ otherwise. These functions are hyperlogarithms with $\Sigma = \{-1,0,1\}$ and can be written as

$$\mathrm{H}(m_1,...,m_n;z) = (-1)^{|\{i|m_i=1\}|}L_{m_1,...,m_n}(z).$$

Harmonic polylogarithms were applied in numerous computations and are implemented for applications with computer algebra systems **[150, 151, 202]**.

In **[182]** it is noted that harmonic polylogarithms contain the so-called *Nielsen polylogarithms* as a subset. These were introduced in **[166]** as

$$S_{n,p}(z) = \frac{(-1)^{n+p-1}}{(n-1)!p!}\int_0^1 \ln^{n-1}(x)\ln^p(1-zx)\frac{dx}{x},$$

studied in **[132]** and received some further attention in the physics literature. The class of Nielsen polylogarithms contains the classical polylogarithms as

$$\mathrm{Li}_n(z) = S_{n-1,1}(z)$$

and is itself contained in the class of harmonic polylogarithms due to

$$S_{n,p}(z) = \mathrm{H}(\underbrace{0,...,0}_{n \text{ times}},\underbrace{1,...,1}_{p \text{ times}};z)$$

and in the class of hyperlogarithms because of

$$S_{n,p}(z) = (-1)^p L_{\underbrace{0,...,0}_{n \text{ times}},\underbrace{1,...,1}_{p \text{ times}}}(z).$$

As Nielsen polylogarithms only involve the differential 1-forms $\frac{dx}{x}$ and $\frac{dx}{x-1}$, they are also contained in the multiple polylogarithms in one variable due to eq. 2.4.2. We schematically summarize the hierarchy on the above classes of functions:

$$-\ln(1-z) \quad \in \quad \{\mathrm{Li}_n(z)\} \subset \{S_{n,p}(z)\} \subset \{\mathrm{Li}_{n_1,...,n_r}(z)\} \subset \{\mathrm{H}(m_1,...,m_r;z)\} \subset \{L_{m_1,...,m_r}(z)\}\,.$$

The success of harmonic polylogarithms has motivated several extensions in the particle physics literature. The *two-dimensional harmonic polylogarithms* defined in [**108**] can be seen as the subset of hyperlogarithms defined by the set $\Sigma = \{0, 1, 1-y, -y\}$ for some $y \in \mathbb{C}$. In [**12**] a generalization with differential 1-forms including certain square-roots in the denominators such as $dx/\sqrt{x\,(4 \pm x)}$ was introduced. In [**51**] it was shown that these functions can be expressed in terms of hyperlogarithms. In [**5**] the definition of *cyclotomic harmonic polylogarithms* extends the set of differential 1-forms by introducing cyclotomic polynomials in the denominator. A computer program allowing for manipulations with cyclotomic harmonic polylogarithms was presented in [**1**]. Furthermore, iterated integrals for iterated binomial sums were introduced in [**2**]. In [**39**], as a generalization of the two-dimensional harmonic polylogarithms, certain 1-forms with quadratic dependences on variables were introduced, which however could be expressed in terms of linear 1-forms by an Euler transformation.

For a last development to be mentioned here, let us turn to the series representations of generalized polylogarithms. In [**159**] multiple polylogarithms are generalized by allowing for a finite upper bound in the summation. This leads to the definition of *Z-sums*

$$Z(m; n_1, ..., n_r; z_1, ..., z_r) = \sum_{m > j_1 > ... > j_r > 0} \frac{z_1^{j_1} ... z_r^{j_r}}{j_1^{n_1} ... j_r^{n_r}}$$

and *S-sums*

$$S(m; n_1, ..., n_r; z_1, ..., z_r) = \sum_{m \geq j_1 \geq ... \geq j_r \geq 1} \frac{z_1^{j_1} ... z_r^{j_r}}{j_1^{n_1} ... j_r^{n_r}}.$$

In [**159**] these series were applied to expand hypergeometric series around certain values of their arguments. Computer programs for this task, based on Z-sums and S-sums, were presented in [**158, 205**]. Every Z-sum can be expressed in term of S-sums and vice versa. The multiple polylogarithms are contained in this class of series as

$$\mathrm{Li}_{n_1,...,n_r}(z_1, ..., z_r) = Z(\infty; n_r, ..., n_1; z_r, ..., z_1).$$

Furthermore, the special cases $Z(m; n_r, ..., n_1; 1, ..., 1)$ are known as Euler-Zagier sums [**104, 209**] and $S(m; n_1, ..., n_r; 1, ..., 1)$ are known as harmonic sums [**201**].

In this chapter we have seen that multiple polylogarithms are a very general framework of functions. Hyperlogarithms provide a representation in terms of iterated integrals and we will discuss an alternative in chapter 4. We have not discussed q-analogues and elliptic generalizations of polylogarithms so far. In contrast to all of the above functions, such generalizations have been very rarely applied in particle physics to this point. In chapter

5 we will discuss one such class of generalizations and its application to the computation of certain Feynman integrals, for which multiple polylogarithms are not sufficient. We will also point out some of the connections between this class of functions and some of the known elliptic generalizations in the literature.

CHAPTER 3

Feynman integrals, periods and some computational methods

In this chapter we recall basic notions of Feynman integrals and briefly review two methods for their analytic computation: the method of parametric integration and the method of differential equations. Both methods will play a central role in the subsequent chapters of the thesis.

3.1. Basic notions

A *Feynman graph* G is a labeled, oriented graph which is allowed to have multiple edges (i.e. each two vertices may be connected by more than one edge) and external edges (i.e. half-edges with only one end attached to a vertex). The orientation is chosen arbitrarily. We assume our Feynman graphs to have one connected component and to be *one-particle irreducible* (1PI), i.e. there is no edge in the graph whose removal would increase the number of connected components. This assumption does not restrict the class of integrals as for graphs which are not 1PI the Feynman integrals factorize and in this sense, every Feynman graph is trivially reduced to 1PI graphs.

Let L be the first Betti-number of the graph, also called the *loop-number*. Let $E+1$ be the number of the external edges and N be the number of the internal edges. Every external edge is labeled by an external momentum p_i, $i = 1, ..., E+1$, which by our convention is said to be incoming at the vertex. Every internal edge is labeled by an internal momentum q_i, $i = 1, ..., N$. We denote the number of space-time dimensions by D and all momenta are D-dimensional Lorentz vectors[1].

Consider an internal edge which is labeled by a momentum q and oriented from vertex v_1 to vertex v_2. Then we say that q is incoming at v_2 and $-q$ is incoming at v_1. In every Feynman graph, momentum conservation is implemented by the condition that at each vertex the sum of all incoming momenta is zero. This implies that only E of the external momenta are linearly independent. Furthermore, every internal momentum q_i can be expressed as a $\mathbb{Q}$-linear combination of a linearly independent set of momenta $\{p_1, ..., p_E, k_1, ..., k_L\}$ where the k_i are called loop-momenta. In general the loop-momenta can be introduced in several ways such that momentum conservation is satisfied. The Feynman integral will not depend on this choice. Finally, each internal edge e_i of the graph is labeled with a particle mass m_i, which is treated as a real-valued variable in this thesis.

[1]Feynman integrals will be considered as functions of scalar quantities and none of our main considerations will make use of Lorentz vectors.

To every internal edge e_i labeled with momentum q_i and mass m_i, we associate a scalar *Feynman propagator*

$$\frac{1}{P_i} = \frac{1}{-q_i^2 + m_i^2 - i\delta}.$$

The term $i\delta$ with a small, real number δ was introduced by Feynman to shift the pole of the propagator away from the integration contour. Equivalently, the contour can be deformed to circumvent the point $q_i^2 = m_i^2$. The sign of the $i\delta$ keeps track of the side on which the contour passes the pole. In the following we omit this term.

Let $M = E + L$. With the momenta $p_1, ..., p_E, k_1, ..., k_L$ we can form $\frac{L(L+1)}{2} + LE$ independent scalar products $l_i l_j = l_j l_i$ with $l_i \in \{k_1, ..., k_L\}$ and $l_j \in \{p_1, ..., p_E, k_1, ..., k_L\}$. In the case of $\frac{L(L+1)}{2} + LE \leq N$, all of these scalar products can be expressed as linear combinations of the q_i^2 and products of external momenta. In the other case, there are $B = \frac{L(L+1)}{2} + LE - N$ remaining scalar-products which can not be expressed in this way. These are called the *irreducible scalar-products* in this context. Let us denote these scalar products by $S_1, ..., S_B$.

To a Feynman graph G we associate the scalar Feynman integrals[2]

$$I = \left(\prod_{j=1}^{L} \int \frac{d^D k_j}{i\pi^{D/2}} \right) \prod_{i=1}^{N} P_i^{-\nu_i} \prod_{j=1}^{B} S_j^{-\nu_{N+j}} \tag{3.1.1}$$

with all $\nu_i \in \mathbb{Z}$. We call this expression the *momentum space representation*.

We consider Feynman integrals in *dimensional regularization* **[50, 78, 193, 199]** (also see **[102]** and chapter 4 of **[86]**), which implies that D is treated as a complex variable[3]. As one is usually interested in the Feynman integral of a theory in four space-time dimensions, one considers the expansion

$$I = \sum_{i=-2L}^{\infty} I_i \epsilon^i \tag{3.1.2}$$

where ϵ is defined by $D = 4 - 2\epsilon$. In this expansion, all the infrared and ultraviolet divergences are manifest as poles in ϵ and no poles worse than ϵ^{-2L} can appear. Therefore it is common practice to compute the relevant Feynman integrals as such an expansion and to use the pole-terms in a renormalization procedure to remove ultraviolet divergences and to make cancellations of infrared divergences explicit.

For some purposes, it is interesting to consider a Feynman integral in a dimension different than four and to define ϵ by $D = 2m - 2\epsilon$ for some positive integer m. Tarasov's method **[196, 197]** provides linear relations between Feynman integrals in different dimensions. We will make use of such relations in chapter 5. Furthermore, this method has

[2]Usually, momenta and masses are assigned a physical mass dimension μ and a general prefactor $\left(\mu^2\right)^{\nu - LD/2}$ with $\nu = \sum_{i=1}^{N+B} \nu_i$ is introduced to define the Feynman integral as dimensionless. While in refs. **[6, 7, 8, 9, 11]** the mass dimension μ is written explicitly, it will be omitted in the present text.

[3]To a reader who is unfamiliar with the general concept of dimensional regularization it may be more instructive to consider eq. 3.1.5 as the definition of the Feynman integral. Here D appears only in exponents of the integrand and in arguments of the gamma-function and it is not necessary to artificially relate a complex number to the dimension of a vector space.

an important implication on Feynman integrals with a tensor structure. Tensor integrals arise in theories with fermions due to the fact that the numerator of the fermion propagator involves a momentum vector with a free Lorentz-index. Tarasov's method allows us to express every Standard Model Feynman integral with a tensor structure as a linear combination of certain standard tensors whose coefficients are scalar Feynman integrals as defined in eq. 3.1.1. (For one-loop integrals, such tensor reductions are already provided in [**156, 173**].) Therefore, the problem of computing a Standard Model Feynman integral can always be reduced to the problem of computing scalar Feynman integrals.

In eq. 3.1.1 the integration is over components of loop-momenta. For many purposes it is very advantageous to express the Feynman integral by integrations over scalar variables which do not play the role of momentum components. Such a representation can be derived with the help of the relation

$$\frac{1}{AB} = \int_0^1 \frac{dx}{(xA + (1-x)B)^{\,2}}$$

which was applied by Feynman in [**105**] and is nowadays called the *Feynman trick*. In [**85, 163**] this formula was generalized to

$$\frac{1}{\prod_{i=1}^n A_i^{\nu_i}} = \frac{\Gamma(\nu)}{\prod_{i=1}^n \Gamma(\nu_j)} \int_0^1 \left(\prod_{i=1}^n dx_i x_i^{\nu_i - 1} \right) \frac{\delta\left(1 - \sum_{i=1}^n x_i\right)}{\left(\sum_{i=1}^n x_i A_i\right)^{\nu}} \tag{3.1.3}$$

where $\nu = \sum_{i=1}^n \nu_i$. Applying this formula to the integrand of eq. 3.1.1, one introduces $N + B$ new integrations over the so-called Feynman parameters x_i. In the resulting denominator on the right-hand side of eq. 3.1.3 one completes the square with respect to the loop-momenta such that these can be integrated out by Gaussian integration. These steps are demonstrated in full detail in [**164**].

In order to express the result of this computation in a convenient way, let us introduce some widely used auxiliary objects. For the propagators P_i and irreducible scalar products S_i of the Feynman integral in eq. 3.1.1 we consider

$$\sum_{a=1}^N x_a P_a + \sum_{b=1}^B x_b S_b = -\sum_{i=1}^L \sum_{j=1}^L \mathcal{M}_{ij} k_i k_j + \sum_{i=1}^L 2 Q_i k_i + J \tag{3.1.4}$$

where the right-hand side is an expansion in loop-momenta by which we define the k-independent coefficients $\mathcal{M}_{ij} = \mathcal{M}_{ji}$, Q_i and J for $i,\ j = 1,\ ...,\ L$. Let $\mathcal{M}$ be the symmetric $L \times L$-matrix whose elements are $\mathcal{M}_{ij}$. All of these coefficients depend on the Feynman parameters and the Q_i and J furthermore depend on external momenta in general. Let us assume that the matrix $\mathcal{M}$ is invertible[4]. Then we define

$$\begin{aligned} \mathcal{U} &= \det(\mathcal{M}), \\ \mathcal{F} &= \det(\mathcal{M}) \left(\sum_{i=1}^L \sum_{j=1}^L \mathcal{M}_{ij}^{-1} Q_i Q_j + J \right). \end{aligned}$$

[4]It is easy to show that this is always the case if the irreducible scalar products are chosen such that none of them is quadratic in the loop-momenta.

With these functions, the Feynman integral can be expressed as

$$I = \Gamma\left(\nu - L\frac{D}{2}\right)\left(\prod_{i=1}^{N+B}\int_0^\infty \frac{dx_i x_i^{\nu_i-1}}{\Gamma(\nu_i)}\right)\delta(H)\,\mathcal{U}^{\nu-(L+1)\frac{D}{2}}\mathcal{F}^{L\frac{D}{2}-\nu} \tag{3.1.5}$$

with $\nu = \sum_{i=1}^{N+B}\nu_i$ and where $H = 1 - \sum_{i=1}^{N+B} c_i x_i$ with $c_i \geq 0$ and not all of the c_i being zero. We refer to this expression as the *parametric representation*. Note that furthermore a closely related representation is obtained by the so-called Schwinger trick and yet another parametric formula was recently introduced in [**145**].

Feynman integrals with irreducible scalar-products play a role in certain computations, for example in integration-by-parts (IBP) reductions [**83**]. However, in many cases one can avoid their presence and deal only with Feynman integrals where no irreducible scalar products are involved, i.e. $\nu_i = 0$ for $i = N+1, ..., N+B$. In this case, we see in eq. 3.1.4 that every Feynman parameter x_i is associated to one propagator P_i and therefore to one edge e_i of the graph.

The functions $\mathcal{U}$ and $\mathcal{F}$ are polynomials in the Feynman parameters, known as the first and second *Symanzik polynomial* respectively. For Feynman integrals without irreducible scalar products they have the following properties: Both polynomials are homogeneous in the Feynman parameters and their degrees are $\deg(\mathcal{U}) = L$ and $\deg(\mathcal{F}) = L+1$. The polynomial $\mathcal{U}$ is always linear in each Feynman parameter while $\mathcal{F}$ is linear in the case of vanishing masses. In $\mathcal{U}$ all coefficients of monomials in the Feynman parameters are 1 while the coefficients in $\mathcal{F}$ involve masses and external momenta.

An elegant construction [**164**] for the Symanzik polynomials is given by

$$\mathcal{U} = \sum_{T\in\mathcal{T}_1}\prod_{e_i\notin T} x_i, \tag{3.1.6}$$

$$\mathcal{F} = \sum_{(T_1,T_2)\in\mathcal{T}_2}\left(\prod_{e_i\notin(T_1,T_2)} x_i\right) s_{(T_1,T_2)} + \mathcal{U}\sum_{i=1}^{N} x_i m_i^2 \tag{3.1.7}$$

with

$$s_{(T_1,T_2)} = -\left(\sum_{p_j\in\mathcal{P}_{T_1}} p_j\right)\cdot\left(\sum_{p_k\in\mathcal{P}_{T_2}} p_k\right). \tag{3.1.8}$$

Here $\mathcal{T}_1$ is the set of *spanning trees* of the Feynman graph G. These are all sub-graphs of G each containing all vertices of G, having one connected component and no loops. The set $\mathcal{T}_2$ is the set of spanning two-forests, which are all sub-graphs with all vertices of G, two connected components and no loops. In eqs. 3.1.7 and 3.1.8 such two-forests are denoted (T_1, T_2) where T_1 and T_2 are the components. By $\mathcal{P}_{T_i}$ we denote the set of incoming external momenta at the component T_i for $i = 1, 2$. Here we see that the Feynman integral depends on the external momenta only in terms of the scalar coefficients $s_{(T_1,T_2)}$ which we will refer to as the *kinematic invariants* of the Feynman graph.

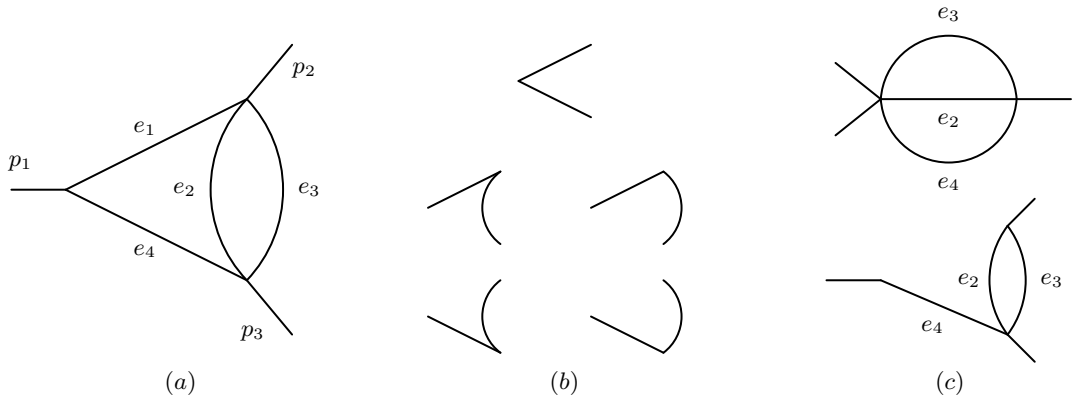


FIGURE 3.1.1. A two-loop example

Let us recall one further feature of Symanzik polynomials. Let $\mathcal{F}_0 = \mathcal{F}|_{m_i=0 \text{ for } i=1,...,N}$ and let $\mathcal{U}(G)$ and $\mathcal{F}_0(G)$ denote the polynomials associated to the graph G. Furthermore let a *regular edge* of G be an edge whose removal does not increase the number of connected components and which furthermore is not a tadpole, i.e. it is not connected to the same vertex at both of its ends. Then for every regular edge e_i of G we have the *deletion-contraction relations*

$$\begin{aligned} \mathcal{U}(G) &= \mathcal{U}(G/e_i) + x_i \mathcal{U}(G\backslash e_i), \\ \mathcal{F}_0(G) &= \mathcal{F}_0(G/e_i) + x_i \mathcal{F}_0(G\backslash e_i), \end{aligned}$$

where the graphs on the right-hand side of these relations are not necessarily 1PI. Here $G\backslash e_i$ is the graph obtained by removing e_i from G and G/e_i is the graph obtained by contracting e_i in G, where the latter means that the end-points of e_i are identified and e_i is removed. These operations will play a certain role in one of the computational methods below. Further properties of Symanzik polynomials such as their relation to certain matrices and matroids are reviewed in [**49**].

EXAMPLE. We illustrate some of the above notions for the two-loop graph G in fig. 3.1.1 (a). In this picture we have labeled the external edges with incoming momenta p_1, p_2, p_3 and we have named the internal edges e_1, e_2, e_3, e_4. We clearly have $L = 2$, $N = 4$, $E = 2$. To the internal edges we associate momenta

$$\begin{aligned} q_1 &= k_1, \\ q_2 &= k_2, \\ q_3 &= k_1 + k_2 + p_2, \\ q_4 &= k_1 - p_1 \end{aligned}$$

and the corresponding propagators $P_i^{-1} = (-q_i^2 + m_i^2)^{-1}$ for $i = 1, ..., 4$. It is easy to check that there is an orientation on G such that momentum conservation is satisfied by this choice. The loop-momenta are involved in $\frac{L(L+1)}{2} + LE = 7$ linearly independent

scalar-products and we may write

$$\begin{aligned} k_1^2 &= q_1^2, \\ k_2^2 &= q_2^2, \\ k_1 \cdot k_2 &= -\frac{1}{2}\left(q_1^2 + q_2^2 + p_2^2 + 2S_1 + 2S_3 - q_3^2\right), \\ k_1 \cdot p_1 &= \frac{1}{2}\left(q_1^2 + p_1^2 - q_4^2\right), \end{aligned}$$

with $S_1 = k_1 \cdot p_2$, $S_2 = k_2 \cdot p_1$, $S_3 = k_2 \cdot p_2$ as irreducible scalar-products.

The generic Feynman integral without irreducible scalar-products reads

$$I = \int \frac{d^D k_1}{i\pi^{D/2}} \int \frac{d^D k_2}{i\pi^{D/2}} \prod_{i=1}^{4} P_i^{-\nu_i}$$

in momentum space representation and

$$I = \Gamma(\nu - D) \left(\prod_{i=1}^{4} \int_0^\infty \frac{dx_i x_i^{\nu_i - 1}}{\Gamma(\nu_i)} \right) \delta\left(1 - \sum_{j=1}^{4} x_j\right) \frac{\mathcal{F}^{D-\nu}}{\mathcal{U}^{\frac{3D}{2}-\nu}}$$

in parametric representation with

$$\begin{aligned} \mathcal{U} &= x_2 x_3 + (x_1 + x_4)(x_2 + x_3), \\ \mathcal{F} &= -p_1^2 x_1 x_4 (x_2 + x_3) - p_2^2 x_1 x_2 x_3 - p_3^2 x_2 x_3 x_4 + \mathcal{U} \sum_{i=1}^{4} x_i m_i^2. \end{aligned}$$

The spanning trees for the construction of $\mathcal{U}$ are indicated in fig. 3.1.1 (b). In fig. 3.1.1 (c) we see an example for graphs which appear in deletion-contraction relations for G. The upper part of this picture shows G/e_1 while the lower part shows $G\backslash e_1$.

3.2. Periods and Feynman integrals

Before we turn to the computational methods which play a main role in this thesis, let us briefly discuss a rather new perspective on Feynman integrals, which has influenced both of these methods in the last decade. In this new viewpoint, Feynman integrals play the role of members of a certain class of numbers called periods or, more generally, of functions evaluating to such numbers at algebraic arguments. These periods are related to periodic functions, satisfying a particular type of differential equations and to spaces on which these functions are defined.

Example. We introduce some of the concepts by a classical example (cf. **[75, 126, 134]**). Consider the complex plane of a variable $z \in \mathbb{C}$ and the lattice of points $L = \mathbb{Z} + \tau\mathbb{Z}$, with $\tau \in \mathbb{C}$, $\mathrm{Im}(\tau) > 0$, see fig. 3.2.1 (a). A function $f(z)$ is called *elliptic* with respect to the lattice L if

$$f(z) = f(z + \lambda) \text{ for } \lambda \in L. \tag{3.2.1}$$

Without loss of information, a function with this property can be restricted to just one cell of the lattice (the grey area in fig. 3.2.1), as it behaves exactly the same way in all the

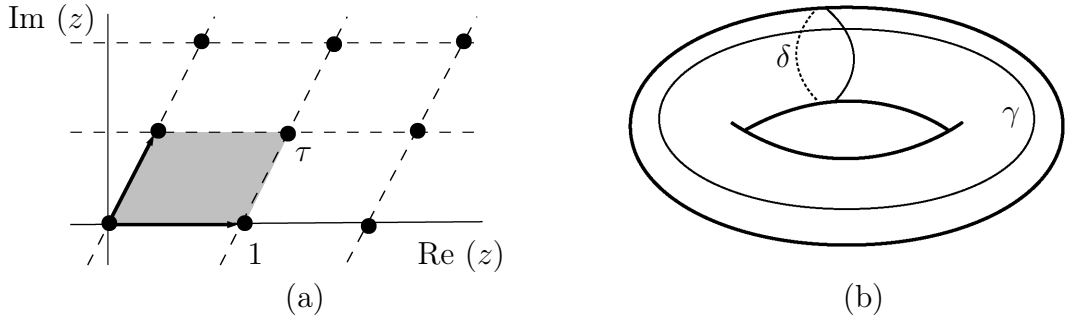


FIGURE 3.2.1. (a) A lattice in the complex plane and (b) a torus

other cells. Such a cell is isomorphic to an elliptic curve E and the periodicity is visualized by gluing the opposite edges of the cell together to obtain a torus $\mathbb{C}/L$.

Instead of one specific elliptic curve, one often considers a family of elliptic curves, parametrized by a complex variable, say t. Here we consider the Legendre family E_t given by the solutions of the cubical equation

$$y^2 = x\,(x-1)\,(x-t)\,.$$

On E_t one considers the differential 1-form

$$\omega = \frac{dx}{y} = \frac{dx}{\sqrt{x\,(x-1)\,(x-t)}}$$

which is closed and has a well-defined cohomology class $[\omega]$. This class can be written in terms of a basis. At first we notice, simply by looking at the torus, that there are two classes of cycles on E_t which can not be contracted to a point or transformed into each other. In other words, the first homology $H_1\,(E_t;\mathbb{Z})$ is generated by two elements and as a basis we can choose two cycles δ and γ as in fig. 3.2.1 (b). Furthermore let $\delta^\star$ and $\gamma^\star$ be the basis of the first cohomology $H^1\,(E_t;\mathbb{Z})$ which is dual to δ and γ, i.e.

$$\int_\delta \delta^\star = \int_\gamma \gamma^\star = 1.$$

With respect to this choice one obtains the basis-decomposition

$$[\omega] = \delta^\star \int_\delta \omega + \gamma^\star \int_\gamma \omega.$$

The coefficients

$$g_1(t) = \int_\delta \omega \text{ and } g_2(t) = \int_\gamma \omega$$

are called *periods* of ω and they indeed determine the periodicity of an elliptic function as E_t corresponds to a lattice as defined above with τ given by

$$\tau = \frac{\int_\gamma \omega}{\int_\delta \omega}.$$

For example one can choose the basis such that we obtain explicitly

$$g_1(t) = \int_{t\leq x\leq 1} \frac{dx}{\sqrt{x\,(x-1)\,(x-t)}}, \tag{3.2.2}$$

$$g_2(t) = \int_{1\leq x\leq \infty} \frac{dx}{\sqrt{x\,(x-1)\,(x-t)}}. \tag{3.2.3}$$

Using the fact that ω and its derivative belong to different cohomology classes, one derives the second order differential equation

$$t\,(t-1)\,\frac{d^2}{dt^2}g(t) + (2t-1)\,\frac{d}{dt}g(t) + \frac{1}{4}g(t) = 0$$

which is solved by the periods. This equation is called *Picard-Fuchs equation* in this context.

In chapter 5 periods of a family of elliptic curves will play an important role in the computation of the massive sunrise integral. In the above example, g_1 and g_2 are functions of t and they evaluate to a certain class of numbers at $t \in \overline{\mathbb{Q}}$. We will use the term period for both, the functions and the numbers they evaluate to at algebraic arguments.

Periods can be defined in a much more general geometrical context as integrals $\int_C \omega$ over n-forms ω and n-chains C defined on varieties with certain properties. In [**134**] Kontsevich and Zagier present a comprehensive theory of these numbers and introduce the following unifying, elementary definition:

Definition 1. (Kontsevich and Zagier [**134**]) A *period* is a complex number whose real and imaginary parts are values of absolutely converging integrals of rational functions with rational coefficients, over domains in $\mathbb{R}^n$ given by polynomial inequalities with rational coefficients.

Equivalently, one obtains the same class of numbers by replacing the word "rational" by "algebraic" in this definition. Let $\mathcal{P}$ denote the set of periods. This set contains all algebraic numbers and many transcendental numbers. However, as the set $\mathcal{P}$ is countable while $\mathbb{C}$ is not, it is clear that not every transcendental number is a period. Therefore periods are an interesting set in between the algebraic and complex numbers:

$$\overline{\mathbb{Q}} \subset \mathcal{P} \subset \mathbb{C}.$$

Clearly, for $t \in \overline{\mathbb{Q}}$ the functions g_1 and g_2 in the above example evaluate to numbers in $\mathcal{P}$. One of many other well-known examples is the number

$$\pi = \iint_{x^2+y^2\leq 1} dx\,dy.$$

From integral representations discussed in the previous chapter, it is furthermore clear that multiple polylogarithms evaluate to periods at algebraic arguments and in particular the set of multiple zeta values is contained in $\mathcal{P}$.

Now let us consider the parametric representation

$$I = \Gamma\left(\nu - L\frac{D}{2}\right)\left(\prod_{i=1}^{N}\int_0^\infty \frac{dx_i x_i^{\nu_i-1}}{\Gamma(\nu_i)}\right)\delta(H)\frac{\mathcal{F}^{L\frac{D}{2}-\nu}}{\mathcal{U}^{(L+1)\frac{D}{2}-\nu}} \tag{3.2.4}$$

for a Feynman integral without irreducible scalar products and let us summarize some of the known correspondences with periods. We distinguish the following cases:

- Assuming a graph without external edges, we set $\mathcal{F} = 1$. We furthermore assume, that for some even integer value of D of interest the integral in (but not necessarily the gamma prefactor) in eq. 3.2.4 is finite. The conditions for this to be the case are well-known from Dyson's power-counting theorem [**101, 204**]. Feynman integrals of this case obviously belong to the set $\mathcal{P}$ and are sometimes called Feynman periods. Due to a correspondence sometimes referred to as "cutting and gluing" (see [**83, 60**]), they are relevant not only for vacuum graphs but also for graphs with one kinematic invariant.
  The idea to view such Feynman integrals as periods of an underlying space arose from the work of Bloch, Esnault and Kreimer [**41**] where a particular Feynman integral was shown to be a period of a motive. This correspondence between Feynman integrals and algebraic geometry was furthermore strengthened in [**14, 15, 16, 87, 60, 61, 155**]. As it was already known from [**55, 56**] that many Feynman periods evaluate to linear combinations of multiple zeta values, the question arose whether this might be a general feature. This question attracted the attention of algebraic geometers as on the other hand multiple zeta values are the periods of certain motives. A related conjecture of Kontsevich on the point-count over finite fields of the zero-set of the first Symanzik polynomial was disproved in [**31**], but the idea to address the mentioned question by such point-counts led to the results of [**69, 66**] which imply, that multiple zeta values are not sufficient to express Feynman periods in general.
  Nevertheless, mathematical properties of Feynman periods are very well studied today [**64, 187, 170, 171**] and for ϕ^4-theory these numbers are known to a very high loop-order [**185**], thanks to the results of Broadhurst and Kreimer [**55, 56**], the numerical methods and the technique of graphical functions invented by Schnetz [**186, 110**] and also thanks to work based on the method of parametric integration [**64, 170, 167, 168**] to be discussed below.
- Let us again set $\mathcal{F} = 1$ but introduce no further assumptions on possible divergences. Viewed as functions of D, such Feynman integrals are known to be Igusa zeta functions. It was shown in [**32**] that the coefficients of the Laurent series (as in eq. 3.1.2) of such integrals are in $\mathcal{P}$.
- Consider the case of generic Symanzik polynomials $\mathcal{U}$ and $\mathcal{F}$. As a trivial consequence of the parametric representation in eq. 3.2.4, every finite number which the Feynman integral evaluates to at some even integer D and algebraic values

of the masses and the kinematic invariants will be in $\mathcal{P}$. In the divergent case, we again consider the Laurent series as in eq. 3.1.2. It was shown in [**48**] that if the integral is evaluated at algebraic values of kinematic invariants and masses in the Euclidean momentum region, i.e. all kinematic invariants non-positive, every coefficient in this series is in $\mathcal{P}$.

We recommend the recent reviews of Brown [**64**] and Todorov [**198**] for further reading.

We already mentioned that the method of parametric integration was influenced by the geometric viewpoint and we will see that it depends strongly on the properties of the Symanzik polynomials whether this method can be applied. Also the method of differential equations benefits from the geometric point of view. We have seen in the example of the Legendre family, that the periods satisfy a differential equation of a particular type, called Picard-Fuchs equations, and it is pointed out in [**134**], that this is true for every period. We refer to [**20**] for a standard reference on Picard-Fuchs equations. In general it is not known how to determine, whether a given linear differential equation is of Picard-Fuchs type. However, Kontsevich and Zagier [**134**] summarize three conjectures, of which one might be particularly interesting with respect to Feynman integrals: A linear differential equation is of Picard-Fuchs type if it only has regular singular points and a monodromy group contained in $SL\left(n, \overline{\mathbb{Q}}\right)$, where n is the order of the equation.

Indeed, the recent literature on differential equations for Feynman integrals has put some emphasis on the property of having only regular singular points and has discussed algorithms to make this property manifest (see [**121**] and references therein). Furthermore, by use of methods for the derivation of Picard-Fuchs equations in algebraic geometry, a new way to derive differential equations was found in [**161, 160**]. We will briefly come back to some of these points below.

At this point let us mention one further interesting aspect of periods, which to the best of our knowledge has not found an explicit application to Feynman integrals so far. It is conjectured in [**134**], that if a period can be expressed by two different integrals, one can pass from one expression to the other by using only the following computational steps, where all functions and domains of integration are algebraic with coefficients in $\overline{\mathbb{Q}}$:

- Additivity:

$$\begin{aligned} \int_a^b \left(f(x)+g(x)\right) dx &= \int_a^b f(x)dx + \int_a^b g(x)dx, \\ \int_a^b f(x)dx &= \int_a^c f(x)dx + \int_c^b f(x)dx. \end{aligned}$$

- Change of variables:

$$\int_{f(a)}^{f(b)} F(y)dy = \int_a^b F\left(f(x)\right) f'(x)dx$$

  for an invertible change of variables $y = f(x)$.

- Newton-Leibniz formula:

$$\int_a^b f'(x)dx = f(b) - f(a).$$

It was shown in [**21**] that if this conjecture is true a similar statement should hold as well for Laurent series, whose coefficients are periods. Therefore we may hope, that this conjecture implies useful restrictions on relations which are possible between Feynman integrals. The standard source of linear relations between Feynman integrals is the IBP method [**83**]. Currently it is not known whether the resulting set of relations is exhaustive or whether other approaches like the ones suggested in [**129, 143**] can provide genuinely new relations.

3.3. The method of differential equations

In [**13**] Almkvist and Zeilberger describe the *method of differentiating under the integral sign* as the following trick, which apparently was one of Feynman's favourite tools to compute integrals [**106**]: Given a function $F(x, y)$ of two variables x and y and being interested in the computation of the integral

$$R(x) = \int_{-\infty}^{\infty} F(x, y)dy,$$

one differentiates $R(x)$ with respect to x, explicitly differentiating $F(x, y)$ under the integral, and, by possibly using changes of variables and integration by parts, one derives a differential equation for $R(x)$. Then one evaluates $R(x)$ and its derivatives at some point, serving for the boundary conditions, and solves the differential equation. In [**13**] a theory of this method is presented for holonomic functions.

A short time later, the same method was introduced to the computation of Feynman integrals by Kotikov [**135**] and Remiddi [**179**] and developed into one of the most powerful techniques in the field since then. Let I be a Feynman integral in momentum space representation and let Φ be its set of inverse scalar propagators P_i and irreducible scalar products S_i and Λ its set of squared particle masses and kinematic invariants. We differentiate I with respect to a chosen $x \in \Lambda$ and (using the same notation as in eq. 3.1.1) we write

$$\frac{d}{dx} I = \left(\prod_{j=1}^{L} \int \frac{d^D k_j}{i\pi^{D/2}} \right) \frac{d}{dx} \frac{1}{\mathcal{D}}$$

with

$$\mathcal{D} = \prod_{i=1}^{N} P_i^{\nu_i} \prod_{j=1}^{B} S_j^{\nu_{N+j}}.$$

We evaluate the differentiation under the integral sign. The result can be expressed as a quotient with the same denominator as the original integrand:

$$\frac{d}{dx} \frac{1}{\mathcal{D}} = \frac{\mathcal{N}}{\mathcal{D}}.$$

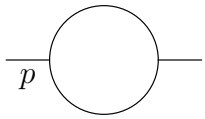


FIGURE 3.3.1. The mass-less one-loop two-point graph

It is a simple but crucial observation that the numerator $\mathcal{N}$ is always a polynomial in Φ whose coefficients are rational functions of $\Lambda \cup \{D\} \cup \{\nu_i\}$. Therefore, we always obtain a differential equation of the type

$$\frac{d}{dx} I = \sum_i c_i I_i$$

where the I_i are scalar Feynman integrals (obtained from I by raising and lowering some of the powers ν_j by integer values) and the coefficients c_i are are rational functions of $\Lambda \cup \{D\} \cup \{\nu_i\}$.

EXAMPLE. For the simple Feynman graph of fig. 3.3.1 we consider the Feynman integral

$$I(\nu_1, \nu_2) = \int \frac{d^D k}{i\pi^{D/2}} \frac{1}{P_1^{\nu_1} P_2^{\nu_2}}$$

with $P_1 = -k^2 + m_1^2$ and $P_2 = -(p-k)^2 + m_2^2$. The integral is a function of p^2, m_1^2, m_2^2 and D. We differentiate with respect to p^2 :

$$\begin{aligned}
\frac{d}{dp^2} I(\nu_1, \nu_2) &= \int \frac{d^D k}{i\pi^{D/2}} \frac{d}{dp^2} \frac{1}{P_1^{\nu_1} P_2^{\nu_2}} \\
&= \frac{1}{2p^2} \int \frac{d^D k}{i\pi^{D/2}} p_\mu \frac{d}{dp_\mu} \frac{1}{P_1^{\nu_1} P_2^{\nu_2}} \\
&= \frac{-\nu_2}{2p^2} \int \frac{d^D k}{i\pi^{D/2}} \frac{-2p^2 + 2k \cdot p}{P_1^{\nu_1} P_2^{\nu_2+1}} \\
&= \frac{-\nu_2}{2p^2} \int \frac{d^D k}{i\pi^{D/2}} \frac{P_1 - P_2 - p^2 + m_1^2 - m_2^2}{P_1^{\nu_1} P_2^{\nu_2+1}} \\
&= \frac{-\nu_2}{2p^2} \left(I(\nu_1 - 1, \nu_2 + 1) - I(\nu_1, \nu_2) + \left(-p^2 + m_1^2 - m_2^2\right) I(\nu_1, \nu_2 + 1) \right).
\end{aligned}$$

We have obtained an ordinary differential equation of the type

$$\frac{d}{dp^2} I + c_0 I = c_1 I_1 + c_2 I_2$$

for $I = I(\nu_1, \nu_2)$, involving new Feynman integrals $I_1 = I(\nu_1 - 1, \nu_2 + 1)$ and $I_2 = I(\nu_1, \nu_2 + 1)$ in the inhomogeneous part.

At this point, the new integrals in the differential equation are usually reduced by use of the IBP method. Without reviewing this method here, let us just focus on the general concept, which is best understood by looking at the bigger picture: As we mentioned

briefly in chapter 1, the typical computation begins with a large number of Feynman integrals which by use of the IBP method are expressed in terms of a smaller set of Feynman integrals, called master integrals. Let us call the latter set M. It depends strongly on the details of the reduction which integrals are in M and the computer programs **[153, 189]** provide ways to choose a preferred selection of integrals. In order to compute the master integrals, we apply the above method to derive a differential equation for each integral in M. We apply the IBP method to the new integrals arising in these equations with the aim to express them in terms of the integrals in M. For this purpose the original set M may have to be extended.

In this way we obtain a system of first order differential equations for the master integrals. Let $\mathcal{I} = (I_1, ..., I_N)^T$ with $N = |M|$ be the vector of all integrals in M in some ordering and let again x be the squared mass or kinematic invariant with respect to which we differentiate. We write the system of differential equations as

$$\frac{d}{dx}\mathcal{I} = A\mathcal{I}$$

where A is an $N \times N$-matrix. Such systems are extensively studied in the recent literature (see e.g. **[121]**). Let us emphasise four relevant questions for such a system:

(1) Are all singular points of A regular?
(2) Is A of Fuchsian type?
(3) Is A triangular?
(4) Is A of the form ϵB where B is an $N \times N$-matrix independent of ϵ?

Questions 1 and 2 are closely related. Let $X = \{x_1, ..., x_n\}$ be the set of singular points of A. A point $x_i \in X$ is regular singular if A has a pole of first order at this point and A is said to be Fuchsian in x_i if this pole is manifest, i.e. if the matrix is of the form $A = \frac{1}{x-x_i}A'$ with A' being regular and non-vanishing at x_i. From the results on Feynman integrals and periods and the conjecture on Picard-Fuchs equations mentioned in section 3.2, we may expect the existence of a system with only regular singular points. This does not necessarily imply, that A is of Fuchsian type. However, if A has only regular singular points, it can always be transformed into a matrix which is Fuchsian with respect to all singular points except for at most one remaining point. We refer to **[144]** and references therein for details. In practice it is very common that A can be transformed into Fuchsian type with respect to all regular singular points, such that we can write

$$A = \sum_{i=1}^{n} \frac{1}{x - x_i} A_i.$$

Let us turn to question 3. If the matrix A is of lower triangular form, i.e.

$$\frac{d}{dx}\begin{pmatrix} I_1 \\ I_2 \\ \vdots \\ I_{|M|} \end{pmatrix} = \begin{pmatrix} A_{11} & 0 & 0 & \dots & 0 \\ A_{21} & A_{22} & 0 & \dots & 0 \\ A_{31} & A_{32} & A_{33} & & \vdots \\ \vdots & & & \ddots & 0 \\ A_{N1} & \dots & & & A_{NN} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \\ \vdots \\ I_N \end{pmatrix},$$

we can attempt to solve the equations for $I_1, ..., I_N$ integral by integral in this ordering. If we have results for the first $n-1$ integrals $I_1, ..., I_{n-1}$, every term in the inhomogeneous part of the differential equation

$$\frac{d}{dx}I_n - A_{nn}I_n = \sum_{i=1}^{n-1} A_{ni}I_i \tag{3.3.1}$$

is determined.

It is very common that these differential equations have to be expanded in the parameter ϵ of dimensional regularization in order to find solutions. This leads to question 4 whose relevance was pointed out by Henn in [**120**]. Let us assume a system of the type

$$\frac{d}{dx}\mathcal{I} = \epsilon B\mathcal{I}$$

where B does not depend on ϵ. In the differential equations

$$\frac{d}{dx}I_n = \epsilon \sum_{i=1}^{n} B_{ni}I_i \tag{3.3.2}$$

for $n = 1, ..., N$ we replace the Feynman integrals by their Laurent series

$$I_n = \sum_{i=a_n}^{\infty} I_n^{(i)}\epsilon^i,$$

each beginning at some integer a_n. We write $I_n^{(i)} = 0$ for $i < a_n$. Separating the orders in ϵ, we obtain differential equations for the coefficients of the integrals:

$$\frac{d}{dx}I_n^{(k)} = \sum_{i=1}^{n} B_{ni}I_i^{(k-1)}$$

for $k \geq a_n$. As the inhomogeneous part in each of these equations only involves coefficients of lower orders one can solve the system iteratively to arbitrary order. The results are built up as iterated integrals. Henn pointed out in [**120**] that many systems of Feynman integrals admit this property and criteria for this to be the case were discussed in [**121**] and references therein. A first algorithm to obtain systems with this explicit property was presented in [**144**] and we mention [**109, 157, 176, 195**] for further recent progress.

Let us now assume a system with regular singular points as expected and the matrix A of Fuchsian type. If also the properties of question 3 and 4 are satisfied, we have a very pleasant situation. Because of the triangular shape of A we can solve the system integral by integral and because of the form $A = \epsilon B$ we obtain solutions order by order

in ϵ in terms of integrals over functions we have already computed in this iteration. As A is of Fuchsian type, we can use a combination of partial fraction decompositions and partial integrations to reduce all integrals which we have to compute to non-elementary integrations of the form

$$I = \int^x \frac{1}{x' - x_i} J(x') dx'. \tag{3.3.3}$$

If all of the functions $J(x')$ are hyperlogarithms, the result is clearly a hyperlogarithm as well. Therefore, by induction, the Feynman integrals satisfying such a system of differential equations can be computed to all orders and the results can be expressed in terms of multiple polylogarithms. Of course we have assumed here, that we know sufficient boundary conditions for each integral.

A systematic solution in terms of hyperlogarithms can still be admissible if only one of the properties of questions 3 and 4 is missing. However, if the answer to both of these questions is "no", i.e. the equations neither decouple nor are they of the form of eq. 3.3.2, we have a substantial problem: We can not use the above concept to build up the solutions in terms of hyperlogarithms by iteratively integrating over results of previous steps.

Let us consider this problem from a slightly different point of view. From every system of N differential equations of first order, we obtain a differential equation of N-th order for the last integral I_N by simple differentiations and eliminations. For example, from

$$\frac{d}{dx} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} I_1 \\ I_2 \end{pmatrix}$$

we obtain the second order differential equation

$$L I_2 = (A'_{21} + A_{21} A_{11})\, I_1$$

with the operator

$$L = \frac{d^2}{dx^2} - A_{22} \frac{d}{dx} - A'_{22} - A_{21} A_{12}$$

and where $A'_{ij} = \frac{d}{dx} A_{ij}$. If $A_{12} = 0$ the above system is of lower triangular form and in this case the operator L factorizes into differential operators of first order:

$$L = \frac{d}{dx} \left(\frac{d}{dx} - A_{22} \right).$$

In the general case of a triangular system of N equations, the corresponding N-th order differential operator for I_N factorizes completely into differential operators of first order. This is another way to see that if the condition of question 3 is satisfied, the solution can be built up in terms of iterated integrals.

The latter perspective is relevant for differential equations for Feynman integrals derived in an alternative approach by Müller-Stach, Weinzierl and Zayadeh [**161, 160**]. Here a given Feynman integral is considered in parametric representation and by use of methods from algebraic geometry [**116**] a Picard-Fuchs differential equation, possibly of

higher order, is derived from the varieties given by the zero-sets of the Symanzik polynomials. If the Picard-Fuchs operator of this equation factorizes into pieces of first order, the result can be constructed as an iterated integral.

In chapter 5 of this thesis, we will consider a system of differential equations for Feynman integrals which fails the conditions of questions 3 and 4. We will see that the corresponding Picard-Fuchs operators do not factorize into operators of first order. However, by use of the elliptic generalizations of polylogarithms to be introduced in chapter 5 we will be able to solve these integrals and even use the concept of iterated integration to provide results to arbitrary order in ϵ.

3.4. The method of parametric integration

The second method for the analytic computation of master integrals which plays a central role in this thesis is the method of parametric integration. Here again the result is built up as an iterated integral. However, in contrast to the method of differential equations, we integrate over Feynman parameters instead of kinematic invariants or squared particle masses. The basic concept was applied early in the literature. However, for a long time, these ideas were applied using quite restricted classes of iterated integrals, for example the Nielsen polylogarithms mentioned in section 2.5, and in general it was not clear for which cases the method would succeed. More recently, Brown presented a comprehensive, modern version of the method [**60**] based on the very general framework of hyperlogarithms and introduced a sufficient, algorithmic criterion for the method to apply to a given integral. The approach is fully implemented in Panzer's program HyperInt [**169**] and in our program MPL [**47, 45**] to be discussed below. Related computational tools were applied in [**3, 4, 58, 92**]. In this section, we briefly recall some main aspects of Brown's work [**60**] and of later refinements.

Before we may apply the method, we have to make sure, that we deal with integrals which are finite at the integer value of the dimension D which we are interested in. For many Feynman integrals this is of course not the case. However, several methods exist by which we can express a given divergent Feynman integral in terms of finite integrals over Feynman parameters. For Feynman integrals with ultraviolet divergences, the method of Brown and Kreimer [**67**] provides a systematic way to introduce counter-terms in the integrand such that the resulting Feynman integral is renormalized. In [**133**] an implementation of this method is reported on and results for the 6-loop beta function and anomalous dimensions of ϕ^4-theory are obtained from parametric integration.

For Feynman integrals with possibly both ultraviolet and infrared divergences, there are methods to expand the integral in ϵ of dimensional regularization such that the coefficients are given as finite integrals over Feynman parameters. One such method widely used for numerical computations is sector decomposition by Binoth and Heinrich [**38**]. We also mention versions of the method of $R^\star$-operations (see [**80, 81, 82, 84, 26**]). For a combination with the method of parametric integration, the method of analytic

regularization by Panzer [**168**], later combined with the IBP-method in [**152**], may be the most appropriate approach. The finite integrals resulting from this decomposition only involve Symanzik polynomials of Feynman graphs in the integrand. Special properties of such polynomials (some of which we mentioned in section 3.1) are usually the reason for the method to succeed.

Let us assume that with the help of one of these methods we have renormalized a given Feynman integral, or we have obtained its Laurent series

$$I = \sum_{k=-2L}^{\infty} I_k \epsilon^k$$

where the I_k are finite integrals over Feynman parameters $x_1, ..., x_N$. The integrands of the latter may be of a slightly more general (however of course D-independent) type compared to the parametric representation of I. Let us consider one of these integrals I_k and let some x_j denote the first Feynman parameter which we want to integrate out. We may assume that the integral is of the type

$$I_k = \int_0^{\infty} \prod_{\substack{i=1 \\ i \neq j}}^{N} dx_i I_k^{(j)} \tag{3.4.1}$$

with

$$I_k^{(j)} = \int_0^{\infty} dx_j \frac{\prod_{Q_i \in \mathcal{Q}} Q_i^{\alpha_i}}{\prod_{P_i \in \mathcal{P}} P_i^{\beta_i}} J(x_j) \tag{3.4.2}$$

where $\mathcal{Q}$, $\mathcal{P} \subset \mathbb{Q}[x_1, ..., x_N]$ are sets of irreducible polynomials whose coefficients possibly depend on squared particle masses and kinematic invariants, all $\alpha_i, \beta_i \in \mathbb{N} \cup \{0\}$ and J is either a constant or a hyperlogarithm whose differential 1-forms are in

$$\Omega_{\text{Hyp}} = \left\{ \frac{dx_j}{x_j}, \frac{dx_j}{x_j - \rho_i} \text{ with } \rho_i = -\frac{P_i|_{x_j=0}}{\frac{\partial P_i}{\partial x_j}}, P_i \in \mathcal{P}_j \right\}$$

where $\mathcal{P}_j \subseteq \mathcal{P} \subset \mathbb{Q}[x_1, ..., x_N]$ is a subset of $\mathcal{P}$ whose polynomials are linear in x_j.

A few remarks about this type of integral are in order. Instead of only two Symanzik polynomials, we allow for an arbitrary number of polynomials in $\mathcal{Q}$, $\mathcal{P}$. We furthermore allow for a hyperlogarithm J whose distinguished variable is x_j. Notice that the differential forms in Ω_{Hyp} are defined such that

$$\frac{dx_j}{P_i} = \frac{dx_j}{x_j - \rho_i} \left(\frac{\partial P_i}{\partial x_j} \right)^{-1} \tag{3.4.3}$$

where $\frac{\partial P_i}{\partial x_j}$ does not depend on x_j due to the condition that P_i is linear in x_j. We can evaluate the integration over x_j and obtain a result in terms of hyperlogarithms if $I_k^{(j)}$

can be reduced to integrands of the type

$$\frac{dx_j}{x_j - a} J\left(x_j\right)$$

where a does not depend on x_j. This is the same integration step as in the method of differential equations with the only difference that here we integrate over a Feynman parameter.

When can this computation be done? The polynomials Q_i are irrelevant for this question, as we can always perform a sequence of partial integrations and partial fraction decompositions such that we only have to consider integrands with unity in the numerator. Only the polynomials in the denominator are relevant for this question. We have to express each dx_j/P_i by in terms of $dx_j/(x_j - a)$ which is only possible if P_i is linear in x_j and leads to eq. 3.4.3. Let us call a polynomial *at most linear* in x_j if it is of degree 0 or 1 in x_j.

Consequently, the integral $I_k^{(j)}$ in eq. 3.4.2 can be computed and the result is obtained in terms of hyperlogarithms if all polynomials in $\mathcal{P}$ are at most linear in x_j. In the computation of the integral I_k in eq. 3.4.1 the result which we obtain for $I_k^{(j)}$ is then an integrand of a next integration and can be written in the same form as the integrand of eq. 3.4.2. We denote the set of polynomials in the denominator of the new integrand by $\mathcal{P}^{(j)}$. More generally, let σ be a permutation on $\{1, ..., N\}$ and let $\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i))}$ denote the set of polynomials in the denominator of the integrand of eq. 3.4.2 after the parameters $x_{\sigma(1)}, x_{\sigma(2)}, ..., x_{\sigma(i)}$ have been integrated out in this order. If a polynomial in $\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i))}$ fails to be at most linear in $x_{\sigma(i+1)}$ then the integration over this variable can not be done with this method and a corresponding set $\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i),\sigma(i+1))}$ does not exist.

By these considerations one arrives at a condition for I_k to be computable with the method of parametric integration: If there is a permutation σ on $\{1, ..., N\}$, defining the ordering of integration variables, such that the sequence of sets

$$\mathcal{P},\ \mathcal{P}^{(\sigma(1))},\ \mathcal{P}^{(\sigma(1),\sigma(2))},\ ...,\ \mathcal{P}^{(\sigma(1),...,\sigma(N))}$$

exists, we can integrate over $x_{\sigma(1)}, x_{\sigma(2)}, ..., x_{\sigma(N)}$ in this order. The condition implies that for every $i = 1, ..., N-1$ every polynomial in $\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i))}$ is at most linear in $x_{\sigma(i+1)}$.

General experience with the method shows, that many Feynman integrals can be computed in this way. A comprehensive overview can be obtained from **[170]**. If an integral I_k can be computed, usually not all permutations $\{1, ..., N\}$ provide an admissible ordering of integration variables. Searching for admissible orderings by trial and error, while not knowing whether they exist at all, would be cumbersome and time consuming in practice.

This search is crucially improved by the *polynomial reduction algorithms* of Brown **[60, 61]**. For a set of irreducible polynomials $\mathcal{P}$ and a permutation σ on $\{1, ..., N\}$, such

an algorithm constructs a sequence

$$S^{\{\sigma(1)\}},\ S^{\{\sigma(1),\sigma(2)\}},\ ...,\ S^{\{\sigma(1),\sigma(2),...,\sigma(k)\}},\ k \leq N, \tag{3.4.4}$$

of sets of irreducible polynomials such that for every $\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i))}$ of the above integration procedure, a corresponding set $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}$ exists and

$$\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i))} \subseteq S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}. \tag{3.4.5}$$

The important advantage of these algorithms is their computational simplicity. The sets $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}$ are constructed just by simple operations on polynomials without evaluating any integral. Therefore, the algorithms can very quickly construct the sequences with respect to all possible permutations σ. Every permutation for which the sequence of eq. 3.4.4 is constructed completely for $k = N$ defines an ordering in which all Feynman parameters can be integrated out.

We recall one of the reduction algorithms [**60**] implemented in Panzer's HyperInt [**169**] and in our program MPL [**45**], which will be discussed in chapter 4 in more detail. For a set $S \subset \mathbb{Q}[x_1, ..., x_N]$ we denote its set of irreducible factors, disregarding constants, by S_{irred}. Following [**60, 61**] and using conventions of [**170**], the basic operations on polynomials P are denoted

$$\begin{aligned}
[P, 0]_i &= P|_{x_i=0}, \\
[P, \infty]_i &= \begin{cases} \frac{\partial P}{\partial x_i} & \text{if } \frac{\partial P}{\partial x_i} \neq 0, \\ P|_{x_i=0} & \text{otherwise,} \end{cases} \\
[P_j, P_k]_i &= \frac{\partial P_j}{\partial x_i} P_k|_{x_i=0} - \frac{\partial P_k}{\partial x_i} P_j|_{x_i=0}.
\end{aligned}$$

Let S be a set of irreducible polynomials at most linear in x_i. One defines the *simple reduction* of S with respect to x_i by

$$S_i = \left\{[P, 0]_i, [P, \infty]_i : P \in S\right\}_{\text{irred}} \cup \left\{[P_j, P_k]_i : P_j, P_k \in S\right\}_{\text{irred}}.$$

By use of this operation, the *Fubini reduction* of the set $\mathcal{P}$ with respect to the permutation σ is constructed as the sequence of sets

$$S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}} = \cap_{k \in \{\sigma(1),\sigma(2),...,\sigma(i)\}} S_k^{\{\sigma(1),\sigma(2),...,\sigma(i)\}\setminus\{k\}}, \tag{3.4.6}$$

where the initial set of the recursion is $S^{\emptyset} = \mathcal{P}$. In the intersection on the right-hand side, only sets $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}\setminus k}$ are included in which all polynomials are at most linear in x_k. If there are none of these sets, $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}$ is not defined.

It is shown in [**60**] that the sets defined by eq. 3.4.6 satisfy eq. 3.4.5. In fact, this statement remains true, if in eq. 3.4.5 we replace $\mathcal{P}^{(\sigma(1),\sigma(2),...,\sigma(i))}$ by $\mathcal{P}^{(\lambda(\sigma(1)),\lambda(\sigma(2)),...,\lambda(\sigma(i)))}$ where λ is any permutation on $\{\sigma(1), \sigma(2), ..., \sigma(i)\}$. In other words, if there is a permutation σ on $\{1, ..., N\}$ such that all sets $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}$ for $i = 1, ..., N$ defined by the Fubini algorithm exist, then the method of parametric integration can be applied and the

Feynman parameters can be integrated out in the ordering given by $x_{\sigma(1)}, ..., x_{\sigma(N)}$. In this case, we say that the initial set $\mathcal{P}$ is *Fubini reducible*.

Notice that according to eq. 3.4.5 the sets $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}$ give an upper bound but might not coincide with the sets of polynomials which will actually appear in the denominators of integrands. In fact it might happen, that a polynomial is contained in some set $S^{\{\sigma(1),\sigma(2),...,\sigma(i)\}}$ but cancels in the integration procedure. If such a polynomial is of degree greater than one in one or several Feynman parameters, the algorithm might stop because of this polynomial and fail to predict the computability of the integral. An attempt to avoid such cases was made in **[61]** with a new algorithm which constructs a more refined upper bound by use of certain compatibilities among the polynomials. A variant of this refined algorithm was later presented in **[170]** and implemented in **[169]**. We have implemented the above Fubini algorithm and the latter version of the refined algorithm in our program MPL.

In conclusion of this chapter, let us briefly return to the question whether a given Feynman integral can be expressed in terms of multiple polylogarithms. We have seen that above methods provide criteria to address this question. The discussion in section 3.3 shows that if the corresponding system of differential equations is of Fuchsian type and can be written in triangular form or admits a special form with respect to ϵ, we can build up the result in terms of hyperlogarithms. In the present section we have furthermore seen that if the Symanzik polynomials (or related polynomials obtained after one of the preliminary procedures to extract the divergences) are Fubini reducible (or reducible with respect to a refined algorithm), then all Feynman parameters can be integrated out and the result is again obtained in terms of hyperlogarithms and can of course be rewritten in terms of multiple polylogarithms (see eq. 2.4.5). Other computational approaches which can not be discussed in detail here provide further criteria. For example if we are able to express a Feynman integral in terms of generalized hypergeometric functions, methods for the expansion of these functions **[71, 70, 124, 125, 159, 128, 127, 130, 206]** imply further sufficient conditions for the integral to be expressible in terms of multiple polylogarithms. For a Feynman integral which can not be expressed in terms of multiple polylogarithms, we expect all of such conditions to fail.

CHAPTER 4

Iterated integrals on moduli spaces of curves and the program MPL

The first direction of our work to be presented in this thesis addresses the computation of a class of Feynman integrals, which can be expressed in terms of multiple polylogarithms, and provides an automatization of the method of parametric integration (see section 3.4). Our main contributions here are our joint article with Brown [**47**] where explicit algorithms for this purpose are presented, and our article [**45**] where the resulting computer program MPL is introduced. Both articles are re-printed in the appendix. In the present chapter, we give an introduction to the main steps of this work.

4.1. Moduli spaces of curves of genus zero

In chapter 2 we have discussed iterated integrals on spaces $\mathbb{C}\backslash\Sigma$ with finite sets $\Sigma \subset \mathbb{C}$ and $0 \in \Sigma$. These integrals were defined by use of differential 1-forms $\frac{dx}{x-\sigma}$ with $\sigma \in \Sigma$ and we have seen that all of these iterated integrals are homotopy invariant by construction. For $\Sigma = \{0, 1\}$ we obtained the classical polylogarithms and multiple polylogarithms in one variable while a generic Σ gives rise to hyperlogarithms, which serve as an integral representation of multiple polylogarithms (see eq. 2.4.5). Due to the fact that hyperlogarithms are defined on a complex one-dimensional space, one of the variables in the arguments of the multiple polylogarithm is distinguished in the latter representation (see section 2.4).

In this chapter, as an alternative to hyperlogarithms, we represent multiple polylogarithms by use of a class of iterated integrals, which are defined on complex m-dimensional spaces with $m \in \mathbb{N}$. These spaces, denoted $\mathcal{M}_{0,n}$ with $n = m+3$, are the moduli spaces of curves of genus zero with n ordered, marked points. Let us briefly introduce these spaces.

Moduli spaces of curves are constructed such that each point of such a space corresponds to an equivalence class of algebraic curves of a given genus, where the equivalence is given by the isomorphisms. There is a canonical bijection between such isomorphism classes and the isomorphism classes of Riemann surfaces (see e.g. [**162**]). Therefore we can equivalently consider each point of the moduli space corresponding to an isomorphism class of Riemann surfaces of the given genus.

Every Riemann surface of genus zero (without further data assigned to it) is isomorphic to the Riemann sphere $\mathbb{C} \cup \{\infty\}$. Hence, there is only one isomorphism class at genus zero and the corresponding moduli space $\mathcal{M}_0$ consists of only one point. More interesting moduli spaces are obtained by marking points on the Riemann surfaces. Let S and S' be two Riemann surfaces of genus zero with n marked points each, $z_1, ..., z_n$ on S and

$z'_1, ..., z'_n$ on S'. We say that S and S' are isomorphic, if there is an isomorphism of Riemann surfaces which maps z_i to z'_i for $i = 1, ..., n$. Despite this restriction, one can show that for Riemann surfaces with $n \leq 3$ marked points such isomorphisms are contained in the group of automorphisms $\mathrm{PGL}_2(\mathbb{C})$ (the Möbius transformations) of the Riemann sphere, and therefore the corresponding moduli spaces still only have one point. However, for $n > 3$ there is more than one isomorphism class.

The moduli spaces of curves of genus zero with n ordered, marked points are

$$\mathcal{M}_{0,n}(\mathbb{C}) = \{(z_1, ..., z_n) \in \mathbb{C}^n \cup \{\infty\} \text{ distinct}\} / \mathrm{PGL}_2(\mathbb{C}).$$

On a Riemann surface with $n \geq 3$ marked points, three of the points can always be mapped to 0, 1 and ∞ by an automorphism in $\mathrm{PGL}_2(\mathbb{C})$. By convention, we can always set

$$z_1 = 0,\ z_{n-1} = 1,\ z_n = \infty.$$

Let us consider the case of $n = 4$ distinct, marked points. The point $z_2 = t_1$ may be located anywhere on the Riemann surface, except of course at $z_1 = 0$, $z_3 = 1$ or $z_4 = \infty$, so we have $t_1 \in \mathbb{C} \setminus \{0, 1\}$. There is an isomorphism class for every possible value, so we can parametrize the corresponding moduli space by t_1 and obtain

$$\mathcal{M}_{0,4} \cong \mathbb{C} \setminus \{0, 1\}.$$

Recall that this is the space on which the iterated integrals for classical polylogarithms and multiple polylogarithms in one variable are defined. For every further marked point on the Riemann surface, every possible location of the point, which of course may not coincide with the previous points, corresponds to a new isomorphism class. One obtains

$$\mathcal{M}_{0,n}(\mathbb{C}) \cong \left\{(t_1, ..., t_{n-3}) \in \mathbb{C}^{n-3} | t_i \neq t_j \text{ and } t_i \notin \{0, 1\} \text{ for } i, j = 1, ..., n-3\right\}.$$

The variables t_i are called *simplicial coordinates*. After the change of variables

$$x_1 = \frac{t_1}{t_2},\ x_2 = \frac{t_2}{t_3}, ...,\ x_{n-4} = \frac{t_{n-4}}{t_{n-3}},\ x_{n-3} = t_{n-3} \tag{4.1.1}$$

the moduli spaces are parametrized as

$$\mathcal{M}_{0,n}(\mathbb{C}) \cong \left\{(x_1, ..., x_{n-3}) \in \mathbb{C}^{n-3} | \prod_{i \leq k \leq j} x_k \notin \{0, 1\} \text{ for all } 1 \leq i \leq j \leq n-3\right\}. \tag{4.1.2}$$

The variables x_i are called *cubical coordinates*. In the following we denote by $m = n - 3$ the dimension of $\mathcal{M}_{0,n}$.

The spaces $\mathcal{M}_{0,n}$ play an important role in algebraic geometry. In [**114**] Goncharov and Manin conjectured, that all periods of these spaces are multiple zeta values. In [**59**] Brown proved this statement and developed a theory of the iterated integrals on $\mathcal{M}_{0,n}$ for this purpose. These integrals are used in the following and our work relies on results of [**59**] to a large extent.

4.2. Differential forms and iterated integrals on $\mathcal{M}_{0,n}$

In simplicial coordinates one considers the differential 1-forms

$$\omega_{ij} = \frac{dt_i - dt_j}{t_i - t_j} \text{ for } 0 \leq i, j \leq m+1 \tag{4.2.1}$$

with $t_0 = 0$ and $t_{m+1} = 1$. They satisfy the linear relations

$$\omega_{ij} = \omega_{ji} \text{ and } \omega_{ii} = 0,$$

and the quadratic relations

$$\omega_{ij} \wedge \omega_{jk} + \omega_{jk} \wedge \omega_{ki} + \omega_{ki} \wedge \omega_{ij} = 0. \tag{4.2.2}$$

The exterior algebra, generated by the $\mathbb{Q}$-span of these 1-forms, modulo the latter quadratic relations is an explicit model for the de Rham cohomology on $\mathcal{M}_{0,n}$ (see [**59**]).

Translating the 1-forms in eq. 4.2.1 to cubical coordinates by eq. 4.1.1 one obtains the set of closed differential 1-forms

$$\Omega_m = \left\{ \frac{dx_1}{x_1}, ..., \frac{dx_m}{x_m}, \frac{d\left(\prod_{a \leq i \leq b} x_i\right)}{\prod_{a \leq i \leq b} x_i - 1} \text{ for } 1 \leq a \leq b \leq m \right\}. \tag{4.2.3}$$

Let $\mathcal{A}_m$ denote the $\mathbb{Q}$-vectorspace spanned by Ω_m. We will work with iterated integrals in these 1-forms.

We define the auxiliary sets

$$\begin{aligned} \bar{\Omega}^F_m &= \left\{ \frac{dx_m}{x_m}, \frac{\left(\prod_{a \leq i \leq m-1} x_i\right) dx_m}{\prod_{a \leq i \leq m} x_i - 1} \text{ for } 1 \leq a \leq m \right\}, \\ \Omega^F_m &= \left\{ \frac{dx_m}{x_m}, \frac{d\left(\prod_{a \leq i \leq m} x_i\right)}{\prod_{a \leq i \leq m} x_i - 1} \text{ for } 1 \leq a \leq m \right\}, \end{aligned}$$

and let $\bar{\mathcal{A}}^F_m$ and $\mathcal{A}^F_m$ denote the $\mathbb{Q}$-vectorspaces spanned by $\bar{\Omega}^F_m$ and Ω^F_m respectively. We notice that

$$\Omega_m = \Omega^F_m \cup \Omega_{m-1} \text{ and } \mathcal{A}^F_m \subseteq \mathcal{A}_m.$$

Furthermore we define the isomorphism

$$\lambda_m : \bar{\mathcal{A}}^F_m \to \mathcal{A}^F_m$$

by

$$\begin{aligned} \frac{dx_m}{x_m} &\mapsto \frac{dx_m}{x_m}, \\ \frac{\left(\prod_{a \leq i \leq m-1} x_i\right) dx_m}{\prod_{a \leq i \leq m} x_i - 1} &\mapsto \frac{d\left(\prod_{a \leq i \leq m} x_i\right)}{\prod_{a \leq i \leq m} x_i - 1}. \end{aligned}$$

For a given m we call λ_m the lift, $\mathcal{A}_m$ the total space, $\bar{\mathcal{A}}^F_m$ the fiber, $\mathcal{A}^F_m$ the lifted fiber and $\mathcal{A}_{m-1}$ the base.

Transforming the quadratic relations to cubical coordinates, we obtain for wedge-products of 1-forms in the lifted fiber:

$$\frac{dx_m}{x_m} \wedge \frac{d\left(x_i ... x_m\right)}{x_i ... x_m - 1} = -\sum_{k=i}^{m-1} \frac{dx_k}{x_k} \wedge \frac{d\left(x_i ... x_m\right)}{x_i ... x_m - 1}, \tag{4.2.4}$$

$$\begin{aligned} \frac{d\left(x_j ... x_m\right)}{x_j ... x_m - 1} \wedge \frac{d\left(x_i ... x_m\right)}{x_i ... x_m - 1} &= \frac{d\left(x_i ... x_{j-1}\right)}{x_i ... x_{j-1} - 1} \wedge \left(\frac{d\left(x_i ... x_m\right)}{x_i ... x_m - 1} - \frac{d\left(x_j ... x_m\right)}{x_j ... x_m - 1} \right) \\ &\quad - \sum_{k=i}^{j-1} \frac{dx_k}{x_k} \wedge \frac{d\left(x_i ... x_m\right)}{x_i ... x_m - 1}. \end{aligned} \tag{4.2.5}$$

Note that on the right-hand side of these relations, one of the factors in each wedge-product is in the base and one is in the lifted fiber. We will make use of this property in the algorithms below.

Let us consider the integrable words of 1-forms in $\mathcal{A}_m$. (Notice that not every word in $\mathcal{A}_m$ is integrable.) According to Chen's theorem [**79**] discussed in section 2.2, every such word defines a homotopy invariant iterated integral for a given path γ. As in section 2.2 we fix all our paths to begin at the origin as a tangential basepoint. As a generalization of eq. 2.3.3 these iterated integrals admit expansions of the type

$$I = \sum_{j=(i_1,...,i_m)} f_j\left(x_1, ..., x_m\right) \prod_{k=1}^{m} \ln\left(x_k\right)^{i_k}$$

where the f_j converge at the origin. Therefore, the regularization of these functions is achieved by re-defining the logarithm at the origin to zero as in section 2.2. We furthermore normalize these functions by the condition that the regularized value vanishes at the origin, i.e.

$$f_{(0,...,0)}\left(0, ..., 0\right) = 0. \tag{4.2.6}$$

Together with these conditions, each integrable word in $\mathcal{A}_m$ determines the iterated integral as a multivalued function on $\mathcal{M}_{0,n}$ whose arguments are given by the end-point of the path. Therefore, using Chen's isomorphism, we will denote each iterated integral $\int_\gamma \omega_1 ... \omega_r$ by the word $\left[\omega_1 | ... | \omega_r\right]$. Recall that according to our conventions, the iterated integration begins with the rightmost 1-form and proceeds to the left.

We define $V\left(\Omega_m\right)$ to be the $\mathbb{Q}$-vectorspace of homotopy invariant iterated integrals of 1-forms in $\mathcal{A}_m$ admitting the above regularization and normalization conditions. Analogously we define $V\left(\bar{\Omega}_m^F\right)$ to be the auxiliary $\mathbb{Q}$-vectorspace of iterated integrals of 1-forms in $\bar{\mathcal{A}}_m^F$, which in fact consists of hyperlogarithms in cubical coordinates.

4.3. The main algorithms

The fact that all iterated integrals in $V\left(\Omega_m\right)$ can be written as words of differential forms in $\mathcal{A}_m$ is a great advantage for practical computations. To give a flavour of how computations are performed in the program MPL, we briefly sketch the main algorithms here, referring to our work with Brown [**47**] for details and to [**59**] for the mathematical foundation.

As a first element of these algorithms we define the map

$$\rho_i : V\left(\bar{\Omega}_m^F\right) \to \Omega_{m-1} \otimes V\left(\bar{\Omega}_m^F\right)$$

as follows: Consider $[\omega_1|...|\omega_r] \in V\left(\bar{\Omega}_m^F\right)$ with 1-forms $\omega_i \in \bar{\Omega}_m^F$ for $i = 1, ..., r$. We take a pair ω_i, ω_{i+1} of neighbouring 1-forms in this word, apply the lift λ_m and then consider the wedge-product of these forms:

$$\lambda_m\omega_i \wedge \lambda_m\omega_{i+1} = \sum_j c_j\eta_j \wedge \alpha_j. \tag{4.3.1}$$

According to the quadratic relations in eqs. 4.2.4 and 4.2.5, this defines certain $\eta_j \in \Omega_{m-1}$, $\alpha_j \in \Omega_m^F$, $c_j \in \mathbb{Q}$ on the right-hand side of the equation. With these terms we define

$$\rho_i\left[\omega_1|...|\omega_r\right] = \sum_j c_j\eta_j \otimes \left[\omega_1|...|\omega_{i-1}|\lambda_m^{-1}\alpha_j|\omega_{i+2}|...|\omega_r\right]. \tag{4.3.2}$$

In other words, the map ρ_i replaces the i-th pair of neighbouring 1-forms by a corresponding wedge-product an pulls the base-factor out of the word. Notice that the words in the second factor on the right-hand side of eq. 4.3.2 are of length $r-1$ and therefore the map ρ_i can serve for recursive computations.

This operation ρ_i is useful for the construction of integrable words in $\mathcal{A}_m$, and hence of homotopy invariant iterated integrals in $V(\Omega_m)$. For this purpose, we define the *symbol map*

$$\Psi : V\left(\bar{\Omega}_m^F\right) \to V(\Omega_m) \tag{4.3.3}$$

by

$$\Psi\left([\omega_i]\right) = [\lambda_n\omega_i], \tag{4.3.4}$$

$$\Psi\left([\omega_{i_1}|...|\omega_{i_r}]\right) = [\lambda_n\omega_{i_1}] \sqcup \Psi\left([\omega_{i_2}|...|\omega_{i_r}]\right) - \sum_{1\le i<r} \sqcup\left((\mathrm{id}\otimes\Psi)\,\rho_i\left[\omega_{i_1}|...|\omega_{i_r}\right]\right), \tag{4.3.5}$$

with $1 < r$ and where $\sqcup w_1w_2 = w_1 \sqcup w_2$ denotes the concatenation of words w_1, w_2. In order to see that $\Psi\left([\omega_1|...|\omega_r]\right)$ is an integrable word for any $w \in V\left(\bar{\Omega}_m^F\right)$, we recall Chen's integrability condition in eq. 2.2.11. As we are working with closed differential forms, the condition simplifies to

$$\sum_{j=1}^{r-1} [\omega_1|...|\omega_{j-1}|\omega_j \wedge \omega_{j+1}|\omega_{j+2}|...|\omega_r] = 0.$$

We see that every $\Psi\left([\omega_1|...|\omega_r]\right)$ satisfies this condition by construction, as by a wedge-multiplication applied to the right-hand side of eq. 4.3.5 we obtain the difference between the left-hand side and the right-hand side of the quadratic relation eq. 4.3.1, and hence obtain zero.

The symbol map Ψ is the unique linear map which satisfies the relation

$$(id \otimes \Psi) \circ \nabla_T = d \circ \nabla_T$$

where the total connection

$$\nabla_T : V\left(\bar{\Omega}_m^F\right) \to \mathcal{A}_m \otimes V\left(\bar{\Omega}_m^F\right) \tag{4.3.6}$$

is computed as

$$\nabla_T [\omega_1|...|\omega_r] = d[\omega_1|...|\omega_r] - \sum_{1\leq i<r} \rho_i [\omega_1|...|\omega_r]$$

with the ordinary differentiation

$$d[\omega_1|\omega_2|...|\omega_r] = \omega_1 \otimes [\omega_2|...|\omega_r]. \tag{4.3.7}$$

An alternative algorithm for Ψ, making use of the correspondence to these differentiations, is discussed in [**46**].

The symbol map is related to the symbol as constructed in [**113, 115, 100**] and was named after this correspondence. The symbol as used in the latter constructions and the image of the symbol map Ψ both have the crucial property to satisfy the differential equations of multiple polylogarithms with respect to all variables. For a hyperlogarithm $w \in V\left(\bar{\Omega}_m^F\right)$ which represents the multiple polylogarithm, this statement is only true with respect to one variable. Furthermore, in contrast to common notions of the symbol, the function $\Psi(w)$ is actually identical to the corresponding multiple polylogarithm due to the above regularization and normalization conditions.

In [**59**] it was shown that there is an isomorphism of algebras

$$V(\Omega_m) \cong V(\Omega_{m-1}) \otimes V\left(\bar{\Omega}_m^F\right). \tag{4.3.8}$$

As a consequence, the vectorspace $V(\Omega_m)$ can be recursively constructed by

$$\mu(id \otimes \Psi) : V(\Omega_{m-1}) \otimes V\left(\bar{\Omega}_m^F\right) \to V(\Omega_m)$$

where μ denotes the multiplication, performed by the shuffle product. Let $V_k(\Omega_m) \subset V(\Omega_m)$ be the subspace of iterated integrals $[\omega_1|...|\omega_r] \in V(\Omega_m)$ with $r \leq k$. Then the mentioned construction provides a unique basis $V_k(\Omega_m)$ for each k. Furthermore in the other direction, each element of $V(\Omega_m)$ can be decomposed into elements of $V(\Omega_{m-1}) \otimes V\left(\bar{\Omega}_m^F\right)$ by a so-called unshuffle map. See [**47, 45**] for details and examples.

The main application of the algorithms is the computation of a certain class of definite integrals and ultimately of Feynman integrals. For this purpose, primitives and limits have to be computed. Let us at first consider the case of hyperlogarithms. For a 1-form $\omega_0 \in \bar{\Omega}_m^F$ and a hyperlogarithm $[\omega_1|...|\omega_r] \in V\left(\bar{\Omega}_m^F\right)$, the primitive is simply obtained by left-concatenation of the 1-form to the word: $\omega_0 \sqcup [\omega_1|...|\omega_r] = [\omega_0|\omega_1|...|\omega_r]$. This is a direct consequence of the differential equation eqs. 2.4.4 and 4.3.7. If we proceeded in the same simple way with functions in $V(\Omega_m)$, we would clearly generate iterated integrals which fail the integrability condition and do not belong to $V(\Omega_m)$ anymore. A theorem of [**59**] implies that $V(\Omega_m)$ is closed under taking primitives, so it is always possible to construct primitives in $V(\Omega_m)$.

A naive computation of such primitives would take a detour via hyperlogarithms: We could use the unshuffle map to express a function in $V(\Omega_m)$ in terms of hyperlogarithms, then we could apply simple left-concatination as above, and finally map the result back to $V(\Omega_m)$ by use of the symbol map. Such a computation would be more cumbersome than necessary.

It is more efficient to use the following auxiliary structures instead: For $0 \leq i < k$ we define $C_i(\Omega_m)_k$ to be the $\mathbb{Q}$-vector space of words $[\omega_1|...|\omega_k]$ of length k with $\omega_1, ..., \omega_i \in \Omega_{m-1}$, $\omega_{i+1} \in \Omega_m^F$ and $\omega_j \in \Omega_m$ for all $i+1 < j \leq k$. In the following construction, these words are not necessarily integrable and therefore they might not represent functions. For $i < k$ we define the map

$$\star_i : C_{i-1}(\Omega_m)_k \to C_i(\Omega_m)_k$$

by

$$\begin{aligned} \star_i[\omega_1|...|\omega_{i-1}|\omega_i|\omega_{i+1}|...|\omega_k] &= [\omega_1|...|\omega_{i-1}|\omega_{i+1}|\omega_i|...|\omega_k] \qquad \text{if } \omega_{i+1} \in \Omega_{m-1}, \\ \star_i[\omega_1|...|\omega_{i-1}|\omega_i|\omega_{i+1}|...|\omega_k] &= -\sum_j c_j[\omega_1|...|\omega_{i-1}|\eta_j|\alpha_j|\omega_{i+2}|...|\omega_k] \qquad \text{if } \omega_{i+1} \in \Omega_m^F, \end{aligned}$$

where the c_j, η_j, α_j are defined by the quadratic relation

$$\omega_i \wedge \omega_{i+1} = \sum_j c_j \eta_j \wedge \alpha_j.$$

Notice the similarities with eqs. 4.3.2 and 4.3.1. By use of this map, the primitive of a function $[\omega_1|...|\omega_k] \in V(\Omega_m)$ with respect to a 1-form $\omega_0 \in \bar{\Omega}_m^F$ is constructed as

$$\omega_0 \star [\omega_1|...|\omega_k] = (1 + \star_1 + \star_2 \star_1 + ... + \star_k ... \star_1)[\lambda_m \omega_0|\omega_1|...|\omega_k]. \tag{4.3.9}$$

A further ingredient for the computation of definite integrals is the derivation of certain limits of functions in $V(\Omega_m)$. In order to compute integrals from 0 to 1, we need to compute limits at these values. Considering the underlying moduli space $\mathcal{M}_{0,n}$ of eq. 4.1.2 we notice that each such point can be reached from inside the m-dimensional unit-cube via a continuous path starting at the origin. Due to our normalization condition eq. 4.2.6, all functions in $V(\Omega_m)$ are defined to vanish at the origin. Another special point is

$$(x_1, ..., x_m) = (1, ..., 1) \notin \mathcal{M}_{0,n}.$$

In order to compute limits at this point, one considers the compactification $\overline{\mathcal{M}}_{0,n}$ which is defined by use of a blow-up of this point to a higher-dimensional hypersurface. For example, in the showcase of $m = 2$, the point $(1, 1)$ is blown-up to a line such that the unit-square is deformed to a pentagon. For our computations, this compactification has the important implication, that multiple limits will depend on the ordering in which they are computed. Different orderings of limits can be thought of as different directions from which the blown-up point is approached. For example in the case $m = 2$, the two-fold limits $\lim_{x_1 \to 1} \lim_{x_2 \to 1}$ and $\lim_{x_2 \to 1} \lim_{x_1 \to 1}$ will lead to different results in general. For details we refer to **[59]** and section 2.4.3 of **[47]**.

We briefly sketch the algorithm for the computation of limits $\lim_{x_i \to u} f$ with $u \in \{0,1\}$, $f \in V(\Omega_m)$, $1 \leq i \leq m$. It is known from **[59]** that every such limit is a $\mathcal{Z}$-linear combination of elements of $V(\Omega_{m-1})$, where $\mathcal{Z}$ is the $\mathbb{Q}$-vectorspace of multiple zeta values (eq. 2.1.10). The main strategy of the computation is to expand f as a series in $x_i = u$ and to evaluate the coefficient of $\ln(x_i - u)^0$. In this computation, one iteratively uses the isomorphism 4.3.8 to reduce the problem to the one-variable case $V(\Omega_1)$, i.e. the multiple polylogarithms in one variable. For the latter case, the limits at $u = 0$ are zero by our normalization and the limits at $u = 1$ can be obtained in terms of multiple zeta values by a well-known procedure (see e.g. **[63]**), relying on basic properties of iterated integrals such as eq. 2.2.2.

With combinations of the above algorithms, we are in the position to compute integrals of the type

$$I = \int_0^1 dx_m \frac{q}{\prod_i p_i^{a_i}} f \tag{4.3.10}$$

analytically. Here $f \in V(\Omega_m)$, the a_i are non-negative integers, q is some polynomial in the x_i and the p_i are in $\left\{x_m, 1 - \prod_{j=1}^m x_i | 1 \leq j \leq m\right\}$, i.e. they coincide with denominators of 1-forms in $\bar{\Omega}_m^F$. We refer to these as *cubical integrals*. Such integrals arise as period integrals of the moduli spaces $\mathcal{M}_{0,n}$ and in many other contexts, such as irrationality proofs for zeta values (see **[35, 65]**) or the expansion of hypergeometric functions. Several of such examples are computed in **[45, 47]**.

However, our main interest in cubical integrals is given by the fact, that they can be used in the computation of Feynman integrals by the method of parametric integration (section 3.4). We apply the following steps:

- We apply one of the techniques mentioned in section 3.4 to express the Feynman integral I in terms of finite parametric integrals of the type

$$I_k = \prod_{i=1}^N \int_0^\infty d\alpha_i \frac{\prod_{Q_i \in \mathcal{Q}} Q_i^{\alpha_i}}{\prod_{P_i \in \mathcal{P}} P_i^{\beta_i}} J(\alpha_j) \tag{4.3.11}$$

  with the integrand defined as in eqs. 3.4.1 and 3.4.2. We use the letter α for Feynman parameters here, to avoid confusion with the cubical coordinates. Each of these integrals gives rise to a set $\mathcal{P} = \{P_1, ...\}$ of relevant polynomials in the denominator of the integrand and in the denominator of the differential 1-forms defining the hyperlogarithm J. If we have used one of the techniques of **[67, 168, 152]**, these polynomials will be Symanzik polynomials.
- We attempt the polynomial reduction of $\mathcal{P}$. If this set is reducible with respect to one of the algorithms discussed in section 3.4, we choose an admissible ordering of Feynman parameters $\alpha_{\sigma(1)}, ..., \alpha_{(N)}$, given by a permutation σ on $\{1, ..., N\}$. It is important to notice, that the reducibility of the polynomials depends strongly on the chosen parametrization of the kinematic invariants. According to the chosen order, we iterate the following steps for each parameter.

- With respect to the next Feynman parameter, say α_j, a change of variables[1] given in [**47**] is applied, such that the integral is partly expressed in terms of cubical integrals as in eq. 4.3.10 and the integration over α_j from 0 to infinity is expressed as integration over x_m from 0 to 1.
- The integral over x_m is computed by use of the above algorithms. The result is a $\mathcal{Z}$-linear combination of functions in $V(\Omega_{m-1})$.
- By the inverted change of variables, we express the result in terms of only Feynman parameters again. There is a subtlety in this step: The functions in $V(\Omega_{m-1})$ and the hyperlogarithms in the Feynman parameters are each normalized to vanish at the origins of the corresponding parameter spaces, but these are two different points in general. Our way of translating iterated integrals on $\mathcal{M}_{0,n}$ to hyperlogarithms has to regard this difference in the normalization conditions, as detailed in [**47**]. In this computation, certain multiple limits of the involved functions have to be computed. As our above algorithms only allow for the computation of limits at variables equal to $u \in \{0, 1\}$, approaching these points from inside the unit-cube, there are cases of integrals, for which a change of variables where only such limits are necessary, can not be constructed. As a consequence, this last step gives rise to a further, technical restriction on the class of Feynman integrals which can be computed with the above algorithms. We say that the set $\mathcal{P}$ is *properly ordered* at the tangential basepoint 0 if this condition is satisfied. The condition is not a restriction to the general method of parametric integration. We have commented on these points in great detail in section 4.2 of [**45**].

For a Feynman integral admitting the mentioned conditions, this procedure provides an analytical result. Except for the first step, the entire computation is automated in the program MPL [**45**] to be discussed as follows.

4.4. The program MPL

MPL is a publicly available computer program based on the computer algebra system Maple for computations with multiple polylogarithms in terms of iterated integrals on the moduli spaces $\mathcal{M}_{0,n}$. A special focus lies on the computation of Feynman integrals by the method of parametric integration. The program is based on the algorithms of [**47**] as summarized above and was introduced in [**45**]. Additional details and examples are given in a user manual obtained with the program. In this section we highlight some main features of MPL.

Let us demonstrate how certain functions are represented in MPL for the example of the multiple polylogarithm

$$\mathrm{Li}_{1,1}(x_1, x_2) = \sum_{0<j_1<j_2} \frac{x_1^{j_1} x_2^{j_2}}{j_1 j_2}.$$

[1] I want to thank Erik Panzer again for his help with this step.

At first we notice, that this function satisfies the differential equations

$$\frac{\partial}{\partial x_1}\mathrm{Li}_{1,1}(x_1,x_2) = -\left(\frac{1}{x_1}+\frac{1}{1-x_1}\right)\mathrm{Li}_1(x_1\cdot x_2)+\frac{1}{1-x_1}\mathrm{Li}_1(x_2), \tag{4.4.1}$$

$$\frac{\partial}{\partial x_2}\mathrm{Li}_{1,1}(x_1,x_2) = \frac{1}{1-x_2}\mathrm{Li}_1(x_1\cdot x_2). \tag{4.4.2}$$

By use of eq. 2.4.5 the function can be expressed as a hyperlogarithm:

$$\mathrm{Li}_{1,1}\left(\frac{\sigma_2}{\sigma_1},\frac{z}{\sigma_2}\right) = L_{\sigma_2,\sigma_1}(z) = \int_0^z \frac{dz'}{z'-\sigma_2}\int_0^{z'}\frac{dz''}{z''-\sigma_1}. \tag{4.4.3}$$

Using

$$x_1 = \frac{\sigma_2}{\sigma_1},\ x_2 = \frac{z}{\sigma_2} \tag{4.4.4}$$

and the bar-notation we obtain the representation

$$\mathrm{Li}_{1,1}(x_1,x_2) = \left[\frac{dx_2}{1-x_2}|\frac{x_1dx_2}{1-x_1x_2}\right]. \tag{4.4.5}$$

The differential 1-forms of the latter expression are in $\bar{\Omega}_2^F$ and we recognize this hyperlogarithm as a function in $V\left(\bar{\Omega}_2^F\right)$.

In order to work with this hyperlogarithm in MPL, we have to declare our set of cubical coordinates at first. After the command

```
>MPLCoordinates(x, 2):
```

we can compute with `x[1]`, `x[2]` as cubical coordinates. Making use of the bar-notation, the above hyperlogarithm is expressed as

```
>f:=bar((d(x[2])/(1-x[2]),x[1]*d(x[2])/(1-x[1]*x[2]);
```

Now we make use of the symbol map ψ of eq. 4.3.3 to obtain the corresponding iterated integral in $V(\Omega_2)$. Applying

```
>MPLSymbolMap(f);
```

the program returns

```
bar(d(x[2])/(1-x[2]), (x[2]*d(x[1])+x[1]*d(x[2]))/(-x[1]*x[2]+1))
-bar(d(x[1])/(1-x[1]), (x[2]*d(x[1])+x[1]*d(x[2]))/(-x[1]*x[2]+1))
+bar(d(x[1])/(1-x[1]), d(x[2])/(1-x[2]))
-bar(d(x[1])/x[1], (x[2]*d(x[1])+x[1]*d(x[2]))/(-x[1]*x[2]+1))
```

So we have the representation

$$\mathrm{Li}_{1,1}(x_1,x_2) = \left[\frac{dx_2}{1-x_2}-\frac{dx_1}{1-x_1}-\frac{dx_1}{x_1}|\frac{d(x_1x_2)}{1-x_1x_2}\right]+\left[\frac{dx_1}{1-x_1}|\frac{dx_2}{1-x_2}\right] \tag{4.4.6}$$

where the latter expression is in $V(\Omega_2)$.

The difference between the representations of eq. 4.4.5 and of eq. 4.4.6 is best understood by differentiating the latter. We have introduced total differentiation of iterated integrals in eq. 4.3.7 as simple de-concatination of the left-most 1-form[2]. Applying this

[2]In MPL, the command `MPLd` serves for this simple operation.

operation to the iterated integral in eq. 4.4.6 we obtain

$$d\left(\left[\frac{dx_2}{1-x_2}-\frac{dx_1}{1-x_1}-\frac{dx_1}{x_1}|\frac{d\left(x_1x_2\right)}{1-x_1x_2}\right]+\left[\frac{dx_1}{1-x_1}|\frac{dx_2}{1-x_2}\right]\right)$$

$$=\left(\frac{dx_2}{1-x_2}-\frac{dx_1}{1-x_1}-\frac{dx_1}{x_1}\right)\otimes\left[\frac{d\left(x_1x_2\right)}{1-x_1x_2}\right]+\frac{dx_1}{1-x_1}\otimes\left[\frac{dx_2}{1-x_2}\right]. \tag{4.4.7}$$

Noticing that

$$\mathrm{Li}_1\left(x_1\cdot x_2\right)=\left[\frac{d\left(x_1x_2\right)}{1-x_1x_2}\right]\text{ and }\mathrm{Li}_1\left(x_2\right)=\left[\frac{dx_2}{1-x_2}\right]$$

we see that eq. 4.4.7 clearly expresses the differential behaviour of $\mathrm{Li}_{1,1}$ with respect to both variables as given in eqs. 4.4.1 and 4.4.2. On the contrary, in the representation of eq. 4.4.5 only the differential behaviour with respect to the second variable x_2 is manifest. We see that it is a special feature of iterated integrals in $V\left(\Omega_m\right)$ to have the differential behaviour of multiple polylogarithms with respect to all m variables, similar to the mentioned constructions of the symbol in the literature. By use of the command `MPLBasis(x,m,w)` a unique basis of the subspace of $V\left(\Omega_m\right)$ including words up to length w can be automatically generated. Let us just mention that further basic operations such as generating the sets of 1-forms $\bar{\Omega}_m^F$ and Ω_m, the shuffle multiplication of iterated integrals, the mentioned unshuffle map and the total connection ∇_T of eq. 4.3.6 are implemented in MPL as well.

We continue this discussion with the computation of primitives. Let us consider the multiple polylogarithm

$$\mathrm{Li}_{1,2}(x_1,x_2)=\sum_{0<j_1<j_2}\frac{x_1^{j_1}x_2^{j_2}}{j_1j_2^2}.$$

This function can be represented by the hyperlogarithm $-L_{0,\sigma_2,\sigma_1}\left(z\right)$, defined by

$$L_{0,\sigma_2,\sigma_1}\left(z\right)=\int_0^z\frac{dz'}{z'}L_{\sigma_2,\sigma_1}\left(z'\right) \tag{4.4.8}$$

with σ_1,σ_2 as in eq. 4.4.4. Notice that L_{σ_2,σ_1} on the right-hand side was used in eq. 4.4.3 to represent the function $\mathrm{Li}_{1,1}$. In bar-notation and cubical coordinates, the hyperlogarithm L_{0,σ_2,σ_1} reads

$$\left[\frac{dx_2}{x_2}|\frac{dx_2}{1-x_2}|\frac{x_1dx_2}{1-x_1x_2}\right]\in V\left(\bar{\Omega}_2^F\right). \tag{4.4.9}$$

We see again that in the bar-notation of hyperlogarithms, the integration on the right-hand side of eq. 4.4.8 is simply done by left-concatenation of the corresponding 1-form, in this case of $\frac{dx_2}{x_2}$.

Let us now consider the integration of a function of $V\left(\Omega_2\right)$ instead. We consider the representation

$$f=\left[\frac{dx_2}{1-x_2}-\frac{dx_1}{1-x_1}-\frac{dx_1}{x_1}|\frac{d\left(x_1x_2\right)}{1-x_1x_2}\right]+\left[\frac{dx_1}{1-x_1}|\frac{dx_2}{1-x_2}\right]\in V\left(\Omega_2\right) \tag{4.4.10}$$

of the function $\mathrm{Li}_{1,1}$ given in eq. 4.4.6 and compute the indefinite integral

$$F = \int \frac{dx_2}{x_2} f.$$

As we mentioned in section 4.3, there are two ways to do this computation. As a first option, we may consider the hyperlogarithm corresponding to f (given in eq. 4.4.5), then perform left-concatenation to obtain eq. 4.4.9 and finally apply the symbol map ψ. Alternatively, we can apply the algorithm for the operator $\star$ of eq. 4.3.9. The latter strategy is implemented in the MPL procedure `MPLPrimitive` by which F is computed as

```
>MPLPrimitive(d(x[2])/x[2],f,3);
```

which leads to the result

$$\begin{aligned} F \;=\; & \left[\frac{dx_2}{x_2}|\frac{dx_2}{1-x_2} - \frac{dx_1}{1-x_1} - \frac{dx_1}{x_1}|\frac{d\,(x_1x_2)}{1-x_1x_2}\right] - \left[\frac{dx_1}{1-x_1} + \frac{dx_1}{x_1}|\frac{dx_1}{x_1} + \frac{dx_2}{x_2}|\frac{d\,(x_1x_2)}{1-x_1x_2}\right] \\ & + \left[\frac{dx_2}{x_2}|\frac{dx_1}{1-x_1}|\frac{dx_2}{1-x_2}\right] + \left[\frac{dx_1}{1-x_1}|\frac{dx_2}{x_2}|\frac{dx_2}{1-x_2}\right]. \end{aligned}$$

The application of the symbol map ψ to eq. 4.4.9 leads to the same expression. Clearly, F is the representation of $\mathrm{Li}_{1,2}(x_1, x_2)$ in $V\,(\Omega_2)$.

Limits of functions in $V\,(\Omega_m)$ are computed with the command `MPLLimit` and more generally, several limits can be conveniently computed with the command `MPLMultipleLimit`. To give an example, let us again consider the iterated integral f of eq. 4.4.10 and let us define the lists of equations

```
>S1:=[x[1]=1, x[2]=1]:
>S2:=[x[2]=1, x[1]=1]:
```

which define two orderings of limits. Computing

```
>MPLMultipleLimit(f,S1);
0
>MPLMultipleLimit(f,S2);
-ζ(2)
```

shows that

$$\lim_{x_j\to 1}\left(\lim_{x_i\to 1} f\right) = \begin{cases} 0 & \text{for } i=1,\, j=2, \\ -\zeta(2) & \text{for } i=2,\, j=1. \end{cases}$$

In all computations of limits and definite integrals, MPL returns exact multiple zeta values in symbolic notation. In order to obtain simplified expressions, it is convenient to use MPL together with a program to express multiple zeta values in terms of a basis. In our computations we have applied the basis of [**37**] for this purpose.

Definite integrals of cubical type as defined in eq. 4.3.10 can be computed by use of the command `MPLCubicalIntegrate`. As an example, let us consider the integrand

$$g = \frac{{x_1}^3\,(1-x_1)\,{x_2}^4\,(1-x_2)\,{x_3}^3\,(1-x_3)\,{x_4}^2\,(1-x_4)^2}{(1-x_1x_2x_3)^2\,(1-x_2x_3x_4)^2\,(1-x_1x_2x_3x_4)^2\,(1-x_1x_2)}.$$

After declaring the four cubical coordinates x_1, x_2, x_3, x_4 by

```
>MPLCoordinates(x, 4):
```

we integrate over all four variables from 0 to 1 by

```
>MPLCubicalIntegrate(g,x[4],4);
```

and obtain

$$\left(\prod_{i=1}^{4}\int_0^1 dx_i\right) g = \frac{5}{3}\zeta(3) + \frac{26}{9}\zeta(2) - \frac{17}{5}\left(\zeta(2)\right)^2 + \frac{22}{9}.$$

As we mentioned above, such integrals arise in many contexts and give rise to possible applications of the program MPL beyond particle physics.

We conclude this chapter with the main purpose of the program: the computation of Feynman integrals. Let us assume that by use of one of the strategies mentioned in section 4.3 we have expressed a given Feynman integral in terms of finite integrals of the type of eq. 4.3.11 over Feynman parameters $a_1, ..., a_N$. Let M furthermore be the number of kinematic invariants and squared particle masses which the Feynman integral depends on and let us denote these variables by $a_{N+1}, ..., a_T$ where $T = N + M$. In order to compute with these variables and corresponding differential 1-forms in Maple, we have to begin with the declaration

```
>defform(a=0):
```

The integrand defines a set of relevant polynomials $\mathcal{P}$ in these variables. In a first step, we apply

```
>R:=MPLPolynomialReduction(P,aList);
```

where the first argument is the set $\mathcal{P}$ of polynomials and the second argument is the list of all Feynman parameters. The program returns a list whose elements correspond to the sets $S^{\{\sigma(1),\sigma(2),...,\sigma(k)\}}$ of polynomials as in eq. 3.4.4. Depending on the value of a global variable which can be changed by the user, these sets are either constructed by use of the Fubini reduction algorithm [**60**] (see section 3.4) or by the refined version which uses compatibility graphs [**61, 170**]. From this result, all orderings with respect to which $\mathcal{P}$ is reducible are easily extracted.

We furthermore check the technical condition of properly ordered $\mathcal{P}$ as mentioned at the end of section 4.3. This condition, which implies that all multiple limits necessary for the changes of variables between Feynman parameters and cubical coordinates can be approached from inside the unit-cube, is tested by use of the command

```
>MPLCheckOrder(R, FP, AP);
```

Here the first argument is the list generated by the previous command `MPLPolynomialReduction`. The second argument is the list of Feynman parameters, ordered such that reducibility is satisfied (assuming the existence of such an ordering). The third argument is the list of all parameters, including the kinematic invariants and particle masses. The program returns a message to inform the user, whether the chosen ordering is permissible.

Assuming that this is the case, the integral can be computed with the command

```
>MPLFeynmanIntegrate(I, FP, AP);
```

Here the first argument is the integrand, written as in eq. 4.3.11 and the second and third argument are the same as in the previous command. The program returns the result as a $\mathcal{Z}$-linear combination of hyperlogarithms which are defined in terms of the kinematic invariants and squared masses. Notice that only the parameters in the second argument are integrated out, so we can easily generate intermediate results by canceling Feynman parameters in this list. Detailed examples of Feynman integral computations with MPL can be found in [**47, 45**] and in the user manual attached to the program. MPL also includes procedures supporting the comparison of results with Panzer's program [**169**].

CHAPTER 5

Elliptic generalizations of polylogarithms and the sunrise and kite integrals

In chapter 3 we have quickly reviewed the method of differential equations and the method of parametric integration which both allow us to compute Feynman integrals in terms of multiple polylogarithms, if certain conditions are satisfied. In the case of the first method, the system of differential equations has to be of triangular shape or admit a certain property with respect to ϵ of dimensional regularization, while in the other case, the polynomials in the integrand have to be reducible. Usually, the integrals can be written in several ways and it will depend on choices of master integrals or parametrizations whether the conditions are satisfied respectively. However, for some Feynman integrals it is quite clear, that these methods will not succeed, as long as they rely on the use of multiple polylogarithms. In order to address such cases, we have to search for an appropriate alternative class of functions. This search motivates our second line of research, summarized in this chapter.

In this search, we take a special point of view which can be motivated by the material of the previous chapters: We have seen that the use of multiple polylogarithms is very advantageous in the computation of Feynman integrals, in particular due to their double-nature as nested sums and iterated integrals. If we have to use a different class of functions, it would be very desirable to still keep these advantages if possible. Therefore, we will prefer functions which are obtained as further generalizations of polylogarithms.

In our joint work with Adams and Weinzierl [**8, 11**] we have introduced such a class of generalizations beyond multiple polylogarithms. By use of these functions, we have been able to compute Feynman integrals associated to the sunrise graph fig. 1.0.2 (a) in [**8, 9, 11**]. In joint work with the same authors and Schweitzer we have applied this framework furthermore to the kite graph of fig. 1.0.2 (b) in [**6**]. These Feynman integrals admit the mentioned problem that they can not be expressed in terms of multiple polylogarithms. In this chapter, we discuss our generalized framework of functions and summarize the main aspects of our sunrise and kite computations.

5.1. A class of elliptic generalizations of polylogarithms

The class of functions introduced in our work with Adams and Weinzierl [**8, 11**] is related to an elliptic curve in a special way. We have already recalled in the example at the beginning of section 3.2 that a cell of points $L = \mathbb{Z} + \tau\mathbb{Z}$ in the complex plane with $\mathrm{Im}(\tau) > 0$ is isomorphic to an elliptic curve E. We mentioned that a function f on the

complex plane is called elliptic with respect to L if it satisfies

$$f(x) = f(x + \lambda) \tag{5.1.1}$$

for λ being a point in the lattice L.

Let us introduce a simple change of variables and consider the function $f'(z)$ of $z \in \mathbb{C}^\star$ given by

$$f'\left(e^{2\pi i x}\right) = f\left(x\right).$$

If f is elliptic with respect to L, the function f' clearly satisfies

$$f'\left(z\right) = f'\left(zq\right) \tag{5.1.2}$$

where $q = e^{2\pi i \lambda}$ for $\lambda \in L$. There is a simple way to construct functions which satisfy the latter equation. If there is an auxiliary function $g(z)$ such that the sum

$$f'(z) = \sum_{n \in \mathbb{Z}} g\left(zq^n\right) \tag{5.1.3}$$

is defined, the latter will satisfy eq. 5.1.2 by construction.

This principle was used to define *elliptic polylogarithms*. A first version of an elliptic dilogarithm was defined by Bloch in [**40**]. For the single-valued Bloch-Wigner dilogarithm

$$D(z) = \mathrm{Im}\left(\mathrm{Li}_2\left(z\right) + \ln\left(1 - z\right)\ln\left|z\right|\right),\ z \in \mathbb{C}\backslash\left\{0, 1\right\},$$

the elliptic dilogarithm of [**40**] is defined as

$$D\left(q; z\right) = \sum_{n \in \mathbb{Z}} D\left(zq^n\right),\ |q| < 1. \tag{5.1.4}$$

The series converges with exponential rapidity for every complex value of z. Based on a generalization of the Bloch-Wigner dilogarithm to single-valued polylogarithms by Ramakrishnan [**178**], elliptic polylogarithms were defined by Zagier in [**208**]. Further versions of elliptic polylogarithms were studied thereafter [**30, 107, 147, 207**]. In particular, let us mention the functions

$$E_m^{\mathrm{BL}}(z; u; q) = \sum_{n \in \mathbb{Z}} u^n \mathrm{Li}_m\left(zq^n\right) \tag{5.1.5}$$

defined by Brown and Levin [**68**], where u is a certain damping factor to guarantee the convergence. In the same reference, the authors furthermore develop a theory of elliptic multiple polylogarithms and a corresponding framework of iterated integrals. In the following discussion, we will use the term *elliptic* more loosely, to distinguish new versions of generalized polylogarithms from the ones discussed in previous chapters. We will use the term for functions given by power series in the nome q of an elliptic curve. Our functions will not necessarily satisfy eq. 5.1.2. We always assume $|q| < 1$.

A first computation of a Feynman integral in terms of an elliptic polylogarithm was achieved by Bloch and Vanhove in [**44**]. Here the sunrise integral (to be discussed below) in $D = 2$ space-time dimensions and in the case of three equal particle masses was expressed

in terms of an elliptic dilogarithm defined as

$$E_\Theta(q) = \sum_{n\geq 0} h\left(q^n\right) - \frac{h\left(1\right)}{2} \tag{5.1.6}$$

where

$$h\left(x\right) = \frac{i}{2}\left(\mathrm{Li}_2\left(xr_6^5\right) + \mathrm{Li}_2\left(xr_6^4\right) - \mathrm{Li}_2\left(xr_6^2\right) - \mathrm{Li}_2\left(xr_6\right)\right)$$

with the n-th root of unity defined as

$$r_n = e^{\frac{2\pi i}{n}}.$$

Differences between this function and the elliptic dilogarithm of eq. 5.1.4 are discussed in the mentioned reference.

The class of elliptic generalizations of polylogarithms defined in our joint work with Adams and Weinzierl is related to the functions above. In [**8**] we define

$$\mathrm{ELi}_{n;m}(x;y;q) = \sum_{j=1}^{\infty}\sum_{k=1}^{\infty}\frac{x^j}{j^n}\frac{y^k}{k^m}q^{jk}. \tag{5.1.7}$$

and in [**11**] we define the multivariate generalization

$$\mathrm{ELi}_{n_1,\ldots,n_l;m_1,\ldots,m_l;2o_1,\ldots,2o_{l-1}}\left(x_1,\ldots,x_l;y_1,\ldots,y_l;q\right)$$

$$= \sum_{j_1=1}^{\infty}\ldots\sum_{j_l=1}^{\infty}\sum_{k_1=1}^{\infty}\ldots\sum_{k_l=1}^{\infty}\frac{x_1^{j_1}}{j_1^{n_1}}\ldots\frac{x_l^{j_l}}{j_l^{n_l}}\frac{y_1^{k_1}}{k_1^{m_1}}\ldots\frac{y_l^{k_l}}{k_l^{m_l}}\frac{q^{j_1k_1+\ldots+j_lk_l}}{\prod_{i=1}^{l-1}\left(j_ik_i+\ldots+j_lk_l\right)^{o_i}}. \tag{5.1.8}$$

We will refer to these as *ELi-functions*. Multiplication of any of these functions with the $(l=1)$-case $\mathrm{ELi}_{n;m}$ and integration over $\frac{dq}{q}$ leads to a result in the same class of functions. Explicitly we have

$$\mathrm{ELi}_{n_1,\ldots,n_l;m_1,\ldots,m_l;2o_1,\ldots,2o_{l-1}}\left(x_1,\ldots,x_l;y_1,\ldots,y_l;q\right)$$

$$= I^{o_1}\mathrm{ELi}_{n_1;m_1}(x_1;y_1;q')\mathrm{ELi}_{n_2,\ldots,n_l;m_2,\ldots,m_l;2o_2,\ldots,2o_{l-1}}\left(x_2,\ldots,x_l;y_2,\ldots,y_l;q'\right) \tag{5.1.9}$$

where the operator I^{o_i} denotes the o_i-fold integration

$$I^{o_i} = \int_0^q \frac{dq_1}{q_1}\int_0^{q_1}\frac{dq_2}{q_2}\ldots\int_0^{q_{o_i-2}}\frac{dq_{o_i-1}}{q_{o_i-1}}\int_0^{q_{o_i-1}}\frac{dq'}{q'} \text{ for } o_i > 0$$

and $I^0 = 1$. This property will be crucial in our use of these functions with the method of differential equations.

In the computations of Feynman integrals discussed below, these functions appear in specific combinations which we will refer to as *E-functions*. They are defined by

$$\mathrm{E}_{n;m}(x;y;q) = \begin{cases} \frac{1}{i}\left(\frac{1}{2}\mathrm{Li}_n(x) - \frac{1}{2}\mathrm{Li}_n(x^{-1}) + \mathrm{ELi}_{n;m}(x;y;q) - \mathrm{ELi}_{n;m}(x^{-1};y^{-1};q)\right) & \text{for } n+m \text{ even}, \\ \frac{1}{2}\mathrm{Li}_n(x) + \frac{1}{2}\mathrm{Li}_n(x^{-1}) + \mathrm{ELi}_{n;m}(x;y;q) + \mathrm{ELi}_{n;m}(x^{-1};y^{-1};q) & \text{for } n+m \text{ odd}, \end{cases} \tag{5.1.10}$$

and for $l > 1$ by

$$\mathrm{E}_{n_1,\ldots,n_l;m_1,\ldots,m_l;2o_1,\ldots,2o_{l-1}}\left(x_1,\ldots,x_l;y_1,\ldots,y_l;q\right) =$$

(5.1.11)
$$I^{o_1}\left(\mathrm{E}_{n_1;m_1}(x_1;y_1;q') - \mathrm{E}_{n_1;m_1}(x_1;y_1;0)\right)\mathrm{ELi}_{n_2,\ldots,n_l;m_2,\ldots,m_l;2o_2,\ldots,2o_{l-1}}\left(x_2,\ldots,x_l;y_2,\ldots,y_l;q'\right).$$

In the case of the kite graph it will be convenient to use a slightly different combination without classical polylogarithms, defined by

$$\overline{\mathrm{E}}_{n;m}(x;y;q) = \begin{cases} \frac{1}{i}\left(\mathrm{ELi}_{n;m}(x;y;q) - \mathrm{ELi}_{n;m}(x^{-1};y^{-1};q)\right) & \text{for } n+m \text{ even}, \\ \mathrm{ELi}_{n;m}(x;y;q) + \mathrm{ELi}_{n;m}(x^{-1};y^{-1};q) & \text{for } n+m \text{ odd}, \end{cases} \tag{5.1.12}$$

$$\overline{\mathrm{E}}_{n_1,\ldots,n_l;m_1,\ldots,m_l;0,2o_2,\ldots,2o_{l-1}}\left(x_1,\ldots,x_l;y_1,\ldots,y_l;q\right) =$$

$$\overline{\mathrm{E}}_{n_1;m_1}(x_1;y_1;q)\overline{\mathrm{E}}_{n_2,\ldots,n_l;m_2,\ldots,m_l;2o_2,\ldots,2o_{l-1}}\left(x_2,\ldots,x_l;y_2,\ldots,y_l;q\right) \tag{5.1.13}$$

and

$$\overline{\mathrm{E}}_{n_1,\ldots,n_l;m_1,\ldots,m_l;2(o_1+1),\ldots,2o_{l-1}}\left(x_1,\ldots,x_l;y_1,\ldots,y_l;q\right) =$$

$$\int_0^q \frac{dq'}{q'}\overline{\mathrm{E}}_{n_1,\ldots,n_l;m_1,\ldots,m_l;2o_1,\ldots,2o_{l-1}}\left(x_1,\ldots,x_l;y_1,\ldots,y_l;q'\right). \tag{5.1.14}$$

We summarize some relations with known functions. Firstly, the $l = 1$ cases of the ELi-functions can be written as the series of classical polylogarithms

$$\mathrm{ELi}_{n;m}(x;y;q) = \sum_{k=1}^{\infty}\frac{y^k}{k^m}\mathrm{Li}_n(q^k x).$$

Notice that the sum here is over the positive integers while the summation in eq. 5.1.3 is over all integers. The negative integers are however included implicitly in the E-functions and we can derive relations with the functions of Brown and Levin of eq. 5.1.5. For example, by use of the functional relation eq. 2.4.6 we obtain [**10**]

$$\begin{aligned} \mathrm{E}_{2;0}(x;y;q) &= \frac{1}{i}\left(E_2^{\mathrm{BL}}(x;y;q) - \frac{1}{2}\frac{1+y}{1-y}\zeta(2) - \frac{1}{4}\frac{1+y}{1-y}\ln^2(-x)\right. \\ &\left. -\frac{y}{(1-y)^2}\ln(-x)\ln(q) - \frac{1}{2}\frac{y\,(1+y)}{(1-y)^3}\ln^2(q)\right). \end{aligned} \tag{5.1.15}$$

Relations between E_Θ of eq. 5.1.6 and the ELi- or E-functions can be derived as well. Furthermore the functions $\mathrm{E}_{n;m}(x;y;q)$ evaluate to Clausen- and Glaisher-functions for q going to zero (see [**9**]). We recall that Clausen functions are defined by

$$\mathrm{Cl}_n(\varphi) = \begin{cases} \frac{1}{2i}\left(\mathrm{Li}_n\left(e^{i\varphi}\right) - \mathrm{Li}_n\left(e^{-i\varphi}\right)\right) & \text{for } n \text{ even}, \\ \frac{1}{2}\left(\mathrm{Li}_n\left(e^{i\varphi}\right) + \mathrm{Li}_n\left(e^{-i\varphi}\right)\right) & \text{for } n \text{ odd}, \end{cases}$$

and Glaisher functions are defined by

$$\mathrm{Gl}(\varphi) = \begin{cases} \frac{1}{2}\left(\mathrm{Li}_n\left(e^{i\varphi}\right) + \mathrm{Li}_n\left(e^{-i\varphi}\right)\right) & \text{for } n \text{ even}, \\ \frac{1}{2i}\left(\mathrm{Li}_n\left(e^{i\varphi}\right) - \mathrm{Li}_n\left(e^{-i\varphi}\right)\right) & \text{for } n \text{ odd}. \end{cases}$$

We have the relations

$$\lim_{q\to 0}\mathrm{E}_{n;m}\left(e^{i\varphi};y;q\right)=\mathrm{Cl}_n\left(\varphi\right)$$

for m being zero or even and

$$\lim_{q\to 0}\mathrm{E}_{n;m}\left(e^{i\varphi};y;q\right)=\mathrm{Gl}_n\left(\varphi\right)$$

for m being odd.

We conclude this quick review of functions with a remark on the q-exponential function

$$e_q(z)=\frac{1}{\prod_{n=0}^{\infty}\left(1-zq^n\right)},\ |z|<1,$$

and its logarithm

$$\ln\left(e_q(z)\right)=\sum_{n=0}^{\infty}\sum_{m=1}^{\infty}\frac{z^m}{m}q^{mn}$$

as studied in **[131, 212]**. Due to a certain resemblance in the limit of q going to 1, the latter function was named *quantum dilogarithm* in **[212]**. This function is obviously related to one of the ELi-functions by

$$\ln\left(e_q(z)\right)=\mathrm{Li}_1(z)+\mathrm{ELi}_{1;0}(z;1;q).$$

We expect many other correspondences between ELi- or E-functions and interesting q-series. In particular, it would be very desirable to exhibit relations to elliptic multiple zeta values (e.g. **[57]**) or other q-analogues of multiple zeta values (e.g. **[22]**) in future work.

5.2. The massive sunrise integral

The massive sunrise graph of fig. 1.0.2 (a) was considered by many authors **[23, 29, 28, 27, 33, 44, 43, 42, 53, 54, 72, 74, 73, 88, 89, 90, 117, 118, 127, 138, 175, 180, 181]**. To this graph we associate the scalar Feynman integral

$$S(D,\,t)=\int\frac{d^Dk_1d^Dk_2}{\left(i\pi^{D/2}\right)^2}\frac{1}{\left(-k_1^2+m_1^2\right)\left(-k_2^2+m_2^2\right)\left(-\left(p-k_1-k_2\right)^2+m_3^2\right)}\tag{5.2.1}$$

where we define the kinematic invariant as

$$t=p^2.$$

For the general case of D space-time dimensions and arbitrary particle masses, a full result was presented in **[33]**. This result is a linear combination of Lauricella functions of type C, which are defined as

$$F_C(a_1,a_2;b_1,b_2,b_3;x_1,x_2,x_2,x_3)=\sum_{0\le j_1}\sum_{0\le j_2}\sum_{0\le j_3}\frac{\left(a_1\right)_{j_1+j_2+j_3}\left(a_2\right)_{j_1+j_2+j_3}}{\left(b_1\right)_{j_1}\left(b_2\right)_{j_2}\left(b_3\right)_{j_3}}\frac{x_1^{j_1}}{j_1!}\frac{x_2^{j_2}}{j_2!}\frac{x_3^{j_3}}{j_3!}$$

with the Pochhammer symbol

$$\left(a\right)_n=\frac{\Gamma\left(a+n\right)}{\Gamma\left(a\right)}.$$

As the Feynman integral is divergent in $D = 4$ dimensions, a Laurent expansion in the regularization parameter is required. As the arguments a_1, a_2 and b_1, b_2, b_3 are rational functions of D, the Lauricella functions F_C would have to be expanded at $D = 4$ for this purpose. Today, several powerful approaches for the expansion of generalized hypergeometric functions are available. The resulting series usually involve multiple polylogarithms in the coefficients. However, to the best of our knowledge, none of these techniques suffices for an expansion of generic Lauricella functions of type C in terms of multiple polylogarithms or another well-understood class of functions[1]. In this sense, it is not possible to extract poles in say $\epsilon = 4 - D/2$ from the mentioned result. The missing expansion of the functions F_C can be seen as one manifestation of the problem, that this integral can not be expressed in terms of multiple polylogarithms alone.

In the Feynman parametric representation of eq. 3.1.5 the sunrise integral reads

$$S(D,\, t) = \Gamma\left(3 - D\right) \left(\prod_{i=1}^{3} \int_0^\infty dx_i \right) \delta\left(H\right) \frac{\mathcal{U}^{3-3\frac{D}{2}}}{\mathcal{F}^{3-D}}$$

where the Symanzik polynomials are

$$\mathcal{U} = x_1 x_2 + x_2 x_3 + x_1 x_3, \tag{5.2.2}$$

$$\mathcal{F} = -x_1 x_2 x_3 t + \left(x_1 m_1^2 + x_2 m_2^2 + x_3 m_3^2\right)\left(x_1 x_2 + x_2 x_3 + x_1 x_3\right). \tag{5.2.3}$$

The second Symanzik polynomial $\mathcal{F}$ is quadratic in each of the three Feynman parameters. Therefore, the set $\{\mathcal{U},\, \mathcal{F}\}$ is obviously not reducible with respect to the algorithms discussed in section 3.4 and the method of parametric integration fails. A change of variables to safe the reducibility could not be found. This is the second manifestation of the mentioned problem.

Thirdly, the differential equations arising from the sunrise integral do not admit the properties discussed in section 3.3 which would be necessary to obtain a solution in terms of multiple polylogarithms. The differential equations involve the tadpole integral

$$T\left(D, m^2\right) = \int \frac{d^D k}{i\pi^{\frac{D}{2}}} \frac{1}{\left(-k^2 + m^2\right)} = \Gamma\left(1 - \frac{D}{2}\right) \left(m^2\right)^{\frac{D}{2}-1}$$

in the inhomogeneous part. For the general case of D dimensions and arbitrary particle masses, one obtains a fourth-order differential equation

$$L_4(D) S(D,\, t) = c_{12} T_{12} + c_{13} T_{13} + c_{23} T_{23} \tag{5.2.4}$$

with a differential operator

$$L_4(D) = P_4 \frac{d^4}{dt^4} + P_3 \frac{d^3}{dt^3} + P_2 \frac{d^2}{dt^2} + P_1 \frac{d}{dt} + P_0$$

and with

$$T_{ij} = T\left(D, m_i^2\right) T\left(D, m_j^2\right).$$

[1] In [**7**] we have derived an expansion in terms of unevaluated infinite sums over Z-sums

The coefficients $P_0, P_1, P_2, P_3, P_4, c_{12}, c_{13}, c_{23}$ are polynomials in the squared particle masses, in D and in t. They are listed explicitly in [**9**]. This differential equation can either be extracted from the results of [**72**], derived by use of the method [**161**] or generated by the program Reduze [**194, 153**].

In the case of three equal particle masses,

$$S^{\rm em}(D,\,t) = S(D,\,t)|_{m_1=m_2=m_3=m},$$

the sunrise integral in D dimensions satisfies a second order differential equation

$$L_2^{\rm em} S^{\rm em}(D,\,t) = -6m^4 T\left(D, m^2\right)^2 \tag{5.2.5}$$

with a differential operator

$$L_2^{\rm em}(D) = P_2^{\rm em}\frac{d^2}{dt^2} + P_1^{\rm em}\frac{d}{dt} + P_0^{\rm em}$$

whose coefficients $P_0^{\rm em}, P_1^{\rm em}, P_2^{\rm em}$ are polynomials in m^2, t, D [**54, 138**].

Differential operators will be denoted by

$$L_{r,i}^{(j)}(D).$$

Here the space-time dimension is indicated in the argument and the subscript r is the order of the operator. In the case that the operator is obtained from an expansion in ϵ at a special value of D, the superscript j denotes the order in ϵ. The number i is an additional label to distinguish several operators whose numbers r, D, j are the same. In the following discussion, we will consider the cases of $D = 2$ and $D = 4$ space-time dimensions. As in these cases neither one of the differential operators in eqs. 5.2.4 and 5.2.5 factorizes into pieces of only first order, the solutions can not be constructed in terms of multiple polylogarithms only. Instead the results are obtained in terms of the generalizations defined above as ELi- and E-functions.

5.3. The case of two dimensions

The starting point of our series of computations is the sunrise integral $S(D,\,t)$ in $D = 2$ dimensions with three non-zero, arbitrary particle masses. Without loss of generality we assume

$$0 < m_1 \leq m_2 \leq m_3.$$

In $D = 2$ dimensions the sunrise integral is finite. Its parametric representation simplifies to

$$S(2,t) = \left(\prod_{i=1}^{3}\int_0^\infty dx_i\right)\delta\left(H\right)\frac{1}{\mathcal{F}},$$

so the integrand involves only the second Symanzik polynomial eq. 5.2.3. We may as well consider this function as an integral in projective space

$$S(2,t) = \int_\sigma \frac{\omega}{\mathcal{F}}$$

with

$$\begin{aligned}\omega &= x_1 dx_2 \wedge dx_3 + x_2 dx_3 \wedge dx_1 + x_3 dx_1 \wedge dx_2, \\ \sigma &= \left\{[x_1 : x_2 : x_3] \in \mathbb{P}^2 | x_i \geq 0, i = 1, 2, 3\right\}.\end{aligned}$$

Using the polynomial $\mathcal{F}$, Müller-Stach, Weinzierl and Zayadeh [**160**] derived a second-order differential equation

$$L_2(2) S(2, t) = p_3 \tag{5.3.1}$$

with a Picard-Fuchs operator

$$L_2(2) = p_2 \frac{d^2}{dt^2} + p_1 \frac{d}{dt} + p_0. \tag{5.3.2}$$

The coefficients p_0, p_1, p_2 are polynomials in the squared masses and t while p_3 furthermore involves logarithms of the squared masses.

A key to a solution of this equation and all further steps is the consideration of an elliptic curve arising from the second Symanzik polynomial. Here we generalize ideas of the work of Bloch and Vanhove [**44**] to the case of arbitrary masses. We consider the variety defined by

$$\mathcal{F} = 0$$

and the Euclidean momentum region where

$$t \leq 0.$$

This condition guarantees that the variety of $\mathcal{F}$ intersects the integration domain only at its boundary. We have an intersection only in the three points

$$Q_1 = [1 : 0 : 0], \, Q_2 = [0 : 1 : 0], \, Q_3 = [0 : 0 : 1]. \tag{5.3.3}$$

We consider these points as three possible choices for an origin. Together with such a choice, the zero-set of $\mathcal{F}$ defines an elliptic curve. We denote the elliptic curve with the origin Q_i by E_i with $i = 1, 2, 3$. In each case, the elliptic curve can be transformed into Weierstrass normal form

$$\hat{E} : \, y^2 z = 4x^3 - g_2 x z^2 - g_3 z^3. \tag{5.3.4}$$

Here x, y, z are polynomials in the squared masses, the Feynman parameters and in t. The explicit changes of variables are given in [**8**].

Following standard literature on elliptic curves, we consider the chart $z = 1$ of the Weierstrass normal form. Here we have

$$\begin{aligned}g_2 &= -4\left(e_1 e_2 + e_2 e_3 + e_1 e_3\right), \\ g_3 &= 4 e_1 e_2 e_3\end{aligned}$$

and the factorization of the cubical polynomial in x

$$y^2 = 4\left(x - e_1\right)\left(x - e_2\right)\left(x - e_3\right)$$

with the three roots

$$\begin{aligned} e_1 &= \frac{1}{24}\left(-t^2+2Mt+\Delta+3\sqrt{\delta}\right), \\ e_1 &= \frac{1}{24}\left(-t^2+2Mt+\Delta-3\sqrt{\delta}\right), \\ e_1 &= \frac{1}{24}\left(2t^2-4Mt-2\Delta\right), \end{aligned}$$

where

$$\begin{aligned} M &= m_1^2+m_2^2+m_3^2, \\ \Delta &= \mu_1\mu_2\mu_3\mu_4, \\ \delta &= \left(t-\mu_1^2\right)\left(t-\mu_2^2\right)\left(t-\mu_3^2\right)\left(t-\mu_4^2\right), \\ 0 &= e_1+e_2+e_3 \end{aligned}$$

with

$$\mu_1 = m_1+m_2-m_3,\ \mu_2 = m_1-m_2+m_3,\ \mu_3 = -m_1+m_2+m_3,\ \mu_1 = m_1+m_2+m_3.$$

We define the period integrals (cf. the standard example in section 3.2)

$$\psi_1 = 2\int_{e_2}^{e_3}\frac{dx}{y} \text{ and } \psi_2 = 2\int_{e_1}^{e_3}\frac{dx}{y}.$$

It is well-known that these integrals can be written as complete elliptic integrals of the first kind

$$K(z) = \int_0^1 \frac{dz}{\sqrt{\left(1-z^2\right)\left(1-x^2z^2\right)}}.$$

We have

$$\psi_1 = \frac{4}{\delta^{\frac{1}{4}}}K(k) \text{ and } \psi_2 = \frac{4i}{\delta^{\frac{1}{4}}}K(k')$$

with

$$k = \sqrt{\frac{e_3-e_2}{e_1-e_2}} \text{ and } k' = \sqrt{\frac{e_1-e_3}{e_1-e_2}}.$$

These period integrals are solutions of the homogeneous differential equation

$$L_2(2)\psi_i = 0 \text{ for } i = 1,2,$$

with the above Picard-Fuchs operator.

In **[7]** we used the period integrals to construct a solution of eq. 5.3.1 as

$$S(2,t) = S(2,0) + S_{\text{special}}(t)$$

where the boundary value $S(2,0)$ is a linear combination of Clausen functions Cl_2 obtained from **[149, 34, 90]**. By classical variation of constants, the special solution reads

$$S_{\text{special}}(t) = \int_0^t dt' \frac{p_3(t')}{p_2(t')W(t')}\left(\psi_1(t)\psi_2(t_1)+\psi_2(t)\psi_1(t_1)\right)$$

with the Wronski determinant

$$W(t) = \psi_1(t)\frac{d}{dt}\psi_2(t) - \psi_2(t)\frac{d}{dt}\psi_1(t).$$

By use of two associated period integrals and the Legendre relation, the special solution is simplified. We arrive at a result in terms of integrals over complete elliptic integrals in [**7**]. Similar functions have been used in the literature before, e.g. in [**138**] and also later in [**52, 180, 181**].

The success of iterated integrals in the computation of Feynman integrals serves as our main motivation to consider elliptic generalizations of polylogarithms as an alternative. We partly follow the mentioned work by Bloch and Vanhove which leads to the mentioned result of the equal-mass case of $S(2,t)$ in terms of the elliptic dilogarithm E_Θ of eq. 5.1.6. In [**8**] we use the above periods ψ_1, ψ_2 to define the ratio

$$\tau = \frac{\psi_2}{\psi_1} \tag{5.3.5}$$

and the nome

$$q = e^{i\pi\tau}$$

of the elliptic curve given by $\mathcal{F}$. The dependence on the kinematic invariant t is now expressed as a dependence of q and by slight abuse of notation we write $S(2,t) = S(2,q)$ and $\psi_1(t) = \psi_1(q)$. One can show that t and q are related by

$$\frac{t}{\delta} = -\frac{\eta\left(\frac{\tau}{2}\right)^{24}\eta\left(2\tau\right)^{24}}{m_1^2 m_2^2 m_3^2 \eta\left(\tau\right)^{48}}$$

with Dedekind's η-function

$$\eta\left(\tau\right) = q^{\frac{1}{12}}\prod_{n=1}^{\infty}\left(1-q^{2n}\right).$$

We find that the sunrise integral in $D = 2$ dimensions can be expressed as

$$S\left(2,q\right) = \frac{\psi_1(q)}{\pi}\sum_{j=1}^{3}\mathrm{E}_{2;0}\left(w_j(q);-1;-q\right) \tag{5.3.6}$$

where $\mathrm{E}_{2;0}$ is the elliptic dilogarithm defined in eq. 5.1.10. The arguments w_1, w_2, w_3 of this function are obtained from the three intersection points of eq. 5.3.3 and the transformations which the elliptic curve has implicitly undergone so far in this discussion. Notice that we started from three elliptic curves E_i, $i = 1,2,3$, given by $\mathcal{F} = 0$ and the three possible choices Q_i as the origin. After a first change of variables, we arrived at the same Weierstrass normal form $\hat{E}$ of eq. 5.3.4 in each case. The periods obtained from this representation define the quotient τ of eq. 5.3.5 which defines a lattice L as in fig. 3.2.1, discussed in the example of section 3.2. Here, gluing together boundaries of the lattice, the elliptic curve $\mathbb{C}/L$ is viewed as a torus. This is the parametrization of the beginning of section 5.1 where we discussed the periodicity of elliptic functions with respect to $x \to x + \lambda$ with $\lambda \in L$. Finally, as we have seen in the further discussion of section 5.1, this condition turns into the periodicity with respect to $z \to zq$ after a change of variables

$z = e^{2\pi i x}$. By this change, we have arrived at the Jacobi uniformization $\mathbb{C}^\star/q^{2\mathbb{Z}}$. It is clear from our discussion in section 5.1 that arguments of elliptic polylogarithms should be given in this parametrization and the arguments w_1, w_2, w_3 are indeed obtained as a result of the mentioned mappings:

$$E_i \to \hat{E} \to \mathbb{C}/L \to \mathbb{C}^\star/q^{2\mathbb{Z}}.$$

The explicit expressions are given in [**8**].

Compared with our previous result in terms of integrals over elliptic integrals, the result of eq. 5.3.6 has numerous obvious advantages. Firstly, the expression is very compact and reveals the nature of the sunrise integral as a product of a period and an elliptic polylogarithm which both are derived from the same elliptic curve. The period is a well-known elliptic integral and no further unevaluated integrations are involved here. The function $\mathrm{E}_{2;0}$ is understood as an elliptic generalization of the dilogarithm, belonging to the class of E-functions discussed in section 5.1 which admits an iterated integral structure due to eq. 5.1.11.

It is worth to emphasize again that the case of $D = 2$ dimensions satisfies the optimal preconditions for the above considerations: The integral is finite and involves only one Symanzik polynomial which defines our elliptic curve. In the remaining sections of this thesis, we will make the remarkable observation, that we can still make use of the above principles in cases where some of these conditions are violated. In sections 5.4 and 5.5 we consider the case $D = 4$ and higher orders in ϵ respectively. Here the integrand involves also the first Symanzik polynomial. In section 5.6 we consider the kite integral whose integrand involves two different Symanzik polynomials. Nevertheless, we will be able to use the same framework of functions and even the same nome q.

5.4. Four dimensions

The dimension shift relations of Tarasov [**196, 197**] relate Feynman integrals of different space-time dimensions and different powers of propagators. To keep track of these propagator powers, let us define the family of sunrise integrals

$$S_{\nu_1\nu_2\nu_3}(D,\, t) = \int \frac{d^D k_1 d^D k_2}{\left(i\pi^{D/2}\right)^2} \frac{1}{\left(-k_1^2+m_1^2\right)^{\nu_1}\left(-k_2^2+m_2^2\right)^{\nu_2}\left(-\left(p-k_1-k_2\right)^2+m_3^2\right)^{\nu_3}}$$

with ν_1, ν_2, ν_3 taking integer values. Obviously, the integral defined in eq. 5.2.1 is the member $S_{111}(D,\, t)$ of this family. In the Feynman parametric representation, the family of integrals reads

$$S_{\nu_1\nu_2\nu_3}(D,\, t) = \Gamma\left(|\nu| - D\right) \int_\sigma \omega \left(\prod_{i=1}^{3} \frac{x_i^{\nu_i-1}}{\Gamma\left(\nu_i\right)}\right) \frac{\mathcal{U}^{\nu-\frac{3}{2}D}}{\mathcal{F}^{\nu-D}}$$

with $\nu = \nu_1+\nu_2+\nu_3$ and with the above definitions for $\omega, \sigma, \mathcal{U}, \mathcal{F}$. For this family, Tarasov's relations read

$$S_{\nu_1\nu_2\nu_3}(D,\, t) = \nu_1\nu_2 S_{(\nu_1+1)(\nu_2+1)\nu_3}\left(D+2, t\right) + \nu_2\nu_3 S_{\nu_1(\nu_2+1)(\nu_3+1)}\left(D+2, t\right) + \nu_1\nu_3 S_{(\nu_1+1)\nu_2(\nu_3+1)}\left(D+2, t\right)$$

and we furthermore have

$$\frac{d}{dt}S_{\nu_1\nu_2\nu_3}(D,\,t) = \nu_1\nu_2\nu_3 S_{(\nu_1+1)(\nu_2+1)(\nu_3+1)}\,(D+2,t)\,.$$

In [**9**] we consider the sunrise integral in $D = 4-2\epsilon$ dimensions:

$$S_{111}(4-2\epsilon,\,t) = S_{111}^{(-2)}(4,t)\epsilon^{-2} + S_{111}^{(-1)}(4,t)\epsilon^{-1} + S_{111}^{(0)}(4,t) + \mathcal{O}\,(\epsilon)$$

with the known pole terms

$$\begin{aligned} S_{111}^{(-2)}(4,t) &= -\frac{1}{2}M, \\ S_{111}^{(-1)}(4,t) &= \frac{1}{4}t - \frac{3}{2}M + \sum_{i-1}^{3} m_i^2 \ln\left(m_i^2\right). \end{aligned}$$

By use of the above dimension shift relations, $S_{111}(4-2\epsilon,\,t)$ can be expressed in terms of four integrals of the sunrise family in $D = 2-2\epsilon$ dimensions. For the coefficient $S_{111}^{(0)}(4,t)$ we obtain a linear combination

$$S_{111}^{(0)}(4,t) = c + \tilde{L}_0 S_{111}^{(0)}(2,t) + \tilde{L}_1 S_{111}^{(1)}(2,t) \tag{5.4.1}$$

where $S_{111}^{(0)}$ and $S_{111}^{(1)}$ are defined by the expansion

$$S_{111}(2-2\epsilon,\,t) = S_{111}^{(0)}(2,t) + S_{111}^{(1)}(2,t)\epsilon + \mathcal{O}\left(\epsilon^2\right) \tag{5.4.2}$$

and where $\tilde{L}_0$ and $\tilde{L}_1$ are differential operators of the type

$$\tilde{L} = C_0 + \sum_{i=1}^{3} C_i m_i^2 \frac{\partial}{\partial m_i^2}.$$

Notice that due to

$$\frac{\partial}{\partial m_i^2} x_i^{\nu_i - 1}\mathcal{F}^{D-\nu}\mathcal{U}^{\nu-\frac{3}{2}D} = (D-\nu)\,x_i^{\nu_i}\mathcal{F}^{D-\nu-1}\mathcal{U}^{\nu-\frac{3}{2}D+1}$$

and

$$\frac{\Gamma\,(\nu-D)}{\Gamma\,(\nu_i)} = -\frac{\nu_i}{(D-|\nu|)}\frac{\Gamma\,(\nu+1-D)}{\Gamma\,(\nu_i+1)}$$

the differentiation with respect to particle masses is related to shifts of propagator powers by

$$\frac{\partial}{\partial m_i^2} S_{\nu_1\nu_2\nu_3}\,(D,t) = -S_{\nu_1\nu_2\nu_3}\,(D,t)\,|_{\nu_i\to\nu_i+1}\cdot\nu_i$$

for $i = 1, 2, 3$. All of the above coefficients c, C_0, C_1, C_2, C_3 are explicitly given in [**9**].

On the right-hand side of eq. 5.4.1 the term $S_{111}^{(0)}(2,t)$ is of course the function $S(2,t)$ of section 5.3 for which we obtained the result in eq. 5.3.6. It remains to compute the ϵ-coefficient $S_{111}^{(1)}(2,t)$. In order to find a suitable differential equation for $S_{111}^{(1)}(2,t)$ we consider the fourth-order differential equation 5.2.4 and replace $S(D,t)$ by the expansion of $S_{111}(2-2\epsilon,\,t)$ (eq. 5.4.2) and the operator $L_4(D)$ by its expansion

$$L_4(2-2\epsilon) = \sum_{j=1}^{5} \epsilon^j L_4^{(j)}(2).$$

In this way we obtain a coupled system of differential equations for the coefficients in eq. 5.4.2 where the inhomogeneous part of the differential equation for $S_{111}^{(k)}(2,t)$ involves coefficients $S_{111}^{(j)}(2,t)$ with $j<k$. In particular we obtain a differential equation

$$L_4^{(0)}(2)S_{111}^{(1)}(2,t) = I_1(t)$$

where

$$I_1(t) = -L_4^{(1)}(2)S_{111}^{(0)}(2,t) + R$$

with R being some polynomial in t, the squared particle masses and their logarithms. We find that the fourth-order differential operator $L_4^{(0)}(2)$ factorizes as

$$L_4^{(0)}(2) = L_{1,a}^{(0)}(2)L_{1,b}^{(0)}(2)L_2^{(0)}(2)$$

where $L_{1,a}^{(0)}(2)$, $L_{1,b}^{(0)}(2)$ are certain first-order operators and $L_2^{(0)}(2)$ is precisely the Picard-Fuchs operator L_2 of eq. 5.3.2. Using this factorization, we obtain the second-order differential equation

$$L_2^{(0)}(2)S_{111}^{(1)}(2,t) = I_2(t)$$

where I_2 is obtained as a two-fold integral over a combination of I_1 and solutions of the homogeneous first-order differential equations given by $L_{1,a}^{(0)}(2)$, $L_{1,b}^{(0)}(2)$. In other words, $S_{111}^{(1)}(2,t)$ satisfies a similar second-order as $S_{111}^{(0)}(2,t)$ with the only difference being a more complicated function in the inhomogeneous part. Therefore we can construct the solution in a similar way as in the previous section. In terms of q-integrals we obtain

$$S_{111}^{(1)}(2,t) = K_1\psi_1 + K_2\psi_2 - \frac{\psi_1}{\pi}\int_0^q \frac{dq'}{q'}\int_0^{q'}\frac{dq''}{q''}\frac{I_2(q'')\psi_1(q'')^3}{\pi p_2(q'')W(q'')^2}$$

where K_1, K_2 are integration constants. By use of this expression we obtain the result as a q-series which allows us to construct the function in closed form in terms of E-functions. This result involves multiple polylogarithms and the E-functions $\mathrm{E}_{1;0}$, $\mathrm{E}_{2;0}$, $\mathrm{E}_{3;1}$, $\mathrm{E}_{0,1;-2,0;4}$ whose arguments again include the terms w_1, w_2, w_3 discussed above. By insertion into eq. 5.4.1 one obtains the desired result for $S_{111}^{(0)}(4,t)$.

5.5. Higher orders in ϵ

In the next step we shed light on the higher orders in the ϵ-expansion of the sunrise integral [**11**]. As the previous section has shown, higher-orders of the four-dimensional case $S_{111}(4-2\epsilon,\, t)$ can be obtained by computing higher orders of the two-dimensional case $S_{111}(2-2\epsilon,\, t)$. For simplicity, we consider the latter integral in the case of equal masses $m_1 = m_2 = m_3 = m$. In this section we drop the above superscript 'em', understanding that all integrals and operators refer to the equal-mass case. It will be convenient to consider the Laurent series of the Feynman integral

$$S_{111}(2-2\epsilon,\, t) = e^{-2\gamma\epsilon}\sum_{j=0}^{\infty}\epsilon^j S_{111}^{(j)}(2,t)$$

where γ is Euler's constant.

Our starting point is the differential equation eq. 5.2.5. In $D = 2 - 2\epsilon$ dimensions, the differential operator can be expanded as

$$L_2(2-2\epsilon,t) = L_2^{(0)}(2) + \epsilon L_2^{(1)}(2) + \epsilon^2 L_2^{(2)}(2)$$

with

$$L_2^{(0)}(2) = t\left(1-m^2\right)\left(t-9m^2\right)\frac{d^2}{dt^2} + \left(3t^2 - 20tm^2 + 9m^4\right)\frac{d}{dt} + t - 3m^2$$

and some further non-zero expressions for $L_2^{(1)}(2), L_2^{(2)}(2)$. It turns out that the expansion of the differential equation simplifies, if we consider it as an equation for an auxiliary integral $\tilde{S}_{111}(2-2\epsilon,t)$ which we define by

$$S_{111}\left(2-2\epsilon,t\right) = \Gamma(1+\epsilon)^2\left(\frac{3\sqrt{t}}{m\left(t-m^2\right)\left(t-9m^2\right)}\right)^{\epsilon}\tilde{S}_{111}(2-2\epsilon,t).$$

This equation reads

$$\tilde{L}_2\tilde{S}_{111}(2-2\epsilon,t) = -6\left(\frac{\left(t-m^2\right)\left(t-9m^2\right)}{3m^3\sqrt{t}}\right)$$

where the differential operator is obtained as

$$\tilde{L}_2(2-2\epsilon,t) = \tilde{L}_2^{(0)}(2) + \epsilon^2\tilde{L}_2^{(2)}(2)$$

with

$$\tilde{L}_2^{(0)}(2) = L_2^{(0)}(2)$$

and

$$\tilde{L}_2^{(2)}(2) = -\frac{\left(t+3m^2\right)^4}{4t\left(t-m^2\right)\left(t-9m^2\right)}.$$

Notice that in contrast to $L_2(2-2\epsilon,t)$ the operator $\tilde{L}_2(2-2\epsilon,t)$ has no ϵ-term. As a consequence, each coefficient of $\tilde{S}_{111}(2-2\epsilon,t)$ satisfies the differential equation

$$L_2^{(0)}(2)\tilde{S}_{111}^{(j)}(2,t) = \frac{6}{j!}\ln^j\left(\frac{\left(t-m^2\right)\left(t-9m^2\right)}{3m^3\sqrt{t}}\right) + \frac{\left(t+3m^2\right)^4}{4t\left(t-m^2\right)\left(t-9m^2\right)}\tilde{S}_{111}^{(j-2)}(2,t).$$

Here we define $\tilde{S}_{111}^{(j)}(2,t) = 0$ for $j < 0$. By use of this differential equation, we can compute $\tilde{S}_{111}(2-2\epsilon,t)$ and hence $S_{111}\left(2-2\epsilon,t\right)$ iteratively to arbitrary order in terms of E-functions. For this purpose it is now crucial that this class of functions admits an iterated integral structure as pointed out in section 5.1.

As $L_2^{(0)}(2)$ is just the equal-mass case of our previous second-order Picard-Fuchs operator, we can construct the solutions in a similar way as in our previous computations as

$$\tilde{S}_{111}^{(j)}(2,t) = C_1\psi_1(t) + C_2\psi_2(t) + \tilde{S}_{111\text{special}}^{(j)}(2,t)$$

where C_1 and C_2 are constants determined from certain boundary conditions and ψ_1, ψ_2 now denote the equal-mass versions of the above period integrals. The special solution

can be expressed as

$$\tilde{S}^{(j)}_{111\text{special}}(2,t) = -\frac{\psi_1}{\pi}\int_0^q \frac{dq'}{q'}\int_0^{q'}\frac{dq''}{q''}\frac{\psi_1\left(q''\right)^3}{\pi p_2\left(q''\right)W\left(q''\right)^2}I\left(q''\right) \tag{5.5.1}$$

with W and p_2 being the equal-mass cases of the previous quantities and with the function I involving $\tilde{S}^{(j-2)}_{111}(2,t)$.

In the computation of these integrals over q we consider a general problem, which will appear again in the discussion of the kite graph below and hopefully of further Feynman integrals in the future: We obtain the solution via integrations of the type

$$S(q) = \int_0^q \frac{dq'}{q'} f\left(q'\right) \mathrm{ELi}_{n_1,...,n_l;m_1,...,m_l;2o_1,...,2o_{l-1}}\left(x_1,...,x_l;y_1,...,y_l;q'\right)$$

where f is some function of q'. If f can be expressed as a linear combination of the $(l=1)$-case of our ELi-functions $\mathrm{ELi}_{n,m}$, then by use of eq. 5.1.9 we obtain a result for S in terms of ELi-functions. A similar concept of course has been central to our computations with multiple polylogarithms discussed in previous chapters as well. For example an integral

$$S'(z) = \int_0^z \omega(x) L_w(x)$$

with L_w being a hyperlogarithm can be expressed in terms of hyperlogarithms, if we are able to express ω in terms of 1-forms of the type $\frac{dx}{x-\sigma}$ (see eq. 2.4.3).

We find that all functions f arising in the computation of $\tilde{S}^{(j)}_{111\text{special}}(2,t)$ by eq. 5.5.1 can be expressed in terms of ELi-functions and therefore every $\tilde{S}^{(j)}_{111\text{special}}(2,t)$ can be computed in terms of ELi-functions by application of eq. 5.1.9. We show in [**11**] that this is true for all orders j and provide explicit results for the lowest orders.

In general, it is not obvious whether a given function of q can be expressed in terms of ELi-functions. As an example arising from our computation of $\tilde{S}^{(j)}_{111\text{special}}(2,t)$ let us mention the logarithm

$$\begin{aligned}\ln\left(\frac{\left(t-m^2\right)\left(t-9m^2\right)}{3m^3\sqrt{t}}\right) &= \frac{1}{2}\ln\left(-q\right) + 12\mathrm{ELi}_{1;0}\left(-1;1;-q\right) + \mathrm{ELi}_{1;0}\left(r_3;-1;-q\right) \\ &\quad + \mathrm{ELi}_{1;0}\left(r_3^{-1};-1;-q\right) - 3\mathrm{ELi}_{1;0}\left(r_3;1;-q\right) - 3\mathrm{ELi}_{1;0}\left(r_3^{-1};1;-q\right).\end{aligned}$$

We notice that the singular points $t \in \{0, m^2, 9m^2\}$ of this logarithm and of the coefficient of $\frac{d^2}{dt^2}$ in $L_2^{(0)}(2)$ coincide. In other words, if we re-write the homogeneous differential equation, solved by the periods, ψ_1, ψ_2, as

$$\left(\frac{d^2}{dt^2} + p_1'\frac{d}{dt} + p_0'\right)\psi_{1/2} = 0$$

then these points are the regular singular points of this equation. This appears to be a reasonable condition for an expression in terms of ELi-functions of q, as this q is implicitly defined by the latter operator via the period integrals. We expect that for functions with further singular points the definition of q has to be altered to allow for such an expression.

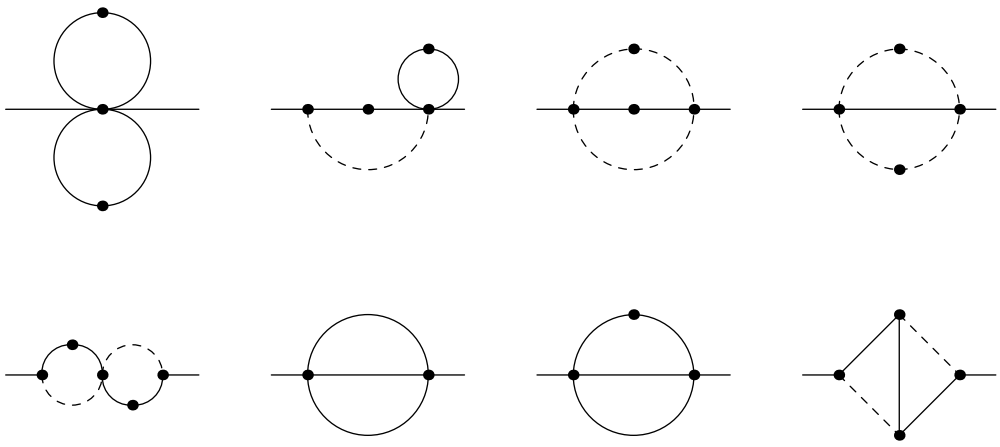


FIGURE 5.6.1. Master integrals for the kite graph

A general method to express functions of q in terms of ELi-functions is currently missing. Such a method may be the key to the systematic application of ELi- and E-functions in the computation of further Feynman integrals. However, we are already able to address one further Feynman graph, to be discussed in the following section.

Concluding our discussion of sunrise integrals, let us mention the recent results of Bloch, Kerr and Vanhove [**43, 42**], including a result for a three-loop extension of the sunrise graph in terms of an elliptic trilogarithm and a new result for the arbitrary mass case of the two-loop graph. Let us also mention the recent computation of Feynman integrals of a conformal scalar field theory by use of elliptic polylogarithms in [**123**].

5.6. The kite integral

We consider the family of the kite integral

$$I_{\nu_1\nu_2\nu_3\nu_4\nu_5}(D,t) =$$

$$\int \frac{d^Dk_1}{i\pi^{\frac{D}{2}}} \int \frac{d^Dk_2}{i\pi^{\frac{D}{2}}} \frac{(-1)^\nu}{(k_1^2-m^2)^{\nu_1}\,(k_2^2)^{\nu_2}\left((k_1-k_2)^2-m^2\right)^{\nu_3}\left((k_1-p)^2\right)^{\nu_4}\left((k_2-p)^2-m^2\right)^{\nu_5}}$$

with $\nu = \sum_{i=1}^5 \nu_i$ and $t = p^2$. We refer to I_{11111} as the kite integral. This graph was already studied in the early sixties by Sabry [**183**] and later in [**54**]. Much more recently, Remiddi and Tancredi computed the integral by use of dispersion relations in terms of integrals over elliptic integrals in [**181**]. This result motivated our re-consideration of the integral by use of our framework of functions in [**6**]. In the first steps we loosely follow Remiddi and Tancredi's work as we consider linear combinations of master integrals for the kite family and a corresponding system of first-order differential equations. Our explicit choice of this system differs from theirs.

We begin with the eight integrals I_{20200}, I_{20210}, I_{02210}, I_{02120}, I_{21012}, I_{10101}, I_{20101}, I_{11111} which form a set of IBP master integrals to express the members of the kite family. The graphs of these integrals are shown in fig. 5.6.1. In this set we recognize the sunrise

integrals

$$I_{10101}(D,t) = S_{111}(D,\,t) \text{ and } I_{20101}(D,t) = S_{211}(D,\,t).$$

The presence of these integrals suggests, that the kite integral can not be expressed in terms of multiple polylogarithms. Now we define eight integrals $I_1, ..., I_8$ as certain linear combinations of these master integrals. The first five integrals $I_1, ..., I_5$ are linear combinations of I_{20200}, I_{20210}, I_{02210}, I_{02120}, I_{21012} (see **[6]**). The integrals I_6 and I_7 involve the sunrise integrals and can be written as

$$\begin{aligned} I_6(D,t) &= (D-4)(D-5)t\, I_{10101}(D-2,t), \\ I_7(D,t) &= 2\,(D-4)\,m^2 t\, I_{20101}(D-2,t). \end{aligned}$$

Notice that by these relations the four-dimensional case $I_6(4-2\epsilon,t)$, $I_7(4-2\epsilon,t)$ is directly obtained from our above results for the sunrise integral in $2-2\epsilon$ dimensions to arbitrary order. The last integral I_8 is directly related to the kite integral by

$$I_8(D,t) = (D-4)(D-5)tI_{02210}(D,t) + (D-3)(D-4)^2(D-5)tI_{11111}(D,t).$$

Our goal is the computation of I_8 in four dimensions.

In the previous sections, the fact that multiple polylogarithms were not sufficient to express the result was visible due to the presence of higher-order differential operators which did not factorize into first-order operators only. Here we see the problem manifesting itself in the system of differential equations which is obtained for the vector $\mathcal{I} = (I_1, ..., I_8)^T$ by the classical approach discussed in section 3.3, for example by use of the program Reduze **[194, 153]**. One obtains

$$\frac{d}{dt}\mathcal{I} = \left(\frac{1}{t}A_0 + \frac{1}{t-m^2}A_1 + \frac{1}{t-9m^2}A_9\right)\mathcal{I} \tag{5.6.1}$$

with

$$A_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \epsilon & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \epsilon & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -4\epsilon & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 2\epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2\epsilon & -\frac{3}{2}-3\epsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{2}{3}+2\epsilon & 2+3\epsilon & 0 \\ 0 & 0 & 0 & 0 & -1-2\epsilon & -3\epsilon & 0 & \epsilon \end{pmatrix},$$

$$A_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\epsilon & -2\epsilon & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -2\epsilon & \epsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & 4\epsilon & -2\epsilon & 0 & 0 & 0 & 0 \\ 0 & -2\epsilon & 0 & 0 & -4\epsilon & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{\epsilon}{4} & 0 & 0 & 0 & 0 & -\frac{1}{2}-\frac{3}{2}\epsilon & -1-2\epsilon & 0 \\ \frac{1}{2}+\epsilon & 0 & -1-2\epsilon & 0 & 0 & \frac{8}{3}\epsilon & 0 & -2\epsilon \end{pmatrix},$$

$$A_9 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{9}{4}\epsilon & 0 & 0 & 0 & 0 & -\frac{1}{6}-\frac{1}{2}\epsilon & -1-2\epsilon & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

Let us recall the criteria discussed in section 3.3. At first we notice that the system has only regular singular points which are given by $t \in \{0, m^2, 9m^2\}$. The fact that these are precisely the singular points we had in the previous section may be seen as an indication that we will be able to use our framework of functions with the same q as above. The system is readily written in Fuchsian form here. The two remaining criteria discussed in section 3.3 are the questions, whether the system is in triangular form and whether its equations factorize in ϵ as eq. 3.3.2. Obviously, the system fails both criteria. However, if we consider the sub-system for the first five integrals $I_1, ..., I_5$ the corresponding blocks in the above matrices satisfy the factorization property in ϵ. Therefore these five integrals are easily computed to arbitrary order in ϵ in terms of multiple polylogarithms and in fact harmonic polylogarithms are sufficient in this case. Even though this computation does not require E-functions, the use of these functions will be advantageous for the further steps.

Therefore we change variables from t to q in the same way as in the previous section. We obtain

$$q\frac{d}{dq}\mathcal{I} = \left(\frac{\psi_1^2}{i\pi W\, t}A_0 + \frac{\psi_1^2}{i\pi W\,(t-m^2)}A_1 + \frac{\psi_1^2}{i\pi W\,(t-9m^2)}A_9\right)\mathcal{I}$$

where the coefficients of all three matrices A_0, A_1, A_9 can be expressed in terms of our functions as

$$\begin{aligned}
\frac{\psi_1^2}{i\pi W\, t} &= 1 - 4\overline{\mathrm{E}}_{0;-1}\left(r_3;-1;-q\right), \\
\frac{\psi_1^2}{i\pi W\,(t-m^2)} &= -\frac{3}{2}\overline{\mathrm{E}}_{0;-1}\left(r_3;-1;-q\right) + \frac{3}{2}\overline{\mathrm{E}}_{0;-1}\left(r_3;1;-q\right) + 3\overline{\mathrm{E}}_{0;-1}\left(-1;1;-q\right), \\
\frac{\psi_1^2}{i\pi W\,(t-9m^2)} &= \frac{1}{2}\overline{\mathrm{E}}_{0;-1}\left(r_3;-1;-q\right) - \frac{9}{2}\overline{\mathrm{E}}_{0;-1}\left(r_3;1;-q\right) + 3\overline{\mathrm{E}}_{0;-1}\left(-1;1;-q\right).
\end{aligned}$$

This property of the coefficients is crucial for our computation and may be expected from the consideration of the regular singular points.

The above system of differential equations comes with one further advantage: The equation for I_8 does not involve I_7. Therefore the consideration of the remaining six integrals is sufficient. The first five integrals $I_1, ..., I_5$ are easily computed due to the mentioned sub-system and I_6 is the known sunrise integral. For convenience we introduce the function E_{111} by

$$S_{111}\left(2-2\epsilon,t\right) = \frac{\psi_1}{\pi}E_{111}\left(2-2\epsilon,q\right).$$

Expanding the differential equation of I_8 we obtain for its jth coefficient the equation

$$\begin{aligned}
q\frac{d}{dq}I_8^{(j)} &= \left(1 - 4\overline{\mathrm{E}}_{0;-1}\left(r_3;-1;-q\right)\right)\left(-2I_5^{(j-1)} - I_5^{(j)} + I_8^{(j-1)}\right) \\
&\quad +3\left(\overline{\mathrm{E}}_{0;-1}\left(-1;1;-q\right) - \overline{\mathrm{E}}_{0;-1}\left(r_6;1;-q\right)\right)\left(I_1^{(j-1)} + \frac{1}{2}I_1^{(j)} - 2I_3^{(j-1)}\right. \\
&\quad \left. -I_3^{(j)} - 2I_8^{(j-1)}\right) - 36\overline{\mathrm{E}}_{0;-1}\left(r_3;1;-q\right)\left(E_{111}^{(j-2)} + 2E_{111}^{(j-3)}\right).
\end{aligned}$$

Assuming that we already know $I_8^{(j-1)}$, all terms on the right-hand side are known in terms of ELi-functions and therefore we can integrate over q by use of eq. 5.1.9. In this way we can compute the integral to arbitrary order in ϵ. We present explicit results for the three lowest orders in **[6]**.

This computation of the kite integral shows, that important advantages of the method of differential equations survive beyond multiple polylogarithms. If the system admits the properties discussed here and in section 3.3, integrals can be computed by use of known results for simpler integrals of the same family, possibly to all orders in ϵ. Our framework of functions has proven to be well-suited for such computations and will hopefully find applications for many further integrals in the future.

CHAPTER 6

Conclusions

This cumulative thesis is dedicated to the analytical computation of Feynman integrals by use of generalizations of polylogarithms. In chapters 2 and 3 we have reviewed some well-established classes of functions and computational methods in this field, providing the basis of our research. In chapters 4 and 5 we have summarized the main aspects of our own work. The corresponding publications are reprinted in the appendix to provide the reader with all details.

We have strongly emphasized the advantages of using multiple polylogarithms in Feynman integral computations. As we have recalled in chapter 2, multiple polylogarithms are usually defined in terms of nested sums and can be represented in terms of iterated integrals known as hyperlogarithms. These functions are deeply studied in the mathematical literature and widely used in particle physics. In chapter 3 we have reviewed the method of parametric integration and the method of differential equations which exploit the strengths of this framework of functions, particularly by use of iterated integrals[1].

Our work summarized in chapter 4 is based on iterated integrals on certain moduli spaces of curves of genus zero, providing an alternative framework to represent multiple polylogarithms. The algorithms presented in our work with Brown serve for various computations with these functions, including the computation of a certain type of definite integrals which we called cubical integrals. Furthermore, by systematically expressing integrals over Feynman parameters in terms of these cubical integrals, the algorithms serve for the analytic computation of a certain class of Feynman integrals. These are Feynman integrals whose integrands involve polynomials which are reducible with respect to the Fubini algorithm or its refined version and which have a further technical property which we described as being properly ordered near a tangential basepoint. We have furthermore discussed the main features of our computer program MPL which is based on these algorithms. Apart from the computation of Feynman integrals, this program may be useful to address problems arising from various other fields of science, as the examples in our publications show.

If a given Feynman integral is expressible in terms of multiple polylogarithms, chances are good that one of the well-established methods and corresponding computer programs

[1]Of course there are further methods for the computation of Feynman integrals which are however less relevant for this thesis. In the context of generalized polylogarithms we have also briefly mentioned the expansion of hypergeometric functions.

can be applied for their computation[2]. On the other hand, if the class of multiple polylogarithms is not sufficient to express the Feynman integral, the situation is usually very different. Alternative classes of functions, which have usually been applied to such cases so far, do not have a representation in terms of known frameworks of iterated integrals. Therefore, computational techniques which at least partly rely on iterated integrals can not be applied to their full capacity. The method of parametric integration can not be applied without iterated integrals at all. The method of differential equations can be useful in such cases, but the systematic computation of integrals of the same family and of higher orders in ϵ of course requires iterated integrals.

In chapter 5 we have summarized our work with Adams and Weinzierl on the massive sunrise integral and with the same authors and Schweitzer on the kite integral. Both integrals belong to the class of Feynman integrals which can not be expressed in terms of multiple polylogarithms. We have computed the lowest orders in ϵ of the sunrise integral in the case of arbitrary masses in two and four dimensions and to arbitrary order in the equal mass case. We have furthermore computed the kite integral to arbitrary order in four dimensions. In all of these computations we have applied the method of differential equations. Considering the elliptic curves defined by the variety of the second Symanzik polynomial of the sunrise graph, we have derived period integrals, serving as homogeneous solutions and defining the corresponding nome q. We were able to express all of our results in terms of a new framework of elliptic generalizations of polylogarithms, defined as power series in q.

Let us emphasize the common philosophy behind the two directions of our research discussed in chapters 4 and 5. In both cases we have started from the parametric representation of the Feynman integral and considered period integrals related to the geometry which is defined by Symanzik polynomials. In our work with Brown, the varieties of these polynomials determine whether the method of parametric integration can be applied and they determine the arguments of the resulting multiple polylogarithms. In this line of research, we were able to avoid a case-by-case study of varieties of certain Symanzik polynomials to extract the corresponding periods. Instead we have mapped a class of such problems, restricted by the mentioned conditions of reducibility and proper ordering, to the well-understood geometry of moduli spaces of curves of genus zero with several marked points. The iterated integrals which include the periods of these spaces were used as our main tool to build up the results of the Feynman integrals. For the integrals addressed in our work with Adams, Weinzierl and Schweitzer, it was clear that we would not be able to use this strategy and it is yet unknown, whether these integrals can be related to moduli spaces of curves of higher genus. Therefore we were forced to study the variety of a particular Symanzik polynomial explicitly. This approach again led to period integrals serving as crucial ingredients to build up the solutions of the Feynman integrals.

[2]Of course the general complexity of the problem reflected in the loop-number and the number of variables will always set limits to practical computability.

In the well-behaved cases were multiple polylogarithms are sufficient to express the results, we have automatized the computation of an entire class of integrals. This approach and the corresponding computer program MPL may be extended in several ways in the future. Firstly, the condition of properly ordered polynomials may be relaxed by a more involved strategy of computing limits. Secondly, the criterion of linear reducibility reflects the fact that the applicability of the method depends on the parametrization of integrations and kinematic invariants. An "optimal" parametrization, such that the polynomials of every Feynman integral which can be expressed in terms of multiple polylogarithms are linearly reducible, is unknown so far.

For Feynman integrals beyond multiple polylogarithms, it would be very desirable to develop algorithms and computer programs based on elliptic generalizations of polylogarithms which serve for whole classes of integrals. Our computation of the kite integral gives rise to the hope that such developments may be possible in the near future. In the computation of this integral, it was not necessary to start from scratch. We have applied the same class of functions which served for the sunrise integral and we have even used the same nome q. It will be interesting to explore ways to proceed to further Feynman integrals. We expect further computations to be possible with the same class of functions by carefully adapting the nome q to the geometry given by the corresponding graphs. Future research may also address more conceptual questions on the class of functions such as their analytical continuation[3], an underlying framework of iterated integrals, possible correspondences between special values and q-analogues of multiple zeta values and the efficient numerical evaluation. Progress in any of these directions would be very desirable in view of future automatizations of Feynman integral computations beyond multiple polylogarithms.

If we wanted to summarize this thesis in just one main message, it could be: Geometry helps us to reveal the functions which are appropriate to compute Feynman integrals, and whenever we are confronted with a new integral, it may be worthwhile to investigate its underlying geometry at first. In some cases, this investigation will show that the problem is solvable with known methods. In other cases, new paths have to be explored, but geometry keeps guiding us.

The work presented in this thesis and many related developments of the recent past show, that the influence of algebraic geometry and number theory in perturbative quantum field theory today not only helps us to understand or classify Feynman integrals. It has become an influence with a strong impact on practical computations with direct relevance for phenomenology at particle colliders. We have all reasons to be very optimistic that many further insights and improvements will come from this source in the future.

[3]A first approach to this problem was very recently presented by Passarino [**172**].

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