Algorithms and Techniques for Finding Canonical Differential Equations of Feynman Integrals

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München 2021

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Dissertation
an der Fakultät für Physik
der Ludwig–Maximilians–Universität
München

vorgelegt von
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München, den 17.12.2021

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Tag der mündlichen Prüfung: 24.02.2022

Zusammenfassung

Die moderne Teilchenphysik stützt sich auf die störungstheoretische Quantenfeldtheorie. Jenseits der führenden Ordnung ist die Berechnung der auftretenden Feynman-Integrale einer der wichtigsten und oft auch kompliziertesten Schritte, die notwendig sind, um Vorhersagen aus der Theorie zu gewinnen. Eine häufig verwendete Methode zur Berechnung der Feynman-Integrale besteht darin, einen Satz gewöhnlicher Differentialgleichungen abzuleiten, die von den Feynman-Integralen erfüllt werden, und diese anschließend in eine kanonische Form zu transformieren, bei der die Lösung in Form bekannter Funktionen auf einfache Weise erhalten werden kann. Diese Arbeit befasst sich mit der entscheidenden Aufgabe, die geeignete Basisänderung zu finden, die den Satz der Differentialgleichungen in die kanonische Form bringt.

Zu diesem Zweck werden zunächst einige der grundlegenden Eigenschaften von Feynman-Integralen und der speziellen Funktionen, die in den Lösungen vorkommen, erläutert. Anschließend erörtern wir, wie das transzendentale Gewicht dieser Funktionen ein wesentliches Leitprinzip bei der Suche nach Teilen der kanonischen Basis darstellt. Insbesondere gehen wir auf die algorithmische Bestimmung der sogenannten dlog-Integrale und ihrer "leading singularities" ein. Außerdem geben wir einen Überblick über heuristische Methoden, die sich in vielen Fällen als ausreichend erweisen, um mit geringem Aufwand eine kanonische Basis zu finden. Anhand eines einfachen Beispiels wird anschließend gezeigt, wie man mit Hilfe von sogenannten "balance"-Transformationen Schritt für Schritt zu den Eigenschaften der kanonischen Form gelangt.

Als Hauptergebnis der Arbeit stellen wir einen neuen Algorithmus vor, mit dem die kanonische Form ausgehend von einem einzigen kanonischen Integral erreicht werden kann. Dieser Algorithmus ermöglicht es ebenfalls, die transzendentalen Gewichtseigenschaften einzelner Integrale zu testen und kann daher auch als Ergänzung zu den anderen in dieser Arbeit beschriebenen Methoden betrachtet werden. Anhand mehrerer univariater Beispiele, sowie eines multivariaten Beispiels, wird die Leistungsfähigkeit und Flexibilität des Algorithmus und der öffentlich zugänglichen Implementierung demonstriert. Schließlich verwenden wir die in dieser Arbeit diskutierten Methoden in drei hochmodernen Anwendungen und zeigen, wie unser Algorithmus die kanonische Form in Fällen finden kann, in denen bestehende Methoden nicht anwendbar sind. Dazu gehören unter anderem Differentialgleichungen mit mehr als 500 Basisintegralen und eine Matrix mit elliptischen Funktionen.

Summary

Modern day particle physics relies on perturbative Quantum Field Theory. Beyond the leading order, the computation of the appearing Feynman integrals is one of the most important and often also most complicated steps necessary to extract predictions from the theory. A prominent method for the latter is to derive a set of ordinary differential equations satisfied by the Feynman integrals and then subsequently transforming them into canonical form where the solution in terms of known functions can be obtained in a straightforward manner. In this thesis, we consider the crucial task of finding the appropriate basis change that transforms the set of differential equations into canonical form.

To this end, we first discuss some of the basic properties of Feynman integrals and the special functions appearing in the solutions. We then show how the transcendental weight of these functions constitutes an essential guiding principle in the search for members of the canonical basis. In particular, we review the algorithmic determination of so-called dlog integrals and their leading singularities. Further, we provide a summary of heuristic methods that, in many cases, prove to be sufficient for finding a canonical basis with little effort. Through a simple example, we then also review how so-called balance transformations can be used to reach the properties of the canonical form step by step.

As the main result of the thesis, we present a new algorithm for attaining the canonical form starting from a single canonical integral. In addition, this algorithm makes it possible to test the transcendental weight properties of individual integrals and can therefore also be seen as complementary to the other methods described in this thesis. Several univariate examples, as well as a multivariate example are used to demonstrate the power and flexibility of the algorithm and our public implementation. Finally, we use the methods discussed in the thesis in three state-of-the-art applications and highlight how our algorithm can find the canonical form in cases where existing methods fail to provide an answer. This includes differential equations with more than 500 basis integrals and a matrix involving elliptic functions.

List of Publications

This thesis is based on the author's work conducted at the Max Planck Institute for Physics in Munich from October 2018 to September 2021. Parts of this work have already been presented in the following publications:

Refereed Research Papers

- **C. Dlapa**, J. M. Henn and K. Yan, *Deriving canonical differential equations for Feynman integrals from a single uniform weight integral*, *JHEP* 05 (2020) 025 [2002.02340];
- R. Brüser, **C. Dlapa**, J. M. Henn and K. Yan, *Full Angle Dependence of the Four-Loop Cusp Anomalous Dimension in QED*, *Phys. Rev. Lett.* 126 (2021) no.2, 021601 [2007.04851];
- **C. Dlapa**, X. Li and Y. Zhang, *Leading singularities in Baikov representation and Feynman integrals with uniform transcendental weight*, *JHEP* 09 (2021) 227 [2103.04638].

Non-Refereed Research Papers

- **C. Dlapa**, G. Kälin, Z. Liu and R. A. Porto, *Dynamics of Binary Systems to Fourth Post-Minkowskian Order from the Effective Field Theory Approach*, 2106.08276.

Contents

1 Introduction and Outline

Any theoretical physicist who had the privilege to participate in some form of public outreach, be it a presentation given to non-scientists or just discussions with family and friends, has probably received either one or both of the questions "Is this theory proven?" or "Will this ever have practical applications?". Both of these questions, of course, express what is generally expected to be the result of a physicist's work and their contribution to human development.

Let us address the first of these questions. It concerns the fact that people have the desire to understand the rules of the world they live in and that scientists are therefore expected to create a model for this purpose, which is then proven through experiment. However, the pitfall in this approach is that the verification of a certain theory would require it to be subjected to every conceivable experiment, which is of course impossible. For example, consider the Standard Model of particle physics (SM) and general relativity (GR), which are arguably the two most important theories of our time. The former describes the interaction of forces and matter and is able to account for nearly all phenomena of everyday live. The latter is the theory of gravity and how it is incorporated into four-dimensional spacetime as a geometric property. Both of these theories have been tested to an enormous extent. Famous measurements that agree with theoretical values within uncertainties are e.g. the magnetic moment of the electron predicted by the SM [5] or the time dilation due a height difference of about one meter predicted by GR [6]. Nevertheless, each theory on its own fails to describe what happens when a large amount of matter is concentrated in an extremely small space, as is e.g. the case in neutron stars. For this, it would be necessary to unify the two theories, a task which has not yet been accomplished.

The failure of the theories in specific cases does however not mean that they are not useful, which brings us to the second question. Within their limitations, each theory is incredibly powerful and their consequences can already be seen in modern day applications. For example, while GR corrections are necessary for GPS devices to reach the accuracy they currently provide to our navigation systems [7], quantum tunneling already affects the development of smaller computer chips [8]. This was however not always the case. At the advent of these theories, practical applications were far out of sight. More likely, they were developed solely to satisfy our curiosity and that of the scientists working on them. Today we are glad that this research was not deemed unnecessary and stopped in its infancy.

After having argued about the importance of physical theories for human development, let us now discuss how these theories are developed. In general, this process involves a long sequence of trial and error. Observations made in laboratories motivate a certain physical model based on postulates and mathematical structures. The model is then

used to make predictions which are tested in experiments. If the outcome differs from the theoretical predictions, this is seen as a hint that the model is not correct or complete and that we can therefore still reach an even better understanding of nature by adjusting the model in some way.

In the case of the SM, our currently most advanced experiments are carried out at particle colliders, specifically the large hadron collider (LHC) situated at CERN, where many properties of the particles of the SM have been measured to very high accuracy. In 2012, this culminated in the discovery of the Higgs boson, which was predicted by the model more than four decades earlier.

On the theory side, the SM is built on the framework of quantum field theory (QFT) which combines special relativity and quantum mechanics in a field theory. Similar to experiments, it is not possible to calculate the quantities we would like to observe to arbitrary precision. Instead, the complexity of the theory requires us to make certain approximations. Consider e.g. the scattering of electrons depicted in figure 1.1 where

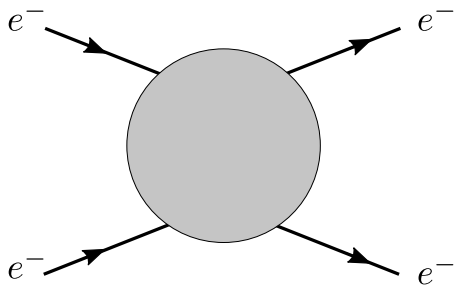


Figure 1.1: Schematic scattering of two electrons.

the gray blob indicates possible unknown interactions. To compute the probability for this process to happen, we assume that the coupling constants of the model are small, specifically the electric charge e. This allows us to carry out the calculation in an expansion in e, which is called perturbation theory. At each order, the contributions can be written in terms of *Feynman diagrams*, which in turn are translated to a mathematical expression through the use of *Feynman rules*. An example diagram contributing to leading order (LO), i.e. $\mathcal{O}(e^2)$, is given in figure 1.2a, where the wavy line indicates the exchange of an intermediate photon that cannot be observed directly at the detector. Note that momentum is conserved at every vertex and therefore the sum of incoming momenta equals the sum of outgoing momenta.

At next-to-leading order (NLO), we see from the example diagram in figure 1.2b that there are now two photons exchanged between the electrons. Again, momentum is conserved at every vertex. However, there is an overall momentum in the loop which is not determined by momentum conservation and the Feynman rules dictate that we therefore integrate over this *loop momentum*. As a result, the contributions beyond the leading order naturally involve so-called *Feynman integrals*, also called loop integrals. For many processes, the computation of the NLO or even NNLO corrections and the corresponding Feynman integrals is highly desired because the estimation given by the LO correction

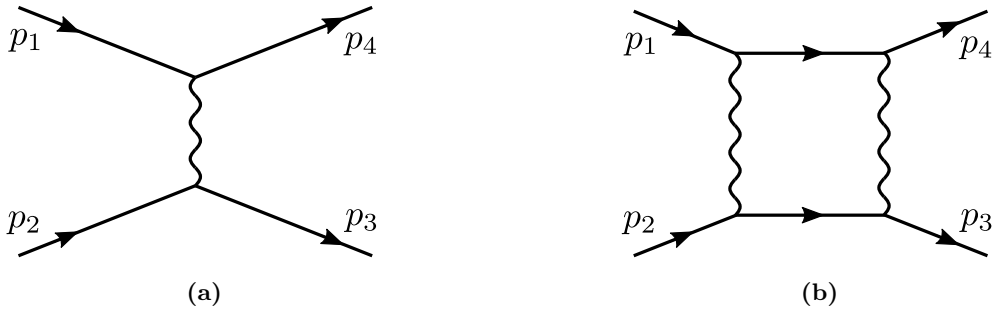


Figure 1.2: Electron-electron scattering in perturbation theory: Example diagram of (a) the leading order and (b) the next-to-leading order in the coupling constant.

is simply not enough to give a satisfying answer on whether the theoretical predictions agree with experimentally measured values [9]. Therefore, since the beginning of perturbative QFT, great effort has been put into the development of methods that allow for the computation of Feynman integrals, see e.g. [10] for a review.

Some of the most prominent of these approaches aim at finding a better integral representation where each of the multi-fold integrals can be performed in terms of known functions. Two of these are the Feynman parametrization and the Mellin-Barnes (MB) representation which are described in many standard textbooks on QFT and Feynman integrals, see e.g. [11, 10]. For both parametrizations there are also public tools for the generation of the representation [12, 13, 14], as well as the direct analytic [15, 16] or numeric [17, 13, 14] integration, see also [18] for an overview of methods that aim at deriving a series representation of the integrals. However, there is another method that is nowadays the most commonly used way of computing Feynman integrals: the method of differential equations (see [19] or [10] for early reviews, and [20] for a modern introduction).

In the '90s [21, 22] the first such differential equations were derived by taking the derivative of massive Feynman integrals w.r.t. the mass. This was then generalized to the derivative w.r.t. any scalar product of external momenta [23, 24]. These first ideas were then made more systematic in an application to complicated two-loop integrals with four external particles [25, 26]. At this point, the differential equations already had the form in which they are still used today and their derivation was completely algorithmic. However, there was still no general recipe for solving them. This changed dramatically in 2013, when it was realized [27] that the solution is straightforward if one can find a basis of integrals that brings the differential equations to a certain *canonical form*.

Finding this canonical form from a given set of integrals and their differential equations is the central theme of this thesis.

Several different techniques and algorithms are already available for this task. A method directly proposed in [27] builds on the conjecture that integrals whose *integrand* admits a so-called dlog form with constant *leading singularities* [28, 29, 30] can be chosen as members of the canonical basis. An algorithm for finding this type of integrals in a systematic way has been given in [31] and implemented in a publicly available package

in [32]. This method is especially useful for integrals with multiple kinematic variables, because the scaling in complexity with an increasing number of variables is relatively low compared to the other methods, see e.g. [33, 34] for an application to two-loop integrals with five external particles. In addition, it is commonly used to choose a canonical basis with special singularity properties, which in turn makes it easier to determine the boundary conditions [29, 35, 32]. However, the appearance of square-roots in the integration variables, which often need to be dealt with manually, can make this method less algorithmic. Further, in many cases it is not possible to furnish a complete basis of canonical integrals exclusively through dlog-form integrals.

This disadvantage can, to some extent, be mitigated by adding candidates to the basis that are found by a more heuristic approach. Here, the two main guiding principles are that canonical integrals satisfy a certain power counting in the loop momentum and that canonical one-loop integrals can often be used as building blocks to construct their higher-loop counter part. Although the success of this method is not guaranteed, experience shows that, in many cases, it is sufficient for finding a canonical form or at least a set of differential equations which is greatly simplified compared to the original one. We refer to [20, 36] and also [31] for examples of this approach.

As the last technique we want to mention, it is possible to reach the properties of the canonical form step by step through so-called balance transformations [37]. This method is completely oblivious to the actual integrals and their integrands and therefore always finds a complete basis of canonical integrals if successful. Because of this and the high degree of automation offered by the implementations [38, 39, 40], this is probably the most used technique for simpler differential equations, see e.g. [4]. However, by construction, the balance transformations are rational functions, and it is therefore again required that one manually rationalizes all appearing square-roots. Although there exist methods for doing this [41, 42], especially in cases with multiple kinematic scales one often needs to rationalize more than one square-root simultaneously. This, together with the need to find a separate transformation for each kinematic invariant, makes it difficult to apply the balance transformations to multivariate problems.

The main goal of this thesis is to present a new method for finding the canonical form which aims to overcome some of the drawbacks of the mentioned techniques. Our algorithm allows to keep the dlog integrals or candidate integrals found through other means and furthermore use them to transform the rest of the basis to canonical integrals. This is not restricted to rational functions and can include square-roots and and more complicated functions if needed. In addition, in the multivariate case, it is sufficient to run the algorithm for only one of the invariants. We also provide a publicly available implementation [1] together with example applications on multiple single-variable cases, as well as a four-variable example.

Before discussing the outline of the thesis, let us note that there are several topics which are likewise of enormous importance to the method of differential equations and are not discussed in this thesis. For instance, solving the differential equations is meaningless if the solutions cannot be evaluated efficiently. Therefore, it is no surprise that the special functions appearing in those solutions have sparked a rapid development both on the mathematical and the computational side of function theory. As an example,

understanding the algebraic structure of these special functions has made it possible to simplify a 17-page result computed in [43, 44] to a few lines of much simpler functions [45]. We refer to [46] for a review on analytic properties and to [47] for numerical evaluation.

Another essential step in solving the differential equations is the determination of boundary conditions. In some cases this proves to be even more difficult than finding the canonical form itself. A common way of acquiring the boundary constants is to consider the integrals in a certain, possibly singular, limit where enough simplifications happen so that an analytic answer can be obtained. We refer to [48] for an example. In addition, it is often possible to restrict the boundary constants through certain physical constraints on the integrals or the full result. To some extent, this approach has already been used since the development of the differential equations method. However, recent work has succeeded in making this more systematic, so that, under certain requirements, it is often possible to determine nearly all boundary conditions even for integrals with multiple kinematic scales and loops, see e.g. [49]. Lastly, we note that it is of course also an option to determine the boundary conditions in a non-analytic way by numerically evaluating the integrals at some regular point. In some cases, it is then also possible to lift the numerical values to analytic constants using the algorithm described in [50].

The outline of the thesis is as follows: In chapter 2 we introduce the reader to the properties of Feynman integrals and differential equations which are essential to this thesis. We assume some basic knowledge of QFT, algebra, complex analysis and special functions. In the following three chapters, we then review the already existing methods mentioned above, i.e. dlog integrals, heuristic techniques and balance transformations, respectively. This is done so that readers can understand how our new algorithm fills an important gap in the existing methods for the canonical form. Note that many concepts introduced in chapter 2 are described in more detail at the beginning of chapter 5, in particular, here we explicitly derive the differential equations for a simple example. Readers who prefer an algebraic approach to the topic of this thesis are invited to read this chapter directly after chapter 2. In chapter 6 we present our algorithm [1] for finding the canonical form and discuss its advantages and disadvantages compared to the techniques of the previous chapters. Further, we apply our algorithm to three different physical processes in chapter 7 and show how it can be used in cases where the other methods fail to find a canonical form. We conclude in chapter 8 and give an outlook for further possible improvements of the methods discussed in the thesis. Appendix A provides additional technical details on the algorithm of chapter 6.

2 Feynman Integrals

In order to find efficient methods for computing Feynman integrals, it is incredibly helpful to understand what properties the integrals have. Some of these properties can already be deduced without knowing the actual solutions. In particular, in this chapter we will give an overview of the singularity structure near special kinematic points and the linear relations satisfied between integrals that share the same denominators. This will be especially important for the differential equations method because it helps us to understand why we generally expect the canonical form to exist. Note that this chapter is meant to give a general overview without discussing technical details. We will derive the differential equations for an explicit example only in chapter 5 and readers may therefore choose to read chapter 5 directly after this chapter if they so prefer.

The goal of this thesis is to introduce a new algorithm for finding the canonical form of the differential equations and compare it to existing methods. Some of these methods, which will be reviewed in subsequent chapters, rely on properties of the special functions appearing in the solutions of the canonical differential equations. At the end of this chapter, we therefore also give a brief overview of this structure and the relevant special functions.

2.1 The Massless One-Loop Box Integral

Let us start with one of the most prominent examples of Feynman integrals, the massless one-loop box integral depicted in figure 2.1. It is the most important integral for massless

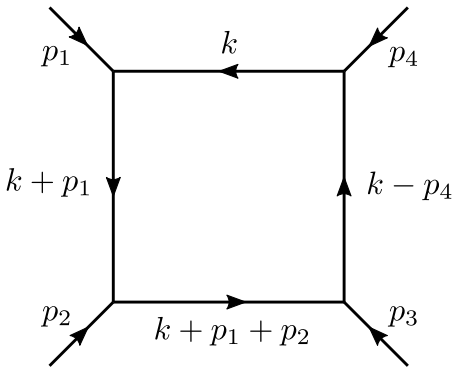


Figure 2.1: One-loop box.

two-to-two scattering at next-to-leading order and appears in many physical processes.

The four external momenta p_i are on-shell, $p_i^2 = 0$, and satisfy momentum conservation $p_1 + p_2 + p_3 + p_4 = 0$. One can see that also at every vertex in the graph of figure 2.1 momentum is conserved. The loop momentum k is not determined by any conservation delta function and is therefore integrated over:

$$I_{\text{box}} = \int \frac{\mathrm{d}^4 k}{i\pi^2} \frac{1}{k^2 (k+p_1)^2 (k+p_1+p_2)^2 (k-p_4)^2}. \tag{2.1}$$

Since the integral is a scalar under Poincaré transformations it can depend on scalar quantities, i.e. the Mandelstam invariants $s = (p_1 + p_2)^2$ and $t = (p_2 + p_3)^2$, only. By momentum conservation we have $u = (p_1 + p_3)^2 = -s - t$. The four propagators have an implicit small imaginary part according to the Feynman prescription, e.g. $k^2 \equiv k^2 - i0$, which shifts the poles slightly away from the real axis and is needed to preserve causality.

2.2 Divergences and Dimensional Regularization

Analyzing the integral in (2.1) more carefully shows that it is actually not well defined because the integrand diverges for parts of the integration region. Consider e.g. the case where $|k|$ becomes very small. Then the integrand behaves as

$$I_{\text{box}} \sim \int \frac{\mathrm{d}|k|}{|k|}. \tag{2.2}$$

To define what we actually mean by I_{box} we need to regularize this divergence. One simple way would be to introduce a cut-off so that the $|k|$ integral starts at Λ instead of zero. The mentioned soft divergence would then appear in the limit $\Lambda \to 0$.

However, we will instead use the much more commonly used method of *dimensional regularization* introduced in [51, 52, 53]. In this procedure, the space-time dimension is slightly shifted away from four dimensions: $D = 4 - 2\epsilon$. The integrand then behaves as

$$I_{\text{box}} \sim \int \frac{\mathrm{d}|k|}{|k|^{1+2\epsilon}} \tag{2.3}$$

and can be integrated to yield a well-defined quantity by assuming $\epsilon < 0$. The result then has poles at $\epsilon = 0$, which can subsequently be removed by redefining the parameters of the theory.

There are several advantages of dimensional regularization over other regulators, the most important one being that it preserves many symmetries of the integral and often also the gauge theory under consideration. In addition, it also regulates divergences coming from the region where the loop momentum becomes very large (ultraviolet, UV) or when it becomes collinear to one of the external momenta, i.e. $k \sim p_i$. Note that soft and collinear divergences are called infrared (IR) divergences and only appear for integrals involving massless particles.

2.3 Behavior of Feynman Integrals Near Singular Points

Another important case occurs when analyzing the integral in certain limits of the kinematic invariants. These limits are often used to gain valuable information without having to deal with the complexity of the full integral. By considering specific integral representations, such as the Feynman parameter representation, it is clear that the behavior in a certain limit is bound by some finite power [20]. In particular, one can use the method of regions [54] to determine that an integral e.g. around $s = 0$ behaves as $s^\alpha \log^k s$ for some constants α and k. This means that Feynman integrals can only have regular singularities in the kinematic invariants and no essential singularities. The latter implies that a behavior such as $e^{1/s}$ is excluded.

We note that the kinematic regions where a particular Feynman integral is potentially singular can be inferred from the *Laundau equations* [55, 56]. This can sometimes be used to constrain the coefficients in an ansatz for the solution, a method which is referred to as a *bootstrap*. Instead of just the Feynman integrals, one can also try to apply this bootstrap procedure to the final answer of the calculation. Especially in the case of scattering amplitudes such an approach has turned out to be incredibly powerful, see e.g. [57, 58].

2.4 Integral Families

In a given scattering problem, the number of Feynman integrals appearing can be quite large, especially at multi-loop order. Fortunately, they can be classified by the integral "family" (also called topology), by which we usually mean integrals with propagators from the same set. At this point it is worth mentioning that the powers of the propagators can take any (integer) value. For example, the box family in dimensional regularization is given by

$$I_{a_1,a_2,a_3,a_4} = e^{\epsilon\gamma_E} \int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{1}{[k^2]^{a_1}[(k+p_1)^2]^{a_2}[(k+p_1+p_2)^2]^{a_3}[(k-p_4)^2]^{a_4}}, \tag{2.4}$$

where the factor of $e^{\epsilon\gamma_E}/i\pi^{D/2}$ is purely conventional and intended to remove constants such as Euler's constant γ_E from the result. The box, triangle and bubble integrals in figures 2.1, 2.2a and 2.2b are then given by $I_{1,1,1,1}$, $I_{1,1,0,1}$ and $I_{1,0,1,0}$, respectively. As in this example of the box family, the integral with all propagators of a family is generally used as a representative and is given by the one whose graph has only three-point vertices and no four-point vertices.

Identifying the relevant families can help reduce the number of needed integrals drastically because the integrals within a family satisfy many relations. The most important relations follow simply from using integration-by-parts (IBP). These are linear relations and lead to a vector-space like structure of the family, meaning that there is a basis of integrals from which all others can be computed. For instance, the three integrals $I_{1,1,1,1}$, $I_{1,1,0,1}$ and $I_{1,0,1,0}$ form a basis for all integrals I_{a_1,a_2,a_3,a_4} in the box family. The IBP relations, as well as the example of the box family will be discussed in more detail

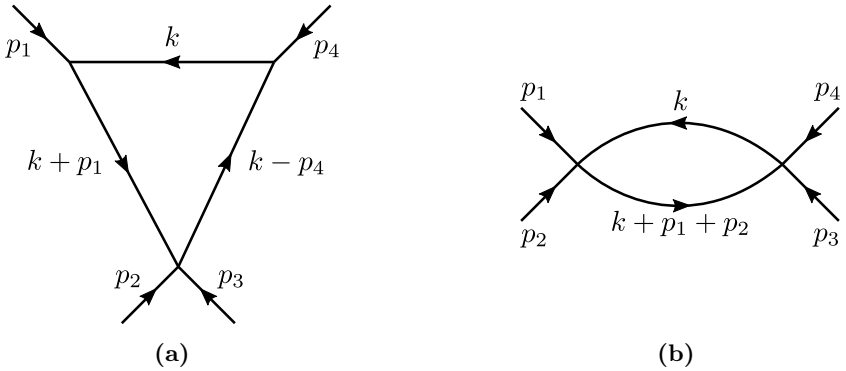


Figure 2.2: The one-loop triangle (a) and bubble (b) integral.

in section 5.1. In the following we will also use the word *master* integrals to refer to such a basis, however, note that the basis is not unique, i.e. we are free to choose any linearly independent set of integrals in a family as master integrals.

2.5 Computation of Master Integrals and the Differential Equations Method

After having reduced our set of Feynman integrals to a basis, it is natural to ask how to actually compute the chosen set of master integrals. As discussed in the introduction, we are going to use the method of differential equations for this calculation. To this end, we take the derivative of the master integrals w.r.t. a kinematic invariant x, which results in

$$\frac{\partial}{\partial x}\vec{f} = A(x,\epsilon)\vec{f}, \tag{2.5}$$

where $\vec{f}$ is the vector of master integrals and $A(x,\epsilon)$ is the coefficient matrix consisting of entries rational in x and ϵ. Note that the fact that the integrals resulting from the derivative of the masters can again be written in terms of the masters is thanks to the IBP identities. This will be discussed in more detail in section 5.2 where we explicitly derive the differential equations for a simple example.

The goal of this thesis is then to find a basis $\vec{g}$, related to $\vec{f}$ by a transformation $\vec{f} = T\vec{g}$, s.t. the dimensional regulator ϵ factorizes:

$$\frac{\partial}{\partial x}\vec{g} = \epsilon\,\tilde{A}(x)\vec{g} \tag{2.6}$$

and the coefficient matrix $\tilde{A}(x)$ has only regular singularities. A differential equation of this type is said to be in canonical form. Note that $\tilde{A}(x)$ might not be rational anymore because the basis $\vec{g}$ can contain non-rational functions as coefficients of the Feynman integrals.

A formal solution of (2.6) is given by

$$\vec{g} = \mathrm{P}\, e^{\epsilon \int_{x_0}^{x} \tilde{A}(x')\,\mathrm{d}x'} \vec{g}_0, \tag{2.7}$$

where $\vec{g}_0$ is a vector of boundary constants. This formula is defined through the series expansion of the matrix-exponential, which, because of the factorization, coincides with the expansion in ϵ. The path-ordering symbol P ensures that each term is ordered with increasing x. The first few orders are

$$\mathrm{P}\, e^{\epsilon \int_{x_0}^{x} \tilde{A}(x')\,\mathrm{d}x'} = 1 + \epsilon \int_{x_0}^{x} \tilde{A}(x_1)\,\mathrm{d}x_1 + \epsilon^2 \int_{x_0}^{x} \int_{x_0}^{x_1} \tilde{A}(x_1)\tilde{A}(x_2)\,\mathrm{d}x_2\,\mathrm{d}x_1 + \mathcal{O}(\epsilon^3). \tag{2.8}$$

The solution as an expansion in ϵ is usually sufficient since only a finite number of terms are required to compute observables in a given integer dimension. Note that, for simplicity, we focus here on the case of a single variable x. The generalization to the multi-variable case can however be easily done by replacing the partial derivative in (2.6) with a total derivative, which leads to $\mathrm{d}\vec{g} = \epsilon\, \mathrm{d}\tilde{A}\, \vec{g}$.

2.6 Canonical Form and Uniform Transcendental Weight Integrals

In order to find the canonical form (2.6) it is helpful to understand what properties the master integrals in the basis $\vec{g}$ have. First, let us look at what class of functions we can expect. Remember from the last section that the canonical differential equations only have regular singularities. Further, we will assume that it is possible to find an appropriate variable change s.t. $\tilde{A}(x)$ is rational in x. As a result, the singularities of $\tilde{A}(x)$ are of the form $1/(x-c)$ for some constant c. Therefore, we see that the term of order ϵ in (2.8) only involves logarithms and that at higher orders in ϵ the following functions become relevant:

$$G(a_1, a_2, \ldots, a_n; x) = \int_0^x \frac{\mathrm{d}t}{t - a_1} G(a_2, \ldots, a_n; t), \qquad G(;x) = 1 \tag{2.9}$$

The logarithm itself is included in this definition:

$$G(\underbrace{a, \ldots, a}_{n}; x) = \frac{1}{n!} \log^n \left(1 - \frac{x}{a}\right) \tag{2.10}$$

In the special case where all indices a_i are zero we define

$$G(\underbrace{0, \ldots, 0}_{n}; x) = \frac{1}{n!} \log^n x. \tag{2.11}$$

We will refer to these functions as multiple polylogarithms[1] (MPLs) or Goncharov polylogarithms (GPLs) [59, 60] (see [47] for their numerical evaluation). The study of these

[1] Some authors use "multiple polylogarithms" to refer to the generalized classical polylogarithms $\mathrm{Li}_{m_1,\ldots,m_k}(x_1, \ldots, x_k)$ which are related to the functions $G(a_1, a_2, \ldots, a_n; x)$ discussed here.

functions and their properties have facilitated the computation of many ground-breaking results in quantum field theory and string theory. On the other hand, the importance of the MPLs in physics has also greatly accelerated the mathematics research on these special functions. Especially for the simplification of lengthy expressions, it is useful to be able to derive relations through the *shuffle algebra*:

$$G(\vec{a};x)G(\vec{b};x) = \sum_{\vec{c}\in(\vec{a}\sqcup\!\sqcup\vec{b})} G(\vec{c};x), \tag{2.12}$$

where we follow [46] and introduce the vector notation $\vec{a} = (a_1, \ldots, a_n)$. The shuffle product $\vec{a}\sqcup\!\sqcup\vec{b}$ denotes all shuffles of $\vec{a}$ and $\vec{b}$, where a shuffle is a combination of two lists that respects the relative ordering within each original list. For instance,

$$(a_1, a_2)\sqcup\!\sqcup(b_1, b_2) = \{(a_1, a_2, b_1, b_2), (a_1, b_1, a_2, b_2), (a_1, b_1, b_2, a_2) \tag{2.13}$$

$$(b_1, a_1, a_2, b_2), (b_1, a_1, b_2, a_2), (b_1, b_2, a_1, a_2)\}. \tag{2.14}$$

In addition, MPLs are invariant under rescaling

$$G(k\,\vec{a}, k\,x) = G(\vec{a}, x), \tag{2.15}$$

if the rightmost index a_n is different from zero. This index is also important when discussing the definition of MPLs in eq. (2.9). We see that they are formally divergent at the lower integration limit $t = 0$ if $a_n = 0$. However, the shuffle product allows us to extract these *trailing zeros*, i.e. we can write any MPL with $a_n = 0$ in terms of MPLs with $a_n \neq 0$ and MPLs where all indices are zero. For instance

$$G(a_1, 0, 0; x) = G(a_1; x)G(0, 0; x) - G(0, a_1; x)G(0; x) + G(0, 0, a_1; x). \tag{2.16}$$

For $G(0; x)$ and $G(0, 0; x)$ we now simply use the definition given in (2.11). This procedure of defining the functions $G(\vec{a}; x)$ is called *shuffle regularization* and is equivalent to modifying the base point in an intricate way. From this definition it follows that MPLs are still logarithmically divergent for $x \to 0$ if $a_n = 0$. Likewise, a similar divergence appears for $x \to a_1$, which can also be extracted through the shuffle algebra.

The functions defined in (2.9) are special instances of more general functions, i.e. iterated integrals [61] (see also [62, 63]). These are defined by

$$I(f_1, f_2, \ldots, f_n; x) = \int_{x_0}^{x} \mathrm{d}t f_1(t)\; I(f_2, \ldots, f_n; t), \qquad I(;x) = 1, \tag{2.17}$$

and have numerous applications whenever the integration kernels $f_i(t)$ cannot be written in terms of the integration kernels of MPLs. An important case occurs when the $f_i(t)$ involve square-roots $\sqrt{y(t)}$ which one failed to rationalize. If $y(t)$ is a polynomial of degree one or two, it is likely that it is in principle still possible to find a representation in terms of MPLs where the a_i now involve square-roots of the kinematic variables. Alternatively, one can directly use *square-root valued iterated integrals* [64, 65].

In the case where $y(t)$ is a polynomial of degree three or four, one can use the definition of the so-called elliptic multiple polylogarithms (eMPLs), see e.g. [66, 67]. However, for the differential equations method, it is often more convenient to use iterated integrals over *modular forms* instead of eMPLs, see [68, 69, 70]. These integration kernels then explicitly involve the elliptic integral of the first kind:

$$\mathrm{K}(x) = \int_0^1 \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-x\,t^2)}} \tag{2.18}$$

Note that eMPLs can be written in terms of iterated integrals over modular forms. We will see an example of a differential equation involving $\mathrm{K}(x)$ in section 6.7.3, however, most of the methods described in this thesis have been developed for integrals that evaluate to multiple polylogarithms and we will discuss possible generalizations to the elliptic case in chapter 8.

For multiple polylogarithms, it is now very convenient to introduce the *transcendental weight* $\mathcal{T}(f)$ of a function f as the number of integrations needed to define it. Therefore, we have

$$\mathcal{T}(G(a_1,\ldots,a_n;x)) = n, \tag{2.19}$$

and e.g. $\mathcal{T}(\log x) = 1$. Following the shuffle algebra of MPLs, we also define $\mathcal{T}(f_1 f_2) = \mathcal{T}(f_1) + \mathcal{T}(f_2)$. Note that $\mathcal{T}(f_1 + f_2)$ only makes sense if $\mathcal{T}(f_1) = \mathcal{T}(f_2)$. Further, algebraic[2] functions have weight zero and numerical constants have the transcendental weight of the function they are derived from, e.g. $G(0,1;1) = -\pi^2/6$ and therefore $\mathcal{T}(\pi) = 1$.

Going back to our solution of the differential equations in (2.8), it is customary to use ϵ as a formal parameter to keep track of the transcendental weight of the expansion. To this end, we assign $\mathcal{T}(\epsilon) = -1$. Then it becomes immediately clear that the terms in the solution (2.8) will all have the same transcendental weight! A function with this property is said to be of uniform transcendental weight (UT). Furthermore, the solutions of the canonical differential equations satisfy

$$\mathcal{T}\left(\frac{\mathrm{d}}{\mathrm{d}x} g_i(x)\right) = \mathcal{T}(g_i(x)) - 1. \tag{2.20}$$

A UT function with this property is said to be a pure function. Roughly speaking, this means that there are no non-constant algebraic functions multiplying the transcendental function. For example the individual functions in (2.9) are all pure, but if we multiply them with an x-dependent factor, they are not pure anymore although they still have uniform transcendental weight.

Comparing eq. (2.20) to the canonical differential equations (2.6) and keeping in mind that $\tilde{A}(x)$ has only regular singularities and that $\mathcal{T}(\epsilon) = -1$, we see why the solutions $\vec{g}$ consist of pure functions.

[2] When referring to an algebraic function, we mean a function that is not transcendental, but can be rational or non-rational. For example, $\sqrt{x}$ is algebraic, but not rational. Therefore, loosely speaking, we have: rational $\subset$ algebraic $\subset$ transcendental.

To summarize, the properties of Feynman integrals suggest that a certain canonical form for their differential equations exists. In the canonical form, the solution in terms of iterated integrals at each order in the ϵ-expansion follows almost by definition. Further, this solution manifestly consists of pure functions, i.e. it has uniform transcendental weight without any rational or algebraic functions.

One very powerful statement made in [27] is that this argument can be reversed. In other words, the canonical form can be reached by finding a basis $\vec{g}$ that consists of pure integrals, i.e. integrals that evaluate to pure functions. In the next chapter, we review a method that allows to find these pure integrals by analyzing the singularities of the integrand of a given Feynman integral.

Let us now discuss recent developments in the computation of Feynman integrals. The main factors that contribute to the complexity of a given integral are the number of loops and the number of kinematic scales [9]. The latter is determined by the number of external and internal masses, as well as the number of external particles. At one loop, the differential equations method and the other techniques mentioned in the introduction are sufficient to analytically compute integrals with nearly any configuration of masses, see [71, 72] for a collection of known results.

At two loops, most state-of-the-art results have been obtained through the differential equations method. In particular, massless integrals with five external particles have been computed in [33, 34] and also results with one external mass are available [73, 74, 75]. Further, two-loop integrals with massive propagators and four external particles have received a lot of attention due to their high phenomenological relevance, see e.g. [76, 77, 78]. However, massive propagators often lead to the appearance of elliptic Feynman integrals, which make it difficult to obtain a form of the differential equations that can be solved analytically. For this reason, most of the mentioned results with massive propagators have been obtained through semi-numeric methods, e.g. by numerically expanding the analytic differential equations [79, 80].

For integrals with zero or one kinematic scale, the number of loops where analytic results are still possible can be impressively high. Zero-scale examples (mostly computed by methods other than differential equations) are given by the five-loop QCD beta-function [81, 82, 83] and the light-like four-loop cusp anomalous dimension [84, 85]. Further, we will give an explicit one-scale four-loop example through the integrals relevant to the computation of the angle-dependent four-loop cusp anomalous dimension in QED [2].

3 Leading Singularities and Uniform Weight Feynman Integrals

The canonical form of the differential equations makes it possible to easily write down their solution order-by-order in ϵ. Furthermore, from their structure, it is clear that this solution will consist of pure functions, i.e. a sum of multiple polylogarithms of the same transcendental weight without algebraic prefactors. Turning this logic around, we see that we can exchange the task of finding a canonical basis with the one of finding pure Feynman integrals.

In this section, we will see that the integrand of a Feynman integral already gives information about the transcendentality of the integrated quantity. More concretely, we will find that so-called *dlog integrals* constitute a basis of UT integrals [29, 30, 27], and that a criterion for selecting this type of integrals naturally involves the computation of *leading singularities* (LS). This method does not require any knowledge of the actual differential equations and the latter are merely used to verify that the determined basis indeed leads to a canonical form. This is in contrast to the balance transformations which we will review in chapter 5.

An essential point is that the dlog integrals we find in this chapter might not be enough to form a complete basis of canonical integrals. However, they can be used as an input for our new algorithm which we will present in chapter 6.

The importance of leading singularities for scattering amplitudes was first shown in [28], where the integrand of the two-loop five-particle amplitude in $\mathcal{N} = 4$ super Yang-Mills (sYM) was determined through an alternative method. This technique is very similar to generalized unitarity [86, 58, 87] where one makes an ansatz for the amplitude in terms of a minimal set of Feynman integrals and then determines the coefficients by matching different multivariate residues on both sides. In particular, these residues are computed by cutting the propagators D_i, i.e. the integration contour is taken to encircle the poles of the propagators:

$$\mathrm{LS}(I_{\mathrm{box}}[N]) = \frac{1}{(2\pi i)^4} \prod_{i=1}^{4} \oint_{D_i=0} \frac{\mathrm{d}D_i}{D_i} \frac{N(k)}{J(k)}, \tag{3.1}$$

where we have used the example of the one-loop box integral. Here, N represents a possible numerator of the integrand and J is the Jacobian from changing to the variables D_i. The resulting LS is therefore just $N(k^*)/J(k^*)$, where k^* is one of the solutions of the four simultaneous equations $D_i = 0$.

Note that, in this example, taking the four residues completely localizes all integrations, because the number of poles is equal to the number of integration variables. The

leading singularities generalize this concept of localizing all integrations to any number of poles and integration variables: If there are more poles than integrations, then there will be multiple, possibly different results depending on which poles we choose to encircle. If there are fewer poles than integrations, new poles will appear through the Jacobian, allowing to iteratively localize all integrations. The leading singularities are then the residues resulting from this computation.

The development of these techniques allowed to derive a very compact recursive formula for the integrand of planar scattering amplitudes in $\mathcal{N} = 4$ sYM [88, 29].

3.1 Leading Singularities, dlog Forms and Uniform Transcendental Weight Integrals

A very convenient form that makes the LS of an integrand manifest is the dlog form. As a simple example, we consider again the one-loop box. Let us state for now that the four-dimensional integrand can be written as [89]

$$\mathcal{I}_{\text{box}} = \frac{1}{st}\text{dlog}\frac{k^2}{(k-k^*)^2} \wedge \text{dlog}\frac{(k+p_1)^2}{(k-k^*)^2} \wedge \text{dlog}\frac{(k+p_1+p_2)^2}{(k-k^*)^2} \wedge \text{dlog}\frac{(k-p_4)^2}{(k-k^*)^2}, \quad (3.2)$$

where k^* is one of the solutions for k to the simultaneous equations $k^2 = (k+p_1)^2 = (k+p_1+p_2)^2 = (k-p_4)^2 = 0$. We will show in the next section how a dlog form for a given integrand can be obtained algorithmically. Here, we only want to discuss the advantages of the form given in (3.2). The wedge product $\wedge$ keeps track of the orientation of the contour and therefore of the overall sign. However, since this will not be important in our further analysis, we will often omit writing it explicitly. In doing so, we have to keep in mind that the differential forms are anti-symmetric, $\mathrm{d}x \wedge \mathrm{d}y = -\mathrm{d}y \wedge \mathrm{d}x$ and therefore $\mathrm{d}x \wedge \mathrm{d}x = 0$.

The dlog form makes the LS of the integrand explicit since the residue of a logarithmic differential form around its pole is trivially one. Therefore, the LS are just the prefactors of the differential forms, i.e. $\text{LS}(I_{\text{box}}) = 1/(st)$. Note that only integrands with logarithmic poles can be written in dlog form. The appearance of a higher order pole[1] $\mathrm{d}x/x^a$, $a \neq 1$, in the integrand immediately implies that a dlog form cannot exist.

This is tied to the following conjecture [29, 30, 27]: Integrals whose integrand admit a dlog form with kinematic independent LS evaluate to pure functions and are therefore pure integrals.

Before trying to understand the origin of this conjecture, let us discuss its consequences for the canonical basis. Since our goal is to find pure integrals, the conjecture states that we can equivalently try to find dlog integrals within a given integral family. As we will see in the next section, this can be done algorithmically by making an ansatz for possible dlog integrals and subsequently determining the coefficients by requiring the absence of double poles, as well as the kinematic independence of all LS. However, note

[1] A non-logarithmic pole can always be mapped to a pole $\mathrm{d}x/x^2$ through a change of variables. Therefore we will refer to this as a double pole.

that also integrals without a dlog form can be pure. Therefore dlog integrals form only a subset of possible pure integrals and it can happen that they are not enough to form a complete basis of master integrals for the given integral family. Because of this, the method in this chapter should be seen as being complementary to the other methods described in this thesis. This becomes especially important for the algorithm described in chapter 6 where a single dlog integral can be utilized to find the rest of the integrals in the canonical basis.

So why do we expect dlog integrals with constant LS to be pure integrals? The idea behind this conjecture is that a double pole is a manifest obstruction in uniformly raising the transcendental weight of the function during integration. Therefore their absence should intuitively give a sufficient (but not necessary) criterion for the uniform transcendental weight property of an integral. However, note that the differential forms in (3.2) are not the same as the ones encountered in the definition of MPLs in eq. (2.9). While the former are differential forms in the loop integration variables, the latter have no such dependence and instead depend only on the kinematic invariants. Deriving a precise relation between the two is far from trivial, see [90] for recent progress in this direction. Finally, the LS of an integral roughly corresponds to the algebraic prefactor of the transcendental functions in the result. Therefore the requirement on the LS to be constant can be understood as the requirement on the integrals to be pure instead of just UT.

Careful readers might have noticed that all LS mentioned so far were computed from integrals defined in strictly four dimensions. However, in the last chapter we saw explicitly that the transcendental weight can also be used for integrals in dimensional regularization. In fact, we even went as far as defining $\mathcal{T}(\epsilon) = -1$. The solution to this is that dlog integrands in dimensional regularization can only to be multiplied by a simple factor with an exponent proportional to ϵ [20, 91]:

$$\mathcal{I} = G(k)^{-\beta\epsilon} \prod_{i=1}^{n} \mathrm{dlog}\, f_i(k), \tag{3.3}$$

where $G(k)$ and f_i are algebraic functions of the integration variables. Since $G(k)^{-\beta\epsilon}$ is a pure function (expand in ϵ to see this), we expect that it does not destroy the uniform weight of the remaining integral and therefore set $\epsilon = 0$.

There is however one caveat to this prescription: While we set $\epsilon = 0$ in the exponent, there are cases were it is incorrect to use a strictly four-dimensional parametrization for the momenta. Explicitly, Gram determinants

$$G(\{n_i\}, \{n_j\}) = \det_{i,j}(2n_i \cdot n_j) \tag{3.4}$$

with more than four different momenta n_i vanish in a four-dimensional parametrization, in contrast to a D-dimensional one. In general, these determinants can play a role in finding dlog integrals [33]. In section 3.4 we will introduce a representation of Feynman integrals that takes these determinants into account.

3.2 4D Momentum-Space Parametrizations

As a first example, let us try to put the integrals of the one-loop box family into dlog form. Recall, that the four propagators of I_{box} are

$$D_1 = k^2, \quad D_2 = (k+p_1)^2, \quad D_3 = (k+p_1+p_2)^2, \quad D_4 = (k+p_1+p_2+p_3)^2, \tag{3.5}$$

with the kinematics being

$$p_i^2 = 0, \qquad p_1 \cdot p_2 = \frac{s}{2}, \qquad p_2 \cdot p_3 = \frac{t}{2} \qquad p_1 \cdot p_3 = -\frac{s+t}{2}. \tag{3.6}$$

Instead of trying to find the result quoted in (3.2) we will use a simple parametrization that allows for a very systematic computation of the leading singularity:

$$k = a_1 p_1 + a_2 p_2 + a_3 q_1 + a_4 q_2, \tag{3.7}$$

with two new massless vectors $q_i^2 = 0$ which are orthogonal to p_1 and p_2, and satisfy

$$q_1 \cdot q_2 = -\frac{s}{2}, \qquad q_1 \cdot p_3 = \frac{t}{2}, \qquad q_2 \cdot p_3 = -\frac{s+t}{2}. \tag{3.8}$$

Note that this is a strictly four-dimensional parametrization, however, the complications mentioned at the end of the previous section will not play a role here.

The Jacobian from the change of variables in (3.7) can be computed by noting that

$$\det_{i,j}(J_i \cdot J_j) = -\det(J)^2, \tag{3.9}$$

with

$$J_i^\mu = \frac{\partial k^\mu}{\partial a_i}, \quad \mu = 0, \ldots, 3, \quad i = 1, \ldots, 4 \tag{3.10}$$

and therefore

$$\det(J) = \sqrt{-\det_{i,j}(J_i \cdot J_j)} = \pm i \frac{s^2}{4}. \tag{3.11}$$

The overall factor of $\pm i$ will not be important for us and we therefore ignore it. The propagators are now

$$\begin{aligned} D_1 &= s b_4, \\ D_2 &= s(a_2 + b_4), \\ D_3 &= s(1 + a_1 + a_2 + b_4), \\ D_4 &= s(a_2 - a_4 + b_4) - t(a_1 - a_2 - a_3 + a_4), \end{aligned} \tag{3.12}$$

where we defined $b_4 = (a_1 a_2 - a_3 a_4)$. Starting with the triangle integral, this leads to

$$\mathcal{I}_{1,1,1,0} = \frac{\mathrm{d}a_1\, \mathrm{d}a_2\, \mathrm{d}a_3\, \mathrm{d}b_4}{s a_3 b_4 (a_2 + b_4)(1 + a_1 + a_2 + b_4)}. \tag{3.13}$$

Using the definition of the total differential

$$\mathrm{d} = \sum_{i=1}^{4} \mathrm{d}a_i \frac{\partial}{\partial a_i}, \tag{3.14}$$

as well as the antisymmetry of the wedge product, it becomes easy to bring this into dlog form:

$$\begin{aligned}
\mathcal{I}_{1,1,1,0} &= \frac{\mathrm{d}a_1\,\mathrm{d}a_2\,\mathrm{d}a_3\,\mathrm{d}b_4}{sa_3b_4(a_2+b_4)} \frac{\partial}{\partial a_1} \log(1+a_1+a_2+b_4) \\
&= -\frac{\mathrm{d}a_2\,\mathrm{d}a_3\,\mathrm{d}b_4}{sa_3b_4(a_2+b_4)} \mathrm{dlog}(1+a_1+a_2+b_4) \\
&= -\frac{\mathrm{d}a_3\,\mathrm{d}b_4}{sa_3b_4} \mathrm{dlog}(a_2+b_4)\mathrm{dlog}(1+a_1+a_2+b_4) \\
&= -\frac{\mathrm{d}a_3}{sa_3} \mathrm{dlog}(b_4)\mathrm{dlog}(a_2+b_4)\mathrm{dlog}(1+a_1+a_2+b_4) \\
&= -\frac{1}{s} \mathrm{dlog}(a_3)\mathrm{dlog}(b_4)\mathrm{dlog}(a_2+b_4)\mathrm{dlog}(1+a_1+a_2+b_4)
\end{aligned} \tag{3.15}$$

We see that the LS of the triangle integral is $-1/s$, and therefore the normalized integral $sI_{1,1,1,0}$ has constant LS and is a pure integral. Notice how we chose to start the dlog construction in the variable a_1 because there was only one factor depending on it. Of course, we could have started also with a different variable, but e.g. for b_4 we would have needed to perform partial fractioning.

Next, consider the bubble integral $I_{1,0,1,0}$. The steps are essentially the same, however, we now encounter an obstruction:

$$\mathcal{I}_{1,0,1,0} = -\frac{\mathrm{d}a_2}{s} \mathrm{dlog}(a_3)\mathrm{dlog}(b_4)\mathrm{dlog}(1+a_1+a_2+b_4) \tag{3.16}$$

This is a double pole at infinity, which can be exposed by performing the change of variables $a_2 \to 1/a_2'$. Therefore, the bubble integral in four dimensions does not admit a dlog form and we a priori don not know whether it is a pure integral or not. The box integral $I_{1,1,1,1}$, on the other hand, is a dlog integral with LS $1/(st)$ and we leave it as an example to check this explicitly.

Square-roots. In state-of-the art computations, reaching the dlog form will hardly ever be as simple as in the above example. The most commonly encountered difficulty is the appearance of square-roots. These arise from the fact that the propagators are often at least quadratic in the integration variables.

As a simple example, consider again the one-loop triangle, but now with all external legs being massive, i.e. $p_1^2 = m_1^2, p_2^2 = m_2^2$ and $p_1 \cdot p_2 = (s - m_1^2 - m_2^2)/2$. We would again like to use a parametrization similar to (3.7). To do this, we introduce four massless auxiliary vectors in the following way:

$$p_1 = q_1 + q_2, \qquad p_2 = q_3 + q_4 \tag{3.17}$$

with $q_i^2 = 0$ and $q_1 \cdot q_4 = q_2 \cdot q_3 = q_2 \cdot q_4 = 0$. From the original kinematics it follows that

$$q_1 \cdot q_2 = \frac{m_1^2}{2}, \qquad q_3 \cdot q_4 = \frac{m_2^2}{2}, \qquad q_1 \cdot q_3 = \frac{s - m_1^2 - m_2^2}{2}. \tag{3.18}$$

After having dealt with a_1 and a_4, we encounter a quadratic denominator:

$$\mathcal{I}^{\text{massive}}_{1,1,1,0} = \frac{\mathrm{d}a_2\,\mathrm{d}a_3}{s(1+a_2)a_3 + (a_2 - a_3)((1+a_2)m_1^2 - a_3 m_2^2)} \times \mathrm{dlog}(\ldots)\mathrm{dlog}(\ldots) \tag{3.19}$$

By using partial fraction w.r.t. a_2, one finds that

$$\mathcal{I}^{\text{massive}}_{1,1,1,0} = \frac{\mathrm{d}a_2\,\mathrm{d}a_3}{m_1^2(a_2 - c_2^+)(a_2 - c_2^-)} \times \mathrm{dlog}(\ldots)\mathrm{dlog}(\ldots) \tag{3.20}$$

$$= -\frac{\mathrm{d}a_3}{m_1^2(c_2^+ - c_2^-)}\mathrm{dlog}\left(\frac{a_2 - c_2^+}{a_2 - c_2^-}\right)\mathrm{dlog}(\ldots)\mathrm{dlog}(\ldots), \tag{3.21}$$

with

$$\begin{aligned} c_2^\pm = -\frac{1}{2m_1^2}\Big(& a_3(s - m_1^2 - m_2^2) + m_1^2 \\ & \pm \sqrt{(a_3(s - m_1^2 - m_2^2) + m_1^2)^2 - 4a_3 m_1^2(s - m_1 + a_3 m_2^2)}\Big) \end{aligned} \tag{3.22}$$

being the two roots of the quadratic denominator in (3.19). The denominator in (3.21) is now the square-root of a polynomial quadratic in a_3:

$$\begin{aligned} \mathcal{I}^{\text{massive}}_{1,1,1,0} = & \frac{1}{\sqrt{s^2 + (m_1^2 - m_2^2)^2 - 2s(m_1^2 + m_2^2)}} \frac{\mathrm{d}a_3}{\sqrt{(a_3 - c_3^+)(a_3 - c_3^-)}} \\ & \times \mathrm{dlog}\left(\frac{a_2 - c_2^+}{a_2 - c_2^-}\right)\mathrm{dlog}(\ldots)\mathrm{dlog}(\ldots) \end{aligned} \tag{3.23}$$

This is immediately a dlog because of [32] (see also [31])

$$\frac{1}{\sqrt{(x - c^+)(x - c^-)}} = \frac{\partial}{\partial x}\log\frac{1 + \sqrt{\frac{(c^+ - x)}{(c^- - x)}}}{1 - \sqrt{\frac{(c^+ - x)}{(c^- - x)}}}. \tag{3.24}$$

As a result, the massive triangle integral is a dlog integral with leading singularity

$$\mathrm{LS}(I^{\text{massive}}_{1,1,1,0}) = \frac{1}{\sqrt{s^2 + (m_1^2 - m_2^2)^2 - 2s(m_1^2 + m_2^2)}} \tag{3.25}$$

and normalizing it by the inverse of this LS gives a pure integral.

For completeness, we list the other two dlog forms that involve square-roots and are often encountered in a computation:

$$\frac{1}{(x-c)\sqrt{(x-c_1)(x-c_2)}} = \frac{1}{\sqrt{(c-c_1)(c-c_2)}} \frac{\partial}{\partial x} \log \frac{1+\sqrt{\frac{(c_2-c)(c_1-x)}{(c_1-c)(c_2-x)}}}{1-\sqrt{\frac{(c_2-c)(c_1-x)}{(c_1-c)(c_2-x)}}} \tag{3.26}$$

$$\frac{1}{(x-c)\sqrt{(x-c_1)}} = \frac{1}{\sqrt{(c-c_1)}} \frac{\partial}{\partial x} \log \frac{1+\sqrt{\frac{(c_1-x)}{(c_1-c)}}}{1-\sqrt{\frac{(c_1-x)}{(c_1-c)}}} \tag{3.27}$$

In [91] it was conjectured that a cubic or higher order polynomial under the square-root leads to an elliptic integral. While it is true that this case cannot be handled by the methods described in this section, we will see in section 3.4 an explicit counterexample to this conjecture.

3.3 Algorithmic Determination of dlog Integrals

Now that we know how to compute LS of individual integrals, let us use this to find all possible dlog integrals in the massless one-loop box family. Here, we will follow [31] closely. The idea is to make an ansatz and then constrain the coefficients by requiring the absence of double poles, as well as the kinematic independence of the LS. Of course, we cannot include all integrals I_{a_1,a_2,a_3,a_4} in the ansatz because this is an infinite number of terms. However, we can already restrict the indices a_i in the following way:

- $a_i \leq 1$, because higher powers in the denominator would immediately lead to a corresponding higher-order pole.
- Bubble integrals immediately lead to a double pole, see eq. (3.16). They can therefore be excluded from the ansatz.
- Likewise, tadpole integrals can easily be shown to lead to a double pole.
- Let $a = a_1 + a_2 + a_3 + a_4$. To keep the ansatz finite, we will for now restrict to integrals with $a \geq 2$. This criterion will be proven and further constrained in the following.

This leaves us with the ansatz

$$\begin{aligned} &n_1 I_{1,1,1,1} + n_2 I_{0,1,1,1} + n_3 I_{1,0,1,1} + n_4 I_{1,1,0,1} + n_5 I_{1,1,1,0} \\ &+ n_6 I_{-1,1,1,1} + n_7 I_{1,-1,1,1} + n_8 I_{1,1,-1,1} + n_9 I_{1,1,1,-1}. \end{aligned} \tag{3.28}$$

Requiring the coefficients of all double poles to be zero leads to

$$n_6 = \ldots = n_9 = 0. \tag{3.29}$$

We see that triangle integrals with a numerator should have vanishing coefficient. A systematic way to understand this [32] can be found by rescaling the loop momentum $k = \tilde{k}/\tilde{k}^2$, where a propagator $D_i = k^2 + k\cdot q_i$ transform as $D_i = \tilde{D}_i/\tilde{k}^2$ with $\tilde{D}_i = 1 + \tilde{k}\cdot q_i$. Then, the integrand is

$$\mathcal{I}_{a_1,a_2,a_3,a_4} = \frac{\mathrm{d}^4\tilde{k}}{[\tilde{k}^2]^{4-a}\tilde{D}_1^{a_1}\tilde{D}_2^{a_2}\tilde{D}_3^{a_3}\tilde{D}_4^{a_4}}, \tag{3.30}$$

and hence $a < 3$ always leads to a double pole. As LS we find

$$\frac{n_1}{st}, \qquad \frac{n_4}{t}, \qquad \frac{n_5}{s} - \frac{n_1}{st}, \qquad -\frac{n_3}{s} + \frac{n_1}{st}, \qquad -\frac{n_2}{t} + \frac{n_1}{st}. \tag{3.31}$$

Five non-trivial solutions for them to be constant are

$$\begin{aligned} &n_1 = st, && n_i = 0, && i \neq 1 \\ &n_2 = t, && n_i = 0, && i \neq 2 \\ &n_3 = s, && n_i = 0, && i \neq 3 \\ &n_4 = t, && n_i = 0, && i \neq 4 \\ &n_5 = s, && n_i = 0, && i \neq 5, \end{aligned} \tag{3.32}$$

which gives five dlog integrals when plugging this into the ansatz (3.28). Note however that IBP identities give only three master integrals and therefore the five dlog integrals are not linearly independent. Specifically, the two s-channel triangles, as well as the two t-channel triangles, are equivalent.

In a multi-loop computation, the number of terms in the ansatz can be considerably larger than in this example. To reduce this number before doing the full computation of the LS it can be advantageous to first analyze the ansatz on certain cuts. In the above example, we could first take residues around the poles $D_1 = D_3 = 0$. This is known as the *maximal cut* of the bubble $I_{1,0,1,0}$, because all propagators of this integral are cut. Note that all integrals without the denominators D_1 and D_3 vanish on this cut. Therefore, although the computation of the LS is simpler, we do not get conditions on n_1, n_3, n_7, n_8 and n_{10}. To get the restrictions on these coefficients, we can repeat the analysis on the maximal cut of integral $I_{0,1,0,1}$ and combine the two systems to recover the results in eqs. (3.29) and (3.31). For this reason, the two cuts are called a *spanning set* of cuts.

All techniques of this section have been described in [31] and implemented in the `Mathematica`-package `DlogBasis` [32]. The most important command is probably `LeadingSingularities`, which computes the LS of a given expression together with the constraints for the absence of double poles.

3.4 Baikov Representation

In the leading singularity computation, it can be very advantageous to use the propagators themselves as integration variables. This e.g. trivializes the operation of taking

cuts, c.f. eq. (3.1). The most systematic way to achieve such a parametrization is the Baikov representation [92, 93, 94, 95]. An L-loop Feynman integral in D dimensions and with E independent external momenta is written as

$$I_{a_1,\ldots,a_n} = C_E^L \int_{\mathcal{D}} \frac{\mathrm{d}z_1 \cdots \mathrm{d}z_n}{z_1^{a_1} \cdots z_n^{a_n}} U^{\frac{E-D+1}{2}} P^{\frac{D-L-E-1}{2}}. \tag{3.33}$$

Let us go through the objects appearing in this equation one at a time. The propagators are now called z_i and form a complete set of linearly independent scalar products. Since we have L loop momenta $k_1, \ldots, k_L$ and E external momenta $p_1, \ldots, p_E$, there are $n = L(L+1)/2 + LE$ such scalar products. For example, the simplest set of independent scalar products is

$$\{k_i \cdot k_j\} \cup \{k_i \cdot p_l\} \qquad i,j = 1,\ldots,L, \quad l = 1,\ldots,E. \tag{3.34}$$

For $L \geq 2$, n is usually bigger than the number of denominators. The z_i that do not appear in the denominator, i.e. $a_i \leq 0$, are called irreducible scalar products (ISPs). Because n is generally not equal to the number of integration variables in four-dimensions, this is an inherently D-dimensional representation. Otherwise the transformation would not be invertible. However, one can often still put $\epsilon = 0$ to simplify the LS computation, see the discussion around eq. (3.3).

The factors C_E^L, U and P are nothing but the Jacobian from changing integration variables. C_E^L is a factor of Gamma-functions:

$$C_E^L = A \frac{\pi^{\frac{L-n}{2}}}{\Gamma(\frac{D-E-L+1}{2}) \cdots \Gamma(\frac{D-E}{2})}, \tag{3.35}$$

where A is the constant Jacobian from switching from the set of scalar products in (3.34) to the propagators z_i. The factor in (3.35) is irrelevant for computing LS and we will mostly omit it. However, note that it can be important for analyzing whether an integral is UT.

U is the Gram determinant of the external momenta,

$$U = G(p_1,\ldots,p_E) \equiv G(\{p_1,\ldots,p_E\},\{p_1,\ldots,p_E\}) = \det_{i,j}(2p_i \cdot p_j) \tag{3.36}$$

and P is the Baikov polynomial

$$P = G(k_1,\ldots,k_L,p_1,\ldots,p_E). \tag{3.37}$$

The integration domain $\mathcal{D}$ can be determined by requiring the integral to be real for certain values of the kinematic invariants [96]. For $L = 1$ this results in the region where P is positive definite. This makes the Baikov representation a popular choice for deriving IBP identities [97, 98, 99] because P vanishes on the integration boundary.

For the one-loop box

$$C_E^L = \frac{1}{8}\frac{1}{\pi^{\frac{3}{2}}\Gamma(\frac{1}{2}-\epsilon)}, \tag{3.38}$$

$$U = -2st(s+t), \tag{3.39}$$

$$\begin{aligned} P = {} & t^2(z_1-z_3)^2 + s^2[t^2+(z_2-z_4)^2 - 2t(z_2+z_4)] \\ & - 2st[-z_2z_3 + t(z_1+z_3) + 2z_2z_4 - z_3z_4 - z_1(z_2-2z_3+z_4)] \end{aligned} \tag{3.40}$$

and

$$I_{a_1,a_2,a_3,a_4} = C_E^L U^\epsilon \int_{\mathcal{D}} \frac{\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3\,\mathrm{d}z_4}{z_1^{a_1}z_2^{a_2}z_3^{a_3}z_4^{a_4}} P^{-\frac{1}{2}-\epsilon}. \tag{3.41}$$

From this parametrization, one can set $\epsilon = 0$ (see the discussion around 3.3) and again compute the LS of the dlog integrals of the previous section. As a quick check, we compute the maximal cut of the 4d box integral:

$$I_{1,1,1,1}^{\text{max-cut}} \sim P^{-\frac{1}{2}}\Big|_{z_1=\cdots=z_4=0} = \frac{4}{st} \tag{3.42}$$

in agreement with its LS.

Example: The Three-Mass Double Box. As an advanced example, we consider the double-box family in figure 3.1 with three massive external legs. The canonical basis for

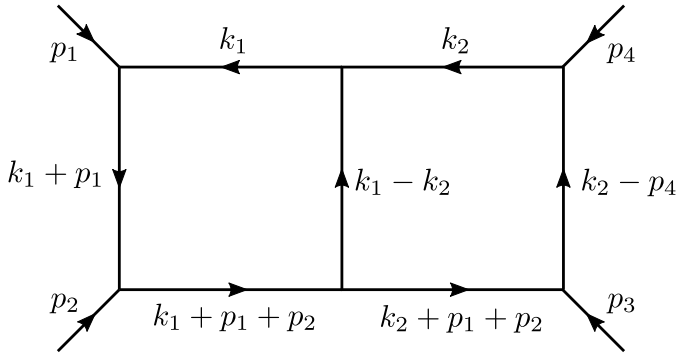


Figure 3.1: The two-loop box integral. We consider the three-mass case where only $p_4 = -p_1-p_2-p_3$ has a vanishing invariant mass.

this family was found by the present author and collaborators in [3], see also section 7.1. The kinematics is

$$\begin{gathered} p_1^2 = m_1^2, \quad p_2^2 = m_2^2, \quad p_3^2 = m_3^2, \quad p_4^2 = 0 \\ p_1\cdot p_2 = \frac{s-m_1^2-m_2^2}{2}, \quad p_2\cdot p_3 = \frac{t-m_2^2-m_3^2}{2}, \quad p_1\cdot p_3 = -\frac{s+t-m_2^2}{2} \end{gathered} \tag{3.43}$$

and the nine propagators are

$$\begin{aligned} z_1 &= k_1^2, & z_2 &= (k_1 + p_1^2), & z_3 &= (k_1 + p_1 + p_2)^2, \\ z_4 &= (k_2 + p_1 + p_2)^2, & z_5 &= (k_2 - p_4)^2, & z_6 &= k_2^2, \\ z_7 &= (k_1 - k_2)^2, & z_8 &= (k_1 - p_4)^2, & z_9 &= (k_2 + p_1)^2 \end{aligned} \tag{3.44}$$

where z_8 and z_9 are ISPs, i.e. they never appear in the denominator of the integrand and are only needed to complete the set of independent scalar products.

We could now proceed to put the integrals in this family into Baikov representation according to eq. (3.33). It is however more efficient to recycle the result for the one-loop box and first only put one of the two loops in figure 3.1 into Baikov representation. Afterwards, we proceed with the remaining diagram. This so-called *loop-by-loop* (LbL) Baikov representation [100] is of course not unique, since it depends on which loop we start with, as well as the chosen momentum-routing.

Starting with the right loop in k_2, the external momenta are k_1, p_3 and p_4. Therefore the representation for the integral at this point is

$$I_{a_1,\dots a_8,0} = \int \frac{\mathrm{d}^D k_1}{i\pi^{D/2}} \frac{1}{z_1^{a_1} z_2^{a_2} z_3^{a_3} z_8^{a_8}} C_3^1 U_2^\epsilon \int \frac{\mathrm{d}z_4\, \mathrm{d}z_5\, \mathrm{d}z_6\, \mathrm{d}z_7}{z_4^{a_4} z_5^{a_5} z_6^{a_6} z_7^{a_7}} P_2^{-\frac{1}{2}-\epsilon} \tag{3.45}$$

with

$$U_2 = G(k_1, p_3, p_4) \qquad \text{and} \qquad P_2 = G(k_1, k_2, p_3, p_4). \tag{3.46}$$

Note that we put $a_9 = 0$ because z_9 cannot appear in this approach. We will comment more on this at the end of this paragraph. We now proceed with the remaining k_1 integration. To decide what the external momenta for this loop are, it is helpful to look at the remaining propagators z_1, z_2, z_3 and z_8. We recognize again the one-loop box with external momenta p_1, p_2 and p_4. Therefore

$$I_{a_1,\dots a_8,0} = C_3^1 U_1^\epsilon \int \frac{\mathrm{d}z_1\, \mathrm{d}z_2\, \mathrm{d}z_3\, \mathrm{d}z_8}{z_1^{a_1} z_2^{a_2} z_3^{a_3} z_8^{a_8}} P_1^{-\frac{1}{2}-\epsilon} C_3^1 U_2^\epsilon \int \frac{\mathrm{d}z_4\, \mathrm{d}z_5\, \mathrm{d}z_6\, \mathrm{d}z_7}{z_4^{a_4} z_5^{a_5} z_6^{a_6} z_7^{a_7}} P_2^{-\frac{1}{2}-\epsilon}, \tag{3.47}$$

where

$$U_1 = G(p_1, p_2, p_4) \qquad \text{and} \qquad P_1 = G(k_1, p_1, p_2, p_4). \tag{3.48}$$

We call this the right-to-left representation of the double-box integral. Another way to arrive at eq. (3.47) is to start from the full two-loop Baikov representation in eq. (3.33) and carry out the integration over variable z_9. This is generally much more complicated than the LbL approach and only possible when $a_9 = 0$ [100].

The advantages of the LbL approach over the full Baikov representation are that 1) there are fewer integration variables, and 2) the integrand factorizes into several smaller pieces. Both of these aid the further analysis of the integral, especially the computation of leading singularities. The downside of this approach is that one cannot analyze integrals with $a_9 \neq 0$, missing potential dlog integrals. To circumvent this issue to some extent, one can subsequently use the left-to-right approach where $a_8 = 0$ instead of a_9.

As an advanced example for the leading singularity computation, consider the integrand

$$\mathcal{I}_{1,1,0,1,1,0,1,0,0} \sim \frac{\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3\,\mathrm{d}z_4\,\mathrm{d}z_5\,\mathrm{d}z_6\,\mathrm{d}z_7\,\mathrm{d}z_8}{z_1 z_2 z_4 z_5 z_7} \frac{1}{\sqrt{P_1}\sqrt{P_2}}. \tag{3.49}$$

We note that $P_1 \equiv P_1(\boldsymbol{z}_1), P_2 \equiv P_2(\boldsymbol{z}_2)$ are quadratic polynomials in the variables $\boldsymbol{z}_1 = \{z_1, z_3, z_4, z_5, z_6, z_7, z_8\}$ and $\boldsymbol{z}_2 = \{z_1, z_2, z_3, z_8\}$. Since P_2 does not depend on z_4, z_5 and z_7 we can immediately use (3.26) to build dlog forms:

$$\frac{\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3\,\mathrm{d}z_6\,\mathrm{d}z_8}{z_1 z_2} \frac{1}{\sqrt{P_{1,457}}\sqrt{P_2}} \times \prod_{i\in\{4,5,7\}} \mathrm{d}z_i \frac{\partial}{\partial z_i} \log(\ldots), \tag{3.50}$$

with $P_{1,457} = P_1(z_4 = z_5 = z_7 = 0)$. Next, we factorize

$$P_{1,457} = f_1(z_3, z_8)(z_6 - c_6^+)(z_6 - c_6^-) \tag{3.51}$$

and use (3.24) to build a dlog in z_6:

$$\frac{\mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3\,\mathrm{d}z_8}{z_1 z_2} \frac{1}{\sqrt{f_1(z_3, z_8)}\sqrt{P_2}} \times \prod_{i\in\{4,5,6,7\}} \mathrm{d}z_i \frac{\partial}{\partial z_i} \log(\ldots) \tag{3.52}$$

Since f_1 does not depend on z_1 and z_2 we can now again use (3.26) to get

$$\frac{\mathrm{d}z_3\,\mathrm{d}z_8}{\sqrt{f_1(z_3, z_8)}\sqrt{P_{2,12}}} \times \prod_{i\in\{1,2,4,5,6,7\}} \mathrm{d}z_i \frac{\partial}{\partial z_i} \log(\ldots), \tag{3.53}$$

with $P_{2,12} = P_2(z_1 = z_2 = 0)$.

f_1 and $P_{2,12}$ are both quadratic polynomials in z_3 and z_8. Therefore it seems that we have reached the limit of our available methods. To proceed, we can try to find a change of variables $\{z_3, z_8\} \to \{x_3, x_8\}$ that rationalizes one of the square roots, e.g. $f_1(x_3, x_8) = g(x_3, x_8)^2$, where $g(x_3, x_8)$ is rational. An approach for finding this change of variables has been described in [41] and implemented in a `Mathematica` package in ref. [42]. We find,

$$z_3 = -m_3^2 x_3(1 + x_8), \qquad z_8 = -m_3^2(1 + x_3)x_8. \tag{3.54}$$

Surprisingly, the Jacobian of this transformation turns out to cancel $\sqrt{f_1(x_3, x_8)}$. Therefore the integrand becomes

$$\frac{\mathrm{d}x_3\,\mathrm{d}x_8}{\sqrt{P_{2,12}(x_3, x_8)}} \times \prod_{i\in\{1,2,4,5,6,7\}} \mathrm{d}z_i \frac{\partial}{\partial z_i} \log(\ldots) \tag{3.55}$$

which can easily be put into dlog form. The resulting LS is

$$\mathrm{LS}\left(I_{1,1,0,1,1,0,1,0,0}\right) = \frac{1}{\sqrt{(s + t - m_2^2)^2 - 4m_1^2 m_3^2}}. \tag{3.56}$$

3.5 Dimensional Recurrence Relations

In section 3.2 we analyzed the bubble integral and found that a double pole in the representation prevents us from finding a dlog form. In section 3.3 we saw that this behavior can be predicted by counting powers of $|k|$ in the integrand. This gives a possible hint on how to improve the situation in cases where no or only few dlog integrals can be found: Since the power explicitly depends on the space-time dimension D, we consider the bubble integral in two instead of four dimensions. The result is that the integrand is now free of double poles and can therefore be put into dlog form with

$$\mathrm{LS}\left(I^{(D=2)}_{1,0,1,0}\right) = \frac{1}{s}. \tag{3.57}$$

However, we were initially interested in integrals in four dimensions and hence we want to translate the 2d-integral back to 4d. This can be done via *dimensional recurrence relations* (DRR) [101, 102], which are derived in the following way: Starting from the Baikov representation in $D+2$ dimensions

$$I^{(D+2)}_{a_1,\dots,a_n} = A\frac{\pi^{\frac{L-n}{2}}}{\prod_{i=1}^{L}\Gamma(\frac{(D+2)-E-i+1}{2})}\int_{\mathcal{D}}\frac{\mathrm{d}z_1\cdots\mathrm{d}z_n}{z_1^{a_1}\cdots z_n^{a_n}}U^{\frac{E-(D+2)+1}{2}}P^{\frac{(D+2)-L-E-1}{2}}, \tag{3.58}$$

we factor out appropriate powers of U, P and Gamma functions, to recognize the D-dimensional integral:

$$\begin{aligned} I^{(D+2)}_{a_1,\dots,a_n} &= \frac{1}{\prod_{i=1}^{L}(\frac{D-E-i+1}{2})}U^{-1}\int_{\mathcal{D}}P \\ &\quad\times A\frac{\pi^{\frac{L-n}{2}}}{\prod_{i=1}^{L}\Gamma(\frac{D-E-i+1}{2})}\frac{\mathrm{d}z_1\cdots\mathrm{d}z_n}{z_1^{a_1}\cdots z_n^{a_n}}U^{\frac{E-D+1}{2}}P^{\frac{D-L-E-1}{2}} \\ &= \frac{1}{\prod_{i=1}^{L}(\frac{D-E-i+1}{2})}U^{-1}P(A_1^-,\dots,A_n^-)I^{(D)}_{a_1,\dots,a_n}, \end{aligned} \tag{3.59}$$

where A_i^- are operators that reduce the index a_i by one, i.e.

$$A_i^- I^{(D)}_{a_1,\dots,a_i,\dots,a_n} = I^{(D)}_{a_1,\dots,a_i-1,\dots,a_n} \tag{3.60}$$

and $P(A_1^-,\dots,A_n^-)$ is the Baikov polynomial with the propagators z_i replaced by the operators A_i. This is a useful way to formally pull the Baikov polynomial $P(z_1,\dots,z_n)$ out of the integral.

Using the explicit form of the polynomials in eqs. (3.39) and (3.40) we can choose to lower the dimension of any integral in the one-loop box family. A convenient choice is to use a set of master integrals, e.g. $\vec{f}^{(D+2)} = \left(I^{(D+2)}_{1,1,1,1}, I^{(D+2)}_{1,1,0,1}, I^{(D+2)}_{1,0,1,0}\right)^{\mathrm{T}}$, s.t.

$$\vec{f}^{(D+2)} = \frac{1}{(\frac{D-3}{2})}U^{-1}P(A_1^-,\dots,A_4^-)\vec{f}^{(D)}. \tag{3.61}$$

Note that the r.h.s. is a linear combination of D-dimensional integrals, which we can again reduce to D-dimensional masters[2]. Therefore the result is a matrix $T^{(D+2)}$ s.t.

$$\vec{f}^{(D+2)} = T^{(D+2)} \vec{f}^{(D)}. \tag{3.62}$$

This enables us to invert the coefficient matrix $T^{(D+2)}$ and get recurrence relations which raise the number of dimensions:

$$\vec{f}^{(D)} = T^{(D-2)} \vec{f}^{(D+2)} \equiv (T^{(D+2)})^{-1} \vec{f}^{(D+2)} \tag{3.63}$$

These raising dimensional recurrence relations can also be directly derived from the parametric representation [101]. For the bubble integral we find

$$I^{(D=2-2\epsilon)}_{1,0,1,0} = 2I^{(D=4-2\epsilon)}_{2,0,1,0}. \tag{3.64}$$

Note that this integral is directly related to the triangle integral via IBP relations:

$$I^{(D=4-2\epsilon)}_{2,0,1,0} = -\epsilon\, I^{(D=4-2\epsilon)}_{1,1,1,0} \tag{3.65}$$

We see that we can search for dlog integrals in any even dimension and then relate them to four dimensional Feynman integrals. The methods reviewed in this chapter enable us to do so algorithmically in different representations. Some representations might be better suited for a specific problem than others. For example, the Baikov representation makes it trivial to take cuts of the integrals, however, the number of integration variables might be larger than in a direct integer-dimensional parametrization.

In general, the main bottleneck in this method is the appearance of square-roots in the integration variables that need to be rationalized, see e.g. the discussion following (3.53). These square-roots can appear even though the final leading singularity might be free of square-roots in the kinematic variables, i.e. only the dlog form depends on the square-roots. However, experience shows that this gets worse mainly with the number of loops, and the impact of an increasing number of kinematic scales is comparatively low.

It is important to realize that dlog integrals are only a subset of all possible UT integrals. In particular, it can happen that not enough linearly independent dlog integrals are found to form a complete canonical basis. However, in chapter 6 we will introduce an algorithm that uses the found dlog integrals to transform the rest of the basis into canonical form.

[2]The IBP-relations are analytic in D and therefore the IBP reduction for $\vec{f}^{(D+2)}$ is the same as for $\vec{f}^{(D)}$, but with D replaced by $D+2$.

4 Heuristic Methods for Finding UT Candidate Integrals

Many of the methods for finding pure integrals aim to be algorithmic, i.e. they require minimal input and work in cases as general as possible. This is ideal for a situation where little is known about the integrals under consideration or if a large number of integrals should be analyzed in an automatic fashion. The downside is however that these algorithms often try to do more than is actually necessary or that they scale badly with the size and complexity of the differential equations. For example, computing leading singularities quickly becomes unfeasible at high loop order, because there are many square-roots appearing during the computation.

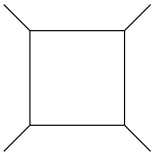
On the other hand, we saw in the last chapter that it is often possible to make statements about the transcendental weight even before integrating or even before analyzing the LS of the integrand. For example, we saw that a too high power of the loop-momentum in the numerator immediately leads to a double pole at infinity, destroying the uniform transcendentality. In this chapter, we try to convince the reader that general UT integrals, not only dlog integrals, follow a certain power counting in the loop momentum and that this can often be used to make educated guesses for uniform weight integrals at multi-loop level. This will go hand-in-hand with the concept of building blocks, i.e. using the result for lower-loop sub-integrals in a multi-loop integral.

Of course it would be meaningless to make guesses for UT integrals without being able to test whether the guess is actually correct. The purity of a full basis can always be proven by deriving the differential equations and showing that they are in canonical form. In addition, in chapter 6, we will introduce a method to perform the test on individual integrals and even find the rest of the canonical basis starting from the tested integral.

The goal of this chapter is to familiarize the reader with some heuristic techniques to quickly decide whether an integral could be UT or not, based on its diagram. It is important to understand that these methods are quite flexible and not limited to standard Feynman integrals. To emphasize this point, we will also extensively analyze integrals with linear (or *eikonal*) propagators, i.e. of the form $D_i = (k \cdot p + m^2)$. These propagators appear frequently in the computation of physical quantities in effective theories such as soft-collinear effective theory (SCET) [103, 104], heave quark effective theory (HQET) [105, 106] or the expansion of quantum gravity around the classical limit [107, 108, 109]. In addition, they have a natural representation in terms of Wilson lines. The latter emerge e.g. from the soft region of the loop integration or through their duality to scattering amplitudes in certain supersymmetric theories [110, 111, 112, 113, 114].

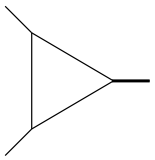
4.1 Summary of Pure One-Loop Integrals

The two most important one-loop UT integrals that we have seen so far are the massless box and the massless triangle. Both admit a dlog form and we know their leading singularities. In dimensional regularization, the integrals evaluate to



$$= \epsilon^{-2}(-s)^{-\epsilon}\frac{1}{st} \times \text{pure} \tag{4.1}$$

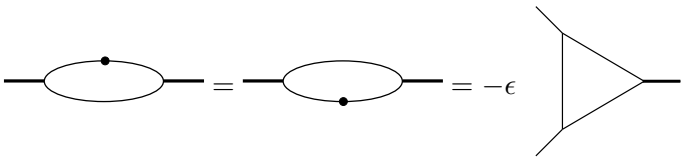
and



$$= \epsilon^{-2}(-s)^{-\epsilon}\frac{1}{s} \times \text{pure}, \tag{4.2}$$

where the thick line denotes a massive external leg. We see that the LS is indeed the prefactor of the pure function. Note that the factor of $\epsilon^{-2}(-s)^{-\epsilon}$ was chosen s.t. the pure function depends only on dimensionless quantities and is of transcendental weight zero. For the LS computation this factor was irrelevant, however, it will be advantageous to keep it for the analysis done in the following sections.

Further, we also found that the scalar bubble integral has a double pole and is no dlog integral. However, we know that the bubble integral is related to the triangle via IBP relations for any powers of the propagators. Therefore there should be a bubble integral with uniform transcendental weight corresponding to the scalar triangle. Indeed, we already found in the previous chapter that



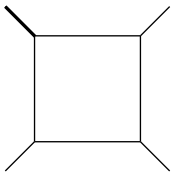
$$= -\epsilon^{-1}(-s)^{-\epsilon}\frac{1}{s} \times \text{pure}. \tag{4.3}$$

A dot on the internal line signifies that the power of the corresponding denominator is raised by one. The additional factor of ϵ is also interesting since it leads to a drop in transcendental weight by one. This drop is actually expected because of the double pole of the bubble integral. Likewise, putting two dots on the same line, meaning a propagator is raised to the third power, also leads to a UT integral but with transcendental weight lowered by two. Raising the powers of the propagators any further does not lead to new UT integrals. This can be seen from the full result for arbitrary powers:

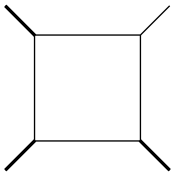
$$I_{a_1,a_2} = (-s)^{D/2-a}\frac{\Gamma(a-D/2)\Gamma(D/2-a_1)\Gamma(D/2-a_2)}{\Gamma(a_1)\Gamma(a_2)\Gamma(D-a)}, \tag{4.4}$$

where $a = a_1 + a_2$.

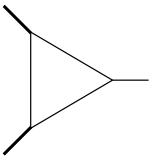
In the following, we list other UT integrals used in the rest of this chapter:



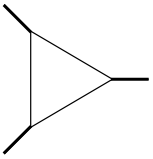
$$= \epsilon^{-2}(-s)^{-\epsilon}\frac{1}{st} \times \text{pure}, \tag{4.5}$$



$$= \epsilon^{-2}(-s)^{-\epsilon}\frac{1}{(st - m_1^2 m_3^2)} \times \text{pure}, \tag{4.6}$$



$$= \epsilon^{-2}(m_1^2)^{-\epsilon}\frac{1}{(m_1^2 - m_2^2)} \times \text{pure}, \tag{4.7}$$



$$= \epsilon^{-2}(-s)^{-\epsilon}\frac{1}{\sqrt{\lambda(m_1^2, m_2^2, s)}} \times \text{pure}, \tag{4.8}$$

where $\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$ is the Källén function. Further results for one-loop integrals with at most four external legs can be found at [71].

4.2 Building Blocks

We already computed the leading singularity of the two-loop box with three external masses of figure 4.1 in chapter 3 through the loop-by-loop Baikov representation. Let us

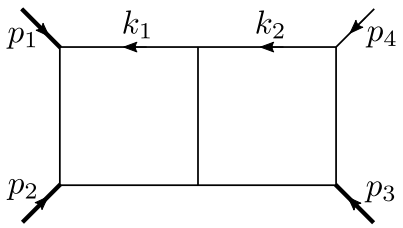
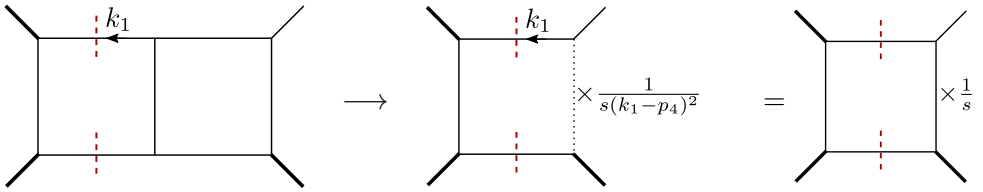


Figure 4.1: The two-loop box integral with three massive external legs.

now use a more pragmatic approach to quickly see that the scalar integral is a potential UT integral. Again we proceed first with the right loop in k_2 where we recognize a box with three of the four external legs being massive. Although we know its leading singularity from eq. (4.6), the masses complicate the subsequent analysis of the rest of

the diagram. To simplify the computation, we consider the maximal cut of the two-loop box, i.e. all internal lines are on-shell. Therefore the right box now only has one massive external leg with $p_3^2 = m_3^2$. Taking the maximal cut of the diagram is more than reasonable to quickly decide whether the integral can be UT or not. In particular, we will see in chapter 5 that this is enough when only considering the corresponding diagonal block of the differential equations, and often one can read off the corrections that are needed when relaxing the cut constraints directly from the off-diagonal blocks of the DEs.

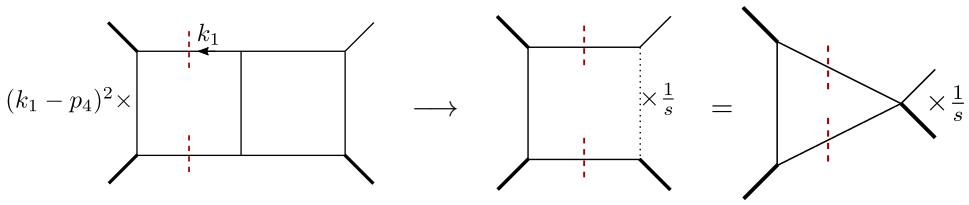
In the kinematics of this sub-diagram, the leading singularity is $1/[(p_3+p_4)^2(k_1-p_4)^2]$ or $1/[s(k_1-p_4)^2]$. The k_1-dependent factor is now exactly the propagator that is missing to complete the one-loop box integral in k_1:



(4.9)

The red dashed lines remind us that the internal lines are cut. According to (4.6) we expect this integral to be UT (on the maximal cut) with leading singularity $1/(s[st - m_1^2 m_3^2])$.

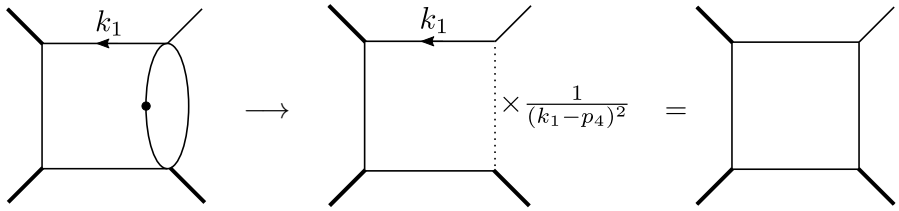
This method actually allows us to immediately find another UT candidate by using a numerator $(k_1 - p_4)^2$ which cancels the leading singularity in the first step:



(4.10)

leading to a UT candidate with leading singularity $1/s$ times the square-root given in (4.8). A third one can be found by starting with the left loop in k_1: Here the leading singularity of the one-loop box is $1/[s(k_2+p_1)^2]$ and therefore the numerator $(k_2+p_1)^2$ again leads to a UT candidate. This explains the choice for the three master integrals made in [3].

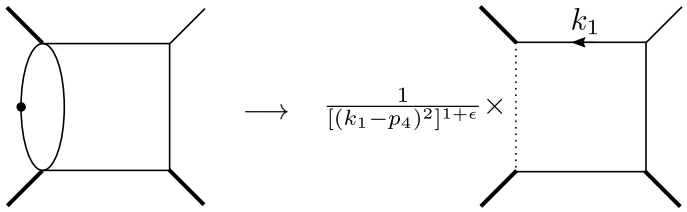
So far our analysis in this section, even when done on the maximal cut, still relied on the computation of leading singularities and is therefore largely equivalent to the one of chapter 3. However, if we consider integrals with viewer propagators we will have to use different building blocks. As an example, consider the box with a bubble attached to it:



(4.11)

Since we know that the scalar bubble integral is not UT, we put a dot on one of its lines. This ensures via (4.3) that this sub-integral is a UT function. Furthermore, the prefactor of this function is again exactly the propagator missing to complete the one-loop box. Overall, we expect this integral to have uniform weight, even if it is not a dlog integral. A second UT integral can again be found by putting a corresponding numerator $(k_1 - p_4)^2$ to cancel the leading singularity.

The example in (4.11) immediately leads us to a similar integral where our heuristic arguments result in an candidate which turns out not to be UT. Consider the case where the bubble is now between two massive lines:



(4.12)

Following the same arguments as in eq. (4.11) we conclude that (4.12) is a good UT candidate, because we neglect the additional factor of $[(k_1 - p_4)^2]^\epsilon$ in the denominator that is caused by the factor of $(-s)^{-\epsilon}$ in eq. (4.3). Here, however, this slight shift actually leads to a box integral which is not UT anymore.[12] Nevertheless, in practice it is far more efficient to ignore such shifts in the denominator powers and just include integrals such as (4.12) into the list of candidates. As mentioned before, the basis can then later be tested for the UT property by inspecting the differential equations or through the algorithm which will be described in chapter 6.

In the examples so far, we have seen that the following integrals are likely to be good building blocks for UT integrals:

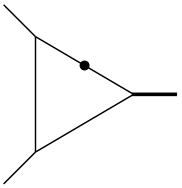
- scalar box and triangle integrals
- box integrals with numerators
- bubble integrals with a dot

This leads to the heuristic rule that integrands which behave as $\mathrm{d}^4k(k^2)^{-3}$ or $\mathrm{d}^4k(k^2)^{-4}$ are generally preferred when trying to find possible candidates. An immediate question is therefore whether the triangle integral also allows for a dot to be placed on one of its internal lines. It turns out that indeed some of these integrals are UT at least on certain

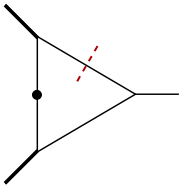
[1] A very simple example of how this can happen is given by the bubble integrals in eq. (4.4) with $a_1 = 2 + \epsilon$ and $a_2 = 1$. This integral is also not UT, although we would naively think that the factor of $1/(k^2)^\epsilon$ in the integrand should be irrelevant.

[2] It is indeed very interesting to observe that dlog integrals never seem to be affected by such shifts, which is why the computation of the leading singularities can be done with $\epsilon = 0$ (see the discussion around eq. (3.3)).

cuts. For example:

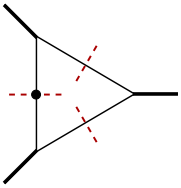


$$= \epsilon^{-1}(-s)^{-\epsilon}\frac{1}{s^2} \times \text{pure}, \tag{4.13}$$



$$= \epsilon^{-1}(m_1^2)^{-\epsilon}\frac{1}{m_1^2(m_1^2-m_2^2)} \times \text{pure}. \tag{4.14}$$

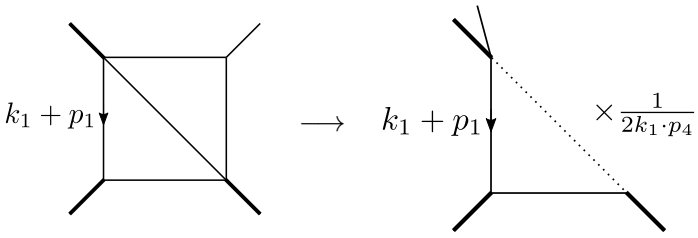
and



$$= \epsilon^{-1}(-s)^{-\epsilon}\frac{(m_1^2-m_2^2+s)}{sm_1^2\sqrt{\lambda(m_1^2,m_2^2,s)}} \times \text{pure}. \tag{4.15}$$

However, most other combinations of placements for the dot and the external masses do not have uniform transcendental weight and are unlikely to be good candidates for the canonical basis.

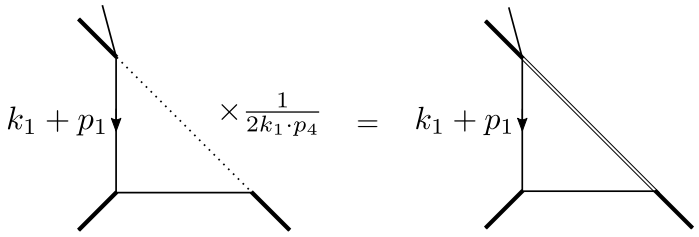
Nevertheless, triangle sub-diagrams with a dot should sometimes be considered as building bocks, especially when they appear in combination with other triangles. To understand why this is the case, consider the following integral of the three-mass double-box family:



(4.16)

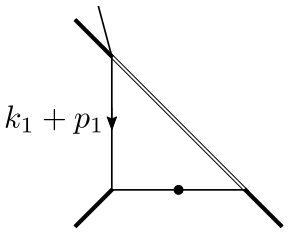
The upper-right triangle has two massive external legs with masses k_1^2 and $(k_1 - p_4)^2$. Therefore its LS, according to eq. (4.7), is $1/[k_1^2 - (k_1 - p_4)^2] = 1/(2k_1 \cdot p_4)$. As a result, the denominator has the correct momentum flow $(k_1 - p_4)$ to complete the triangle in k_1, however, it has been linearized, i.e. the k_1^2 part was removed. We will indicate such

linear propagators using a double-line in the diagram:



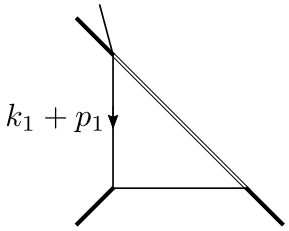
(4.17)

Since this line is now not quadratic in the loop-momentum anymore, the power counting behavior of the integrand changes. Therefore we expect that it is now safer to put a dot on one of the lines when trying to find UT integrals. Indeed, we find that the three-mass case with a dot is now UT also without cuts,



$$= \epsilon^{-1}(-s)^{-\epsilon} \frac{1}{m_2^2(m_3^2 - s)} \times \text{pure}, \tag{4.18}$$

and that the leading singularity of the scalar integral simplifies compared to (4.8):



$$= \epsilon^{-1}(-s)^{-\epsilon} \frac{1}{(m_1^2 + m_3^2 - s - t)} \times \text{pure} \tag{4.19}$$

As a result, the scalar integral in (4.16) and also the integral with a dot on the lower-left triangle are UT.

4.3 Wilson Line Integrals

Linear propagators, like the one coming from the leading singularity of the triangle, are conventionally not found in standard Feynman integral computations. The Lagrangian and the ensuing Feynman rules usually dictate that propagators should be quadratic in the loop momentum. However, linear propagators appear e.g. when considering the soft region of Feynman integrals, which is important when analyzing the IR divergences of scattering amplitudes. The latter are known to factorize in a universal way from the process-dependent finite part [115, 116] and can be studied in terms of Wilson lines [117, 118].

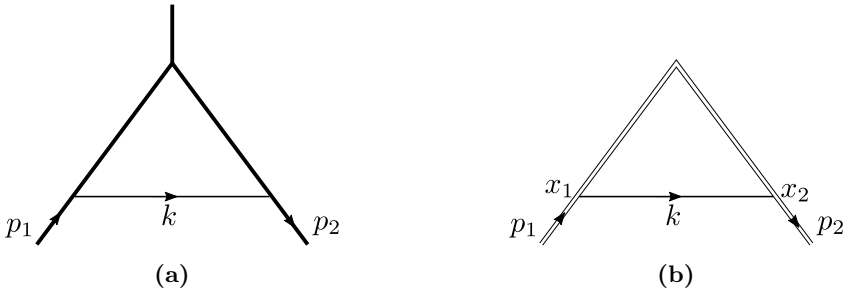


Figure 4.2: (a) The massive one-loop triangle integral. (b) The integral in the soft region can be approximated by a Wilson line integral.

As an example, we follow [119, 120] and consider the massive triangle integral in figure 4.2a, which appears e.g. in the computation of the massive quark form factor. The integral is given by

$$I_\Gamma = \int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{1}{k^2[(k-p_1)^2-m^2][(k-p_2)^2-m^2]}, \tag{4.20}$$

where $p_1^2 = p_2^2 = m^2$. In the soft region, we can approximate the denominators by

$$(k-p_1)^2 - m^2 \approx -2k\cdot p_1 \qquad \text{and} \qquad (k-p_2)^2 - m^2 \approx -2k\cdot p_2. \tag{4.21}$$

The integral in this region is therefore

$$I_\Gamma^{\mathrm{IR}} = \frac{1}{4}\int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{1}{k^2(-k\cdot p_1)(-k\cdot p_2)}, \tag{4.22}$$

and shown in figure 4.2b, where we used the diagrammatic notation for linear propagators introduced in the last section.

We can now use the simple identity

$$\frac{1}{-k\cdot p} = -i\int_0^\infty \mathrm{d}s\, e^{is(-k\cdot p)}, \tag{4.23}$$

to write the integral as

$$I_\Gamma^{\mathrm{IR}} = \frac{1}{4}\int_0^\infty \mathrm{d}s_1 \int_0^\infty \mathrm{d}s_2 \int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{e^{ik\cdot(-s_1p_1-s_2p_2)}}{k^2} \tag{4.24}$$

$$= \frac{\Gamma(1-\epsilon)}{2^{4-D}} \int_0^\infty \mathrm{d}s_1 \int_0^\infty \mathrm{d}s_2 \frac{1}{[-(s_1p_1+s_2p_2)^2]^{1-\epsilon}}, \tag{4.25}$$

where in the second line we used the Fourier transform of the propagator:

$$D(x) = -i\int \frac{\mathrm{d}^D k}{(2\pi)^D} \frac{e^{ik\cdot x}}{k^2} = \frac{\Gamma(1-\epsilon)}{4\pi^{D/2}} \frac{1}{(-x^2)^{1-\epsilon}} \tag{4.26}$$

In position space, the interpretation of (4.25) is now the following (see also figure 4.2b): The k^2 propagator has endpoints x_1 and x_2. They are integrated along a contour C formed by the external legs p_1 and p_2, i.e. $x_1 = -s_1 p_1$ and $x_2 = s_2 p_2$. Up to an overall factor, this is exactly the integral appearing in the $\mathcal{O}(g^2)$ correction of the following Wilson line:

$$W(C) = \langle 0| \operatorname{Tr} \mathrm{P} \exp\left(ig \int_C \mathrm{d}x_\mu A^\mu(x) \right) |0\rangle \tag{4.27}$$

There is however one caveat to this: The integral in (4.22) has not only IR but also UV divergences when integrated over the full space $\mathbb{R}^D$. In dimensional regularization these divergences cancel so that the integral vanishes. Therefore we need to disentangle the two divergences in order to study them separately, however, since they are equivalent, we can choose to study either IR or UV. It will be convenient for us to remove the IR divergence by adding a mass δ to the linear propagators:

$$\frac{1}{-2k \cdot p_i} \quad \longrightarrow \quad \frac{1}{-2k \cdot p_i + \delta} \tag{4.28}$$

We will see in the next section that the effect of this on the position space representation is very mild and does not alter the transcendental weight properties of the integral. Further, we can set $\delta = 1$, since the dependence of the integral on this scale can always be deduced from dimensional analysis. In addition, from (4.22) we see that we can rescale $p_1 = v_1 m$ and $p_2 = v_2 m$ and then factor out the overall dependence of the integral on m^2. This enables us to also set $m^2 = 1$ since we know the overall factor from counting powers of p_1 and p_2. As a result, the integral becomes

$$I_\Gamma^{\mathrm{IR}} = \int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{1}{k^2(-2k \cdot v_1 + 1)(-2k \cdot v_2 + 1)}, \tag{4.29}$$

and depends only on the Euclidean cusp angle $\cos\phi = v_1 \cdot v_2$.

Let us now start analysing the Wilson line integrals and try to find pure integrals which can be used as building blocks at higher-loop order. First, by using the methods of chapter 3, we easily find that (4.29) has a dlog form with leading singularity $(1 - \cos^2\phi)^{-1/2}$. It is advantageous to rationalize this square root through the change of variables

$$x = e^{i\phi}, \tag{4.30}$$

s.t.

$$\cos\phi = \frac{1}{2}\left(x + \frac{1}{x}\right), \tag{4.31}$$

and

$$\sin\phi = \sqrt{1 - \cos^2\phi} = \frac{1}{2i}\left(x - \frac{1}{x}\right). \tag{4.32}$$

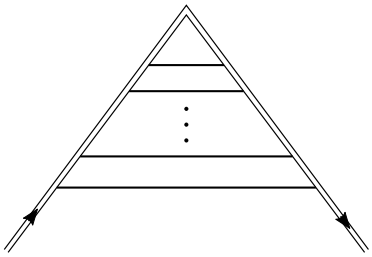
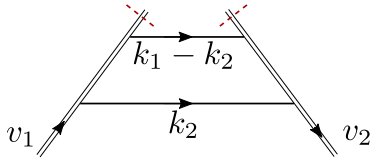


Figure 4.3: The L-loop Wilson line ladder with L rungs is UT.

Second, this allows us to see that all L-loop Wilson line ladder integrals in figure 4.3 are candidates for UT integrals, by also using the following building block:



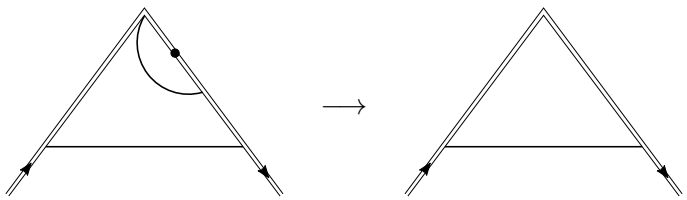
$$= \epsilon^{-2}(-k_1^2)^{-\epsilon}\frac{1}{\sin\phi}\frac{1}{k_1^2} \times \text{pure} \tag{4.33}$$

Here, the red dashed lines indicate again that the corresponding propagators are on shell. Since these propagators are $(-2k_1 \cdot p_{1,2} + 1)$, this means that $k_1 \cdot p_{1,2} = 1/2$. It turns out that all of these integrals do indeed have a dlog form [121, 36] with leading singularity $(\sin\phi)^{-L}$ at L-loops.

Another important building block is the bubble integral where one of the propagators is linear. This can be computed for arbitrary indices and the result is [36]

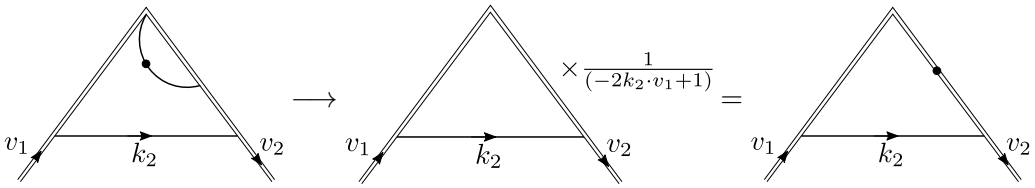
$$\begin{aligned}\int \frac{\mathrm{d}^D k}{i\pi^{D/2}} &\frac{1}{[(k_1-k_2)^2]^{a_1}[-2k_1\cdot v_1+1]^{a_2}} \\ &= (-2k_2\cdot v_1+1)^{D-2a_1-a_2}\frac{\Gamma(2a_1+a_2-D)\Gamma(D/2-a_1)}{\Gamma(a_1)\Gamma(a_2)},\end{aligned} \tag{4.34}$$

which gives UT integrals for $\{a_1, a_2\}$ being $\{1,2\}, \{1,3\}$ or $\{2,1\}$. Therefore one again needs to put a dot on one of the lines to make this bubble integral UT. Note however, that the result, and especially the power of the prefactor, now depends on which propagator is squared. This is important when using this integral as a building block. For example, we find that the following integral is a good candidate for the canonical basis:



(4.35)

On the other hand, putting the dot on the other line of the bubble integral leads to



(4.36)

which is less likely to be a good candidate. Indeed, deriving the differential equations shows that (4.35) is a pure integral when normalized by $\sin\phi$, but that (4.36) does not have uniform transcendental weight.

4.4 Position-Space Parametrization

In chapter 3 we saw that different parametrizations can be used to analyze the transcendental weight properties of Feynman integrals. In particular, we computed leading singularities through four-dimensional momentum space parametrizations and through the Baikov representation. The latter was especially suited for doing computations on certain cuts of the integral. For Wilson line integrals, however, we have already seen that linear propagators naturally lead to a simple position space representation, and we can therefore expect that this simplifies the computation of leading singularities. A systematic way to analyze the uniform weight property of Wilson line integrals in position space, together with some examples presented also in this section, has been given e.g. in [36] and [121].

First, consider again the one-loop integral in figure 4.2b and eq. (4.29). We derived the corresponding line integral in eq. (4.24), however, the introduction of the IR regulator $\delta = 1$, leads to an additional exponential inside the integral:

$$\int_0^\infty \mathrm{d}s \int_0^\infty \mathrm{d}t \frac{e^{i(s_1+s_2)/2}}{[(s_1 v_1 + s_2 v_2)^2]^{1-\epsilon}}, \tag{4.37}$$

where we omitted overall factors that do not affect the uniform weight properties. We now change variables according to $s_1 = \rho z, s_2 = \rho \bar{z}$ with $\bar{z} = 1 - z$, which leads to

$$-\int_0^\infty \frac{\mathrm{d}\rho}{\rho^{1-2\epsilon}} e^{i\rho} \int_0^1 \mathrm{d}z \left[\frac{x}{(zx+\bar{z})(z+\bar{z}x)}\right]^{1-\epsilon}. \tag{4.38}$$

In this form, the integral over the overall scale ρ is completely factorized. Note how the exponential correctly regularizes the IR divergence of this integral, s.t. in the result only the UV divergence appears in the form of a Gamma function $\Gamma(2\epsilon) \sim 1/(2\epsilon)$. This structure continues at higher loop orders, i.e. we can always separate the ρ integral which leads to a pure function and is therefore not relevant for finding uniform weight integrals.

The computation of the leading singularity is now straightforward since the rest of the integrand has the following dlog-form:

$$\int_0^1 \mathrm{d}z \left[\frac{x}{(zx+\bar{z})(z+\bar{z}x)}\right]^{1-\epsilon} = \frac{x}{1-x^2}\int_0^1 \mathrm{d}\log\left(\frac{z+\bar{z}x}{zx+\bar{z}}\right)\times \left[\frac{x}{(zx+\bar{z})(z+\bar{z}x)}\right]^{-\epsilon} \tag{4.39}$$

Neglecting again the factor with exponent proportional to ϵ, we find the leading singularity $x/(1-x^2) = -2i/\sin\phi$.

An interesting feature of the position space representation is that doubled propagators do not immediately lead to a double pole. For example, the Fourier transform of a doubled quadratic propagator is

$$-i\int \frac{\mathrm{d}^D k}{(2\pi)^D}\frac{e^{ik\cdot x}}{(k^2)^2} = -\frac{1}{\epsilon}\frac{\Gamma(1-\epsilon)}{16\pi^{D/2}}\frac{1}{(-x^2)^{-\epsilon}}, \tag{4.40}$$

which effectively removes the corresponding line from the computation and leads to a weight drop by one. As an example, consider the position space representation of the integral in figure 4.4a with $x_1 = -s_1 v_1, x_2 = s_2 v_2$ and $x_3 = s_3 v_2$:

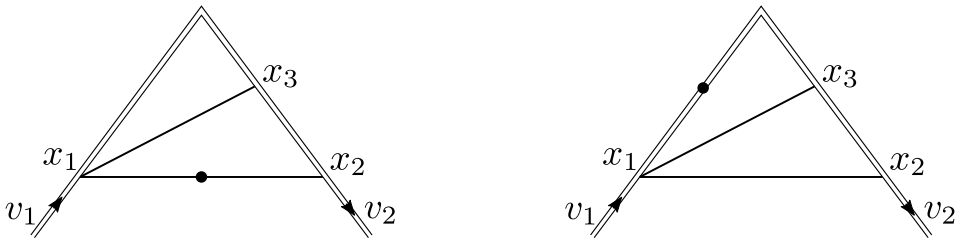


Figure 4.4: Two-loop Wilson line integrals with doubled propagators.

$$\frac{1}{\epsilon}\int_0^\infty \mathrm{d}s_1\,\mathrm{d}s_2\,\mathrm{d}s_3 \frac{e^{i(s_1+s_2)/2}}{[(s_1v_1+s_2v_2)^2]^{-\epsilon}[(s_1v_1+s_3v_2)^2]^{1-\epsilon}} \tag{4.41}$$

Again we separate the overall scale ρ through $s_1 = \rho z, s_2 = \rho\bar{z}$ and $s_3 = \rho\bar{z}y$. This leads to

$$\frac{1}{\epsilon}\int_0^\infty \frac{\mathrm{d}\rho}{\rho^{-4\epsilon}} e^{i\rho/2}\int_0^1 \mathrm{d}z\,\mathrm{d}y\,\bar{z}\left[\frac{x}{(zx+\bar{z})(z+\bar{z}x)}\right]^{-\epsilon}\left[\frac{x}{(zx+\bar{z}y)(z+\bar{z}yx)}\right]^{1-\epsilon}. \tag{4.42}$$

While the ρ integral can be evaluated in terms of a Gamma function (this time without pole in ϵ), the rest of the integrand has the dlog form

$$\frac{x}{1-x^2}\int_0^1 \mathrm{d}\log\left(\frac{y\bar{z}+xz}{xy\bar{z}+z}\right)\mathrm{d}\log z \times\left[\frac{x}{(zx+\bar{z})(z+\bar{z}x)}\right]^{-\epsilon}\left[\frac{x}{(zx+\bar{z}y)(z+\bar{z}yx)}\right]^{-\epsilon}. \tag{4.43}$$

Likewise, the integral in figure 4.4b, which has a doubled linear propagator, can also be put into dlog form. To see this, we first use

$$\frac{1}{\left(-k\cdot p+\frac{1}{2}\right)^2} = -\int_0^\infty \mathrm{d}s\; s\, e^{is\left(-k\cdot p+\frac{1}{2}\right)} \tag{4.44}$$

and then proceed in the same way as for the other examples:

$$\begin{aligned}&\int_0^\infty \frac{\mathrm{d}\rho}{\rho^{1-4\epsilon}} e^{i\rho/2} \int_0^1 \mathrm{d}z\,\mathrm{d}y\, z\bar{z}\left[\frac{x}{(zx+\bar{z})(z+\bar{z}x)}\right]^{1-\epsilon}\left[\frac{x}{(zx+\bar{z}y)(z+\bar{z}yx)}\right]^{1-\epsilon}\\ &= \left(\frac{x}{1-x^2}\right)^2 \int_0^1 \mathrm{d}\log\left(\frac{y\bar{z}+xz}{xy\bar{z}+z}\right)\mathrm{d}\log\left(\frac{z+\bar{z}x}{zx+\bar{z}}\right)\times\Big(\dots\Big)^{-\epsilon}\end{aligned} \tag{4.45}$$

Both of the integrals in figure 4.4 have been shown to be UT integrals by deriving the corresponding differential equations in canonical form [36].

We see that, for Wilson line integrals, the position space parametrization is indeed very powerful when trying to find pure Feynman integrals. Another advantage of this representation is that the integration boundaries are very simple as compared to e.g. the Baikov representation. In many cases, this allows one to explicitly carry out the integrals through direct integration. Especially for integrands in dlog form, writing down the solution in terms of multiple Polylogarithms often reduces to a sequence of algebraic manipulations and the identification of a suitable integration order. This is implemented in the `HyperInt` package [15], see also [121] for examples and other methods regarding the direct integration of Wilson line integrals.

5 Algebraic Simplifications of Differential Equations

The transcendental weight of Feynman integrals is an immensely useful guiding principle when trying to find a basis which brings the differential equations into canonical form. Often, it is possible to find a complete UT basis before ever looking at the differential equations, and upon subsequent analysis the latter then turn out to indeed be in canonical form.

However, in many cases it is necessary to perform at least some algebraic manipulations on the integrals based on the specific entries of the coefficient matrix $A(s,\epsilon)$. In particular, this is expected when using the heuristic methods of the previous chapter, because the found candidate integrals often still require some slight "corrections" to make them proper pure integrals. As a simple example, consider the case where our analysis found a candidate which is a uniform weight function, but we did not manage to compute what the correct normalization (leading singularity) is. A typical differential equation for such an integral (i.e. the entry $A_{1,1}$) is

$$\frac{\partial}{\partial s} f_1 = \frac{a+b\epsilon}{s} f_1 + \dots, \tag{5.1}$$

where the dots indicate the dependence of the derivative on the other integrals of the basis. Anticipating that the normalization of this integral is not correct, we define $f_1 = n(s) g_1$. The resulting equation for g_1 is

$$\begin{aligned} \frac{\partial}{\partial s} g_1 &= n(s)^{-1} \left(\frac{a+b\epsilon}{s} n(s) - n(s)' \right) g_1 + \dots, \\ &= \frac{b\epsilon}{s} g_1 + n(s)^{-1} \left[\frac{a}{s} n(s) - n(s)' \right] g_1 + \dots . \end{aligned} \tag{5.2}$$

Here we make two observations: First, we see that the homogeneous term linear in ϵ does not depend on $n(s)$ since we chose this normalization to be independent of ϵ. Second, to make (5.2) proportional to ϵ, we have to solve the differential equation $n(s)' = (a/s)n(s)$ which is similar to the original equation in (5.1) but with $\epsilon = 0$. This equation can easily be solved and we find $n(s) = s^a$. Therefore, $g_1 = f_1/s^a$ is the correctly normalized integral, which we obtained by *integrating out* the ϵ^0 part of the homogenous differential equation (5.1).

In practice, the differential equations will often be too complicated to manually find a suitable transformation for the whole basis. In addition, there are cases where it is not possible to find enough independent dlog integrals to form a complete set of master integrals. Therefore it is important to have an algorithm available that, in principle,

can bring the differential equations for an arbitrary basis into canonical form. In this chapter, we will review the method of balance transformations, which is one of the most commonly used algorithms for this task. At the same time, this is also a good opportunity to make some concepts more concrete that we have so far mentioned only in passing. This includes the determination of master integrals through the integration-by-parts identities (IBPs), the derivative of Feynman integrals w.r.t. a kinematic variable, the matrix structure of the differential equations, as well as the algebraic structure of its entries.

All of these concepts will be crucial as a starting point for the presentation of our new algorithm for the canonical form in chapter 6. Further, the balance transformations make many properties of the canonical differential equations manifest and realizing how these properties can be reached step by step will likewise be helpful in understanding the principles of our new algorithm. We will also discuss the limitations of the method of balance transformations and how, in this thesis, we strive to fill an important gap among the available techniques for the canonical form.

Throughout this chapter, we will again use the massless one-loop box integral family to serve as an explicit example for all introduced concepts, however, we will frequently also refer to the three-mass two-loop box of section 3.4 to point out additional complications in the multi-loop case.

5.1 Revisiting Integration-by-Parts

As a reminder, the integrals in the massless one-loop box-family are defined through

$$I_{a_1,a_2,a_3,a_4} = e^{\epsilon\gamma_E} \int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{1}{D_1^{a_1} D_2^{a_2} D_3^{a_3} D_4^{a_4}} \tag{5.3}$$

where the propagators are

$$D_1 = k^2, \qquad D_2 = (k+p_1)^2, \qquad D_3 = (k+p_1+p_2)^2, \qquad D_4 = (k-p_4)^2. \tag{5.4}$$

The integrals in this family are related by the integration-by-parts identities[1]

$$0 = e^{\epsilon\gamma_E} \int \frac{\mathrm{d}^D k}{i\pi^{D/2}} \frac{\partial}{\partial k^\mu} \frac{v^\mu}{D_1^{a_1} D_2^{a_2} D_3^{a_3} D_4^{a_4}}, \tag{5.5}$$

where v can be any of the available vectors, i.e. k, p_1, p_2 or p_4. We can also choose $v = p_3$, but the resulting relation will obviously not be independent of the others. The derivative inside the integral will now lead to a linear combination of terms where the powers a_i are in general different from the original ones. In addition, numerators in the form $v^\mu \partial_{k^\mu} D_i$ will appear. However, since the propagators D_i form a complete set of

[1] Note that the vanishing of total derivatives is special to dimensional regularization and other regulators might require careful consideration of boundary terms.

independent scalar products, these numerators can again be written as propagators. For example, for $v = k$ we have

$$\begin{aligned} k^\mu \partial_{k^\mu} D_1 &= 2D_1, & k^\mu \partial_{k^\mu} D_2 &= D_1 + D_2, \\ k^\mu \partial_{k^\mu} D_3 &= D_1 + D_3 - s, & k^\mu \partial_{k^\mu} D_4 &= D_1 + D_4 \end{aligned} \tag{5.6}$$

so that eq. (5.5) becomes

$$\begin{aligned} 0 =& (D - 2a_1 - a_2 - a_3 - a_4) I_{a_1,a_2,a_3,a_4} - s a_3 I_{a_1,a_2,a_3+1,a_4} - a_2 I_{a_1-1,a_2+1,a_3,a_4} \\ & - a_3 I_{a_1-1,a_2,a_3+1,a_4} - a_4 I_{a_1-1,a_2,a_3,a_4+1}. \end{aligned} \tag{5.7}$$

We note that, starting from two-loops, it is necessary to introduce auxiliary propagators into the integral family since the denominators coming from the Feynman diagram are not sufficient to form an independent set of scalar products[2]. These auxiliary propagators are the irreducible scalar products (ISPs) and we already made use of them at the beginning of section 3.4.

Additional relations, which are not expressible through integration-by-parts, come from diagram symmetries. For example, since the kinematic variables, $s = (p_1 + p_2)^2$ and $t = (p_1 + p_3)^2$, are invariant under the simultaneous exchange $\{p_1 \leftrightarrow p_3, p_2 \leftrightarrow p_4\}$, the integrals have to have the symmetry $I_{a_1,a_2,a_3,a_4} = I_{a_3,a_2,a_1,a_4}$. This can easily be verified by performing the momentum shift $k \to k + p_1 + p_2$ after the exchange of the external momenta or by comparing the parametric representation of the two integrals. The latter is also used to automatically detect scaleless integrals which vanish in dimensional regularization.

All relations together can then be solved in terms of a finite number [124] of master integrals. Since this is a very important task in modern particle physics, there are various implementations that aim at doing this as efficiently as possible. In particular, LiteRed [125] is able to solve the relations with analytic indices a_i, which is useful if a large number of relatively simple integrals should be computed. On the other hand, for more complicated integrals, it has become standard practice to use the Laporta algorithm [126], where a system of equations with integer values for the indices is generated before attempting to solve it. Common implementations of this are for example `FIRE` [127], `Kira` [128], FiniteFlow [129], `Reduze 2` [130] and AIR [131].

In the present case of the massless one-loop box integral, we find that there are only three independent master integrals. However, since the basis is not unique, we have to make a choice, which is commonly done by requiring the following numbers to be as small as possible:

- ℓ, the number of denominators, i.e. positive exponents a_i with $a_i > 0$

[2] When deriving these relations, the external momenta are usually considered in D dimensions. However, there also exist methods which restrict the external momenta to four dimensions [122, 123] in which case the number of independent scalar products further reduces due to the vanishing of certain Gram determinants.

- d, the number of dots, i.e.

$$d = -\ell + \sum_{j|a_j>0} a_j \tag{5.8}$$

- r, the total power of the numerator, i.e.

$$r = -\sum_{j|a_j\leq 0} a_j. \tag{5.9}$$

In general, the order of importance varies between different implementations, although the first criterion is usually taken to be the most important one.[3] The idea behind this is that integrals with higher ℓ, d and r are considered to be more complex. Following these criteria, we find

$$\vec{f} = \begin{pmatrix} I_{0,1,0,1} \\ I_{1,0,1,0} \\ I_{1,1,1,1} \end{pmatrix} \tag{5.10}$$

to be a suitable basis.

To discuss this choice of master integrals further, it is advantageous to introduce the concept of *sectors*: A sector is the set of all integrals with the same denominators, but possibly raised to different powers or with different numerators. In other words, two integrals are in the same sector if they have the same lines in their diagram. It is common practice to represent a sector by its *corner integral*, i.e. the integral with no numerators and all denominators raised to power one. For example, $I_{1,0,1,-1}$ and $I_{2,-1,1,0}$ are both in the same sector which is called the s-channel bubble sector and denoted by $J_{1,0,1,0}$. Further, a sub-sector is obtained by removing one or more denominators from a sector. For instance, $J_{1,0,1,0}$ is a sub-sector of $J_{1,1,1,0}$. Lastly, the sector with all possible lines, i.e. the highest number of denominators, is called the top sector.[4]

Using this terminology, we see that our basis includes one integral from the top sector $J_{1,1,1,1}$ which cannot be further reduced to only integrals from its sub-sectors. This leads to the concept of master integrals of a sector: In general we say that a sector has n master integrals if all integrals from this sector can be written as a linear combination of n integrals from this sector plus integrals from sub-sectors. Therefore the box sector, as well as the two bubble sectors $J_{0,1,0,1}$ and $J_{1,0,1,0}$, each have one master integral. For example the integrals $I_{1,1,2,2}$ and $I_{1,0,2,0}$ reduce to

$$\begin{aligned} I_{1,1,2,2} =& \frac{(D-5)(D-6)}{st} I_{1,1,1,1} - \frac{4(D-5)(D-3)}{s^3 t} I_{1,0,1,0} \\ & - \frac{4(D-5)(D-3)}{st^3} I_{0,1,0,1}, \end{aligned} \tag{5.11}$$

$$I_{1,0,2,0} = -\frac{(D-3)}{s} I_{1,0,1,0}. \tag{5.12}$$

[3] An algorithmic implementation will of course define further criteria so that no two integrals have the same importance.

[4] The diagram of the top sector typically has only three-point vertices and no four- or higher-point vertices.

On the other hand, the triangle sectors $J_{1,1,1,0}, J_{1,1,0,1}, J_{1,0,1,1}$ and $J_{0,1,1,1}$ have zero master integrals, which can be seen e.g. in

$$I_{1,1,1,0} = \frac{2(D-3)}{(D-4)s} I_{1,0,1,0}. \tag{5.13}$$

Of course, the terminology of master integrals per sector is mainly useful when combined with the criterion of a small number of denominators because otherwise a master integral can always be replaced by an integral from one of its super-sectors that is linearly independent from the rest of the basis.

5.2 Differential Equations for the Massless One-Loop Box Integral

The next step in the computation of the integrals of the massless one-loop box family is the computation of the master integrals. To this end, we take the derivative of the basis $\vec{f}$ w.r.t. the kinematic invariants s and t. However, since the propagators in eq. (5.4) do not explicitly depend on these variables, we make the ansatz

$$\partial_s = (\alpha_1 p_1 + \alpha_2 p_2 + \alpha_4 p_4) \cdot \partial_{p_2}, \tag{5.14}$$
$$\partial_t = (\beta_1 p_1 + \beta_2 p_2 + \beta_4 p_4) \cdot \partial_{p_4}. \tag{5.15}$$

The coefficients can be found by requiring that the derivatives are compatible with the kinematics. The result is

$$\alpha_1 = \frac{1}{2s}, \qquad \alpha_2 = \frac{2s+t}{2s(s+t)}, \qquad \alpha_4 = \frac{1}{2(s+t)}, \tag{5.16}$$
$$\beta_1 = \frac{1}{2t}, \qquad \beta_2 = \frac{1}{2(s+t)}, \qquad \beta_4 = \frac{s+2t}{2t(s+t)}. \tag{5.17}$$

A general formula for this change of variables has been given in [125]:

$$\frac{\partial}{\partial(p_1 \cdot p_2)} = \sum_{i=1}^{3} [\mathbb{G}^{-1}]_{i2}\, p_i \cdot \partial_{p_1} = \sum_{i=1}^{3} [\mathbb{G}^{-1}]_{i1}\, p_i \cdot \partial_{p_2}, \tag{5.18}$$
$$\frac{\partial}{\partial(p_1^2)} = \frac{1}{2} \sum_{i=1}^{3} [\mathbb{G}^{-1}]_{i1}\, p_i \cdot \partial_{p_1}, \tag{5.19}$$

where $\mathbb{G}$ is the Gram matrix, $\mathbb{G}_{ij} = p_i \cdot p_j$.[5]

Applying these derivatives to our master integrals yields linear combinations very similar to the ones coming from the derivative in the integration-by-parts identities.

[5] Eqs. (5.18) and (5.19) make it clear that there is some freedom in defining the derivative. However, the result will always be the same after IBP reduction.

However, all appearing integrals can again be written in terms of master integrals through a subsequent IBP reduction. The resulting differential equations are

$$\partial_s \vec{f} = A_s \vec{f}, \tag{5.20}$$

$$\partial_t \vec{f} = A_t \vec{f}, \tag{5.21}$$

with

$$A_s = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -\frac{\epsilon}{s} & 0 \\ -\frac{2(1-2\epsilon)}{st(s+t)} & \frac{2(1-2\epsilon)}{s^2(s+t)} & -\frac{s+t+\epsilon t}{s(s+t)} \end{pmatrix}, \tag{5.22}$$

$$A_t = \begin{pmatrix} -\frac{\epsilon}{t} & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{2(1-2\epsilon)}{t^2(s+t)} & \frac{2(1-2\epsilon)}{st(s+t)} & -\frac{s+t+\epsilon s}{t(s+t)} \end{pmatrix}. \tag{5.23}$$

Note that the matrices are rational functions in the kinematic variables and ϵ, which follows simply from the structure of the integrand and the IBP identities. An immediate check of the two equations can be obtained through $\partial_s \partial_t \vec{f} = \partial_t \partial_s \vec{f}$, which, for the coefficient matrices, translates to

$$\partial_t A_s - \partial_s A_t + [A_s, A_t] = 0. \tag{5.24}$$

This is known as the *integrability* condition and it implies that the differential equations can be unambiguously integrated, meaning that the result does not depend on the chosen integration contour. In canonical form one can collect powers of ϵ in this equation, s.t.

$$\partial_t A_s - \partial_s A_t = 0 \qquad \text{and} \qquad [A_s, A_t] = 0 \tag{5.25}$$

hold separately. The first of these equations implies that there is a matrix A s.t. its total differential is $\mathrm{d}A = \mathrm{d}s A_s + \mathrm{d}t A_t$.

Another useful check is to compute

$$(s\partial_s + t\partial_t)\vec{f} = (sA_s + tA_t)\vec{f} = \begin{pmatrix} -\epsilon & 0 & 0 \\ 0 & -\epsilon & 0 \\ 0 & 0 & -2-\epsilon \end{pmatrix} \vec{f}. \tag{5.26}$$

As one can readily check, the entries on the diagonal correspond to the scaling dimensions of the master integrals. Since this matrix can easily be inferred from the integrals themselves, it is actually redundant to compute both A_s and A_t. Instead, we should normalize our integrals to have mass-dimension zero

$$\vec{f}' = \begin{pmatrix} (-t)^{\epsilon} I_{0,1,0,1} \\ (-t)^{\epsilon} I_{1,0,1,0} \\ (-t)^{2+\epsilon} I_{1,1,1,1} \end{pmatrix}, \tag{5.27}$$

so that they can only depend on the dimensionless variable $x = s/t$. In practice, we set $x = -s, t = -1$ since the overall factor of t can always be inferred from the mass dimension of the integrals. The differential equations are therefore

$$\partial_x \vec{f} = A(x,\epsilon)\vec{f}, \tag{5.28}$$

with

$$A(x,\epsilon) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{\epsilon}{x} & 0 \\ \frac{2(1-2\epsilon)}{x(1+x)} & \frac{2(1-2\epsilon)}{x^2(1+x)} & \frac{1+x+\epsilon}{x(1+x)} \end{pmatrix}. \tag{5.29}$$

5.3 Algorithmic Reduction to Canonical Form

Now that we have obtained the differential equations for the master integrals we would like to find a transformation $\vec{f} = T\vec{g}$ that brings them into canonical form

$$\partial_x \vec{g} = \epsilon\, \tilde{A}(x)\vec{g}, \tag{5.30}$$

where

$$\epsilon\tilde{A}(x) = T^{-1}\left[A(x,\epsilon)T - \partial_x T\right] \tag{5.31}$$

has only logarithmic singularities. We have already seen how the transcendental weight can be used to achieve this. In this section, however, we will use the algorithm introduced in [37] to reach the same result. This is done in multiple steps where each step will change the properties of $A(x,\epsilon)$ to be closer to the ones of the canonical form. In particular, the steps are

1) Fuchsification: Removal of essential singularities

2) Normalization: Shifting the eigenvalues of the residue-matrices, s.t. they are proportional to ϵ

3) Factorization: Factorizing ϵ

and they will be described in more detail further below. Here we only mention that each step requires certain criteria to be met in order to succeed, giving us the opportunity to discuss in which cases a canonical form is unobtainable. The algorithm has already been implemented in the packages `Libra` [38], `epsilon` [40] and `Fuchsia` [39] and we refer to the respective papers for their usage.

5.3.1 Fuchsification

As discussed in section 2.3, Feynman integrals are free of essential singularities, i.e. they only have regular singularities. In the present case, this means that it should be possible to make this property manifest by reaching the form

$$\mathrm{d}\vec{f} = \left(\sum_i a_i(\epsilon)\frac{\mathrm{d}x}{(x-c_i)}\right)\vec{f} = \left(\sum_i a_i(\epsilon)\,\mathrm{d}\log(x-c_i)\right)\vec{f} \tag{5.32}$$

where c_i are constants and a_i are matrices independent of x. Differential equations of this type are called *Fuchsian*. Often one also speaks of the *dlog* form. We can see from (5.29) that the one-loop box integrals have potential singularities at $x = 0$ and $x = -1$. In addition, $x = \infty$ is also a singular point, which is visible through the change of variables $x = 1/y$.

Inspecting eq. (5.29), it becomes clear that we need to remove the double pole at $x = 0$. This can be achieved by letting T be a so-called *balance* transformation

$$T = \mathcal{B}(P, x_1, x_2; x) = \bar{P} + \frac{x - x_2}{x - x_1} P, \tag{5.33}$$

where P is a projector, $P^2 = P$, and $\bar{P} = \mathbb{1} - P$. Note that, because $\bar{P}P = 0$, the inverse of (5.33) is simply $\mathcal{B}(P, x_2, x_1; x)$ and hence the transformation only has the singular points $x = x_1$ and $x = x_2$. Therefore, either x_1, x_2 or both will be chosen to be a singular point that we would like to affect trough the transformation. In addition, it is also possible to choose the point at infinity by defining

$$\mathcal{B}(P, x_1, \infty; x) = \bar{P} + \frac{1}{x - x_1} P, \qquad \mathcal{B}(P, \infty, x_2; x) = \bar{P} + (x - x_2) P. \tag{5.34}$$

Now, without loss of generality, let $x_1 = 0$ and assume that the coefficient matrix $A(x, \epsilon)$ has the following expansion around this singular point:

$$A(x, \epsilon) = \frac{A_0}{x^{r+1}} + \frac{A_1}{x^r} + \mathcal{O}(1/x^{r-1}), \tag{5.35}$$

where r is called the Poincaré rank of $A(x, \epsilon)$. Computing the transformed matrix

$$A_F(x, \epsilon) = T^{-1} \left[A(x, \epsilon) T - \partial_x T \right] \tag{5.36}$$

and collecting the most singular terms results in

$$A_F(x, \epsilon) = -\frac{x_2 \bar{P} A_0 P}{x^{r+2}} + \frac{P A_0 P + \bar{P}(A_0 - x_2 A_1 P)}{x^{r+1}} + \mathcal{O}(x^r). \tag{5.37}$$

Therefore, the first requirement on the projector P is $\bar{P} A_0 P = 0$, so that the Poincaré rank of the matrix at $x = 0$ is not increased. This can easily be achieved by noting that an $n \times n$ projector matrix can always be constructed from an $n \times k$ matrix $\mathcal{U}$ and an $k \times n$ matrix $\mathcal{V}^{\mathrm{T}}$ in the following way:

$$P = \mathcal{U} (\mathcal{V}^{\mathrm{T}} \mathcal{U})^{-1} \mathcal{V}^{\mathrm{T}} \tag{5.38}$$

Choosing $\mathcal{U}$ s.t. $A_0 \mathcal{U} = \mathcal{U} C$ for some matrix $C \equiv C(\epsilon)$, one can easily show that the resulting projector satisfies $\bar{P} A_0 P = 0$. Note that $A_0 \mathcal{U} = \mathcal{U} C$ means that we should choose the columns of $\mathcal{U}$ to be the (generalized) eigenvectors of the matrix A_0. Likewise, one can show that $\mathcal{V}^{\mathrm{T}}$ with $\mathcal{V}^{\mathrm{T}} A_0 = C' \mathcal{V}^{\mathrm{T}}$ ensures that the Poincaré rank at $x = x_2$ is not increased.

Next, for Fuchsification, we would like to decrease the rank of the coefficient matrix at $\mathcal{O}(1/x^{r+1})$ so that repeated application of such a transformation eventually leads to

the vanishing of this coefficient. An algorithm for constructing a suitable projector has been given in [132] section E.8. The general idea is to first choose only the eigenvectors with eigenvalues zero, so that $A_0\mathcal{U} = 0$ and therefore $A_0 P = 0$. Then one ensures that $(A_0 - x_2 A_1 P)$ has a non-zero overlap with the direction of the projector P, so that the complementary projector $\bar{P}$ necessarily removes these components and therefore reduces the rank of the coefficient-matrix. This can again be done solely through the choice of $\mathcal{U}$. Similarly, $\mathcal{V}^{\mathrm{T}}$ can be chosen to reduce the rank of the coefficient matrix at the singular point x_2.

In total, this gives an algorithm to systematically bring the differential equations into dlog form by constructing appropriate balance transformations that decrease the Poincaré rank at one singular point while not affecting the other. Even more, it is often possible to choose $\mathcal{U}$ and $\mathcal{V}^{\mathrm{T}}$ in such a way that the Poincaré rank at both singular points is decreased simultaneously.

Applied to $A(x, \epsilon)$ in (5.29) we find that the coefficient-matrix of the $1/x^2$ pole has rank one. Therefore, a single balance transformation with $x_1 = 0$ and e.g. $x_2 = -1$ is enough to Fuchsify the matrix at $x = 0$ while not affecting the Poincaré rank at $x = -1$. The result is

$$A_F(x, \epsilon) = \frac{a_0(\epsilon)}{x} + \frac{a_{-1}(\epsilon)}{1 + x} \tag{5.39}$$

with

$$a_0(\epsilon) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \epsilon & 0 \\ \frac{2(2+\epsilon)(1-2\epsilon)}{\epsilon} & \frac{2(2-\epsilon)(1-2\epsilon)}{\epsilon} & 2 + \epsilon \end{pmatrix}, \tag{5.40}$$

and

$$a_{-1}(\epsilon) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ -\frac{2(2+\epsilon)(1-2\epsilon)}{\epsilon} & -\frac{2(2-\epsilon)(1-2\epsilon)}{\epsilon} & -1 - \epsilon \end{pmatrix}. \tag{5.41}$$

Further, by the global residue theorem, we have $a_\infty(\epsilon) = -a_0(\epsilon) - a_{-1}(\epsilon)$.

Let us note that this algorithm will always succeed in finding an appropriate transformation to reduce the Poincaré rank at a given singular point, if such a transformation exists [133]. In other words, the existence of the appropriate eigenvectors that decrease the rank of the leading term in the expansion gives a necessary and sufficient criterion for the possibility of removing an essential singularity [134]. However, since Feynman integrals only have regular singularities, we expect this to be always the case.[6]

5.3.2 Normalization

The next step is to normalize the matrix residues $a_i(\epsilon)$, which means that their eigenvalues should be proportional to ϵ. The reason for doing this will become clear in the next

[6] An exception to this may be when the IBP reduction failed to completely reduce all integrals, so that some relations between the master integrals are not implemented into the differential equation system.

section. We note that all eigenvalues are of the form $n + k\epsilon$, which can be seen from the parametric representation and proven by using the method of regions [54]. Moreover, we will assume that n is an integer, which is the case for our example where the eigenvalues are

$$a_{-1}(\epsilon): \quad \{0, 0, -1-\epsilon\} \tag{5.42}$$
$$a_{0}(\epsilon): \quad \{0, 2+\epsilon, \epsilon\} \tag{5.43}$$
$$a_{\infty}(\epsilon): \quad \{0, -1, -\epsilon\} \tag{5.44}$$

The case where n is not an integer will be discussed in section 5.5.

Constructing an appropriate transformation is now very simple since we already introduced all necessary tools in the last section. As an example, we can shift the third eigenvalue of $a_{-1}(\epsilon)$ by $+1$ while simultaneously shifting the second eigenvalue of $a_0(\epsilon)$ by -1. This is done through a balance transformation with $x_1 = -1$ and $x_2 = 0$, where $\mathcal{U}$ is now the right eigenvector of the corresponding eigenvalue at x_1 and $\mathcal{V}^{\mathrm{T}}$ is the left eigenvector of the corresponding eigenvalue at x_2.

To understand why e.g. $\mathcal{U}$ is chosen in this way, one can consider a basis where $a_{-1}(\epsilon)$ is in Jordan form. Then the projector P will have a 1 one the diagonal entry corresponding to the position of the eigenvalue we want to shift. Using this projector in the balance transformation then leads to the desired shift in the Jordan form of the coefficient matrix.

In summary, the balance transformation will always increase an eigenvalue at x_1 by one, while decreasing an eigenvalue at x_2 by one. In principle, successive application of this always leads to a completely normalized matrix, since we know that the sum of all eigenvalues has to be zero by the global residue theorem. However, it can happen that the two eigenvectors are orthogonal, in which case $\mathcal{V}^{\mathrm{T}}\mathcal{U}$ in eq. (5.38) is not invertible. Then one can try to choose a different pair of eigenvectors. Note that it might be necessary to artificially shift an already normalized eigenvalue, so that it can then be balanced with a different eigenvalue.

If at some point it is not possible to find a suitable pair of eigenvectors anymore, one can conclude that the ϵ-factorized form cannot be reached using rational transformations only. A typical case of where this happens is when the result involves elliptic functions, see e.g. [68]. We will give an example of such a differential equation in the next chapter.

For our current example however, this obstruction does not occur and we can completely balance the second eigenvalue of $a_0(\epsilon)$ first with the third eigenvalue of $a_{-1}(\epsilon)$ and then with the second eigenvalue of $a_{\infty}(\epsilon)$. This results in a differential equation which is both Fuchsian and normalized. Note that, to some extent, it is possible to combine the Fuchsification with the normalization procedure by e.g. choosing $\mathcal{U}$ to affect a matrix rank at one singular point, while choosing $\mathcal{V}^{\mathrm{T}}$ to shift an eigenvalue of a matrix residue at another singular point.

5.3.3 Factorization

The last step of the algorithm is to find a transformation matrix which completely factorizes ϵ from the residue-matrices $a_i(\epsilon)$. If there was only one singular point, this

would be an easy task since we could just transform $a_i(\epsilon)/\epsilon$ to Jordan form through a simple similarity transformation. Because this is not the case, we will have to allow for a more general transformation $T(\epsilon)$ to factor ϵ from all $a_i(\epsilon)$ simultaneously.

This task can be stated as finding a $T(\epsilon)$ s.t. there exist constant matrices s_k with

$$T^{-1}(\epsilon)\frac{a_i(\epsilon)}{\epsilon}T(\epsilon) = s_k = T^{-1}(\mu)\frac{a_i(\mu)}{\mu}T(\mu). \tag{5.45}$$

We can make this system of equations linear by multiplying with $T(\epsilon)$ from the left and $T^{-1}(\mu)$ from the right:

$$\frac{a_i(\epsilon)}{\epsilon}T(\epsilon,\mu) = T(\epsilon,\mu)\frac{a_i(\mu)}{\mu}, \tag{5.46}$$

where $T(\epsilon,\mu) = T(\epsilon)T^{-1}(\mu)$ and there are as many such equations as there are singular points. In practice, one can set μ to an arbitrary number so long as $T(\mu)$ remains well defined and invertible. This is because ϵ-factorized differential equations

$$\partial_x \vec{g} = \epsilon \tilde{A}(x)\vec{g}, \tag{5.47}$$

remain factorized when performing an arbitrary constant, i.e. x and ϵ-independent transformation $T(\mu)$. In fact, in [135] it was proven that the canonical form is unique up to exactly such transformations.

For the example of the massless one-loop box, the factorization step results in

$$\partial_x \vec{g} = \epsilon \left(\frac{\tilde{a}_{-1}}{1+x} + \frac{\tilde{a}_0}{x} \right), \tag{5.48}$$

with

$$\tilde{a}_{-1} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \text{and} \qquad \tilde{a}_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}. \tag{5.49}$$

Although our example only depends on a single variable x, all steps of the algorithm in principle also work in the multi-variables case. One simply applies each step to one variable at a time while treating the others as constant. However, after having brought the differential equations w.r.t. one variable into canonical form, the transformations for the other variables should be independent of the first variable. In practice, the ability to find such transformations mainly depends on an educated choice of variables and the correct order of variables for which to apply the algorithm. Because of this, as well as the increasing algebraic complexity, the leading singularity analysis is usually preferred in the multivariate case.

We note that it is also possible to directly make an ansatz for $\tilde{A}(x)$ and $T(x,\epsilon)$ and solve the transformation law

$$\epsilon T(x,\epsilon)\tilde{A}(x) = A(x,\epsilon)T(x,\epsilon) - \partial_x T(x,\epsilon) \tag{5.50}$$

order-by-order in ϵ. In doing so, one has to deal with the fact that the equations are not linear in the unknowns due to the term $T(x,\epsilon)\tilde{A}(x)$. However, in [136] it was shown that they can be linearized by utilizing the above mentioned freedom of a constant transformation. This approach is implemented in the package *CANONICA* [135]. In chapter 6 we describe another method to reach the canonical form through an ansatz for $\tilde{A}(x)$ but without the need of an ansatz for $T(x,\epsilon)$.

5.4 The Block Structure of the Differential Equations

In section 5.1 we argued that it is advantageous to introduce the concept of sectors for the IBP reduction. In doing so, we also showed how the integrals of a specific sector are reduced to the master integrals of that sector plus master integrals from its sub-sectors. Since the coefficients of the master integrals in the differential equations directly come from an IBP reduction, it is natural to expect that this dependence is also visible in the coefficient matrix A.

Indeed, we observe from eqs. (5.22) and (5.23) the following structure:

$$\partial_{s,t} \begin{pmatrix} I_{0,1,0,1} \\ I_{1,0,1,0} \\ I_{1,1,1,1} \end{pmatrix} = \begin{pmatrix} \boxed{\star} & \cdots & 0 \\ \vdots & \boxed{\star} & 0 \\ \star & \star & \boxed{\star} \end{pmatrix} \begin{pmatrix} I_{0,1,0,1} \\ I_{1,0,1,0} \\ I_{1,1,1,1} \end{pmatrix} \tag{5.51}$$

First, we have marked the diagonal blocks, i.e. the homogenous part of the differential equations for each sector, through solid lines. The size of a diagonal block directly corresponds to the number of master integrals in the sector. Importantly, it is easy to see that a diagonal block corresponds to the maximal cut of the integrals in that sector. Indeed, the differential equation for the top sector is

$$\partial_{s,t} \left(I_{1,1,1,1} \right) = \left(\boxed{\star} \right) \left(I_{1,1,1,1} \right) + \cdots \tag{5.52}$$

where the dots correspond to integrals that vanish on the maximal cut.

Second, the derivative of the box integral depends on the master integrals in its sub-sectors through off-diagonal blocks. On the other hand, the bubble integrals do not have sub-sectors and therefore their derivative only depends on themselves. Moreover, the bubble sectors do not depend on each other, since one cannot be a sub-sector of the other.

In total, sorting the master integrals by sector and by increasing number of denominators leads to the following structure of the differential equations:

1. They are lower block triangular.
2. The size of a diagonal block corresponds to the number of master integrals in the sector.
3. The derivative of a sector can only depend on its sub-sectors.
4. Sectors with the same number of denominators cannot depend on each other because they cannot be sub-sectors of each other.

We have emphasized the last point through the dotted lines in eq. (5.51). Note that the outlined structure simply follows from the fact that a derivative of the integrand cannot introduce new denominators into the integrand. This is true for both the derivative w.r.t. an external variable and w.r.t. the loop momentum.

As an advanced example, in figure 5.1 we present the structure of the differential equations for the three-mass two-loop box of section 3.4. We can immediately see that

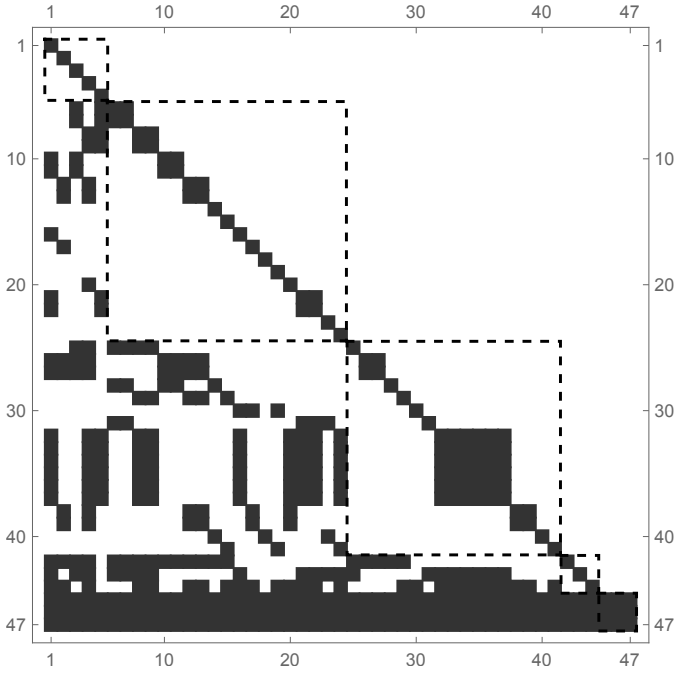


Figure 5.1: Block structure of the differential equations for the three-mass two-loop box integral family. There are 47 master integrals. Black elements indicate non-zero blocks. Dashed lines group together sectors with the same number of denominators.

there are several sectors with one or two master integrals. In addition, there is a single sector with six master integrals, for which we found a suitable dlog integral in eq. (3.56). Again we observe that sectors with the same number of propagators, which are grouped together by the dashed lines, do not depend on each other. In general, the matrix is quite sparse due to the limited dependence of the sectors on each other. The latter dependence can simply be inferred from the denominators present in the sectors while also taking symmetries of the integrand into account.

The block structure of the differential equations simplifies the process of finding a canonical basis enormously. First, we note that, if the diagonal blocks are Fuchsian and normalized, then the whole differential equation matrix is automatically normalized. Therefore, if the diagonal blocks are in canonical form, all we need to do is Fuchsify the off-diagonal blocks and then factorize ϵ from the whole matrix.

Second, Fuchsifying the off-diagonal blocks is much easier than doing the same for the

diagonal blocks. Consider the differential equation matrix

$$A(x,\epsilon) = \begin{pmatrix} \epsilon C(x) & 0 \\ B(x,\epsilon) & \epsilon D(x) \end{pmatrix}, \tag{5.53}$$

where the diagonal blocks C and D are in canonical form[7] and $B(x,\epsilon)$ has the following expansion around $x = 0$:

$$B(x,\epsilon) = \frac{B_0(\epsilon)}{x^{r+1}} + \mathcal{O}(1/x^r), \tag{5.54}$$

with $r > 0$. Since $C(x)$ and $D(x)$ are canonical, they are of the form

$$C(x) = \frac{C_0}{x} + \mathcal{O}(x^0), \qquad D(x) = \frac{D_0}{x} + \mathcal{O}(x^0). \tag{5.55}$$

The transformation

$$T = \begin{pmatrix} \mathbb{1} & 0 \\ \frac{M(\epsilon)}{x^r} & \mathbb{1} \end{pmatrix} \tag{5.56}$$

has the inverse

$$T^{-1} = \begin{pmatrix} \mathbb{1} & 0 \\ -\frac{M(\epsilon)}{x^r} & \mathbb{1} \end{pmatrix} \tag{5.57}$$

and therefore only affects the singular point $x = 0$. Using this transformation on $A(x,\epsilon)$, the diagonal blocks remain unchanged, whereas the result for the off-diagonal block is

$$B(x,\epsilon)' = \frac{B_0(\epsilon) + rM(\epsilon) + \epsilon[D_0 M(\epsilon) - M(\epsilon)C_0]}{x^{r+1}} + \mathcal{O}(1/x^r). \tag{5.58}$$

Demanding that the numerator vanishes gives a set of linear equations for the entries of the matrix $M(\epsilon)$. Moreover, one can show that this equation will actually always have a solution [37] and we can therefore easily Fuchsify the off-diagonal block $B(x,\epsilon)$.

To illustrate the global strategy on larger matrices, consider

$$A(x,\epsilon) = \begin{pmatrix} \epsilon D_{11}(x) & 0 & 0 \\ A_{21}(\epsilon,x) & \epsilon D_{22}(x) & 0 \\ A_{31}(\epsilon,x) & A_{32}(\epsilon,x) & \epsilon D_{33}(x) \end{pmatrix}, \tag{5.59}$$

where the diagonal blocks are again in canonical form. One can then first Fuchsify $A_{21}(\epsilon,x)$ where the only other block this affects is $A_{31}(x,\epsilon)$. Next, we transform $A_{32}(x,\epsilon)$ which likewise affects $A_{31}(x,\epsilon)$. Therefore $A_{31}(x,\epsilon)$ should be considered last, because changes on this block do not alter the other blocks in any way. To summarize the steps:

1. Transform the diagonal blocks into canonical form.

[7] Transformations done on one diagonal block cannot influence any other diagonal block. Also note that the differential equation for the integrals in block $\epsilon C(x)$ can already be solved.

2. Subsequently Fuchsify the off-diagonal blocks by working from top to bottom and right to left.[8]

3. Factorize ϵ from the whole matrix.

Obviously, the factorization can already be done for parts of the matrix at an earlier stage if this simplifies the analysis. In the above example, one could already factorize the matrix consisting of $\epsilon D_{11}(x), \epsilon D_{22}(x)$ and $A_{21}(\epsilon, x)$ after having brought $A_{21}(\epsilon, x)$ into dlog form.

5.5 Variable Changes and Rationalization

In this section we want to comment on the case when the eigenvalues of the residue matrices are not of the form $n + k\epsilon$ with n being an integer. Of particular interest is the case of half integers, but other cases, though more difficult, can be studied analogously. Therefore let us assume that the coefficient matrix $a_{x_1}(\epsilon)$ of the singular point $x = x_1$ has an eigenvalue of the form $1/2 + n + k\epsilon$, with n being again an integer. Since the balance transformations can only shift the eigenvalues by ± 1 they cannot be used to normalize this eigenvalue.

Instead, we should perform a change of variables $x = y(x)$ that rationalizes the square-root $\sqrt{x - x_1}$. One way to see this is by considering the solution of the differential equations around x_1 (see e.g. [137, 138]), which is

$$\vec{f} = (x - x_1)^{a_{x_1}} \left[\mathbb{1} + \mathcal{O}(x - x_1)\right] \vec{f}_0(\epsilon), \tag{5.60}$$

where $\vec{f}_0$ is a vector of boundary constants. By choosing a basis in which a_{x_1} is in Jordan form, we find that at least one of the integrals will behave as $(x - x_1)^{1/2+n+k\epsilon}$ and therefore involves the above mentioned square-root. In the case where only one singular point is affected, we can just use $x = y^2 + x_1$, which causes the solution to behave as $y^{1+2n+2k\epsilon}$ and therefore we can apply balance transformations in the variable y.

However, it is often the case that not one but multiple singular points are affected through a single square-root, which e.g. happens in the case of $\sqrt{1 - x^2}$. Especially for multivariate differential equations it can be very difficult to find an appropriate change of variables[9] due to the increasing complexity of the argument of the square-root. And even if such a variable change is found, it usually increases the polynomial degree of the other denominators drastically, making a subsequent analysis very tedious. Because of this, approaches based on the transcendental weight or on an ansatz for the canonical form are usually preferred for multivariate kinematics.

[8] Note that, when Fuchsifying the off-diagonal blocks of a sector, one can remove all other sectors with the same number of propagators because they cannot depend on the considered sector. Another way to think about this is that sectors with the same number of denominators can always be reordered among each other in the basis, without destroying the block-triangular form.

[9] We refer to [41, 42] for an algorithmic approach to the question of rationalization.

5.6 Relaxing the Canonical Form: Importance of the ϵ^0-Part and Normalization Factors

The canonical form is arguably the most useful form when trying to solve the differential equations in an expansion in ϵ in terms of iterated integrals. First, the factorized ϵ allows one to compute each order in ϵ as an integral over the coefficient matrix multiplied by the previous order. Second, since the integration kernels are in dlog form, it is trivial to identify the iterated integrals with the multiple polylogarithms

$$G(a_1, a_2, \ldots, a_n; x) = \int_0^x \frac{\mathrm{d}t}{t - a_1} G(a_2, \ldots, a_n; t), \qquad G(; x) = 1 \tag{5.61}$$

of section 2.6.

In this section, however, we would like to consider the question what properties of the canonical form we can relax and still retain the ability to solve it in a straightforward, albeit more difficult, way. First, we note that double and higher order poles as integration kernels are in principle no problem, since one can always use integration-by-parts to reduce the order of the pole[10]. For example,

$$\begin{aligned}\int_0^x \frac{\mathrm{d}t}{(t+1)^2} G(1, a_2, \ldots, a_n; t) = &\int_0^x \frac{\mathrm{d}t}{(t+1)(t-1)} G(a_2, \ldots, a_n; t) \\ &- \frac{1}{(t+1)} G(1, a_2, \ldots, a_n; t)\Big|_{t=0}^{t=x} \\ = &\frac{1}{2} G(1, a_2, \ldots, a_n; x) - \frac{1}{2} G(-1, a_2, \ldots, a_n; x) \\ &- \frac{1}{1+x} G(1, a_2, \ldots, a_n; x) + G(1, a_2, \ldots, a_n; 0).\end{aligned} \tag{5.62}$$

Second, it is still possible to iteratively solve the differential equations order-by-order in ϵ, if they are in the form $\partial_x \vec{f} = \epsilon A(x, \epsilon) \vec{f}$ and the ϵ-expansion of $A(x, \epsilon)$ starts at ϵ^0. This is simply because the integrals at a fixed order in ϵ can still be computed through an integral over (a linear combination of) the previous orders. However, one might potentially have to consider very high orders in ϵ to compute all contributions to the order in ϵ one is interested in.

Moreover, it is possible to relax this condition even further to the form

$$\partial_x \vec{f} = A(x, \epsilon) \vec{f}, \qquad A(x, \epsilon) = \sum_{i=0} \epsilon^i A^{(i)}(x), \tag{5.63}$$

where $A^{(0)}(x)$ is strictly lower-triangular. To see this, consider the differential equation for the very first integral. Because $A^{(0)}(x)$ is strictly lower-triangular, the equation for this integral is $\partial_x f_1 = \mathcal{O}(\epsilon)$. Therefore the lowest order of this integral is simply given by the boundary constants. Likewise, the second integral has the differential equation

[10] In the case where the lower integration boundary leads to a potential divergence, one has to use shuffle-regularization, see e.g. [46].

$\partial_x f_2 = A^{(0)}_{21} f^{(0)}_1 + \mathcal{O}(\epsilon)$, which can be computed because the first order of f_1, here denoted by $f^{(0)}_1$, is known. Repeating this for all integrals shows that the form (5.63), with $A^{(0)}(x)$ being strictly lower-triangular is in principle enough to solve the differential equations in an expansion in ϵ.[11]

An algorithm for reaching this form has been given in [139] and we will give a very short overview of the main steps, because this allows us to show the importance of the normalization factors considered at the beginning of this chapter. The first step is to reach (5.63) without $A^{(0)}(x)$ being strictly lower-triangular. This can always be achieved by multiplying the integrals with appropriate powers of ϵ so that their solutions start at the same order in ϵ. In a second step, one finds a transformation rational in x and ϵ which transforms $A^{(0)}(x)$ into a lower triangular form. The details of finding this transformation go beyond what we want to consider in this text and we note that in general this step is only possible for integrals that evaluate to multiple polylogarithms. We refer the reader to [139] for details of the algorithm.

The important point is then that the diagonal elements of the lower triangular $A^{(0)}(x)$ can be regarded as diagonal blocks of size 1×1, and we have already seen that transformations on one diagonal block do not influence other diagonal blocks (at this order in ϵ). Therefore one can immediately integrate out the ϵ^0-part of the diagonal elements by choosing an appropriate normalization $n_i(x)$ for each integral, as was done for f_1 in eqs. (5.1) and (5.2). Therefore, using the algorithm of [139], solving the differential equations can be reduced to the task of finding the correct normalization factors.

This in turn shows how the ϵ^0-part of the differential equations influences the functions appearing in the solutions of the integrals to a large degree. For example, we have already seen how half-integer numbers in the ϵ^0 part can lead to the appearance of square-roots in the kinematic variables. As another example, there are cases where it is not possible to determine a transformation s.t. the diagonal blocks of $A^{(0)}(x)$ are of size 1×1 only. In particular, an irreducible 2×2 block can only be integrated out by solving a second-order differential equation, which in general involves elliptic integrals in the solution. These elliptic integrals will then necessarily appear in the transformation matrix, as well as the integration kernels. An example of this will be discussed in the next chapter.

[11] If one does not sort the master integrals by sectors so that the differential equations are not block-triangular, it is necessary to consider the more general condition of $A^{(0)}(x_1) \dots A^{(0)}(x_k) = 0$ for some degree k, which is a criterion for the integrals to have a Dyson series with a finite number of terms at fixed order in ϵ.

6 The Canonical Basis from a Single Uniform Weight Integral

At this point, we have described two very different approaches for finding a basis of pure integrals. The first is only concerned with the integrals themselves and is oblivious to the actual differential equation matrix. The second is meant to directly transform a given set of differential equations into canonical form while not caring about the transcendental structure of the original Feynman integrals.

Each of these approaches has certain advantages over the other. For example transformations on the coefficient matrix $A(x, \epsilon)$ can in principle be found for any number of master integrals, whereas the analysis of the integrands and diagrams of the Feynman integrals in a family is sometimes simply not enough to find a complete basis of UT candidates. On the other hand, especially in the multivariate case, writing down UT candidates and computing leading singularities is usually easier than finding a transformation matrix for each individual variable.

A natural question to ask is therefore whether a method exists that allows us to

1) keep the already known UT candidates

2) do transformations on the rest of the basis in order to complete the set of pure master integrals.

In addition, such a method should

3) work for any number of master integrals (in principle)

4) not require to find a transformation for each kinematic variable separately.

The first two points require that we find a transformation that does not change the part of the basis that is already pure. The third is automatically satisfied if the approach is based on the coefficient matrix $A(x, \epsilon)$. The last requirement can be met by working with an ansatz for the canonical differential equation matrix. This is because the transformation is completely determined if the coefficients in the ansatz are fixed.

In this chapter, we will present a method that satisfies all of the above criteria. The idea of this method is the following: First, we use $A(x, \epsilon)$ to derive a higher-order differential equation which only depends on the UT candidates and their derivatives. Second, we derive the same equation starting from an ansatz for the canonical matrix $\epsilon\tilde{A}(x)$ s.t. the UT candidates are the same as the ones from the first step. Lastly, we require that the two resulting higher-order differential equations agree and use this to determine the unknown constants in the ansatz.

We note that, for this method to work, the number of UT candidates has to be greater than zero, i.e. we need at least one integral from the canonical basis. At the same time this gives an algorithmic way to test whether an individual candidate integral is indeed pure or not (provided the ansatz for the canonical form is correct).

In the following, we first describe the case of one dimensionless variable x and a basis $\vec{f}$ with

$$\frac{\partial}{\partial x}\vec{f} = A(x,\epsilon)\vec{f}, \tag{6.1}$$

where f_1 is a candidate UT integral. The case of more kinematic scales and multiple UT candidates will be described in sections 6.5 and 6.6, respectively. Throughout this chapter, we will largely follow the presentation given in [1], and in particular, some of the equations are taken from this reference. However, on several occasions, we aim to give additional important details about the algorithm and try to clarify the concepts beyond what is given in [1].

6.1 The Picard-Fuchs Equation

Starting from eq. (6.1), one can derive the following relation between the basis $\vec{f}$ and its derivatives:

$$\begin{pmatrix} f_1' & \cdots & f_1^{(n)} \\ f_2' & \cdots & f_2^{(n)} \\ \vdots & \ddots & \vdots \\ f_n' & \cdots & f_n^{(n)} \end{pmatrix} = \left(A^{[1]}\vec{f}, \ldots, A^{[n]}\vec{f}\right), \tag{6.2}$$

where

$$A^{[1]} := A, \tag{6.3}$$

$$A^{[j]} := \frac{\partial}{\partial x}A^{[j-1]} + A^{[j-1]}A \qquad \text{for } j > 1 \tag{6.4}$$

and n is the number of master integrals. Without loss of generality, we can pick one of the integrals in $\vec{f}$, e.g. f_1, and project the above equation on this subspace using the vector $\vec{v}_1 = (1, 0, \ldots, 0)$. This leads to $f_1^{(j)} = \vec{v}_1 A^{[j]}\vec{f}$ and hence we can define the basis change

$$\begin{pmatrix} f_1' \\ \vdots \\ f_1^{(n)} \end{pmatrix} = \Psi\vec{f} \tag{6.5}$$

with

$$\Psi := \begin{pmatrix} \vec{v}_1 A^{[1]} \\ \vdots \\ \vec{v}_1 A^{[n]} \end{pmatrix}. \tag{6.6}$$

In the case that the derivatives are linearly independent[1], we can invert Ψ and project (6.5) on f_1 to get

$$f_1 + \sum_{m=1}^{n} b_m f_1^{(m)} = 0, \tag{6.7}$$

where the coefficients are

$$(b_1, \ldots, b_n) \equiv -\vec{v}_1 \Psi^{-1}. \tag{6.8}$$

The n-th order differential equation in (6.7) is called the Picard-Fuchs equation and it solely depends on the integral f_1. Therefore we could apply any basis transformation to eq. (6.1) that leaves f_1 unchanged and still end up with the same Picard-Fuchs equation for f_1.

Note that, in the basis $(f_1', \ldots, f_1^{(n)})^{\mathrm{T}}$ of eq. (6.5), the differential equation matrix is [139]

$$\left(\frac{\partial}{\partial x}\Psi + \Psi A\right)\Psi^{-1} = \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \\ \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_n \end{pmatrix}, \tag{6.9}$$

as is evident from eq. (6.7). The elements of the last row are $\hat{b}_m = (b_{m-1} + b_m')/b_n$.

6.2 Determining the Canonical Form

In the previous section, we have derived a higher-order differential equation depending only on a single integral in the basis, namely f_1. In the following, we are going to assume that this integral evaluates to a pure function. We show in appendix A.1 that this assumption can be used to derive degree bounds on the coefficients b_i. Further, if the integral is not yet normalized correctly, one can use these degree bounds to determine the overall factor needed to make f_1 a pure integral. This is the subject of appendix A.2.

However, here in the main text, we will show that the assumption that f_1 is a pure integral is even more powerful. In particular, it is enough to determine a complete basis $\vec{g}$ of uniform weight integrals, i.e.

$$\frac{\partial}{\partial x}\vec{g} = B(x,\epsilon)\vec{g}, \qquad B(x,\epsilon) = \epsilon \tilde{A}(x). \tag{6.10}$$

This may be surprising at first, but becomes more understandable when looking at eq. (6.5). According to this equation, any possible basis containing f_1 can immediately be

[1] The case of linearly dependent derivatives will be dealt with in section 6.6.

related to the basis formed by the derivatives of f_1. Since we want $\vec{g}$ to be a uniform weight basis, we can pick $g_1 = f_1$. It is then clear that one can also compute the basis change

$$\begin{pmatrix} f_1' \\ \vdots \\ f_1^{(n)} \end{pmatrix} = \Phi \vec{g}, \qquad \text{with} \qquad \Phi := \begin{pmatrix} \vec{v}_1 B^{[1]} \\ \vdots \\ \vec{v}_1 B^{[n]} \end{pmatrix}, \tag{6.11}$$

where $B^{[j]}$ is defined in the same way as $A^{[j]}$:

$$B^{[1]} := B, \tag{6.12}$$

$$B^{[j]} := \frac{\partial}{\partial x} B^{[j-1]} + B^{[j-1]} B \qquad \text{for } j > 1 \tag{6.13}$$

Recall that f_1 having uniform transcendental weight is a statement about the functions at each order in an infinite expansion in ϵ. This information is contained in eq. (6.11) through the fact that the derivatives of f_1 still contain multiple pieces of uniform transcendental weight multiplied by rational functions. The transformation Φ in eq. (6.11) is then telling us how to remove the rational functions in each derivative and restore the uniform transcendentality. We therefore see why f_1 carries enough information to determine a canonical basis.

Continuing the results of the previous section, we can use $(f_1', \ldots, f_1^{(n)})^{\mathrm{T}}$ as an intermediate basis to find

$$\vec{f} = T \vec{g}, \qquad \text{where} \qquad T \equiv \Psi^{-1} \Phi. \tag{6.14}$$

Therefore we have a way of determining the transformation T to the canonical basis once the matrix B is known. To determine the latter, we can use the fact that $f_1 = g_1$ and therefore the first line of T must equal $\vec{v}_1$:[2]

$$\vec{v}_1 \Psi^{-1} \Phi = \vec{v}_1 \tag{6.15}$$

From eq. (6.11) we see that Φ contains higher-order derivatives of the entries of B and therefore solving this equation would be just as complicated as the initial problem. Fortunately, we can remove the derivatives by making an ansatz for B. In the case of multiple polylogarithms, we write

$$B(x, \epsilon) = \epsilon \sum_l \mathbf{m}_l \frac{\partial}{\partial x} \log \alpha_l(x), \tag{6.16}$$

where $\alpha_l(x)$ are called the *letters* and the set of all letters is called the *alphabet* $\vec{\alpha} = \{\alpha_l\}$. A reasonable guess for the letters $\alpha_l(x)$ can be obtained by the set of irreducible denominators of $A(x, \epsilon)$ that are independent of ϵ. Using this form, the only unknowns

[2] This is equivalent to requiring the coefficients in the Picard-Fuchs equations to agree, i.e. $\vec{v}_1 \Psi^{-1} = \vec{v}_1 \Phi^{-1}$.

in eq. (6.15) are the constant matrices $\mathbf{m}_l$, however, due to (6.13), the equations are highly non-linear. To circumvent this issue, one can expand (6.15) in ϵ and solve one order at a time. We explain this highly technical procedure in great detail in appendix A.3.

In summary, this gives an algorithm to compute the canonical form starting from a single pure integral. Assuming that the ansatz for $B(x)$ is correct, this also allows us to test f_1 for the uniform weight property, i.e. if f_1 is not pure, then there will be no solution to eq. (6.15).

6.3 Implementation

The above algorithm is implemented in the MATHEMATICA package INITIAL (an INITial Integral ALgorithm) [1] and publicly available at

https://github.com/UT-team/INITIAL

It uses the FINITEFLOW library [129] to perform the sampling over different kinematic variables and subsequently solve the equation system over finite fields. The library then automatically lifts the result from the finite field to the field of rational numbers and reconstructs the rational functions in the solution. In this way, it also greatly reduces the size of intermediate expressions, particularly when inverting the Ψ-matrix and performing repeated matrix multiplications.

6.4 Single-Variable Examples

In this section we show three Feynman integral families that depend only on a single dimensionless scale and how the corresponding differential equations can be brought into canonical form by using the algorithm described in the previous section. The three examples have been chosen to highlight the applicability of the algorithm (and its implementation) to the following three types of problems:

1. A large total number of integrals.

2. A large number of directly coupled integrals.

3. An initial integral is not known.

The IBP reductions for deriving the differential equations were done through the methods and algorithms described in section 5.1. Apart from the initial integral $f_1 = g_1$ the basis of master integrals used as an input to our algorithm is always given by the reduction codes, i.e. no further optimizations were done. A summary of the performance, including the multi-variable example of the next section, can be found in table 6.1.

6.4.1 Full Differential Equations for Planar Three-Loop Integrals

The so-called "tennis-court" integral family is defined by the following propagators

$$\begin{aligned}
D_1 &= -(k_1-k_3)^2, & D_2 &= -(k_1+p_1)^2, & D_3 &= -(k_1+p_1+p_2)^2,\\
D_4 &= -(k_2+p_1+p_2)^2, & D_5 &= -(k_2-p_3)^2, & D_6 &= -(k_2-k_3)^2,\\
D_7 &= -(k_1-k_2)^2, & D_8 &= -k_3^2, & D_9 &= -(k_3+p_1)^2,\\
D_{10} &= -(k_3-p_3)^2, & D_{11} &= -(k_3+p_1+p_2)^2, & D_{12} &= -(k_2+p_1)^2,\\
D_{13} &= -(k_1-p_3)^2, & D_{14} &= -k_1^2, & D_{15} &= -k_2^2,
\end{aligned} \tag{6.17}$$

where the top-sector is given by $J_{1,1,1,1,1,1,1,1,1,1,0,0,0,0,0}$ and shown in figure 6.1. It is

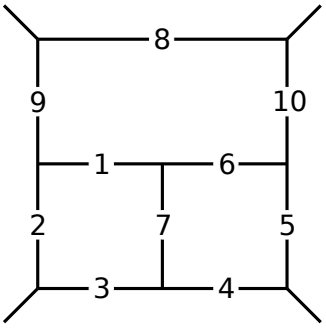


Figure 6.1: Planar three-loop four-point integrals. The number of MIs for this family is 41.

straightforward to find a complete UT basis and compute the master integrals [140]. Nevertheless, we will use the corresponding DEs to show that our implementation of the algorithm is relatively fast in determining the canonical form even in the case of a basis of 41 master integrals.

As an initial integral we choose the dlog-integral

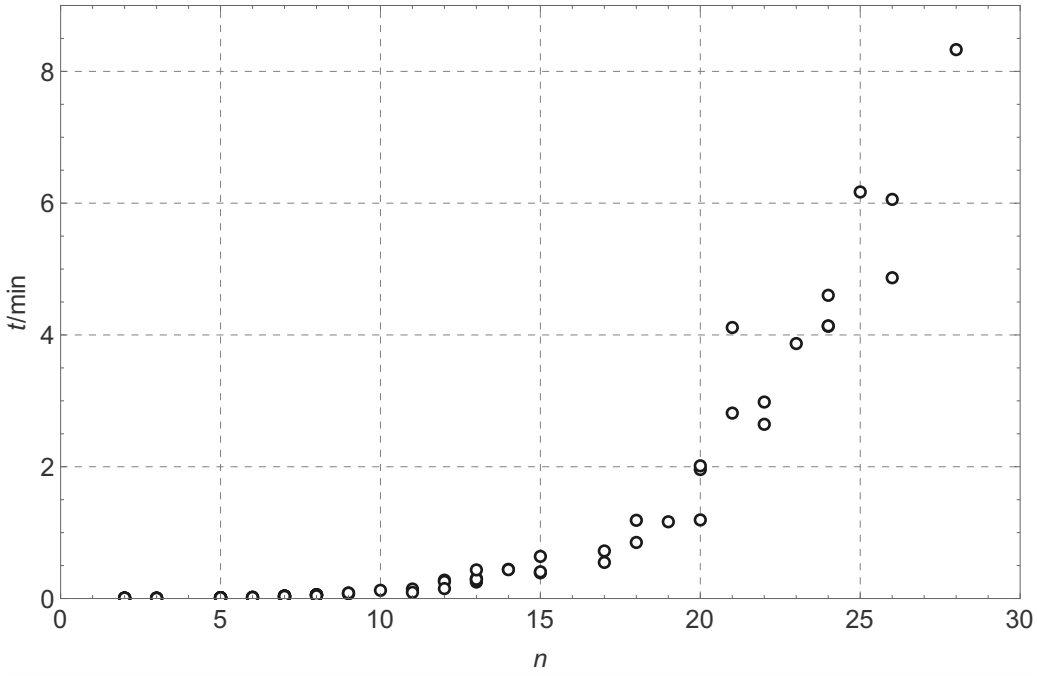
$$f_1 = g_1 = \epsilon^6 x^2 I_{1,1,1,1,1,1,1,1,1,1,-1,0,0,0,0}, \tag{6.18}$$

where $x = s/t$. f_1 can easily be found by applying the methods of chapter 3. The differential equations suggest the alphabet $\vec{\alpha} = \{x, 1+x\}$. Computing the Ψ-matrix takes about 7 min. As described in the previous section, the equations are iteratively solved order-by-order in ϵ by introducing auxiliary vectors $\vec{v}_j$. The number of independent vectors steadily increases until $\mathcal{O}(\epsilon^6)$ where all 41 independent vectors are determined. However, testing eq. (A.16) shows that there are still missing relations between the vectors $\vec{v}_j \mathbf{m}_l$ and $\vec{v}_j$. These relations are then determined by going to $\mathcal{O}(\epsilon^7)$ at which point the problem is solved and the $\mathbf{m}_l$ can be computed by making a suitable choice for the auxiliary vectors. In total, building and solving the system of equations takes 22 min. Finally, we compute the matrix Φ in about 3 min, and the transformation T in about 30 s.

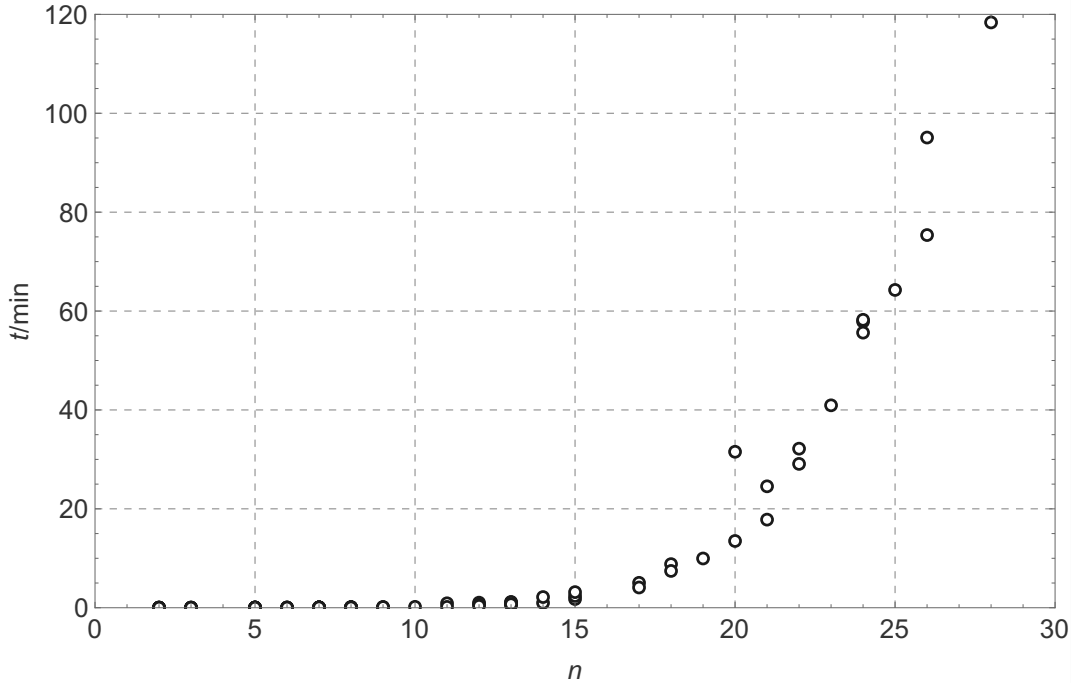
6.4.2 Scaling with the Number of Master Integrals

At this point, it is interesting to analyze the scaling of the time the algorithm takes to compute the transformation matrix with the matrix size. In figure 6.2a we apply our algorithm to different systems of differential equations that are already in canonical form. We can see that the algorithm is relatively fast even for state-of-the-art problem sizes. However, since the scaling behavior is exponential, the computing time increases drastically when going beyond a certain point. This exponential behavior is expected, since the matrix multiplications in the computation of Ψ follow the same behavior, i.e. $A^{[n]} \sim A^n$. Therefore the complexity of the rational functions in Ψ and the equation system also scales exponentially with the matrix size.

In figure 6.2b we show the application to systems that have artificially been transformed away from the canonical form. As a result, the entries of the matrices are rational functions with numerators and denominators being polynomials up to degree 21 in ϵ and 23 in x. We see that the scaling behavior is similar, however the overall scale (the base of the exponential) is about 13 times larger.



(a)



(b)

Figure 6.2: Scaling of the time it takes to find a transformation matrix with the matrix size. The scaling is exponential but depends on the complexity of the matrix: In (a) systems already in canonical form were analyzed, whereas (b) shows the application to systems with high-degree rational functions in ϵ and x.

6.4.3 Non-Planar Four-Loop Sector with 17 Master Integrals

Next, we consider the diagonal block of a specific sector in the DEs of the following integral family (see also section 7.3 for a further discussion of this integral family):

$$\begin{aligned}
D_1 &= 1 - 2k_1 \cdot v_1, & D_2 &= 1 - 2k_2 \cdot v_1, & D_3 &= 1 - 2k_2 \cdot v_2, \\
D_4 &= 1 - 2k_3 \cdot v_2, & D_5 &= -k_1^2, & D_6 &= -k_3^2, \\
D_7 &= -k_4^2, & D_8 &= -(k_1 - k_2)^2, & D_9 &= -(k_1 - k_4)^2, \\
D_{10} &= -(k_2 - k_3)^2, & D_{11} &= -(k_3 - k_4)^2, & D_{12} &= -(k_1 - k_2 + k_3 - k_4)^2, \\
D_{13} &= -(k_2 - k_4)^2, & D_{14} &= -(k_2 - k_3 - k_4)^2, & D_{15} &= 1 - 2k_4 \cdot v_1, \\
D_{16} &= 1 - 2k_4 \cdot v_2, & D_{17} &= 1 - 2k_3 \cdot v_1, & D_{18} &= 1 - 2k_1 \cdot v_2,
\end{aligned} \tag{6.19}$$

where the sector integral is given by $J_{1,0,1,1,0,1,1,1,1,0,0,1,0,0,0,0,0,0}$ and shown in figure 6.3. As discussed in section 5.4, looking at the diagonal block is equal to considering the

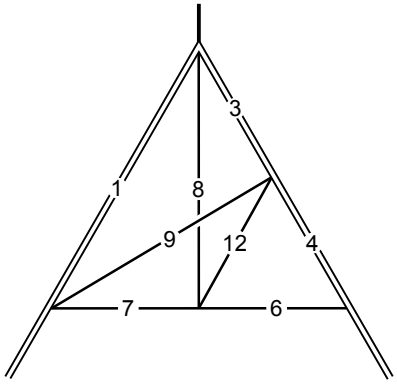


Figure 6.3: An integral sector with 17 master integrals.

maximal cut of this integral. Therefore all integrals of the block directly couple to each other, which leads to a dense matrix without the usual block-triangular structure. This means that blocks like this will be the smallest "sub-problems" that we have to deal with when trying to bring the differential equations of a full integral family into canonical form.

In the case at hand, the diagonal block is a 17×17 matrix and, in fact, it is the largest diagonal block in this family. Hence, it is reasonable to assume, that we might be able to solve the full differential equations if our algorithm can handle this sector (and the alphabet is not vastly more complicated in other sectors). We want to stress that the typical sector size of the other sectors of this family, as well as those of the other examples given in this thesis, is significantly smaller, meaning that the number of master integrals per sector is usually between two and seven.

The initial integral is easily found by making a guess (see e.g. [140, 36] as well as chapter 4) for a list of UT integrals, and then systematically testing them with our algorithm. In this way we find that the following integral is a pure integral on the

maximal cut:

$$f_1 = g_1 = \epsilon^6 \left(\frac{1-x^2}{x}\right)^2 I_{1,0,1,1,0,1,1,2,2,0,0,1,0,0,0,0,0,0}, \tag{6.20}$$

where x is defined by $2v_1 \cdot v_2 = x + 1/x$. The singular points of the differential equations suggest $\vec{\alpha} = \{x, 1+x, 1-x\}$ as ansatz for the alphabet. With this input, our implementation takes less than two minutes to find a transformation to canonical form.

6.4.4 Four-Loop Four-Point Integrals

In this example, we analyze previously unknown four-loop integrals. Again we are only concerned with the differential equations and not with the actual solution for the integrals, which can be found in [1]. The integral family is defined by

$$\begin{aligned}
&D_1 = -k_4^2, && D_2 = -(k_1+p_1)^2, && D_3 = -(k_2+p_1+p_2)^2,\\
&D_4 = -(k_3+p_1+p_2+p_3)^2, && D_5 = -(k_1-k_2)^2, && D_6 = -(k_2-k_3)^2,\\
&D_7 = -(k_3-k_4)^2, && D_8 = -(k_1-k_4)^2, && D_9 = -k_1^2,\\
&D_{10} = -(k_2+p_1)^2, && D_{11} = -(k_3+p_1+p_2)^2, && D_{12} = -(k_4+p_1+p_2+p_3)^2,\\
&D_{13} = -k_2^2, && D_{14} = -k_3^2, && D_{15} = -(k_1-k_3)^2,\\
&D_{16} = -(k_1+p_1+p_2)^2, && D_{17} = -(k_1+p_1+p_2+p_3)^2, && D_{18} = -(k_2-k_4)^2,\\
&D_{19} = -(k_2+p_1+p_2+p_3)^2, && D_{20} = -(k_3+p_1)^2, && D_{21} = -(k_4+p_1)^2,\\
&D_{22} = -(k_4+p_1+p_2)^2.
\end{aligned} \tag{6.21}$$

and we consider the sector $J_{1,1,1,1,1,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0}$, shown in figure 6.4, together with its sub-sectors. In total there are 19 master integrals and we take $\vec{\alpha} = \{x, 1+x\}$

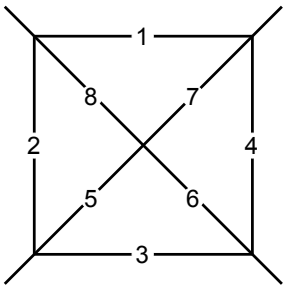


Figure 6.4: Planar four-loop four-point integral. The number of master integrals is 19.

as an ansatz for the alphabet.

This example is interesting because it is not straightforward to find an initial integral. The reason is the following: From power counting, one can show that the integrand of the scalar integral always exhibits a double pole. As a consequence, there are no dlog integrals in four dimensions. While there are other possibilities to determine a

UT integral, we here want to exploit our algorithm's ability to test a list of candidate integrals.

The scalar integral itself turns out to be UT up to an overall normalization in ϵ, however only 18 of its derivatives are linearly independent. As will be discussed in section 6.6, we could proceed by first bringing an 18×18 block into canonical form, and then apply the methods of chapter 5 to the last row. Instead, we choose to test further suitable candidates. In particular, we investigate integrals with one doubled propagator. From figure 6.4 we see that there are only two inequivalent ways of doubling a propagator. We find that both lead to UT integrals, but that only one of them gives an invertible 19×19 Ψ-matrix:

$$f_1 = g_1 = \epsilon^7(1+x)I_{1,1,1,1,1,1,1,1,2,0,0,0,0,0,0,0,0,0,0,0,0,0,0} \tag{6.22}$$

In this case, the overall factor in x was easily determined by demanding that $\tilde{b}_0 = \mathcal{O}(\epsilon)$. Using this as an input, our implementation takes less than one minute to find a transformation to canonical form.

6.5 Generalization to Multi-Variable Case

Many algorithms that aim at finding a canonical basis do not scale very well with the number of scales involved or cannot handle more than one variable at all. As we will see in the following, this is not the case for our algorithm, and the number of scales is only limited by the complexity of the rational functions appearing in the differential equations, which increases the needed computing power. The latter difficulty can often be overcome by using some tricks that are described in a state-of-the-art example in the last part of this section.

6.5.1 General Considerations

Starting from a set of partial differential equations

$$\frac{\partial}{\partial x_i}\vec{f} = A_i(\vec{x},\epsilon)\vec{f}, \qquad i = 1,\ldots,m \tag{6.23}$$

our goal is to achieve the canonical form

$$\mathrm{d}\vec{g}(\vec{x},\epsilon) = \mathrm{d}B(\vec{x},\epsilon)\vec{g}(\vec{x},\epsilon), \qquad \mathrm{d}B(\vec{x},\epsilon) = \epsilon\left[\sum_l \mathbf{m}_l \,\mathrm{d}\log\alpha_l(\vec{x})\right], \tag{6.24}$$

where $\vec{x} = \{x_1,\ldots,x_m\}$ denotes the set of variables and as usual $\mathrm{d} = \sum_i \mathrm{d}x_i\partial_{x_i}$. Without loss of generality, we first consider the differential equations in x_1, treating the other variables as constants. The steps for these differential equations are then essentially the same as in the single-variable case, except that we now need to make sure our solutions for the $\mathbf{m}_l$ are independent of all variables, instead of just x_1. This can be achieved either by sampling over an array of values for $\vec{x}$, by successively series expanding in

the x_i or by finding an independent basis of functions, e.g. through generalized partial fractioning, see [141].

Following this procedure results in the differential equations w.r.t. x_1 being in canonical form:

$$\frac{\partial}{\partial x_1}\vec{g}'(\vec{x},\epsilon) = B_1(\vec{x},\epsilon)\vec{g}', \tag{6.25}$$

where $B_i = \partial_{x_i} B$. As in the single-variable case, this ϵ-factorized form is unique up to transformations that are independent of x_1, as well as an overall factor in ϵ. However, the ansatz (6.24) together with the choice of the independent vectors in the matrix Q in the solution

$$\mathbf{m}_l = Q^{-1}\beta^l Q \tag{6.26}$$

completely determines the canonical form (6.25) in x_1. Therefore the only freedom that is left are transformations that leave (6.25) invariant, i.e. multiplication by an overall factor in ϵ and $x_2, \ldots, x_m$:

$$\vec{g}(\vec{x},\epsilon) = \hat{N}(\epsilon, x_2, \ldots, x_m)\vec{g}'(\vec{x},\epsilon) \tag{6.27}$$

We want to stress that, compared to the method of balance transformations, $\hat{N}(\epsilon, x_2, \ldots, x_m)$ is not a matrix but a scalar function. In practice, we found that this normalization factorizes as $\hat{N}(\epsilon, x_2, \ldots, x_m) = n(\epsilon)N(x_2, \ldots, x_m)$ and that $N(x_2, \ldots, x_m)$ can easily be determined by integrating out the ϵ^0 part of the differential equations w.r.t. the variables $x_2, \ldots, x_m$. However, it is conceivable that a very bad choice of initial integral does not lead to this factorization.

6.5.2 Four-Variable Example: Non-Planar Double Pentagon Integrals

To demonstrate the application of our algorithm to a multi-scale problem, we consider the top sector $J_{1,1,1,1,1,1,1,1,0,0,0}$ of the non-planar double pentagon integral family, shown in figure 6.5 and defined by the propagators [33, 34]

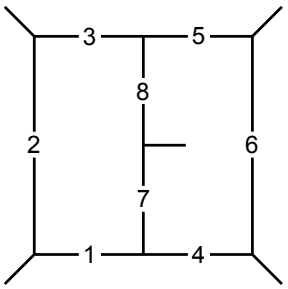


Figure 6.5: Top sector of the non-planar double pentagon integral family. The number of master integrals on the maximal cut is nine.

$$\begin{aligned}
D_1 &= -k_1^2, & D_2 &= -(k_1-p_1)^2, & D_3 &= -(k_1-p_1-p_2)^2,\\
D_4 &= -k_2^2, & D_5 &= -(k_2+p_4+p_5)^2, & D_6 &= -(k_2+p_5)^2,\\
D_7 &= -(k_1-k_2)^2, & D_8 &= -(k_1-k_2+p_3)^2, & D_9 &= -(k_1+p_5)^2,\\
D_{10} &= -(k_2-p_1)^2, & D_{11} &= -(k_2-p_1-p_2)^2.
\end{aligned} \tag{6.28}$$

An ansatz for the alphabet in terms of 31 letters $\{\alpha_i\}$ has been suggested in [142, 143]. To rationalize the external kinematics and thereby also the alphabet, we employ a (variation of) momentum-twistor parametrization, see e.g. [144]:

$$s_{12} = b_1, \qquad s_{23} = b_1 b_4, \qquad s_{34} = \frac{b_1(1+b_3)b_4}{b_2} - b_1 b_3 (1-b_5), \tag{6.29}$$

$$s_{45} = b_1 b_5, \qquad s_{15} = b_1 b_3 (b_2 - b_4 + b_5), \tag{6.30}$$

where b_1 is the only dimensionfull variable. Hence, the 9×9 differential equation matrix depends on the four dimensionless variables $\vec{b} = \{b_2, \ldots, b_4\}$. An initial integral can easily be found using the methods of section 3.4 and 3.5, as was done in [33] and [34], respectively.

We start by determining the canonical form w.r.t. b_2, i.e.

$$B_2(\vec{b}, \epsilon) = \epsilon \sum_{l=1}^{22} \mathbf{m}_l \frac{\partial}{\partial b_2} \log \alpha_l(\vec{b}), \tag{6.31}$$

where the sum runs only over the 22 letters that depend on b_2. The solutions for $\mathbf{m}_1, \ldots, \mathbf{m}_{22}$ are easily found by solving the equations after sampling over different values for the variables. In fact, it turns out that, after sampling over different values for b_2, the solution is automatically independent of $b_3, \ldots, b_5$ and therefore only a single evaluation in these variables is necessary.

In principle, one can now compute the analytic transformation matrix $T(\vec{b}, \epsilon)$ from analytic expressions for Ψ_2 and Φ_2. However, the higher-order derivates in the computation of these matrices lead to complicated rational functions. Therefore this step would be quite time consuming, and we prefer to take a different path by actually exploiting the fact that we have multiple variables for the derivatives available. First, we determine the other matrices B_i, and therefore the full differential, analytically in the following way:

1. Compute Ψ_2, Φ_2 and T without setting b_3 to a constant. This allows us to transform the differential equations in b_3 into canonical form where b_4 and b_5 are constant values.

2. Determine the analytic $B_3(\vec{b}, \epsilon)$ by matching the canonical form from the previous step to the ansatz for B_3.

3. Repeat in b_4 and b_5 to get $B_4(\vec{b}, \epsilon)$ and $B_5(\vec{b}, \epsilon)$.

We note that the analytic matrix $\mathrm{d}B(\vec{b},\epsilon)$ depends on only 17 of the 31 letters. Using this result, we can also compute the Φ-matrix for any basis we like. Therefore we can choose e.g. to use the intermediate basis

$$\vec{h} = (f_1, \partial_{b_2} f_1, \partial_{b_2}^2 f_1, \partial_{b_3} f_1, \partial_{b_3}^2 f_1, \partial_{b_4} f_1, \partial_{b_4}^2 f_1, \partial_{b_5} f_1, \partial_{b_5}^2 f_1) \tag{6.32}$$

instead of a basis that consists of only derivatives w.r.t. one variable but to n-th order as in (6.5) and (6.11). The fact that $\vec{h}$ contains at most second-order derivatives greatly simplifies the matrices Ψ_h and Φ_h defined through

$$\begin{aligned} \vec{h} &= \Psi_h \vec{f}, \\ \Psi_h &:= (\vec{v}_1, \vec{v}_1 A_2^{[1]}, \vec{v}_1 A_2^{[2]}, \vec{v}_1 A_3^{[1]}, \vec{v}_1 A_3^{[2]}, \vec{v}_1 A_4^{[1]}, \vec{v}_1 A_4^{[2]}, \vec{v}_1 A_5^{[1]}, \vec{v}_1 A_5^{[2]})^{\mathrm{T}} \end{aligned} \tag{6.33}$$

and

$$\begin{aligned} \vec{h} &= \Phi_h \vec{g}, \\ \Phi_h &:= (\vec{v}_1, \vec{v}_1 B_2^{[1]}, \vec{v}_1 B_2^{[2]}, \vec{v}_1 B_3^{[1]}, \vec{v}_1 B_3^{[2]}, \vec{v}_1 B_4^{[1]}, \vec{v}_1 B_4^{[2]}, \vec{v}_1 B_5^{[1]}, \vec{v}_1 B_5^{[2]})^{\mathrm{T}}. \end{aligned} \tag{6.34}$$

Finally, the transformation matrix is computed through $T(\vec{b},\epsilon) = \Psi_h^{-1}\Phi_h$.

In total, our implementation takes only a few minutes for all steps outlined above. A summary for all examples is given in table 6.1.

type of problem	#MI	#vars	#letters	time [min]	mem. [MB]
three-loop four-point tennis court	41 — 3	1	2	34	1710
four-loop four-point crossed box	19 — 12	1	2	1	240
non-planar four-loop HQET	17 — 17	1	3	2	390
non-planar two-loop five-point	9 — 9	4	17	5	510

Table 6.1: Approximate evaluation time and memory usage of the different examples on a desktop computer with twelve logical CPU cores. The second column shows the total number of master integrals, as well as the maximum sector size. The third column shows the number of dimensionless variables and the fourth column gives the number of (relevant) letters in the alphabet.

It is remarkable that the number of scales only marginally influences the time it takes to compute the canonical form, and that a higher number of scales actually seems to aid the computation of the transformation matrix. Note that it is also possible to directly and analytically determine the matrix $B(\vec{b},\epsilon)$ through an intermediate basis similar[3] to $\vec{h}$. However, we found that the above mentioned procedure is still by far the most efficient way of computing the canonical form.

[3]The basis $\vec{h}$ itself cannot be used for this task since the entries of $\vec{v}_1\Psi^{-1}$ are not the coefficients of a Picard-Fuchs equation and, in fact, $\vec{v}_1\Psi^{-1}\Phi = \vec{v}_1$ is trivially fulfilled.

6.6 Degenerate Ψ-Matrix

In the example of section 6.4.4 we saw that for some initial integrals not all derivatives were linearly independent and hence Ψ was not invertible. In this section we discuss possible reasons for linearly dependent derivatives, as well as ways to deal with such a case.

As probably the most obvious example, consider the following differential equation matrix

$$A(x,\epsilon) = \begin{pmatrix} A_{1,1} & 0 \\ A_{2,1} & A_{2,2} \end{pmatrix} \tag{6.35}$$

consisting of only two sectors with diagonal blocks $A_{1,1}$ and $A_{2,2}$. We can see that $A_{2,2}$ corresponds to the top sector and therefore we should consider an initial integral from this sector. Instead, we use f_1 as initial integral, which is the first integral in sector $A_{1,1}$. This will immediately lead to a non-invertible Ψ-matrix, as can be seen by recalling that each row of the Ψ-matrix is computed through

$$\Psi_1 = \vec{v}_1 A, \tag{6.36}$$

$$\Psi_m = \frac{\partial}{\partial x}\Psi_{m-1} + \Psi_{m-1}A, \qquad m = 2, \ldots, n, \tag{6.37}$$

with n being the number of master integrals. Therefore the columns corresponding to the sector $A_{2,2}$ are always zero and hence the rows are linearly dependent. This in turn means that the derivatives of f_1 are linearly dependent because

$$f_1^{(m)} = \Psi_m \vec{f}. \tag{6.38}$$

This result is of course not very surprising, because the matrix structure in eq. (6.35) makes it immediately clear that f_1 does not carry enough information to determine all integrals in the basis.

Another interesting case is given by a differential equation matrix without top-sector:

$$A(x,\epsilon) = \begin{pmatrix} A_{1,1} & 0 & 0 \\ A_{2,1} & A_{2,2} & 0 \\ A_{3,1} & 0 & A_{3,3}. \end{pmatrix} \tag{6.39}$$

An initial integral in any of the three sectors leads to a non-invertible Ψ-matrix. This problem can be resolved by realizing that we should actually look separately at the two differential equations

$$A_2(x,\epsilon) = \begin{pmatrix} A_{1,1} & 0 \\ A_{2,1} & A_{2,2} \end{pmatrix} \qquad \text{and} \qquad A_3(x,\epsilon) = \begin{pmatrix} A_{1,1} & 0 \\ A_{3,1} & A_{3,3} \end{pmatrix}. \tag{6.40}$$

Taking initial integrals from the respective new top-sectors $A_{2,2}$ and $A_{3,3}$ will result in linearly independent derivatives for each of the two integrals.

However, in doing so we consider the sector $A_{3,3}$ twice. Therefore, it might be advantageous to use the two known pure integrals to directly bring $A(x,\epsilon)$ in (6.39) into canonical form. This can be done in the following way:

Let us call the two pure integrals f_2 and f_3. These two integrals are from sectors $A_{2,2}$ and $A_{3,3}$ of size n_2 and n_3 respectively. Further, let the two unit vectors that project on these two integrals be $\vec{v}_2$ and $\vec{v}_3$, respectively. Then we can define the following basis of n linearly independent derivatives:

$$(f_2', \ldots, f_2^{(n_2)}, f_3', \ldots, f_3^{(n-n_2)})^{\mathrm{T}} = \Psi \vec{f}, \tag{6.41}$$

where

$$\Psi \equiv \begin{pmatrix} \vec{v}_2 A^{[1]} \\ \vdots \\ \vec{v}_2 A^{[n_2]} \\ \vec{v}_3 A^{[1]} \\ \vdots \\ \vec{v}_3 A^{[n-n_2]}, \end{pmatrix} \tag{6.42}$$

Here it is important that the basis includes n_2 derivatives of f_2 and n_3 derivatives of f_3. The remaining $n - n_2 - n_3$ integrals can be filled in any convenient way, as long as they are linearly independent. In this example we filled them with higher order derivatives of f_3. Using this intermediate basis, we can also compute a Φ-matrix, where now A is replaced by the ansatz B for the canonical form. The latter is computed by requiring that $f_2 = g_2$ and $f_3 = g_3$, which results in the simultaneous constraints

$$\begin{pmatrix} \vec{v}_2 \\ \vec{v}_3 \end{pmatrix} \Psi^{-1} \Phi = \begin{pmatrix} \vec{v}_2 \\ \vec{v}_3 \end{pmatrix}, \tag{6.43}$$

which can be solved in the usual way by expanding in ϵ and grouping terms of equal transcendental weight. The transformation matrix to canonical form is then $T = \Psi^{-1}\Phi$.

Note that the knowledge of multiple pure integrals is not only helpful in the case of a non-invertible Ψ-matrix, but also to reduce the highest order of derivatives present in the intermediate basis[4]. This is somewhat similar to the multi-variable case, where derivatives w.r.t. different variables was used to reduce this order.

Finally, it is important to understand that the block-structure in eq. (6.35) or (6.39) can be hidden, so that it is not obvious whether all derivatives will be independent. In particular, a diagonal block can have this hidden structure. This explains why sometimes even an integral from the top sector leads to a non-invertible Ψ-matrix.

Fortunately, the linear dependence of the derivatives gives a convenient way to make the block-structure manifest [139]: Consider a basis $\vec{f}$ of integrals, where only the first r

[4] We note that it is often also possible to artificially couple the two differential equations by using $f_2 + f_3$ as initial integral. However, the order of derivatives in this case is still higher than through the method described here.

derivatives of f_1 are linearly independent. Therefore, f_1 satisfies a Picard-Fuchs equation of the form

$$f_1 + \sum_{m=1}^{r} b_m f_1^{(m)} = 0. \tag{6.44}$$

A basis that makes the block-structure manifest is given by

$$\vec{f}_B = (f_1', \ldots, f_1^{(r)}, f_{\sigma_{r+1}}, \ldots, f_{\sigma_n})^{\mathrm{T}}, \tag{6.45}$$

where we added $(n-r)$ integrals from the original basis, i.e. $f_{\sigma_{r+1}}, \ldots, f_{\sigma_n} \in \vec{f}$. These integrals need to be linearly independent of the first r derivatives of f_1. Since the integrals in $\vec{f}$ are linearly independent, such a subset of integrals always exists.

As we have seen in eq. (6.9), the differential equations in this basis now have the form

$$\frac{\partial}{\partial x}\vec{f}_B = A_B(x,\epsilon)\vec{f}_B, \qquad A_B(x,\epsilon) = \begin{pmatrix} 0 & 1 & 0 & \ldots & 0 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \ldots & 0 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 1 & 0 & \ldots & 0 \\ \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \ldots & \hat{b}_r & 0 & \ldots & 0 \\ * & * & * & \ldots & * & \bullet & \ldots & \bullet \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \vdots \\ * & * & * & \ldots & * & \bullet & \ldots & \bullet \end{pmatrix}, \tag{6.46}$$

where $*$ and $\bullet$ are arbitrary, i.e. possibly non-zero, entries. Depending on whether the entries $*$ are zero or not, we arrive at the cases of eq. (6.39) or (6.35), respectively.

6.7 Generalizations of the Ansatz

In this section we discuss how the logarithmic ansatz for the canonical form

$$B(\vec{x},\epsilon) = \epsilon \left[\sum_l \mathbf{m}_l \log \alpha_l(\vec{x}) \right] \tag{6.47}$$

can be modified to incorporate more general letters.

6.7.1 Algebraic Singularities

First, we can allow for rational functions instead of just $\log \alpha_l(\vec{x})$. As an example, consider a differential equation with singular points at $\pm i$. Instead of $\log(x \pm i)$ we can equivalently use two linearly independent functions with the same poles but without explicit appearance of complex numbers:

$$B(x,\epsilon) = \epsilon \left[\mathbf{m}_1 \frac{1}{1+x^2} + \mathbf{m}_2 \frac{x}{1+x^2} \right] \tag{6.48}$$

The advantage of this is that the transformation matrix $T(x, \epsilon)$ does not explicitly depend on $\pm i$ and we can therefore still solve the equations over $\mathbb{Q}$ instead of $\mathbb{C}$. This is particularly helpful when combining the algorithm with finite-field methods.

In general, the appearance of letters of the form $x - x_i$, where x_i is one of the (algebraic) roots of a degree-k polynomial $P_k(x)$ with real and rational coefficients suggests adding

$$\epsilon \sum_{l=1}^{k} \mathbf{m}_l \frac{x^{l-1}}{P_k(x)} \tag{6.49}$$

to the ansatz for $B(x, \epsilon)$. This avoids the explicit appearance of the roots x_i in the equations and the transformation matrix, which is expected to be possible if the kinematics of the Feynman-integrals do not explicitly introduce these algebraic numbers. The same is true in the multi-variable case, however one should make sure that the basis of rational functions used in the ansatz is still linearly independent, see e.g. [141].

6.7.2 Algebraic Letters

As discussed in section 5.5, rational transformations are not always sufficient to reach the canonical form. In particular, if the eigenvalues of the residue matrices at a singular point x_i are half-integer for $\epsilon = 0$, one should either try to find a change of variables which rationalizes $\sqrt{x - x_i}$ [37] or incorporate this square root into the ansatz.

An example of this is given by the maximal cut of the sector shown in figure 6.6. There are two master integrals and the differential equations suggest

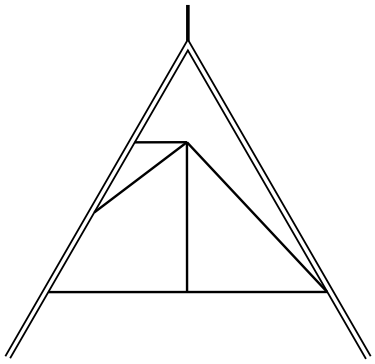


Figure 6.6: Wilson line sector requiring algebraic letters. The number of master integrals is two.

$$B(x, \epsilon) = \epsilon \left[\mathbf{m}_1 \frac{1}{x} + \mathbf{m}_2 \frac{1}{\sqrt{x}} + \mathbf{m}_3 \frac{1}{x-1} + \mathbf{m}_4 \frac{\sqrt{x}}{x-1} + \mathbf{m}_5 \frac{1}{x+1} + \mathbf{m}_6 \frac{\sqrt{x}}{x+1} \right] \tag{6.50}$$

as the ansatz for the canonical form. The scalar integral, normalized by $(1 - x^2)/x$, is a suitable initial integral. The algorithm proceeds in the same way as in the rational case, however, we do not use finite-field techniques to sample over x. For this reason,

square-roots are currently not supported by our implementation. The ensuing canonical form turns out to be very simple. In particular, the result can be written in terms of the alphabet $\{x, 1+x, (1-\sqrt{-x})/(1+\sqrt{-x})\}$.

6.7.3 Non-Polylogarithmic Case

So far we assumed that the canonical form can be reached through algebraic transformations. However, there are cases when the solution to the integrals cannot be written in terms of only MPLs, but more general iterated integrals are required. One example is the so-called two-loop sunrise graph shown in figure 6.7. In [68] a basis of integrals was

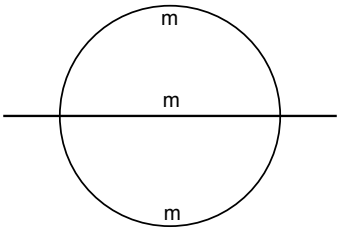


Figure 6.7: Two-loop sunrise graph. There are two master integrals on the maximal cut. All internal lines are massive, e.g. $D_1 = k_1^2 - m^2$.

found where the dimensional regulator still factorizes in the differential equation matrix and consequently the solution can be straightforwardly written in terms of iterated integrals and subsequently also in terms of so-called *elliptic* multiple polylogarithms.

Here we want to demonstrate that this form can still be found by our algorithm, as long as an initial integral and an ansatz for the desired differential equations is known. For the purpose of this example, we simply take this information from [68]:

$$f_1 = g_1 = \frac{1}{\Psi_1} I^{(2-2\epsilon)}_{1,1,1,0,0} \tag{6.51}$$

$$\begin{aligned} B(x,\epsilon) = \epsilon \Bigg[& \mathbf{m}_1 \frac{1}{x(x-1)(x-9)\Psi_1^2} + \mathbf{m}_2 \frac{3x^2-10x-9}{x(x-1)(x-9)} \\ & + \mathbf{m}_3\, \Psi_1 + \mathbf{m}_4 \frac{(3+x)^4 \Psi_1^2}{x(x-1)(x-9)} \Bigg], \end{aligned} \tag{6.52}$$

where

$$\Psi_1 = \frac{4\,\mathrm{K}\left(\frac{16\sqrt{x}}{(1+\sqrt{x})^3(3-\sqrt{x})}\right)}{\pi(1+\sqrt{x})^{\frac{3}{2}}(3-\sqrt{x})^{\frac{1}{2}}} \tag{6.53}$$

with

$$\mathrm{K}(k) = \int_0^1 \frac{\mathrm{d}t}{\sqrt{(1-t^2)(1-k\,t^2)}} \tag{6.54}$$

being the complete elliptic integral of the first kind. $I^{(2-2\epsilon)}_{1,1,1,0,0}$ is the scalar integral near two dimensions, which can be related to the four-dimensional basis through the dimensional recurrence relations discussed in section 3.5. The only dimensionless kinematic variable x is defined by $x = s/m^2$. We note that the functions in $B(x, \epsilon)$ are modular forms, see [69]. For example, it is straightforward to verify the absence of essential singularities in (6.52).

The algorithm then proceeds in the usual manner, however, we again need to assure that the solutions to the equations are independent of x. To do this, we prefer to treat Ψ_1 and its derivative as additional independent variables to sample over. This results in expressions that are easier to handle with `Mathematica` compared to sampling only over x or expanding the equations around $x = 0$. Once a solution for the $\mathbf{m}_i$ is known, it becomes straightforward to compute the transformation matrix in the usual way.

This example demonstrates how flexible the algorithm is w.r.t. the functions appearing in the ansatz. Compared to the other techniques discussed in previous chapters, there is no need to rationalize square-roots in the kinematic variables and one can even use elliptic integrals if required. Further, in the multivariate case, running the algorithm for just one variable is enough to determine the canonical basis up to a rotation in the other variables.

However, there is arguably more input needed than in the leading singularity or the balance transformation methods. Especially the ansatz for the canonical form can be difficult to find in the multivariate case. We refer to [143] for an example of how the letters can be bootstrapped by using information on branch cuts. Further, the algorithm requires the knowledge of at least one UT integral and its normalization. In practice, it is usually relatively easy to find suitable candidates through the methods of chapter 3 and 4. One can then test the integrals w.r.t. the UT property and also find the appropriate normalization as discussed in appendix A.2.

In contrast to the balance transformations of chapter 5, the algorithm is able to use already found pure integrals to simplify the computation. Consider e.g. the extreme case where all but a single integral of the basis are pure. First, without our ability to test individual integrals, there would be no way of knowing which of the integrals needs to be replaced. Second, after having determined which of the integrals is not pure, our algorithm then allows us to find a transformation to canonical form where only a single row is different from the identity matrix. This is an enormous simplification compared to the method of balance transformations.

7 Applications

In this chapter, we present the application of the canonical differential equations method to three different physical processes. Although we could use our algorithm for all three examples, we will see that the leading singularity analysis or the balance transformation method are better suited for certain problems. The main point of this chapter will be however, that we can apply our algorithm in cases where the other methods fail. This justifies our statement that our algorithm fills an important gap in the existing techniques for the canonical form.

We note that the three examples have already been presented in the publications [3], [4] and [2], respectively, from where we also take a large portion of the equations and figures of this chapter.

7.1 Three-Mass Two-Loop Box Integral Family

This section is dedicated to the computation of the complete canonical basis for the two-loop box with three external masses of figure 3.1. The propagators are given in eq. (3.44). The canonical basis for this family has been computed by the present author and collaborators in [3]. Figure 7.1 shows all unique non-zero sectors together with the number of master integrals. As described in section 5.1, these sectors are found during the IBP reduction.

The list of all UT integrals ordered by sector is given in table 7.1. The square roots are defined as

$$\begin{aligned} r_1 &= \sqrt{\lambda(m_1^2, m_2^2, s)}, \quad r_2 = \sqrt{(m_2^2 m_3^2 - m_3^2 s + st)^2 - 4 m_1^2 m_2^2 m_3^2 s}, \\ r_3 &= \sqrt{\lambda(m_2^2, m_3^2, t)}, \quad r_4 = \sqrt{\lambda(m_1^2, m_3^2, u)}, \end{aligned} \tag{7.1}$$

where we have used $s + t + u = \sum_{i=1}^{3} m_i^2$. Recall that $\lambda(x, y, z) = x^2 + y^2 + z^2 - 2xy - 2xz - 2yz$ is the Källén function.

Let us discuss how these integrals were found through the methods described in this thesis:

- Most integrals without bubble sub-integrals are dlog integrals with unit leading singularity. These have been determined in the loop-by-loop Baikov representation as discussed in section 3.4.

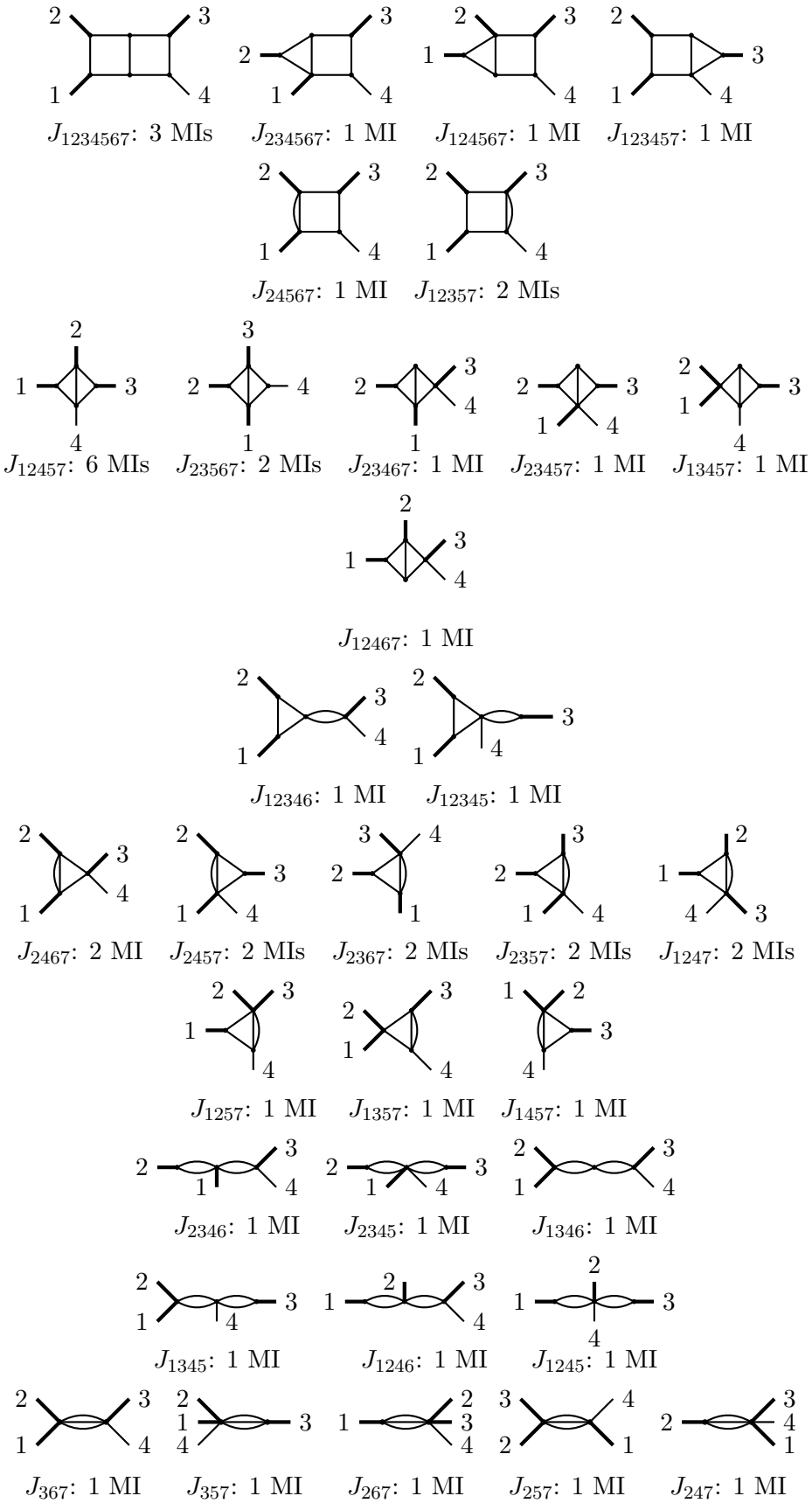


Figure 7.1: The different sectors of the three-mass double-box. Thick lines represent massive external momenta. The sectors J are labeled by the lines that are present in the diagram and we also show the number of master integrals (MIs) in each sector.

$$
\begin{aligned}
J_{1234567} &: g_1 = -\epsilon^2 s(st - m_1^2 m_3^2) I_{1,1,1,1,1,1,1,0,0}, \\
&\quad g_2 = \epsilon^2 r_1(-m_3^2 I_{0,1,1,1,1,1,1,0,0} + s I_{1,1,1,1,1,1,1,-1,0}), \\
&\quad g_3 = \epsilon^2 (m_3^2 - s)(-m_1^2 I_{1,1,1,0,1,1,1,0,0} - m_2^2 I_{1,1,1,1,1,0,1,0,0} + s I_{1,1,1,1,1,1,1,0,-1}), \\
J_{234567} &: g_4 = \epsilon^2 (m_1^2 m_3^2 + m_2^2 s - m_2^2 m_3^2 - st) I_{0,1,1,1,1,1,1,0,0}, \\
J_{124567} &: g_5 = \epsilon^2 s(m_1^2 - t) I_{1,1,0,1,1,1,1,0,0}, \\
J_{123457} &: g_6 = \epsilon^2 r_2 I_{1,1,1,1,1,0,1,0,0}, \\
J_{24567} &: g_7 = \epsilon(1-2\epsilon)(m_3^2 - s) I_{0,1,0,1,1,1,1,0,0}, \\
J_{12357} &: g_8 = \epsilon r_1 I_{1,1,1,0,2,0,1,-1,0}, \quad g_9 = \epsilon(m_1^2 m_3^2 - st) I_{1,1,1,0,2,0,1,0,0}, \\
J_{12457} &: g_{10} = -\epsilon m_1^2 (m_3^2 - s) I_{2,1,0,1,1,0,1,0,0}, \quad g_{11} = -\epsilon m_1^2 r_3 I_{1,2,0,1,1,0,1,0,0}, \\
&\quad g_{12} = -\epsilon m_3^2 r_1 I_{1,1,0,2,1,0,1,0,0}, \quad g_{13} = -\epsilon m_3^2 (m_1^2 - t) I_{1,1,0,1,2,0,1,0,0}, \\
&\quad g_{14} = \epsilon(m_3^2 m_1^2 - st) I_{1,1,0,1,1,0,2,0,0}, \quad g_{15} = \epsilon^2 r_4 I_{1,1,0,1,1,0,1,0,0}, \\
J_{23567} &: g_{16} = \epsilon^2 (m_1^2 + m_3^2 - s - t) I_{0,1,1,0,1,1,1,0,0}, \quad g_{17} = 2\epsilon m_2^2 (t - m_1^2) I_{0,2,1,0,1,1,1,0,0}, \\
J_{23467} &: g_{18} = \epsilon^2 r_1 I_{0,1,1,1,0,1,1,0,0}, \\
J_{23457} &: g_{19} = \epsilon^2 r_3 I_{0,1,1,1,1,0,1,0,0}, \\
J_{13457} &: g_{20} = \epsilon^2 (m_3^2 - s) I_{1,0,1,1,1,0,1,0,0}, \\
J_{12467} &: g_{21} = \epsilon^2 r_1 I_{1,1,0,1,0,1,1,0,0}, \\
J_{12345} &: g_{22} = \epsilon^2 (m_3^2 - s) r_1 I_{1,1,1,1,1,1,0,0,0}, \\
J_{12346} &: g_{23} = \epsilon r_1 m_3^2 (-2\epsilon I_{1,1,1,1,1,1,0,0,0} + s I_{1,1,1,2,1,1,0,0,0}), \\
J_{2467} &: g_{24} = \epsilon r_1 I_{0,2,0,1,0,1,1,0,0}, \quad g_{25} = 3\epsilon(s - m_1^2 - m_2^2) I_{0,2,0,1,0,1,1,0,0} + m_2^2 m_1^2 I_{0,2,0,1,0,1,2,0,0}, \\
J_{2457} &: g_{26} = \epsilon r_3 I_{0,2,0,1,1,0,1,0,0}, \quad g_{27} = 3\epsilon(m_3^2 - m_2^2 - t) I_{0,2,0,1,1,0,1,0,0} + m_2^2 t I_{0,2,0,1,1,0,2,0,0}, \\
J_{2367} &: g_{28} = \epsilon r_1 I_{0,1,1,0,0,2,1,0,0}, \quad g_{29} = 3\epsilon(m_2^2 - m_1^2 - s) I_{0,1,1,0,0,2,1,0,0} + m_1^2 t I_{0,1,1,0,0,2,2,0,0}, \\
J_{2357} &: g_{30} = \epsilon r_3 I_{0,1,1,0,2,0,1,0,0}, \quad g_{31} = 3\epsilon(m_2^2 - m_3^2 - t) I_{0,1,1,0,2,0,1,0,0} + m_3^2 t I_{0,1,1,0,2,0,2,0,0}, \\
J_{1247} &: g_{32} = \epsilon r_1 I_{1,1,0,2,0,0,1,0,0}, \quad g_{33} = 3\epsilon(m_1^2 - m_2^2 - s) I_{1,1,0,2,0,0,1,0,0} + s m_2^2 I_{1,1,0,2,0,0,2,0,0}, \\
J_{1257} &: g_{34} = (1-2\epsilon)(1-3\epsilon) I_{1,1,0,0,1,0,1,0,0}, \\
J_{1357} &: g_{35} = (1-2\epsilon)(1-3\epsilon) I_{1,0,1,0,1,0,1,0,0}, \\
J_{1457} &: g_{36} = (1-2\epsilon)(1-3\epsilon) I_{1,0,0,1,1,0,1,0,0}, \\
J_{2346} &: g_{37} = (1-2\epsilon)^2 I_{0,1,1,1,0,1,0,0,0}, \quad J_{2345} : \ g_{38} = (1-2\epsilon)^2 I_{0,1,1,1,1,0,0,0,0}, \\
J_{1346} &: g_{39} = (1-2\epsilon)^2 I_{1,0,1,1,0,1,0,0,0}, \quad J_{1345} : \ g_{40} = (1-2\epsilon)^2 I_{1,0,1,1,1,0,0,0,0}, \\
J_{1246} &: g_{41} = (1-2\epsilon)^2 I_{1,1,0,1,0,1,0,0,0}, \quad J_{1245} : g_{42} = (1-2\epsilon)^2 I_{1,1,0,1,1,0,0,0,0}, \\
J_{367} &: g_{43} = s I_{0,0,2,0,0,2,1,0,0}, \quad J_{357} : \ g_{44} = m_3^2 I_{0,0,2,0,2,0,1,0,0}, \quad J_{267} : \ g_{45} = m_1^2 I_{0,2,0,0,0,2,1,0,0}, \\
J_{247} &: g_{46} = t I_{0,2,0,0,2,0,1,0,0}, \quad J_{247} : \ g_{47} = m_2^2 I_{0,2,0,2,0,0,1,0,0}.
\end{aligned}
$$

Table 7.1: Complete canonical basis for the three-mass two-loop box integral family. The integrals are ordered according to the sector they belong to.

- To reduce the number of integration variables, it is very beneficial to first perform a general search for dlog integrals on the maximal cut of each sector (see also the discussion at the end of section 3.3). To determine possible corrections when relaxing the cut constraints, one can then further reduce the number of cut propagators in the leading singularity analysis or examine the off-diagonal blocks of the differential equations, see section 5.4. Examples where such corrections are necessary are the integrals g_2 and g_3.

- The master integrals with a bubble can be processed through the heuristic rule of putting a dot on one of the lines of the bubble. An example of this is given by g_8 and g_9 which have also been discussed in equation (4.11). Since most of these sectors only have a single master integral, one can alternatively infer the relative factor in ϵ from the off-diagonal blocks. This leads to the factors of $(1-2\epsilon)$ and $(1-3\epsilon)$ in some of the integrals.

- An exception to this are the triangle-bubble sectors where only one of the two master integrals can be found in this way. However, in this case the corresponding diagonal blocks turn out to be linear in ϵ, and we therefore determine the second canonical integral by simply integrating out the ϵ^0 term.

- Finally, there is one sector with six master integrals: J_{12457}. Because of the position of the massless leg, the leading singularity of one of the triangles is a square-root and therefore we cannot proceed along the lines of sector J_{23567}, see eqs. (4.16)-(4.19). However, we can still guess that the integrals with a single dot on any line are potential UT integrals. Indeed, it turns out that all of them are UT and that we can infer the correct normalization through the ϵ^0-part of the homogeneous differential equation. Alternatively, one can consider super sectors to determine these integrals. For example, a dlog integral in sector J_{124567}[1] is

$$(m_3^2-s)(-I_{1,1,0,1,1,0,1,0,0}+I_{1,1,0,1,1,1,1,0,-1}-m_1^2 I_{1,1,0,1,1,1,1,1,0,0}) \tag{7.2}$$

$$=-\frac{m_1^2(m_3^2-s)}{\epsilon}I_{2,1,0,1,1,0,1,0,0}, \tag{7.3}$$

  and it completely reduces to an integral in sector J_{12457}.

We see that it is straightforward to find a canonical basis using standard techniques and that it is not necessary to apply our new algorithm. The reason is that most sectors have only one or two master integrals and therefore the few UT integrals that are usually used as an input to our algorithm already provide enough information. An exception to this might be sector J_{12457} which has six master integrals. Indeed, one can use the dlog integral found in eq. (3.56) as an input to our algorithm to bring the corresponding diagonal block into canonical form. However, the effort needed to correctly deduce the ansatz for the alphabet is far higher than it is to just guess the remaining five UT integrals by putting dots on the lines of the triangle sub-integrals. In addition, the latter

[1] Note that this sector has zero master integrals.

integrals do not require any corrections through off-diagonal blocks, which would not be the case for integrals found by applying our algorithm to the diagonal block only.

Using the canonical basis results in the following differential equations:

$$\mathrm{d}\vec{g} = \epsilon(\mathrm{d}\tilde{A})\vec{g}, \qquad \tilde{A} = \sum_l \mathbf{m}_l \log \alpha_l, \tag{7.4}$$

where $\mathbf{m}_l$ are 47×47 matrices containing rational numbers. The matrix $\tilde{A}$ can be obtained from the five partial differential equation matrices $\partial_i \tilde{A}$ by subsequently integrating them in each variable, similar to how one can find the potential associated to a conservative force, see e.g. [77]. The alphabet $\vec{\alpha}$ of the three-mass two-loop box integral family consists of 30 letters. They can be ordered according to their behavior under the change of the sign of the square roots r_i:

- Even letters:

$$\begin{gathered}
\alpha_1 = m_1^2, \quad \alpha_2 = m_2^2, \quad \alpha_3 = m_3^2, \quad \alpha_4 = s, \quad \alpha_5 = t \quad \alpha_6 = m_3^2 - s, \\
\alpha_7 = m_1^2 - t, \quad \alpha_8 = m_1^2 m_3^2 - st, \quad \alpha_9 = m_1^2 + m_3^2 - s - t, \\
\alpha_{10} = m_2^2 s + m_1^2 m_3^2 - m_2^2 m_3^2 - st, \\
\alpha_{11} = -2m_1^2 s - 2m_2^2 s + m_1^4 + m_2^4 - 2m_1^2 m_2^2 + s^2 \\
\alpha_{12} = -2m_2^2 t - 2m_3^2 t + m_2^4 + m_3^4 - 2m_2^2 m_3^2 + t^2, \\
\alpha_{13} = -2m_2^2 s - 2m_2^2 t + m_2^4 - 4m_1^2 m_3^2 + s^2 + 2st + t^2, \\
\alpha_{14} = -2m_3^2 s^2 t + m_3^4 s^2 + 2m_2^2 m_3^2 st - 2m_2^2 m_3^4 s - 4m_1^2 m_2^2 m_3^2 s + m_2^4 m_3^4 + s^2 t^2, \\
\alpha_{15} = -m_1^2 st - m_2^2 st - m_3^2 st + m_1^2 m_2^2 s - m_1^2 m_3^2 s - m_1^2 m_3^2 t + m_2^2 m_3^2 t \\
+ m_1^2 m_3^4 + m_1^4 m_3^2 - m_1^2 m_2^2 m_3^2 + s^2 t + s t^2
\end{gathered} \tag{7.5}$$

- Odd letters:

$$\begin{aligned}
\alpha_{16} &= \frac{m_1^2 - m_2^2 + s - r_1}{m_1^2 - m_2^2 + s + r_1}, \quad \alpha_{17} = \frac{m_2^2 - m_3^2 + t - r_3}{m_2^2 - m_3^2 + t + r_3}, \\
\alpha_{18} &= \frac{m_1^2 - m_2^2 - s - r_1}{m_1^2 - m_2^2 - s + r_1}, \quad \alpha_{19} = \frac{m_2^2 - m_3^2 - t - r_3}{m_2^2 - m_3^2 - t + r_3}, \\
\alpha_{20} &= \frac{m_2^2 - s - t + r_4}{m_2^2 - s - t - r_4}, \quad \alpha_{21} = \frac{-m_3^2 s + m_2^2 m_3^2 + st + r_2}{-m_3^2 s + m_2^2 m_3^2 + st - r_2}, \\
\alpha_{22} &= \frac{m_2^2 s + m_3^2 s - m_3^2 t + 2m_1^2 m_3^2 - m_2^2 m_3^2 - s^2 - st - r_4\left(m_3^2 - s\right)}{m_2^2 s + m_3^2 s - m_3^2 t + 2m_1^2 m_3^2 - m_2^2 m_3^2 - s^2 - st + r_4\left(m_3^2 - s\right)}, \\
\alpha_{23} &= \frac{m_2^2 s - m_3^2 s + m_2^2 t - m_1^2 t - m_2^4 + m_1^2 m_2^2 + m_3^2 m_2^2 + m_1^2 m_3^2 + st - r_1 r_3}{m_2^2 s - m_3^2 s + m_2^2 t - m_1^2 t - m_2^4 + m_1^2 m_2^2 + m_3^2 m_2^2 + m_1^2 m_3^2 + st + r_1 r_3}, \\
\alpha_{24} &= \frac{-m_2^2 s + m_3^2 s - 2m_2^2 t - m_3^2 t + m_2^4 - 2m_1^2 m_3^2 - m_2^2 m_3^2 + st + t^2 - r_3 r_4}{-m_2^2 s + m_3^2 s - 2m_2^2 t - m_3^2 t + m_2^4 - 2m_1^2 m_3^2 - m_2^2 m_3^2 + st + t^2 + r_3 r_4},
\end{aligned} \tag{7.6}$$

$$\begin{aligned}
\alpha_{25} &= \frac{m_1^2 s + 2m_2^2 s - m_1^2 t + m_2^2 t - m_2^4 + m_1^2 m_2^2 + 2m_1^2 m_3^2 - s^2 - st - r_1 r_4}{m_1^2 s + 2m_2^2 s - m_1^2 t + m_2^2 t - m_2^4 + m_1^2 m_2^2 + 2m_1^2 m_3^2 - s^2 - st + r_1 r_4}, \\
\alpha_{26} &= \frac{f_{26} - r_1 r_2}{f_{26} + r_1 r_2}, \quad \alpha_{27} = \frac{f_{27} - r_2 r_3}{f_{27} + r_2 r_3}, \quad \alpha_{28} = \frac{f_{28} - (m_1^2 m_3^2 - st) r_2}{f_{28} + (m_1^2 m_3^2 - st) r_2}, \\
\alpha_{29} &= \frac{f_{29} - (m_2^2 s + m_1^2 m_3^2 - m_2^2 m_3^2 - st) r_1}{f_{29} + (m_2^2 s + m_1^2 m_3^2 - m_2^2 m_3^2 - st) r_1}, \\
\alpha_{30} &= \frac{f_{30} - (-m_2^2 t + m_1^2 m_2^2 - m_1^2 m_3^2 + st) r_3}{f_{30} + (-m_2^2 t + m_1^2 m_2^2 - m_1^2 m_3^2 + st) r_3}
\end{aligned} \tag{7.7}$$

where

$$\begin{aligned}
f_{26} =& - m_3^2 s^2 - m_1^2 st - m_2^2 st + 2m_1^2 m_2^2 s + m_1^2 m_3^2 s \\
&+ 2m_2^2 m_3^2 s - m_2^4 m_3^2 + m_1^2 m_2^2 m_3^2 + s^2 t, \\
f_{27} =& m_2^2 st + 2m_3^2 st - m_3^4 s + m_2^2 m_3^2 s - m_2^2 m_3^2 t \\
&+ m_2^2 m_3^4 - m_2^4 m_3^2 + 2m_1^2 m_2^2 m_3^2 - st^2, \\
f_{28} =& - m_3^2 s^2 t - m_1^2 m_3^2 st + m_2^2 m_3^2 st + m_1^2 m_3^4 s \\
&- 2m_1^2 m_2^2 m_3^2 s + m_1^2 m_2^2 m_3^4 + s^2 t^2, \\
f_{29} =& m_2^2 s^2 - m_1^2 st + m_2^2 st - m_2^4 s + m_1^2 m_2^2 s - m_1^2 m_3^2 s \\
&- m_2^2 m_3^2 s + m_1^4 m_3^2 + m_2^4 m_3^2 - 2m_1^2 m_2^2 m_3^2 + s^2 t, \\
f_{30} =& m_2^2 st - m_3^2 st + m_2^2 t^2 - m_2^4 t - m_1^2 m_2^2 t - m_1^2 m_3^2 t \\
&+ m_2^2 m_3^2 t + m_1^2 m_2^4 + m_1^2 m_3^4 - 2m_1^2 m_2^2 m_3^2 + st^2.
\end{aligned} \tag{7.8}$$

One can also explicitly check that the alphabet of the three-mass one-loop box is a subset of this alphabet.

7.2 Three-Loop Classical Gravitational Potential of Binary Systems

Feynman integrals are not only useful for the computation of cross-sections at particle colliders, but they can also be used to extract classical observables through an effective field theory approach. In recent years, this has led to an acceleration of new results in the field of gravitational waves [145, 146, 147, 148, 149, 150]. An example is the dynamics of a binary system, where a specific case is the inspiral phase of two black holes. The powerful techniques developed for particle physics have made it possible to perform this computation to fourth order in Newton's constant for the conservative contribution. This was derived by the present author and collaborators in [4], but has first been obtained in [151] through a different method.

Let us discuss the integrals appearing in the computation. First, since there are two particles going in and two particles going out, we are dealing with four-point kinematics which are characterized by two momenta p_1 and p_2, and one momentum transfer q with $p_i \cdot q = 0$. Second, we are interested in the classical part and therefore work in the

framework of an effective field theory. This leads to linear propagators $(k_i + p_j) - m_1^2 \approx 2k_i \cdot p_j$ very similar to the Wilson lines we encountered in section 4.3.

The integral families relevant to the computation can be summarized as

$$\begin{aligned}
D_1 &= \pm k_1 \cdot v_1, & D_2 &= \pm k_2 \cdot v_1, & D_3 &= \pm k_3 \cdot v_1, \\
D_4 &= \pm k_1 \cdot v_2, & D_5 &= \pm k_2 \cdot v_2, & D_6 &= \pm k_3 \cdot v_2, \\
D_7 &= -k_1^2, & D_8 &= -k_2^2, & D_9 &= -k_3^2, \\
D_{10} &= -(k_1 - q)^2, & D_{11} &= -(k_2 - q)^2, & D_{12} &= -(k_3 - q)^2, \\
D_{13} &= -(k_1 - k_2)^2, & D_{14} &= -(k_2 - k_3)^2, & D_{15} &= -(k_1 - k_3)^2,
\end{aligned} \tag{7.9}$$

where we again factored out the overall masses as $p_i = v_i m_i$. Therefore q^2 is the only variable which is not dimensionless and we can infer it through dimensional analysis. As a result, the integrals only depend on $v_1 \cdot v_2 = (x + 1/x)/2$ in a non-trivial way. The signs of the first six propagators can be different in each integral family[2]. Another interesting property of the integrals is that certain propagators are cut, i.e. they are replaced by delta functions of the same argument. From the point of few of the differential equations this is a simplification because we can simply set all integrals with non-positive powers for the cut propagators to zero. An example diagram representing an integral family is given in figure 7.2.

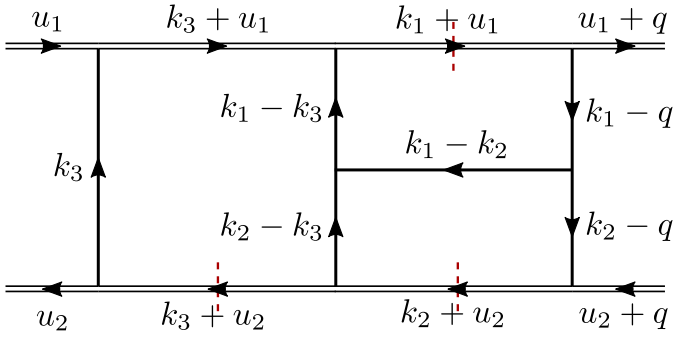


Figure 7.2: Example appearing in the computation of the conservative binary dynamics to fourth post-Minkowskian order.

The most important simplification, however, comes from the fact that not all integrals are needed to compute the result. Therefore, these integrals can be removed from the differential equations if non of the needed integrals depend on them. In some cases, e.g. when the top-sector integrals of a family are removed, this leads to a decoupling of the differential equations into several smaller closed systems, c.f. section 6.6.

Let us now discuss how we bring the largest of these systems with 40 master integrals into canonical form:

[2]Recall that we omit the Feynman prescription, $D_i \equiv D_i - i0$, and therefore different choices for the signs generally give different results.

- Because of the relatively small size of sectors ($n \leq 4$), we prefer to use balance transformations on the diagonal blocks and then subsequently transform the off-diagonal blocks through the transformations discussed in section 5.4.
- There is one sector with three master integrals that cannot be brought into canonical form through algebraic transformations. This can be revealed in the following way: we first multiply all integrals by factors of ϵ s.t. the differential equation matrix is $A(x,\epsilon) = A_0(x) + \mathcal{O}(\epsilon)$. From this, we derive a third order Picard-Fuchs equation for the scalar integral that can easily be solved through the methods discussed in [152]. Three independent solutions of this equation are $x\mathrm{K}(x^2)^2, x\mathrm{K}(x^2)\mathrm{K}(1-x^2)$ and $x\mathrm{K}(1-x^2)^2$.
- Using the knowledge about the elliptic functions in our algorithm, we bring the diagonal block into canonical form in the same way as for the sunrise integral in section 6.7.3. As initial integral we use the scalar integral normalized by $1/(x\mathrm{K}(1-x^2)^2)$.

The resulting differential equations are

$$\frac{\partial}{\partial x}\vec{g} = \epsilon\tilde{A}(x)\vec{g}, \tag{7.10}$$

with

$$\begin{aligned}\tilde{A}(x) = {} & \mathbf{m}_1\frac{\pi^2}{\mathrm{K}(1-x^2)^2(1-x)x(1+x)} + \mathbf{m}_2\frac{1}{1-x} + \mathbf{m}_3\frac{1}{x} + \mathbf{m}_4\frac{1}{1+x} \\ & + \mathbf{m}_5\frac{x}{1+x^2} + \mathbf{m}_6\frac{\mathrm{K}(1-x^2)^2}{\pi^2(1-x)x(1+x)} + \mathbf{m}_7\frac{\mathrm{K}(1-x^2)^2}{\pi^2(1-x)(1+x)} \\ & + \mathbf{m}_8\frac{\mathrm{K}(1-x^2)^2}{\pi^2 x} + \mathbf{m}_9\frac{\mathrm{K}(1-x^2)^2}{\pi^2} + \mathbf{m}_{10}\frac{\mathrm{K}(1-x^2)^2(1-x)(1+x)}{\pi^2 x} \\ & + \mathbf{m}_{11}\frac{\mathrm{K}(1-x^2)^4}{\pi^4(1-x)x(1+x)} + \mathbf{m}_{12}\frac{\mathrm{K}(1-x^2)^4}{\pi^4 x} \\ & + \mathbf{m}_{13}\frac{\mathrm{K}(1-x^2)^4(1-x)(1+x)}{\pi^4 x} + \mathbf{m}_{14}\frac{\mathrm{K}(1-x^2)^4(1-x)^2(1+x)^2}{\pi^4 x},\end{aligned} \tag{7.11}$$

where the $\mathbf{m}_i$ are 40×40 matrices consisting of rational numbers. We note that all of the functions appearing in eq. (7.11) are modular forms and therefore the solution in terms of iterated integrals of modular forms is straightforward. However, using the solutions of the integrals to obtain the final answer shows that only simple elliptic integrals and multiple polylogarithms are relevant for the required order in ϵ.

In this example, we again see that our new algorithm is not necessary for a large portion of the differential equation matrix. This is mostly because of the small size of the diagonal blocks, but also due to the fact that there is only one kinematic variable. For more kinematic variables, the preferred standard approach would have been the computation of leading singularities, however, this can become computationally rather expensive at three loops because of the higher number of integration variables. The most important contribution of our algorithm is to the non-polylogarithmic sector, which cannot be handled by the other methods.

7.3 Four-Loop Cusp Anomalous Dimension in QED

As discussed in section 4.3, IR divergences of scattering amplitudes are known to factorize in a universal way from the process-dependent finite part [115, 116]. Understanding the universal divergent part is crucial for deriving IR finite observables. Further, it is determined by a set of anomalous dimensions, one of which is the so-called cusp anomalous dimension. Because of the universal nature of the cusp anomalous dimension, it can be computed from the divergent part of several different quantities, in particular, from the $1/\epsilon$ pole coefficient of a Wilson line [117] similar to the one considered in section 4.3.

Here, we want to discuss the computation of a particular color structure at four loops, which was first presented in [2]. This color structure, called the matter-dependent quartic Casimir, appears for the first time at four loops and constitutes the first corrections involving non-planar Feynman diagrams. Further, it determines an important part of the four-loop cusp anomalous dimension in QCD and, before the appearance of [2], was the last missing piece for the answer in QED.

There are six necessary Feynman diagrams, which are depicted in figure 7.3. These diagrams are also representative of the integral families that appear in each diagram. The largest and most complicated family is given in figure 7.3e and has 521 master integrals in 154 different sectors. The propagators for this family are given in eq. (6.19). Let us discuss the computation of the integrals of this family through the method of

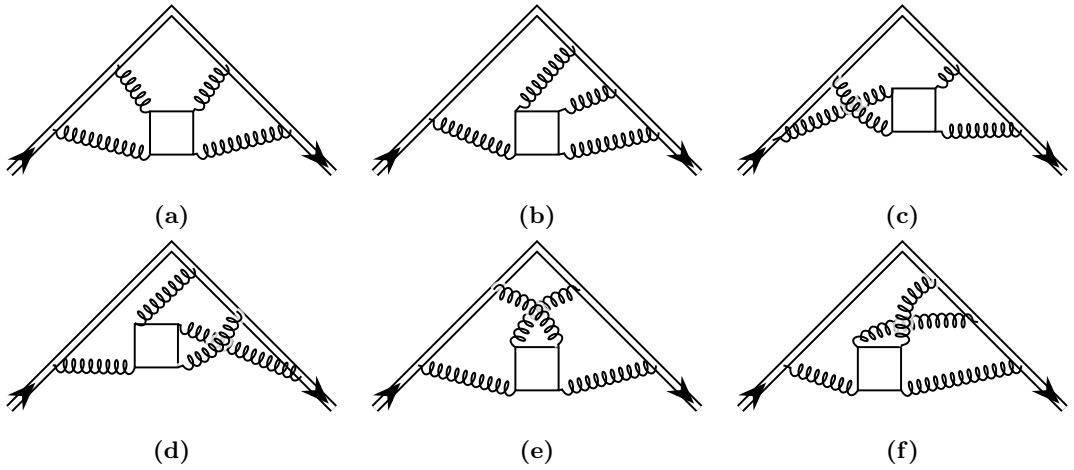


Figure 7.3: Feynman diagrams contributing to the quartic Casimir term of the angle-dependent cusp anomalous dimensions. The diagrams are also representative of the Feynman integral topologies appearing in the computation of each diagram. For this, one can simply replace the gluonic curly lines by scalars, whereas heavy-quark lines depicted by double lines represent linear propagators.

differential equations:

- Because of the large number of sectors, it would be convenient to apply the highly automatized method of balance transformations to each diagonal block and then

subsequently transform the off-diagonal blocks through the transformations discussed in section 5.4. However, the size of the diagonal blocks often goes beyond what the implementations of the method can handle. We observe that sectors with around six master integrals often take several hours to complete, and that for many sectors with more than seven master integrals, the computation fails to advance beyond a certain point.

- Due to the large number of integration variables and the UV behavior of the integrals, it is difficult to find a complete dlog basis for the whole family or even individual sectors. However, by employing different parametrizations, e.g. the position-space parametrization of section 4.4, it is still possible to find a few dlog integrals or UT candidates in each sector.
- We then use these dlog integrals and UT candidates to transform each diagonal block into canonical form through our new algorithm. Here we want to highlight again the ability of the algorithm to test a given list of integrals for the UT property.
- For the sector depicted in figure 7.4, we fail to find a canonical form through algebraic transformations. In fact, an irreducible two-by-two system in this sector at ϵ^0 suggests that elliptic functions are necessary to achieve a canonical form. Instead of trying to find these elliptic functions, we proceed in a more pragmatic way: The boundary constants can be used to infer which integrals actually contribute to the $1/\epsilon$ pole of the final answer. In this way, we find that the potentially elliptic integrals can be discarded, so that a new differential equation system is formed that can now be solved in terms of multiple polylogarithms.

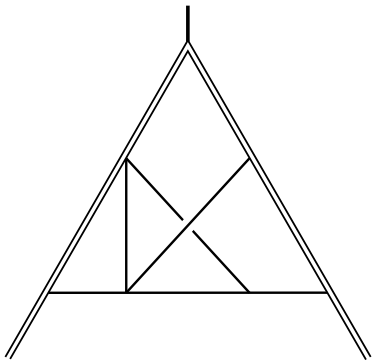


Figure 7.4: Wilson line sector involving functions beyond multiple polylogarithms. The number of master integrals is eleven.

The functions appearing in the solutions of the integrals then depend on the following alphabet:

$$\vec{\alpha} = \{x, 1+x, 1-x, 1+x^2, 1-x+x^2, \frac{1-\sqrt{-x}}{1+\sqrt{-x}}, \frac{1-\sqrt{-x}+x}{1+\sqrt{-x}+x}\}. \tag{7.12}$$

However, due to cancellations between different terms, the cusp anomalous dimension itself only depends on the first four letters.

This example shows how our algorithm is perfectly suited for the case where both the dlog integral method and the balance transformations fail to give a complete canonical basis. A particular example of this is the sector with 17 master integrals discussed in section 6.4.3, whose canonical form seemed to be unobtainable through the use of existing methods. Another important case is the sector discussed in section 6.7.2, which involves algebraic letters and can be transformed through our algorithm without any rationalization.

8 Conclusions and Outlook

The method of differential equations is currently the predominant tool for computing Feynman integrals analytically [153, 154, 9]. However, one of the main bottlenecks in applying it is still to simplify the differential equations enough so that the solutions can be obtained. The canonical form takes this to the point where the solutions in terms of iterated integrals follow almost by definition. One can argue that it is the simplest and most natural form of the differential equations. Not only are the transcendental properties of the iterated integrals in the ϵ-expanded solutions completely manifest, but the behavior around singular points also explicitly follows the behavior that is expected from the parametric representation.

In this thesis, we have reviewed several methods for finding a canonical basis. We have then presented our new method which aims to overcome some of the drawbacks of the already existing techniques. Our algorithm allows us keep the pure integrals found through other means and furthermore use them to transform the rest of the basis to pure integrals. The ansatz for the canonical form is not restricted to rational functions and can include square-roots and even elliptic functions if needed. In addition, in the multivariate case, it is sufficient to run the algorithm for only one of the invariants. The determined UT integrals can then only differ from pure integrals by an overall factor in the remaining invariants. To demonstrate the power of our implementation, we have applied the algorithm to multiple single-variable cases, as well as a four-variable example, see table 6.1 for approximate time and memory usage on a desktop computer. Further, we used the algorithm to derive the canonical form of two example matrices involving elliptic integrals.

We want to emphasize that our algorithm also allows us to test a candidate integral for the UT property by analyzing only the differential equation matrix. This is not possible through any of the other described methods, as they either do not take this matrix into account or are only able to make statements about the basis as a whole. The ability to test integrals opens the possibility to also automatize the step of finding an initial pure integral which the algorithm needs as an input. One simply creates a list of candidate integrals (aided e.g. by a power counting criterion) and then checks one candidate after another until a viable integral is found. As described in section 7.3, this approach was used in [2] to determine the canonical form of most of the diagonal blocks, where the full basis consists of about 521 master integrals.

There are several possible future applications and generalizations of the methods discussed in this thesis:

Using multiple UT integrals in the algorithm: The algorithm of section 6 has so far been mainly applied by using a single canonical integral as input. Because of the high-

degree polynomials appearing in the derivatives, this limited the algorithm to problems with less than about 100 master integrals. Only in the case of linearly dependent derivatives we also used the derivatives of a second canonical integral in order to complete the basis. However, in principle, one could use multiple canonical integrals, e.g. one from each sector, to bring the differential equations for hundreds of master integrals into canonical form.

Simplifications for finite loop integrals: Although the integrals can have divergences that are regularized through dimensional regularization, the desired outcome of the computation is usually a finite four-dimensional quantity. In some cases, it is possible to already choose the integral basis to consist of manifestly finite integrals. One can then try to apply the method of differential equations also for $\epsilon = 0$, where many simplifications happen [155]. The canonical form would then be equivalent to a block triangular matrix with zeros on the diagonal, where the blocks group together integrals of equal transcendental weight. This can e.g. easily be seen by deriving the differential equations for a basis of MPLs $\vec{f} = (G(a_1, a_2, \ldots, a_n; x), G(a_2, \ldots, a_n; x), \ldots,$
$G(a_n; x), 1)^{\mathrm{T}}$. Finding this form can e.g. be done through the leading singularities approach, where it is already very natural to classify the integrals according to their IR properties [29, 35, 32]. It would however be very interesting to generalize the methods based on the explicit differential equation matrix to the case of $\epsilon = 0$.

Loop-by-loop Baikov representation for a complete dlog basis: It is known that the number of master integrals within an integral family can be related to the number of critical points of certain polynomials in the integrand of a specific representation of the integral. In [91] it was shown that each of these critical points can be used to construct a specific, linearly independent dlog integral, which suggests that there is a way to find exactly as many dlog integrals as are needed to complete the canonical basis! However, these dlog integrals do not necessarily have standard Feynman propagators and it would be interesting to analyze when a translation of these integrals to the integrals of the considered family is possible. See [3] for recent progress in this direction.

Generalizations to elliptic integrals: Here, we want to discuss how the methods discussed in this thesis can be generalized to the case where a canonical form cannot be reached through rational or even algebraic transformations [68]. Differential equations of this type have become increasingly important in the last decade and there has been tremendous progress towards understanding the special functions appearing in the results [69, 66, 67, 70]. First, when computing leading singularities, one usually tries to localize all integrations by taking residues around the poles of the integrand. However, for an elliptic Feynman integral, one is left with a denominator that is an unrationalizable square-root in the last integration variable [156, 157]. Therefore, one cannot take the residue in this variable but is forced to explicitly keep this last integration. Depending on the integration contour, the resulting leading singularity is one of two possible elliptic integrals [158], which reflects the fact that a second-order differential equation

has two independent solutions. This approach is already used routinely to determine the elliptic functions appearing in the solutions, as well as to find individual elliptic dlog integrals. However, it remains extremely challenging to find a complete basis in this way. Moreover, the differential equations found in this way often not only depend on the elliptic integral of the first kind, but also on the elliptic integral of the second kind [159]. The latter is a major obstruction to finding a representation in terms of modular forms.

Next, it would be interesting to see if the balance transformations of chapter 4 can be modified to incorporate elliptic integrals. For example, in the case of a rationalizable square-root $y = \sqrt{x}$, one can see that either the numerator or denominator of the transformation will involve the pole $x = 0$ exactly through this square-root. It is conceivable that one can similarly represent the pole through an elliptic integral which then appears explicitly in the numerator or denominator of the transformation.

Analyzing our new algorithm, we have already seen how elliptic integrals can be incorporated by modifying the ansatz for the canonical form accordingly. However, in contrast to the leading singularity computation, it is not possible to determine which type of elliptic functions appear or what arguments they have. Therefore, a promising approach is to try to generalize the algorithm s.t. it can find differential equations linear in ϵ:

$$\mathrm{d}\vec{f} = (\mathrm{d}A_0 + \epsilon\,\mathrm{d}A_1)\,\vec{f}, \tag{8.1}$$

see also [20, 160]. As described in section 5.6, integrating out A_0, or at least its diagonal blocks, would make it possible to solve the differential equations in a straightforward way. If integrating out A_0 leads to elliptic integrals of the second kind, one can then also use the newly won knowledge about the function space in an ansatz for a canonical form in terms of modular forms only. The main difficulty in generalizing the algorithm to the form (8.1) is that the equations are not linearized by expanding in ϵ. This can also be observed when trying the same in the approach of [135].

A The ϵ-Expansion of the Picard-Fuchs Equation

In this appendix, we give details on the ϵ-expansion of the coefficients of the Picard-Fuchs equation derived in chapter 6. After obtaining bounds on the polynomial degrees appearing in the rational functions, we discuss the algorithmic solution of eq. (6.15) for the matrices $\mathbf{m}_l$.

A.1 Degree Bounds on the Coefficients

Assuming that f_1 is a pure integral leads to degree bounds in ϵ on the coefficients of the Picard-Fuchs equation. As a corollary, this yields a necessary condition for an integral to be pure. To derive these degree bounds, let us normalize the coefficients b_m through a common minimal denominator $\tilde{b}_0$

$$\tilde{b}_0 f_1 + \sum_{m=1}^{n} \tilde{b}_m f_1^{(m)} = 0, \tag{A.1}$$

s.t. the $\tilde{b}_m$ are polynomials in ϵ and x. Let us also assume that f_1 is not only of uniform transcendental weight, but specifically of weight zero. This can always be achieved by multiplying it with a suitable power in ϵ which in turn does not change its differential equations because they are homogeneous. As a result, f_1 starts at ϵ^0 with constant coefficients, and its m-th derivative is a sum of functions whose transcendental weights range between -1 and $-m$, i.e.

$$f_1^{(m)} = \sum_{k=1}^{m} f_1^{(m,k)}, \quad m \geq 1 \tag{A.2}$$

where $f_1^{(m,k)}$ has weight $-k$ and is of $\mathcal{O}(\epsilon^1)$. Similarly, we can expand the coefficients as

$$\tilde{b}_m = \sum_{k=0}^{p_m} \epsilon^k \tilde{b}_m^{(k)}. \tag{A.3}$$

Note that this is also an expansion in transcendental weight, since the polynomials $\tilde{b}_m^{(k)}$ have weight zero.

Grouping together terms of equal transcendental weight in eq. (A.1) results in the equations

$$\tilde{b}_0^{(0)} f_1 = 0, \tag{A.4}$$

$$\epsilon^k \tilde{b}_0^{(k)} f_1 + \sum_{m=1}^{n} \sum_{l=0}^{k-1} \epsilon^l \tilde{b}_m^{(l)} f_1^{(m,k-l)} = 0, \qquad k = 1, \ldots, p_{\max}, \tag{A.5}$$

where $p_{\max}$ is minus the minimum transcendental weight of eq. (A.1) and therefore it is the maximum value of $p_m + m$ for all m. Eqs. (A.4) and (A.5) define $p_{\max} + 1$ equations in the $1 + \sum_{m=1}^{n} m = 1 + n(n+1)/2$ unknowns $\{f_1, f_1^{(m,k)}\}$. Hence, for non-trivial solutions to exist, we must therefore have $p_m + m \leq p_{\max} \leq n(n+1)/2$. Further, from the equation at weight zero in (A.4), we see that $\tilde{b}_0^{(0)} = 0$.

In summary, if f_1 is a pure integral, then the following conditions must hold:

$$\tilde{b}_0 = \mathcal{O}(\epsilon), \tag{A.6}$$

$$p_m \leq \frac{n(n+1)}{2} - m, \quad m = 0, \ldots, n. \tag{A.7}$$

This gives a bound on the maximal ϵ-degree p_m of the coefficient $\tilde{b}_m$.

A.2 The Normalization and the ϵ^0-Part

Next, we want to consider the case of an integral that is UT but not pure. However, we assume that this integral can be made pure by a suitable ϵ-independent normalization factor, i.e. we consider the integral $h_1 = f_1/n(x)$, where f_1 is pure. The result is that the derivatives of h_1 now have a non-vanishing weight-zero term $h_1^{(m,0)} = n^{(m)}(x)\, f_1$. Eq. (A.4) changes to

$$\left(\tilde{b}_0^{(0)} n(x) + \sum_{m=1}^{n} \tilde{b}_m^{(0)} n^{(m)}(x) \right) f_1 = 0 \tag{A.8}$$

which immediately gives a method to determine $n(x)$ from a given set of coefficients $\tilde{b}_m$. Note that the necessary condition (A.7) for h_1 to have uniform transcendental weight is unchanged.

A.3 Solving for the Unknowns

In this section, we want to solve eq. (6.15), i.e.

$$\vec{v}_1 \Psi^{-1} \Phi = \vec{v}_1, \tag{A.9}$$

by expanding it in ϵ. We already discussed the expansion of $\vec{v}_1\Psi^{-1} = -(b_1, \ldots, b_n)$ in appendix A.1, see eq. (A.3). On the other hand, the expansion of each row of Φ is

$$\Phi_m \equiv \vec{v}_1 B^{[m]} \equiv \sum_{r=1}^{m} \epsilon^r \Phi_m^{(r)}, \tag{A.10}$$

where each coefficient can be computed recursively

$$\Phi_m^{(r)} = \frac{\partial}{\partial x}\Phi_{m-1}^{(r)} + \sum_l \Phi_{m-1}^{(r-1)}\mathbf{m}_l \frac{\partial}{\partial x}\log\alpha_l(x), \tag{A.11}$$

and we also defined $\Phi_0 \equiv \vec{v}_1$. Plugging the ϵ-expansions into eq. (A.9) results in

$$\sum_{r=1}^{k}\sum_{m=r}^{n} \tilde{b}_m^{(k-r)}\Phi_m^{(r)} = \tilde{b}_0^{(k)}\vec{v}_1, \qquad k = 1, \ldots, p_{\max}. \tag{A.12}$$

Let us use (A.11) to explicitly write down this equation for $k = 1$:

$$\sum_l \sum_{m=1}^{n} \tilde{b}_m^{(0)}\vec{v}_1\mathbf{m}_l \frac{\partial^m}{\partial x^m}\log\alpha_l(x) = \tilde{b}_0^{(1)}\vec{v}_1 \tag{A.13}$$

which is a linear equation if we treat $\{\vec{v}_1\mathbf{m}_l\}$ as unknown constants. Since we want the solutions to be independent of x, we can either expand (A.13) in x and treat each order as an independent equation, or we can simply sample the equation over different rational values of x until the rank of the system no longer increases. The solution to the $k = 1$ equation will then be of the form

$$\vec{v}_1\mathbf{m}_l = \sum_{j=1}^{l-r_1+1} \beta_{1j}^l \vec{v}_j, \tag{A.14}$$

where r_1 is the mentioned rank of the x-independent system of equations and we introduced $l - r_1$ independent vectors $\{\vec{v}_2, \ldots, \vec{v}_{l-r_1+1}\}$ to parametrize the solutions. For example, if $r_1 = l$ then there are no new vectors and all of the unknowns could be determined in terms of $\vec{v}_1$.

Using these solutions at $k = 2$, we find that the resulting equation depends on $\{\vec{v}_j\}$ as well as $\{\vec{v}_j\mathbf{m}_l\}$ due to the term $\Phi_{m-1}^{(r-1)}\mathbf{m}_l$ in (A.11). Assuming that the system has rank r_2, we can again solve it by introducing a new set of independent vectors, similarly to the previous step.

In general, we introduce $N_k = lN_{k-1} - r_k$ new vectors at each step, with $N_0 = 1$. At a certain step $k = k_f$ we will have a set of $S = \sum_{j=1}^{k_f} N_j$ independent vectors

$$Q \equiv \begin{pmatrix} \vec{v}_1 \\ \vdots \\ \vec{v}_S \end{pmatrix} \tag{A.15}$$

that are closed under multiplication with $\mathbf{m}_l$, i.e.

$$Q\mathbf{m}_l = \beta^l Q \tag{A.16}$$

for some constant matrices β^l. We can check (A.16) explicitly by using the solutions obtained from the previous steps. This relation also means that no new vectors can be introduced at further steps and hence Φ is completely determined by the set of vectors in Q.

In fact, if non-trivial solutions exist, than we must have $S = n$. S cannot be greater than n because the vectors $\vec{v}_j$ are linearly independent. Further, S cannot be smaller than n because the rows of Φ, or equivalently the derivatives of f_1, are linearly independent. Hence Q is an $n \times n$ invertible matrix and we can determine the unknowns in $B(x)$ through

$$\mathbf{m}_l = Q^{-1}\beta^l Q. \tag{A.17}$$

Recall that the $\vec{v}_j$ parametrize the solution to eq. (A.9) and therefore we can choose them to be any set of linearly independent constant vectors. In particular, a convenient choice for the vectors $\vec{v}_j$ are the unit vectors, s.t. Q is the identity matrix and $\mathbf{m}_l = \beta^l$. Different choices of Q generate constant similarity transformations on the canonical form through eq. (A.17).

In total, this gives an algorithm to solve the equation $\vec{v}_1\Phi^{-1}\Phi = \vec{v}_1$ in an expansion in ϵ, which reduces the non-linear problem of determining the $\mathbf{m}_l$ to a linear problem of solving in terms of n independent vectors $\vec{v}_1, \ldots, \vec{v}_n$. The fact that the canonical form is only defined modulo a constant similarity transformation poses no problem and is reflected in the choice of the independent vectors.

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Bibliography

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Acknowledgments

I want to thank my supervisor Johannes Henn for introducing me to the fields of scattering amplitudes, Feynman integrals, differential equations and many more. I am especially indebted to him for teaching me how to manage my projects while also being able to work at my own pace. Without his guidance I would certainly still be lost in one of the details of my computations without ever advancing towards the actual goal.

During my PhD I was blessed with having wonderful colleagues. Among them, I particularly want to thank Daniele Lombardi, Leila Maestri and Simone Zoia for making my time at the office so enjoyable and creating a perfect working environment. I am especially thankful to Simone Zoia for sharing his knowledge about the administrative part of writing and defending a PhD thesis in Munich.

Further, I am grateful to Taushif Ahmed, Long Chen, Dmitry Chicherin, Ekta, Amando Hala, Gudrun Heinrich, Stephan Jahn, Gabriël Koole, Ebert Markus, Javier Mazzitelli, Tiziano Peraro, Vasily Sotnikov, William Torres Bobadilla, Alexander Tumanov, Pascal Wasser, Marius Wiesemann and Giuila Zanderighi for enlightening discussions regarding physics, research and everyday life. Special thanks also to Robin Brüser, Gregor Kälin, Xiado Li, Zhengwen Liu, Kai Yan, Yang Zhang and Rafael Porto from whom I learned a lot during our collaborations. In addition, I am thankful to Ralph Blumenhagen for helping me as external supervisor in the advisory panel system.

I would like to express my gratitude to Vera Kudrin, Annette Sturm and Frank Steffen for helping me with the various organizational tasks one frequently encounters at a research institution and within a PhD programme. Also, I am still amazed by the IT skills of Thomas Hahn, who seemingly solved any computer related problem within minutes. Therefore, I want to thank him for being the most irreplaceable person at the institute for me.

Further, I want to thank Johannes Henn, Sorana Scholtes and Barbara Wankerl for showing me how important outreach is to science. I am particularly grateful to Sorana Scholtes for helping me with this task and also for always being open to a chat about the thrills of being a parent.

Lastly, I am truly thankful to my family and friends, and especially my fiancé and my son, for their continuous support during this journey and generally making life enjoyable.

This work received funding from the European Union's Horizon 2020 research and innovation programme *Novel structures in scattering amplitudes* (grant agreement No 725110).