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On General Algorithms to Manipulate Multiple Polylogarithms

Über allgemeine Algorithmen zur Manipulation von Vielfach-Polylogarithmen

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Abstract

In the analytical treatment of particle-physical processes in the context of perturbative quantum field theory, a special class of functions often arises at higher order: the so-called multiple polylogarithms. The present thesis is concerned with these, and, using the concrete example of the Integration of Symbols algorithm decribed in [1], shows how algebraic structures on the set of multiple polylogarithms can be used to find functional relations between individual elements, and rewrite expressions by as simple functions as possible, such as logarithms and classical polylogarithms Li_n. This is important for at least two reasons. First, a reduction to simpler functions allows for a simpler discussion of the analytic properties of the expression under consideration, for example, with respect to the branching structure in the complex plane or the analytic continuation into the scattering region. Second, this also often allows for a faster numerical evaluation.

The thesis is divided into three parts. The first chapter deals with the mathematical framework relevant for the applications. First, the iterated integral after K.-T. Chen is introduced and its properties are discussed, before multiple polylogarithms are identified as a special case of those iterated integrals and statements about their special properties are made. Following the theory of A.B. Goncharov, the perspective on multiple polylogarithms changes from an analytic to an algebraic one. The introduction of a Hopf algebra structure on the set of multiple polylogarithms finally allows for the introduction of the symbol map as the central object of this work. Most of the essential statements are proved. In the appendix the mathematical background usually not taught in undergraduate courses is explained.

The second chapter builds on the knowledge established in the first chapter and discusses the Integration of Symbols algorithm from [1] and its implementation in Mathematica by the author in detail. The implementation can be found at `https://github.com/maxlouda/IntegrationOfSymbols`.

Finally, the third chapter deals with two applications of the Integration of Symbols algorithm. First, minimal spanning sets consisting of the simplest possible functions are constructed for two special classes of multiple polylogarithms - the one- and two-dimensional harmonic polylogarithms up to and including weight four. Such a basis is known for one-dimensional harmonic polylogarithms in the literature (see [1]), but to the author's knowledge not yet for two-dimensional harmonic polylogarithms in the explicit form presented here (see, however, [2] and [3] for related results). Second, the minimal spanning sets obtained before are used to rewrite expressions for the probability amplitudes describing, for example, the Higgs boson decay $H \to ggg$.

Bei der analytischen Behandlung von teilchenphysikalischen Prozessen im Rahmen der perturbativen Quantenfeldtheorie tritt in höherer Ordnung häufig eine spezielle Klasse von Funktionen auf: die sogenannten Multiplen Polylogarithmen. Die vorliegende Arbeit befasst sich mit diesen und zeigt dabei anhand des konkreten Beispiels des Integration of Symbols-Algorithmus ([1]) auf, wie man algebraische Strukturen auf der Menge der Multiplen Polylogarithmen verwenden kann, um funktionale Beziehungen zwischen einzelnen Elementen zu finden und hiermit Ausdrücke durch möglichst einfache Funktionen wie Logarithmen und klassische Polylogarithmen Li_n umzuschreiben. Dies ist aus mindestens zwei Gründen von Bedeutung. Erstens erlaubt eine Reduktion auf einfachere Funktionen eine einfachere Diskussion der analytischen Eigenschaften des betrachteten Ausdrucks beispielsweise in Hinsicht auf die Verzweigungsstruktur in der komplexen Ebene oder die analytische Fortsetzung in die Streuregion. Zweitens erlaubt dies auch in vielen Fällen eine schnellere numerische Evaluierung der auftretenden Ausdrücke.

Die Arbeit ist in drei Teile aufgeteilt. Das erste Kapitel befasst sich mit dem für die Anwendungen relevanten mathematischen Rahmenwerk. Zunächst wird das iterierte Integral nach K.-T. Chen eingeführt sowie dessen Eigenschaften diskutiert, bevor Multiple Polylogarithmen als Spezialfall jener iterierten Integrale identifiziert und Aussagen über deren spezielle Eigenschaften getroffen werden. Der Theorie A.B. Goncharovs folgend verändert sich danach die Perspektive auf die Multiplen Polylogarithmen weg von einer analytisch hin zu einer algebraisch geprägten. Die Einführung einer Hopf-Algebra-Struktur auf der Menge der Multiplen Polylogarithmen erlaubt schließlich die Einführung der Symbol-Abbildung als zentrales Objekt dieser Arbeit. Die meisten wesentlichen Aussagen werden bewiesen. Im Anhang werden mathematische Begrifflichkeiten, die normalerweise im Grundstudium nicht eingeführt werden, erklärt.

Das zweite Kapitel baut auf den im ersten Kapitel etablierten Zusammenhängen auf und diskutiert den Integration of Symbols-Algorithmus aus [1] sowie dessen Implementierung in Mathematica durch den Autor im Detail. Die Implementierung ist unter `https://github.com/maxlouda/IntegrationOfSymbols` zu finden.

Das dritte Kapitel schließlich behandelt zwei Anwendungen des Integration of Symbols-Algorithmus. Erstens werden minimale Erzeugendensysteme bestehend aus möglichst einfachen Funktionen für zwei spezielle Klassen von Multiplen Polylogarithmen - den ein- und zweidimensionalen harmonischen Polylogarithmen bis inklusive Gewicht vier - konstruiert. Jene Basis ist für eindimensionale harmonische Polylogarithmen in der Literatur bekannt (s. [1]), für zweidimensionale harmonische Polylogarithmen nach Wissen des Autors in der hier präsentierten expliziten Form allerdings noch nicht (s. jedoch [2] und [3] für verwandte Ergebnisse). Zweitens werden die minimalen Erzeugendensysteme benutzt, um Ausdrücke für die Wahrscheinlichkeitsamplituden, welche zum Beispiel den Higgs-Boson-Zerfall $H \to ggg$ beschreiben, umzuschreiben.

Chapter 1

Iterated Integrals, Multiple Polylogarithms and the Symbol Map

This thesis deals with special algorithms for working with multiple polylogarithms. In this first chapter we will introduce the mathematical framework and basic properties of these objects and define the essential operation for this work - the symbol map. Throughout this first chapter, I have made an effort to use mathematically precise terminology.

1.1 General Theory of Iterated Integrals

Multiple polylogarithms are a special class of iterated integrals and inherit some properties of those, as we will see. Therefore, it is worthwhile to remain within this more general framework for the moment. In the following $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ applies.

1.1.1 Definition and Basic Properties of Iterated Integrals

Definition 1.1.1. Iterated Integrals ([4], p.833 and [5]. p.2). Let M be a differentiable real or complex manifold [1], $I = [a, b] \subseteq \mathbb{R}$ an interval and $\gamma : I \to M$ a piecewise differentiable curve. For $\mathbb{K}$-valued 1-forms $\omega_1, ..., \omega_r$ on the manifold M whose pullback along γ is given by

$$\forall i \in \{1, ..., r\} : \quad (\gamma^* \omega_i)_t = f_i(t)\,\mathrm{d}t \tag{1.1}$$

with functions $f_i : I \to \mathbb{K}$, one defines recursively

$$\begin{aligned} \int_\gamma \omega_1 \cdots \omega_r &:= \int_a^b f_1(t_1)\,\mathrm{d}t_1 \cdots f_r(t_r)\,\mathrm{d}t_r := \\ &:= \int_a^b \left(\int_a^{t_r} f_1(t_1)\,\mathrm{d}t_1 \cdots f_{r-1}(t_{r-1})\,\mathrm{d}t_{r-1} \right) f_r(t_r)\,\mathrm{d}t_r. \end{aligned} \tag{1.2}$$

The iterated integral in brackets is taken as a function on $[a, b]$ depending on the parameter t_r, this is multiplied by the differential form $f_r(t_r)\,\mathrm{d}t_r$ and the result is integrated over the interval $[a, b]$. To simplify notation, the indices at t_i are sometimes suppressed. For the case $r = 1$ one thus obtains the special case of line integrals; in the case $r = 0$ one

[1] A collection of some important definitions regarding differential geometry and algebra relevant to this thesis can be found in the appendix.

sets $\int_\gamma \omega_1 \cdots \omega_r =: 1$. The quantity r is called the weight of the iterated integral. More generally, one also refers to $\mathbb{K}$-linear combinations of iterated integrals as iterated integrals and defines ($\lambda, \mu \in \mathbb{K}$):

$$\int\limits_\gamma (\lambda\omega_1 \cdots \omega_r + \mu\sigma_1 \cdots \sigma_s) := \lambda \int\limits_\gamma \omega_1 \cdots \omega_r + \mu \int\limits_\gamma \sigma_1 \cdots \sigma_s. \tag{1.3}$$

Remark. (i) One can relatively easily obtain the following explicit form of 1.2:

$$\int\limits_a^b \left(\int\limits_a^t f_1(s)\,\mathrm{d}s \cdots f_{r-1}(s)\,\mathrm{d}s \right) f_r(t)\,\mathrm{d}t = \int\limits_{a \le t_1 \le \cdots \le t_r \le b} f_1(t_1) \cdots f_r(t_r)\,\mathrm{d}t_1 \cdots \mathrm{d}t_r = \\ = \int\limits_a^b \mathrm{d}t_r f_r(t_r) \int\limits_a^{t_r} \mathrm{d}t_{r-1} f_{r-1}(t_{r-1}) \cdots \int\limits_a^{t_2} \mathrm{d}t_1 f_1(t_1). \tag{1.4}$$

To do this, simply resolve the recursion step by step, consider the resulting ordering relations of the integration variables and apply Fubini's theorem.

(ii) It is sometimes helpful (for example in Theorem 1.1.2 (iv)) to not just think of $\omega_1 \cdots \omega_r$ as a merely symbolic expression but rather as an element of the free algebra $K\langle X \rangle$ consisting of all (formal) linear combinations of words over some number field K generated by the letters $X = \{\omega_1, ..., \omega_r\}$ (cf. appendix B.2.12 (i)). Alternatively, one may view those expressions as elements of the tensor algebra over some vector space such as $T(\Omega^1(M))$ (described in the appendix in B.2.12 (ii)) as for example in [6]. In both cases, operations like the addition and scalar multiplication in equation 1.3 are well defined. We will use all three interpretations, depending on which one seems most appropriate at the time.

(iii) Another quite elegant way of thinking about iterated integrals is the following ([7], p.5). Given a curve $\gamma : [a, b] \to M$ let

$$\gamma_{\times r} : [a, b]^r \to M^{\times r},\ (t_1, ..., t_r) \mapsto (\gamma(t_1), ..., \gamma(t_r)) \tag{1.5}$$

be the r-fold product map. Then we can write

$$\int\limits_\gamma \omega_1 \cdots \omega_r = \int\limits_{\Delta_r(a,b)} \gamma^*_{\times r} \left(\pi^*_1(\omega_1) \wedge \cdots \wedge \pi^*_r(\omega_r)\right), \tag{1.6}$$

where $\pi_i : M^{\times r} \to M,\ (p_1, ..., p_i, ..., p_r) \mapsto p_i$ denote the canonical projection maps and

$$\Delta_r(a, b) := \{(t_1, ..., t_r) \in \mathbb{R}^r \mid a \le t_1 \le \cdots \le t_r \le b\} \tag{1.7}$$

is a bounded simplex between $a < b$. The right hand side is just an ordinary integral over a real domain. This equation 1.6 can be proven as follows. Let

$$\omega_i = \sum_{j=1}^n f^{(i)}_j\,\mathrm{d}x^j, \quad i \in \{1, ..., r\} \tag{1.8}$$

with functions $f_j^{(i)} : U \to \mathbb{K}^n$ on a coordinate domain $U \subseteq M$. The local coordinates on U are given by functions $x^j : U \to \mathbb{K}$ which constitute a coordinate map $\varphi = (x^1, ..., x^n) : U \to \mathbb{K}^n$. As mentioned in the appendix (cf. paragraph above equation A.7), the product manifold $M^{\times r}$ possesses a differentiable structure which includes the chart $(U^{\times r}, \varphi^{\times r})$ we are going to work with. The map $\varphi^{\times r}$ is defined by

$$\begin{aligned}
&\varphi^{\times r} : U^{\times r} \to \mathbb{K}^{n \cdot r}, \\
&(p_1, ..., p_r) \mapsto (\varphi(p_1), ..., \varphi(p_r)) = \Big(x^1_{(1)}(p_1), ..., x^n_{(1)}(p_1), ..., x^1_{(r)}(p_r), ..., x^n_{(r)}(p_r) \Big) =: \\
&\qquad =: \Big(\hat{x}^1_{(1)}(p_1, ..., p_r), ..., \hat{x}^n_{(1)}(p_1, ..., p_r), ..., \hat{x}^1_{(r)}(p_1, ..., p_r), ..., \hat{x}^n_{(r)}(p_1, ..., p_r) \Big).
\end{aligned} \tag{1.9}$$

with the local coordinates on the product manifold $\hat{x}^j_{(q)} : U^{\times r} \to \mathbb{K}$ given by

$$\hat{x}^j_{(q)}(p_1, ..., p_q, ..., p_r) := (x^j \circ \pi_q)(p_1, ..., p_q, ..., p_r) = x^j_{(q)}(p_q). \tag{1.10}$$

The subscripts in brackets have been added to simplify further discussion; but it should be kept in mind that $x^j_{(q)} = x^j_{(p)}$ as maps on U for $q, p \in \{1, ..., r\}$. First, notice that

$$\pi_i^*(\omega_i) = \pi_i^* \left(\sum_{j=1}^n f_j^{(i)} \, \mathrm{d}x^j \right) = \sum_{j=1}^n \left(f_j^{(i)} \circ \pi_i \right) \mathrm{d} \left(x^j \circ \pi_i \right) = \sum_{j=1}^n \left(f_j^{(i)} \circ \pi_i \right) \mathrm{d}\hat{x}^j_{(i)}. \tag{1.11}$$

Thus it follows

$$\begin{aligned}
&\gamma^*_{\times r} \left(\pi_1^*(\omega_1) \wedge \cdots \wedge \pi_r^*(\omega_r) \right) = \\
&\quad = \gamma^*_{\times r} \left(\sum_{j_1=1}^n \left(f^{(1)}_{j_1} \circ \pi_1 \right) \mathrm{d}\hat{x}^{j_1}_{(1)} \right) \wedge \cdots \wedge \gamma^*_{\times r} \left(\sum_{j_r=1}^n \left(f^{(r)}_{j_r} \circ \pi_r \right) \mathrm{d}\hat{x}^{j_r}_{(r)} \right) = \\
&\quad = \bigwedge_{q=1}^r \sum_{j_q=1}^n \left(f^{(q)}_{j_q} \circ \pi_q \circ \gamma_{\times r} \right) \mathrm{d} \left(\hat{x}^{j_q}_{(q)} \circ \gamma_{\times r} \right) = \\
&\quad = \bigwedge_{q=1}^r \sum_{j_q=1}^n \left(f^{(q)}_{j_q} \circ \gamma \right) \mathrm{d} \left(\hat{x}^{j_q}_{(q)} \circ \gamma_{\times r} \right) = \\
&\quad = \bigwedge_{q=1}^r \sum_{j_q=1}^n \left(f^{(q)}_{j_q} \circ \gamma \right) \sum_{p=1}^r \frac{\partial(\hat{x}^{j_q}_{(q)} \circ \gamma_{\times r})}{\partial t_p} \, \mathrm{d}t_p = \\
&\quad = \bigwedge_{q=1}^r \sum_{j_q=1}^n \left(f^{(q)}_{j_q} \circ \gamma \right) \sum_{p=1}^r \frac{\partial(x^{j_q}_{(q)} \circ \gamma)}{\partial t_p} \delta_{qp} \, \mathrm{d}t_p = \\
&\quad = \bigwedge_{q=1}^r \sum_{j_q=1}^n \left(f^{(q)}_{j_q} \circ \gamma \right) \frac{\partial(x^{j_q}_{(q)} \circ \gamma)}{\partial t_q} \, \mathrm{d}t_q \equiv \bigwedge_{q=1}^r \sum_{j_q=1}^n \left(f^{(q)}_{j_q} \circ \gamma \right) \frac{\partial(x^{j_q} \circ \gamma)}{\partial t_q} \, \mathrm{d}t_q.
\end{aligned} \tag{1.12}$$

In the last expression we can immediately identify

$$f_q : [a,b] \to \mathbb{K},\ t \mapsto \sum_{j=1}^{n} \left(f_j^{(q)} \circ \gamma \right) \frac{\partial (x^j \circ \gamma)}{\partial t}(t) \tag{1.13}$$

such that $(\gamma^* \omega_q)_t = f_q(t)\,\mathrm{d}t$ as in 1.1.1. This means, we have shown:

$$\begin{aligned}\int\limits_{\Delta_r(a,b)} \gamma_{\times r}^* \left(\pi_1^*(\omega_1) \wedge \cdots \wedge \pi_r^*(\omega_r)\right) = \int\limits_{\Delta_r(a,b)} (f_1(t_1)\,\mathrm{d}t_1) \wedge \cdots \wedge (f_r(t_r)\,\mathrm{d}t_r) = \\ = \int\limits_{a \le t_1 \le \cdots \le t_r \le b} f_1(t_1) \cdots f_r(t_r)\,\mathrm{d}t_1 \cdots \mathrm{d}t_r,\end{aligned} \tag{1.14}$$

where the last equality comes from the definition of the integral of differential forms. Hence, the assertion follows.

(iv) It is interesting to note that the definition of iterated integrals can be significantly generalised, as was done by Kuo-Tsai Chen in the 1970s (cf. for example [8] for an explicit construction or [4] for a more abstract description). Indeed, iterated integrals as defined above are often called Chen's iterated integrals. The generalisation consists, first, in weakening the conditions for the underlying space - instead of a differentiable manifold, Chen considers only a construction which he calls differentiable space and which includes smooth manifolds as a special case. Secondly, the differential forms need by no means to be only 1-forms. And third, the generalised integral takes on a variational aspect by considering not just one curve γ but a certain parameterized set of curves.

We will now discuss some properties of iterated integrals.

Theorem 1.1.2. *Properties of iterated integrals ([7], pp.4f. and [9], pp.361ff. and [10] pp.215f.).*

(i) The value of an iterated integral over a curve $\gamma : [a,b] \to M$ does not depend on the parametrization of γ as long as the orientation of the curve is the same. Hence, we will mainly consider $[a,b] = [0,1]$ thereafter.

(ii) If $\gamma^- : [0,1] \to M, t \mapsto \gamma(1-t)$ denotes the reversal of the curve γ, then

$$\int\limits_{\gamma^-} \omega_1 \cdots \omega_r = (-1)^r \int\limits_{\gamma} \omega_r \cdots \omega_1. \tag{1.15}$$

(iii) Let $\gamma_1, \gamma_2 : [0,1] \to M$ be two piecewise differentiable curves in M such that $\gamma_1(1) = \gamma_2(0)$. Then the composed path $\gamma_1\gamma_2$ defined in the obvious way is piecewise differentiable and one has

$$\int\limits_{\gamma_1\gamma_2} \omega_1 \cdots \omega_r = \sum_{i=0}^{r} \int\limits_{\gamma_1} \omega_1 \cdots \omega_i \int\limits_{\gamma_2} \omega_{i+1} \cdots \omega_r. \tag{1.16}$$

As a reminder, $\int_\gamma \omega_1 \cdots \omega_r := 1$ for $r = 0$.

(iv) Define the set of (l, r)-shuffles by

$$\Sigma(l,r) := \{\sigma \in S_{l+r} \mid \sigma^{-1}(1) < \cdots < \sigma^{-1}(l) \wedge \sigma^{-1}(l+1) < \cdots < \sigma^{-1}(l+r)\}. \tag{1.17}$$

Here, S_n denotes the symmetric group of order n and it is taken to act on $\{1, ..., n\}$. Then, the shuffle product formula holds:

$$\int_\gamma \omega_1 \cdots \omega_l \int_\gamma \omega_{l+1} \cdots \omega_{l+r} = \sum_{\sigma \in \Sigma(l,r)} \int_\gamma \omega_{\sigma(1)} \cdots \omega_{\sigma(l+r)}. \tag{1.18}$$

Proof. To get familiar with iterated integrals, the proof of this theorem will be in a rather detailed manner. The proof ideas were inspired by the exercise sheets in [11] unless stated otherwise.

(i) We prove this statement by induction. Let $\phi : [0,1] \to [a,b]$ a C^1-diffeomorphism with $\phi' > 0$. The properties of the pullback immediately imply

$$((\gamma \circ \phi)^* \omega_i)_u = \phi^*(\gamma^* \omega_i)_u = \phi^*(f_i(u)\,\mathrm{d}u) = (f_i \circ \phi)(u)\mathrm{d}\phi_u = f_i(\phi(u))\phi'(u)\,\mathrm{d}u. \tag{1.19}$$

Since line integrals are independent of the parametrization so are iterated integrals of weight one. Now suppose the statement is true for an iterated integral of weight $r-1$, i.e. for $t \in [a,b]$:

$$\int_a^t f_1(s)\,\mathrm{d}s \cdots f_{r-1}(s)\,\mathrm{d}s = \int_{\phi^{-1}(a)}^{\phi^{-1}(t)} f_1(\phi(u))\phi'(u)\,\mathrm{d}u \cdots f_{r-1}(\phi(u))\phi'(u)\,\mathrm{d}u. \tag{1.20}$$

Then (via the usual substitution rule):

$$\begin{aligned}
\int_\gamma \omega_1 \cdots \omega_r &= \int_a^b f_1(t)\,\mathrm{d}t \cdots f_r(t)\,\mathrm{d}t = \int_a^b \left(\int_a^t f_1(s)\,\mathrm{d}s \cdots f_{r-1}(s)\,\mathrm{d}s \right) f_r(t)\,\mathrm{d}t = \\
&= \int_{\phi^{-1}(a)}^{\phi^{-1}(b)} \left(\int_a^{\phi(u)} f_1(s)\,\mathrm{d}s \cdots f_{r-1}(s)\,\mathrm{d}s \right) f_r(\phi(u))\phi'(u)\,\mathrm{d}u = \\
&= \int_0^1 \left(\int_0^u f_1(\phi(\bar{u}))\phi'(\bar{u})\,\mathrm{d}\bar{u} \cdots f_{r-1}(\phi(\bar{u}))\phi'(\bar{u})\,\mathrm{d}\bar{u} \right) f_r(\phi(u))\phi'(u)\,\mathrm{d}u = \\
&= \int_{\gamma\circ\phi} \omega_1 \cdots \omega_r.
\end{aligned} \tag{1.21}$$

(ii) First, note that $\gamma^- = \gamma \circ \phi$ where $\phi : [0,1] \to [0,1]$, $t \mapsto 1-t$. The pullback of the differential forms along γ^- hence evaluates to $((\gamma^-)^*\omega_i)_u = -f_i(1-u)\,\mathrm{d}u$. Hence:

$$\int_{\gamma^-} \omega_1 \cdots \omega_r = \int_0^1 \mathrm{d}s_r(-f_r(1-s_r)) \int_0^{s_r} \mathrm{d}s_{r-1}(-f_{r-1}(1-s_{r-1})) \cdots \int_0^{s_2} \mathrm{d}s_1(-f_1(1-s_1)) =$$

$$
\begin{aligned}
&= (-1)^r \int_0^1 \mathrm{d}s_r f_r(1-s_r) \int_0^{s_r} \mathrm{d}s_{r-1} f_{r-1}(1-s_{r-1}) \cdots \underbrace{\int_{1-s_2}^1 \mathrm{d}t_1 f_1(t_1)}_{=:\, F_1(1-s_2)} = \\
&= (-1)^r \int_0^1 \mathrm{d}s_r f_r(1-s_r) \int_0^{s_r} \mathrm{d}s_{r-1} f_{r-1}(1-s_{r-1}) \cdots \int_0^{s_3} \mathrm{d}s_2 f_2(1-s_2) F_1(1-s_2) = \\
&= (-1)^r \int_0^1 \mathrm{d}s_r f_r(1-s_r) \int_0^{s_r} \mathrm{d}s_{r-1} f_{r-1}(1-s_{r-1}) \cdots \underbrace{\int_{1-s_3}^1 \mathrm{d}t_2 f_2(t_2) F_1(t_2)}_{=:\, F_{1,2}(1-s_3)} = \\
&= \cdots = (-1)^r \int_0^1 \mathrm{d}t_r f_r(t_r) F_{1,\ldots,r-1}(t_r) = \qquad (1.22) \\
&= (-1)^r \int_0^1 \mathrm{d}t_r f_r(t_r) \int_{t_r}^1 \mathrm{d}t_{r-1} f_{r-1}(t_{r-1}) \cdots \int_{t_3}^1 \mathrm{d}t_2 f_2(t_2) \int_{t_2}^1 \mathrm{d}t_1 f_1(t_1) = \\
&\overset{\text{Fubini}}{=} (-1)^r \int_{0 \le t_r \le \cdots \le t_1 \le 1} f_r(t_r) \cdots f_1(t_1)\, \mathrm{d}t_r \cdots \mathrm{d}t_1 = \\
&\overset{\text{Fubini}}{=} (-1)^r \int_0^1 \mathrm{d}t_1 f_1(t_1) \int_0^{t_1} \mathrm{d}t_2 f_2(t_2) \cdots \int_0^{t_{r-1}} \mathrm{d}t_r f_r(t_r) = \\
&= (-1)^r \int_\gamma \omega_r \cdots \omega_1.
\end{aligned}
$$

(iii) Define

$$
\delta : [0,1] \to M, \quad t \mapsto \begin{cases} \gamma_1(2t) & \text{if} \quad 0 \le t \le 1/2 \\ \gamma_2(2t-1) & \text{if} \quad 1/2 < t \le 1 \end{cases} \qquad (1.23)
$$

as a parametrization for the composed path $\gamma_1\gamma_2$. If $(\gamma_1^*\omega_i)_t = f_i^{(1)}(t)\,\mathrm{d}t$ and $(\gamma_2^*\omega_i)_t = f_i^{(2)}(t)\,\mathrm{d}t$, then the pullback along δ can be easily evaluated:

$$
\begin{aligned}
\forall t \in \left[0, \frac{1}{2}\right] : &\quad (\delta^*\omega_i)_t = f_i^{(1)}(2t) \cdot 2\,\mathrm{d}t, \\
\forall t \in \left(\frac{1}{2}, 1\right] : &\quad (\delta^*\omega_i)_t = f_i^{(2)}(2t-1) \cdot 2\,\mathrm{d}t. \qquad (1.24)
\end{aligned}
$$

In summary [2]:

$$(\delta^*\omega_i)_t = 2\left[f_i^{(1)}(2t)1_{[0,1/2]}(t) + f_i^{(2)}(2t-1)1_{(1/2,1]}(t)\right]\mathrm{d}t. \tag{1.26}$$

The main idea is that on the simplex $\Delta^{(r)} = \{(t_1,...,t_r) \in \mathbb{R}^r \mid 0 \le t_1 \le \cdots \le t_r \le 1\}$ only the following products of indicator functions are non-zero:

$$\begin{aligned}
&1_{[0,1/2]}(t_1)1_{[0,1/2]}(t_2)\cdots 1_{[0,1/2]}(t_{r-1})1_{[0,1/2]}(t_r),\\
&1_{[0,1/2]}(t_1)1_{[0,1/2]}(t_2)\cdots 1_{[0,1/2]}(t_{r-1})1_{(1/2,1]}(t_r),\\
&1_{[0,1/2]}(t_1)1_{[0,1/2]}(t_2)\cdots 1_{(1/2,1]}(t_{r-1})1_{(1/2,1]}(t_r),\\
&\qquad\vdots\\
&1_{[0,1/2]}(t_1)1_{(1/2,1]}(t_2)\cdots 1_{(1/2,1]}(t_{r-1})1_{(1/2,1]}(t_r),\\
&1_{(1/2,1]}(t_1)1_{(1/2,1]}(t_2)\cdots 1_{(1/2,1]}(t_{r-1})1_{(1/2,1]}(t_r).
\end{aligned} \tag{1.27}$$

Hence:

$$\begin{aligned}
\int_\delta \omega_1\cdots\omega_r &= 2^r \int_{\Delta^{(r)}} \prod_{i=1}^r \left[f_i^{(1)}(2t_i)1_{[0,1/2]}(t_i) + f_i^{(2)}(2t_i-1)1_{(1/2,1]}(t_i)\right]\mathrm{d}t_r\cdots dt_1 =\\
&= 2^r \int_{\Delta^{(r)}} \sum_{k=0}^r f_1^{(1)}(2t_1)\cdots f_k^{(1)}(2t_k) f_{k+1}^{(2)}(2t_{k+1}-1)\cdots f_r^{(2)}(2t_r-1)\times\\
&\qquad \times 1_{[0,1/2]}(t_1)\cdots 1_{[0,1/2]}(t_k)1_{(1/2,1]}(t_{k+1})\cdots 1_{(1/2,1]}(t_r)\,\mathrm{d}t_r\cdots\mathrm{d}t_1 =\\
&= 2^r \sum_{k=0}^r \int_{1/2}^{1} \mathrm{d}t_r f_r^{(2)}(2t_r-1)\cdots \int_{1/2}^{t_{k+2}} \mathrm{d}t_{k+1} f_{k+1}^{(2)}(2t_{k+1}-1)\times\\
&\qquad \times \int_0^{1/2} \mathrm{d}t_k f_k^{(1)}(2t_k)\cdots \int_0^{t_2} \mathrm{d}t_1 f_1^{(1)}(2t_1).
\end{aligned} \tag{1.28}$$

By substituting $s_i := 2t_i - 1$ for $i > k$ and $s_i := 2t_i$ for $i \le k$ we get:

$$\begin{aligned}
\int_\delta \omega_1\cdots\omega_r &= 2^r\cdot 2^{-r} \sum_{k=0}^r \int_0^1 \mathrm{d}s_r f_r^{(2)}(s_r)\cdots \int_0^{s_{r+2}} \mathrm{d}s_{r+1} f_{r+1}^{(2)}(s_{r+1})\times\\
&\qquad \times \int_0^1 \mathrm{d}s_k f_k^{(1)}(s_k)\cdots \int_0^{s_2} \mathrm{d}s_1 f_1^{(1)}(s_1) =\\
&= \sum_{k=0}^r \int_{\gamma_2} \omega_{k+1}\cdots\omega_r \int_{\gamma_1} \omega_1\cdots\omega_k.
\end{aligned} \tag{1.29}$$

[2] Recall, that for any subset A of some space Ω the indicator functions are defined by

$$1_A : \Omega \to \{0,1\},\ x \mapsto \begin{cases} 1 & \text{if} \quad x \in A,\\ 0 & \text{if} \quad x \notin A. \end{cases} \tag{1.25}$$

(iv) First, note that we can define the shuffle product of two words $\omega_1 \cdots \omega_l$ and $\omega_{l+1} \cdots \omega_{l+r}$ recursively by ([12], p.1)

$$\begin{aligned}(\omega_1 \cdots \omega_l) \sqcup\!\sqcup (\omega_{l+1} \cdots \omega_{l+r}) &:= [(\omega_1 \cdots \omega_{l-1}) \sqcup\!\sqcup (\omega_{l+1} \cdots \omega_{l+r})]\, \omega_l + \\ &\quad + [(\omega_1 \cdots \omega_l) \sqcup\!\sqcup (\omega_{l+1} \cdots \omega_{l+r-1})]\, \omega_{l+r}, \\ \emptyset \sqcup\!\sqcup (\omega_{l+1} \cdots \omega_{l+r}) &:= \omega_{l+1} \cdots \omega_{l+r} \quad \text{and} \quad (\omega_1 \cdots \omega_l) \sqcup\!\sqcup \emptyset := \omega_1 \cdots \omega_l.\end{aligned} \tag{1.30}$$

This shows the identity

$$\int_\gamma (\omega_1 \cdots \omega_l) \sqcup\!\sqcup (\omega_{l+1} \cdots \omega_{l+r}) = \sum_{\sigma \in \Sigma(l,r)} \int_\gamma \omega_{\sigma(1)} \cdots \omega_{\sigma(l+r)}, \tag{1.31}$$

which we will use to construct an inductive proof of (iv) reminiscent of the original proof of Ree in [10], pp.215f. The notation $\gamma|_t$ for the restriction of $\gamma : [0,1] \to M$ to the interval $[0,t]$ will be helpful.

- Base case $l = r = 1$ ($l = 1, r = 0$ and $l = 0, r = 1$ are trivial). Let $x \in [0,1]$ be arbitrary. We make use of the decomposition of the square into two disjoint triangles

$$[0,x]^2 = \{(t_1,t_2) \in [0,x] \mid t_1 \leq t_2\} \cup \{(t_1,t_2) \in [0,x] \mid t_1 > t_2\} \tag{1.32}$$

  and write:

$$\begin{aligned}\int_{\gamma|_x} \omega_1 \int_{\gamma|_x} \omega_2 &= \int_0^x \int_0^x f_1(t_1) f_2(t_2)\, \mathrm{d}t_1\, \mathrm{d}t_2 = \\ &= \int_0^x \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 f_1(t_1) f_2(t_2) + \int_0^x \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_1 f_1(t_1) f_2(t_2) = \\ &= \int_{\gamma|_x} \omega_2\omega_1 + \int_{\gamma|_x} \omega_1\omega_2 = \int_{\gamma|_x} \omega_1 \sqcup\!\sqcup \omega_2.\end{aligned} \tag{1.33}$$

- Induction hypothesis. Suppose that $r \geq 1$ and $l \geq 1$ (the cases $r = 0$ or $l = 0$ are trivial) and that

$$\int_{\gamma|_{t_l}} \omega_1 \cdots \omega_{l-1} \int_{\gamma|_{t_l}} \omega_{l+1} \cdots \omega_{l+r} = \int_{\gamma|_{t_l}} \omega_1 \cdots \omega_{l-1} \sqcup\!\sqcup \omega_{l+1} \cdots \omega_{l+r} \quad \text{and} \tag{1.34}$$

$$\int_{\gamma|_{t_l}} \omega_1 \cdots \omega_l \int_{\gamma|_{t_l}} \omega_{l+1} \cdots \omega_{l+r-1} = \int_{\gamma|_{t_l}} \omega_1 \cdots \omega_l \sqcup\!\sqcup \omega_{l+1} \cdots \omega_{l+r-1} \tag{1.35}$$

  have already been proven.

– Induction step. Calculate:

$$\int_\gamma \omega_1 \cdots \omega_l \int_\gamma \omega_{l+1} \cdots \omega_{l+r} = \left(\int_0^1 \mathrm{d}t_l f_l(t_l) \underbrace{\int_{\gamma|_{t_l}} \omega_1 \cdots \omega_{l-1}}_{=:I_{1,\dots,l-1}(t_l)} \right) \times$$

$$\times \left(\int_0^1 \mathrm{d}t_{l+r} f_{l+r}(t_{l+r}) \underbrace{\int_{\gamma|_{t_{l+r}}} \omega_{l+1} \cdots \omega_{l+r-1}}_{=:I_{l+1,\dots,l+r-1}(t_{l+r})} \right) =$$

$$= \int_0^1 \mathrm{d}t_l \int_0^{t_l} \mathrm{d}t_{l+r} f_l(t_l) I_{1,\dots,l-1}(t_l) f_{l+r}(t_{l+r}) I_{l+1,\dots,l+r-1}(t_{l+r}) +$$

$$+ \int_0^1 \mathrm{d}t_{l+r} \int_0^{t_{l+r}} \mathrm{d}t_l f_l(t_l) I_{1,\dots,l-1}(t_l) f_{l+r}(t_{l+r}) I_{l+1,\dots,l+r-1}(t_{l+r}) =$$

$$= \int_0^1 \mathrm{d}t_l f_l(t_l) I_{1,\dots,l-1}(t_l) I_{l+1,\dots,l+r}(t_l) +$$

$$+ \int_0^1 \mathrm{d}t_{l+r} f_{l+r}(t_{l+r}) I_{1,\dots,l}(t_{l+r}) I_{l+1,\dots,l+r-1}(t_{l+r}) =$$

$$= \int_0^1 \mathrm{d}t_l f_l(t_l) \int_{\gamma|_{t_l}} \omega_1 \cdots \omega_{l-1} \sqcup\!\sqcup\, \omega_{l+1} \cdots \omega_{l+r} +$$

$$+ \int_0^1 \mathrm{d}t_{l+r} f_{l+r}(t_{l+r}) \int_{\gamma|_{t_{l+r}}} \omega_1 \cdots \omega_l \sqcup\!\sqcup\, \omega_{l+1} \cdots \omega_{l+r-1} =$$

$$= \int_\gamma \left([\omega_1 \cdots \omega_{l-1} \sqcup\!\sqcup\, \omega_{l+1} \cdots \omega_{l+r}]\, \omega_l + [\omega_1 \cdots \omega_l \sqcup\!\sqcup\, \omega_{l+1} \cdots \omega_{l+r-1}]\, \omega_{l+r} \right) =$$

$$= \int_\gamma \omega_1 \cdots \omega_l \sqcup\!\sqcup\, \omega_{l+1} \cdots \omega_{l+r}. \tag{1.36}$$

This concludes the proof.

□

Remark. Using the representation of Chen iterated integrals as an ordinary integral over a simplex (cf. equation 1.6)

$$\int_\gamma \omega_1 \cdots \omega_r = \int_{\Delta_r(0,1)} \gamma^*_{\times r}(\pi_1^*(\omega_1) \wedge \cdots \wedge \pi_r^*(\omega_r)), \tag{1.37}$$

one can give another, more concise proof of (iii) and (iv) which relies on dissections of simplices and Fubini's theorem ([7], p.5 and [13], p.174). In particular, (iii) follows from

$$\begin{aligned} \Delta_r(0,1) = \bigcup_{i=0}^{r} \left\{ (t_1, ..., t_r) \in \mathbb{R}^r \mid 0 \le t_1 \le \cdots \le t_i \le \frac{1}{2} \le t_{i+1} \le \cdots \le t_r \le 1 \right\} \cong \\ \cong \bigcup_{i=0}^{r} \Delta_i \left(0, \frac{1}{2}\right) \times \Delta_{r-i} \left(\frac{1}{2}, 1\right). \end{aligned} \tag{1.38}$$

and (iv) can be read off from

$$\Delta_l(0,1) \times \Delta_r(0,1) = \bigcup_{\sigma \in \Sigma(l,r)} \left\{ (t_1, ..., t_{l+r}) \in \mathbb{R}^{l+r} \mid 0 \le t_{\sigma^{-1}(1)} \le \cdots \le t_{\sigma^{-1}(l+r)} \le 1 \right\}. \tag{1.39}$$

1.1.2 Homotopy Functionals

Definition 1.1.3. Homotopy functionals ([7], p.6) Let M be a smooth manifold over the field $\mathbb{K}$ and $\gamma_1, \gamma_2 : [0,1] \to M$ be continuous curves that share the same start- and endpoints $p, q \in M$. We say that γ_1 and γ_2 are homotopic relative to p, q and write $\gamma_1 \sim_h \gamma_2$ if there is a continuous map $\phi : [0,1] \times [0,1] \to M$ with the properties

$$\forall t \in [0,1] : \begin{cases} \phi(0,t) = \gamma_1(t), \\ \phi(1,t) = \gamma_2(t) \end{cases} \quad \text{and} \quad \forall s \in [0,1] : \begin{cases} \phi(s,0) = p, \\ \phi(s,1) = q. \end{cases} \tag{1.40}$$

One can show that every continuous path is homotopic to a piecewise smooth path. Define PM to be the set of all piecewise smooth paths and let $F : PM \to \mathbb{K}$. F is a homotopy functional if the following implication holds:

$$\gamma_1 \sim_h \gamma_2 \implies F(\gamma_1) = F(\gamma_2). \tag{1.41}$$

In this subsection we will answer the question under which circumstances the iterated integral gives rise to a homotopy functional. This is important in that it allows the mapping

$$\tilde{F} : M \to \mathbb{K},\ \tilde{F}(q) := F(\gamma) \quad \text{where } p \in M \text{ is fixed and } \gamma \in PM \text{ with } \gamma(0) = p, \gamma(1) = q \tag{1.42}$$

to be thought of as a well-defined multivalued function on a connected and locally simply connected manifold M ([7], pp.6f.).

The answer to this problem is given by the so-called reduced bar construction.

Definition 1.1.4. Reduced Bar Construction ([14], p.468 and [15], p.5 and [7], p.22 and [13], pp.237ff.). Let $(A^*, \wedge, \mathrm{d})$ be a connected differential graded algebra (definition in appendix B.4.6) over a field K. Using the notation

$$A^+ := \bigoplus_{p>0} A^p \tag{1.43}$$

the reduced bar construction $B^*(A)$ associated with the differential graded algebra is defined as the tensor algebra

$$B^*(A) = \bigoplus_{k\geq 0} (A^+)^{\otimes k}, \tag{1.44}$$

where $(A^+)^{\otimes 0} := K$. It is equipped with some further structure that makes it a differential graded Hopf algebra (notice that the Hopf-algebra structure is basically identical to the one discussed in B.3.9):

(i) Grading: Let $x_i \in A^+,\ i \in \{1, ..., r\}$, be homogeneous (i.e. there is a $p_i \in \mathbb{N}$ such that $x_i \in A^{p_i}$). Then $[x_1|...|x_r] \in B^*(A)$ is homogeneous (the bar notation is customary and replaces the tensor product symbol to distinguish it from external tensor products appearing in elements of, e.g., $B^*(A) \otimes B^*(A)$) and its degree is defined as

$$\deg_B([x_1|...|x_r]) := \sum_{i=1}^{r} \deg_A(x_i) - r. \tag{1.45}$$

Caution: if $x \in A^p$, then $\deg_A(x_i) = p$ but $\deg_B([x_i]) = p - 1$.

(ii) Differential: The differential $\mathrm{d}_B : B^*(A) \to B^*(A)$ is defined as

$$\begin{aligned}\mathrm{d}_B[x_1|...|x_r] :=& \sum_{i=1}^{r} (-1)^i [Jx_1|...|Jx_{i-1}|\mathrm{d}x_i|x_{i+1}|...|x_r] + \\ &+ \sum_{i=1}^{r-1} (-1)^{i+1} [Jx_1|...|Jx_{i-1}|(Jx_i) \wedge x_{i+1}|x_{i+2}|...|x_r],\end{aligned} \tag{1.46}$$

where $J : A^* \to A^*,\ x \mapsto (-1)^{\deg_A(x)} x$.

(iii) Product: The product $\mu : B^*(A) \otimes B^*(A) \to B^*(A)$ is given by the shuffle product as follows:

$$\mu([x_1|...|x_l] \otimes [x_{l+1}|...|x_{l+r}]) := \sum_{\sigma \in \Sigma(l,r)} \eta(\sigma) [x_{\sigma^{-1}(1)}|...|x_{\sigma^{-1}(l+r)}], \tag{1.47}$$

where the sign $\eta(\sigma) \in \{-1, 1\}$ is determined by

$$x_1 \wedge \cdots \wedge x_{l+r} = \eta(\sigma) x_{\sigma^{-1}(1)} \wedge \cdots \wedge x_{\sigma^{-1}(l+r)}. \tag{1.48}$$

(iv) Coproduct: $\Delta : B^*(A) \to B^*(A) \otimes B^*(A)$ is given by the deconcatenation operation

$$\Delta[x_1|...|x_r] := \sum_{i=0}^{r} [x_1|...|x_i] \otimes [x_{i+1}|...|x_r]. \tag{1.49}$$

(v) Antipode: It is given by the map

$$S : B^*(A) \to B^*(A), \quad [x_1|...|x_r] \mapsto (-1)^r \eta(\tau_r)[x_r|...|x_1], \tag{1.50}$$

where the permutation τ_r is defined by $\tau_r(i) := r - i$.

We will now specialize to the case relevant for iterated integrals. Here, we would like to use the de Rham differential graded algebra $(\Omega^*(M), \wedge, \mathrm{d})$ (defined in appendix B.4.7) as the fundamental objects of interest are differential forms. However, this differential graded algebra is not connected which presents a technical difficulty. The reduced bar construction can be adapted to tackle this difficulty (cf. [16]), but this complication is often circumvented as follows ([7], p.22 and [13], p.243 and [15], p.5): Let $A^* \subset \Omega^*(M)$ be a differential graded algebra and $\phi : A^* \to \Omega^*(M)$ the corresponding inclusion map such that

(i) A^* is connected (i.e. $A^0 = K$ and $A^p = 0$ for $p < 0$).

(ii) ϕ is an quasi-isomorphism (i.e. the induced map in cohomology $H(\varphi) : H^*(A^*) \to H^*(\Omega^*(M))$ is an isomorphism).

A^* is called a connected model for $\Omega^*(M)$. Furthermore, we are in this thesis only concerned with iterated integrals over one-forms. Because A^* is connected, this translates to restricting ourselves to elements $[x_1|...|x_r] \in B^*(A^*)$ with $\deg_B([x_1|...|x_r]) = 0$. In other words, we only consider the component

$$B^0(A^*) := \{\xi \in B^*(A) \mid \deg_B(\xi) = 0\} = \bigoplus_{p\geq 0} (A^1)^{\otimes p}. \tag{1.51}$$

Consequently, the only de Rham cohomology group we are interested in, is

$$H^0(B(A^*)) = \mathrm{Ker}(\mathrm{d}_B : B^0(A^*) \to B^1(A^*)) = \left\{\xi \in B^0(A^*) \mid \mathrm{d}_B(\xi) = 0\right\}. \tag{1.52}$$

The elements of $H^0(B(A^*))$ are called integrable words ([17], p.186). Notice, that the restriction of d_B as defined in equation 1.46 to $B^0(A^*)$ is equal to

$$\begin{aligned} \mathrm{d}_B[x_1|...|x_r] = &-\sum_{i=1}^{r} [x_1|...|x_{i-1}|\mathrm{d}x_i|x_{i+1}|...|x_r] - \\ &-\sum_{i=1}^{r-1} [x_1|...|x_{i-1}|x_i \wedge x_{i+1}|x_{i+2}|...|x_r]. \end{aligned} \tag{1.53}$$

The following theorem is important and solves the question of homotopy invariance:

Theorem 1.1.5. *Condition for homotopy invariance of iterated integrals ([13], p.245 and [17], p.186). To every element $x \in B^0(A^*)$ which can be written as*

$$x = \sum_{j=1}^{r} \sum_{i_1,...,i_j} c_{i_1,...,i_j} [\omega_{i_1}|...|\omega_{i_j}] \quad (c_{i_1,...,i_j} \in K) \tag{1.54}$$

for some (arbitrary) $r \in \mathbb{N}_0$ we associate a functional on the space of piecewise smooth paths PM via

$$F : \gamma \mapsto \sum_{j=1}^{r} \sum_{i_1,\ldots,i_j} c_{i_1,\ldots,i_j} \int_\gamma \omega_{i_1} \cdots \omega_{i_j}. \tag{1.55}$$

If $\mathrm{d}_B x = 0$, then F is a homotopy functional and gives rise to a well-defined multivalued function on M.

1.1.3 Regularisation of Logarithmic Divergences

It is often the case that some of the functions f_i with $(\gamma^*\omega_i)_t = f_i(t)\,\mathrm{d}t$ have singularities on the boundary of their domain $I \subseteq \mathbb{R}$ and that the iterated integral as defined in 1.1.1 does not converge. We will now discuss a regularisation scheme for the special case of logarithmic divergences which is of relevance for the subsequent introduction of multiple polylogarithms.

Definition 1.1.6. Shuffle-regularisation or tangential basepoint regularisation ([18], p.38 and [19], pp.14ff.). Let M be a one-dimensional smooth complex manifold and $p, x \in M$. Let $\gamma : [0, 1] \to M$ be a smooth path such that $\gamma(0) = p$ and $\gamma(1) = x$. Let $\omega_i, i \in \{1, ..., r\}$ be meromorphic one-forms on M with at most a logarithmic singularity at p; i.e. in local coordinates z centered at p

$$\omega_i = \underbrace{a_i \,\mathrm{d}\log(z)}_{=:\ \omega_i^\infty} + \hat{\omega}_i = a_i \frac{\mathrm{d}z}{z} + \hat{\omega}_i \quad (a_i \in \mathbb{C}) \tag{1.56}$$

where $\hat{\omega}_i$ is well-behaved at p. The regularisation scheme is as follows.

(i) Let $\epsilon > 0$ and define $\gamma_\epsilon := \gamma|_{[\epsilon,1]}$. We write

$$\int_{\gamma_\epsilon} \omega_1 \cdots \omega_r =: \int_\epsilon^x \omega_1 \cdots \omega_r. \tag{1.57}$$

By assumption, this integral converges.

(ii) One can show that

$$\int_\epsilon^x \omega_1 \cdots \omega_r = I_0(x) + \sum_{k=1}^{r} I_k(x) \log^k(\epsilon) + \mathcal{O}(\epsilon) \quad (\epsilon \to 0). \tag{1.58}$$

(iii) The regularized value of the iterated integral is defined as

$$\mathrm{Reg}_\epsilon \int_\gamma \omega_1 \cdots \omega_r := I_0(x). \tag{1.59}$$

Remark. This procedure yields in fact a sensible regularization as the following statements to be found in [18], pp.38f. and [7], pp.7f. show.

- Consistency: If the ω_i are such that the iterated integral along γ converges (i.e. $I_k(x) = 0$ for $k \geq 1$), we have

$$\int_\gamma \omega_1 \cdots \omega_r = \lim_{\epsilon \to 0} \int_{\gamma_\epsilon} \omega_1 \cdots \omega_r = I_0(x). \tag{1.60}$$

- Properties: Since $\int_{\gamma_\epsilon} \omega_1 \cdots \omega_r$ converges, all properties (i) - (iv) of the theorem 1.1.2 hold for this integral. Hence and by using the fact that the regularization procedure commutes with multiplication in the sense that

$$\mathrm{Reg}_\epsilon \left(\int_\gamma \omega_1 \cdots \omega_l \cdot \int_\gamma \omega_{l+1} \cdots \omega_{l+r} \right) = \mathrm{Reg}_\epsilon \int_\gamma \omega_1 \cdots \omega_l \cdot \mathrm{Reg}_\epsilon \int_\gamma \omega_{l+1} \cdots \omega_{l+r}, \tag{1.61}$$

the regularized iterated integral inherits those properties.

- Uniqueness: Consider a change of variables $\eta = \lambda_1 \epsilon + \lambda_2 \epsilon^2 + \cdots$ where $\lambda_1 \neq 0$. This yields in the limit $\epsilon \to 0 \iff \eta \to 0$

$$\int_\eta^x \omega_1 \cdots \omega_r = I_0(x) + \sum_{k=1}^r I_k(x) \log^k(\eta) + \mathcal{O}(\eta). \tag{1.62}$$

Now,

$$\begin{aligned} \log(\eta) &= \log(\lambda_1 \epsilon + \lambda_2 \epsilon^2 + \cdots) = \log((\lambda_1 \epsilon)(1 + \lambda_2 \lambda_1^{-1} \epsilon + \cdots)) = \\ &= \log(\lambda_1) + \log(\epsilon) + \log(1 + \lambda_2 \lambda_1^{-1} \epsilon + \cdots), \end{aligned} \tag{1.63}$$

where the last term is of order ϵ because

$$\log(1+x) = \sum_{k=1}^\infty (-1)^{k+1} \frac{x^k}{k} \quad (|x| < 1). \tag{1.64}$$

As $\epsilon \log^k(\epsilon) \to 0 \quad (\epsilon \to 0)$ for all $k \geq 0$, we finally conclude that the value of the regularized integral depends on λ_1 and that

$$\lambda_1 = \frac{\partial \eta}{\partial \epsilon} = 1 \implies \mathrm{Reg}_\epsilon \int_\gamma \omega_1 \cdots \omega_r = \mathrm{Reg}_\eta \int_\gamma \omega_1 \cdots \omega_r. \tag{1.65}$$

This result also explains the name tangential basepoint regularisation. Think of ϵ and η as local coordinates on the one-dimensional real manifold $I = [0, x]$. Let $\frac{\partial}{\partial \epsilon}|_0, \frac{\partial}{\partial \eta}|_0 \in T_0 I$ denote the tangent vectors to $0 \in I$ corresponding to the different coordinate systems on I. Since

$$\gamma'_\epsilon(0) = \mathrm{d}\gamma \left(\frac{\partial}{\partial \epsilon}|_0 \right) = \mathrm{d}\gamma \left(\frac{\partial \eta}{\partial \epsilon}|_0 \, \frac{\partial}{\partial \eta}|_0 \right) = \frac{\partial \eta}{\partial \epsilon}|_0 \, \mathrm{d}\gamma \left(\frac{\partial}{\partial \eta}|_0 \right) = \frac{\partial \eta}{\partial \epsilon}|_0 \, \gamma'_\eta(0), \tag{1.66}$$

we deduce that the value of the regularized iterated integral depends solely on the tangent vector to the curve γ at the point p. We will always choose ϵ to mean the standard coordinate on I (i.e. the identity map on $\mathbb{R}$ restricted to this interval) and define the regularization with respect to this standard coordinate. In general, a tangential basepoint at p is defined as a tangent vector v at p together with p itself. Furthermore, a curve starting from this tangential base point satisfies $\gamma(0) = p$ and $\gamma'(0) = v$.

- Last but not least, there is also an explicit formula for the regularized values: Let $\omega_i = a_i \,\mathrm{d}\log(z) + \hat{\omega}_i$ as before and define ω_i^∞ as the part with the logarithmic divergence. Then

$$\begin{aligned} \mathrm{Reg}_\epsilon \int\limits_\gamma \omega_1 \cdots \omega_r &= \sum_{k=0}^{r} \left(\mathrm{Reg}_\epsilon \int\limits_\gamma \omega_1^\infty \cdots \omega_k^\infty \right) \left(\int\limits_\gamma R(\omega_{k+1} \cdots \omega_r) \right) = \\ &= \sum_{k=0}^{r} \frac{a_1 \cdots a_k}{k!} \log^k(x) \int\limits_\gamma R(\omega_{k+1} \cdots \omega_r). \end{aligned} \tag{1.67}$$

The map R acts on the words $\omega_i \cdots \omega_n$ as follows:

$$R : \omega_1 \cdots \omega_n \mapsto R(\omega_1 \cdots \omega_n) := \sum_{k=0}^{n} (-1)^k (\omega_k^\infty \cdots \omega_1^\infty) \sqcup\!\sqcup (\omega_{k+1} \cdots \omega_n). \tag{1.68}$$

An example of this regularization technique will be discussed in the next section.

1.2 Definition and Properties of Multiple Polylogarithms

Definition 1.2.1. Multiple Polylogarithms (MPLs) ([17], pp.187,296 and [20], p.19 and [21], p.64). Let $\{\sigma_1, ..., \sigma_r\} =: \Sigma \subseteq \mathbb{C}$ and consider the manifold $M = \mathbb{C} \setminus \Sigma$ with standard coordinate z. Let $\gamma : [0,1] \to M$ be a piecewise smooth path connecting $\gamma(0) = 0$ and $\gamma(1) = x$ and define

$$\omega_i := \frac{\mathrm{d}z}{z - \sigma_i}, \quad i \in \{1, ..., r\} \tag{1.69}$$

as meromorphic differential forms on M.

(i) Case 1: $\Sigma \cap \{0\} = \emptyset$. One then defines:

$$G(\sigma_1, ..., \sigma_r; x) := \int\limits_\gamma \omega_{\sigma_r} \cdots \omega_{\sigma_1} \tag{1.70}$$

as the multiple polylogarithm with weight r and the so-called vector of singularities $\boldsymbol{\sigma} = (\sigma_1, ..., \sigma_r)$. Note the reversed order of the differential forms in the iterated integral. This amounts to the often cited recursive definition (as in [22] for example):

$$G(;x) \;:=\; 1, \tag{1.71}$$

$$G(\sigma_1, ..., \sigma_r; x) \;:=\; \int\limits_0^x \frac{\mathrm{d}z_1}{z_1 - \sigma_1} G(\sigma_2, ..., \sigma_r; z_1). \tag{1.72}$$

The notation $\int_0^x$ without any reference to the integration path γ will be addressed below. Another popular notation is:

$$G(\sigma_1, ..., \sigma_r; x) = \int_0^x \frac{\mathrm{d}z}{z - \sigma_1} \circ \cdots \circ \frac{\mathrm{d}z}{z - \sigma_r}. \tag{1.73}$$

(ii) Case 2: $\Sigma \cap \{0\} \neq \emptyset$. In this case, one has to resort to the regularization procedure discussed in the previous section above. For example,

$$G(\underbrace{0, ..., 0}_{n}; x) = \frac{1}{n!} \log^n(x) \tag{1.74}$$

as will be proven below.

Remark.

(i) Homotopy invariance ([21], pp.65f.). The integrability condition is trivially fulfilled since M is one-dimensional such that $\mathrm{d}\omega_i = 0$ and $\omega_i \wedge \omega_j = 0$ for all $i, j \in \{1, ..., r\}$. Hence, G gives rise to a multivalued function of x as the endpoint of γ which depends only on the homotopy class of γ. This (together with the standard choice of the path given in (ii)) justifies the notation $\int_0^x$ as used in equation 1.71.

(ii) Implementation. Clearly, a multivalued function is not ideal for an implementation in a computer program. In practice, one often chooses the following convention: Let $\gamma : [0, 1] \to \mathbb{C}$ be the straight line connecting 0 with x. If there is an $i \in \{1, ..., r\}$ such that $\sigma_i \in \gamma([0, 1])$ one adopts the convention to perturb x a little by multiplying it with a factor $1 - i\delta$ with $\delta > 0$ being sufficiently small ([23], p.19 and [3], p.6).

The following theorem collects some important properties of multiple polylogarithms.

Theorem 1.2.2. *Properties of Multiple Polylogarithms ([17], pp.286ff. and [22], pp.12ff. and [5], pp.8ff.).*

(i) Analytic properties: $z \mapsto G(\sigma_1, ..., \sigma_r; z)$ *is divergent whenever* $z = \sigma_1$*. Due to the singularities at* σ_i *(which are here taken to be fixed complex numbers),* $z \mapsto G(\sigma_1, ..., \sigma_r; z)$ *has at most branch cuts extending from* $z = \sigma_i$ *to* $z = \infty$ *for all* $i \in \{1, ..., r\}$*.*

(ii) Sum Representation: Let $m_1, ..., m_k \in \mathbb{N}$ *and define*

$$G_{m_1,...,m_k}(\sigma_1, ..., \sigma_k; z) := G(\underbrace{0, ..., 0}_{m_1 - 1}, \sigma_1, ..., \sigma_{k-1}, \underbrace{0, ..., 0}_{m_k - 1}, \sigma_k; z). \tag{1.75}$$

as well as

$$\mathrm{Li}_{m_1,...,m_k}(z_1, ..., z_k) := \sum_{n_1 > n_2 > ... > n_k > 0}^{\infty} \frac{z_1^{n_1} \cdots z_k^{n_k}}{n_1^{m_1} \cdots n_k^{m_k}}. \tag{1.76}$$

Caution: there exists a different summing convention $0 < n_1 < n_2 < \cdots < n_k$ *(e.g. in [1]). This series converges absolutely if* $|z_j| < 1$ *for all* $j \in \{1, ..., k\}$*. The integer*

k is called depth and $m_1 + \cdots + m_k$ is called weight. Whenever the series converges, we have

$$\mathrm{Li}_{m_1,...,m_k}(z_1, ..., z_k) = (-1)^k G_{m_1,...,m_k}\left(\frac{1}{z_1}, \frac{1}{z_1 z_2}, ..., \frac{1}{z_1 \cdots z_k}; 1\right), \tag{1.77}$$

$$G(\sigma_1, ..., \sigma_k; z) = (-1)^k \mathrm{Li}_{m_1,...,m_k}\left(\frac{y}{z_1}, \frac{z_1}{z_2}, ..., \frac{z_{k-1}}{z_k}\right). \tag{1.78}$$

(iii) *Total differential of G: For convenience, set $\sigma_0 = z$ and $\sigma_{r+1} = 0$. Then:*

$$\mathrm{d}G(\sigma_1, ..., \sigma_r; z) = \sum_{j=1}^{r} G(\sigma_1, ..., \hat{\sigma}_j, ..., \sigma_r; y)\left[\mathrm{d}\log(\sigma_{j-1} - \sigma_j) - \mathrm{d}\log(\sigma_{j+1} - \sigma_j)\right]. \tag{1.79}$$

In order to be consistent with the regularization procedure, we set $\mathrm{d}\log(z_{j+1} - z_j) = 0$ if $z_{j+1} - z_j = 0$.

(iv) *Functional relations. The MPLs display an extremely rich structure of functional relations among each other. For example,*

- *Scaling Relation: For $\sigma_r \neq 0$ and $\lambda \neq 0$ it holds:*

$$G(\sigma_1, ..., \sigma_r; z) = G(\lambda\sigma_1, ..., \lambda\sigma_r; \lambda z). \tag{1.80}$$

- *Hölder convolution: Let $\sigma_1 \neq 1$ and $\sigma_r \neq 0$ as well as $\lambda \neq 0$. Then:*

$$G(\sigma_1, ..., \sigma_r; 1) = \sum_{k=0}^{r} (-1)^k G\left(1 - \sigma_k, ..., 1 - \sigma_1; 1 - \frac{1}{\lambda}\right) G\left(\sigma_{k+1}, ..., \sigma_r; \frac{1}{\lambda}\right). \tag{1.81}$$

  Note, that for $|\lambda| \to \infty$ this becomes

$$G(\sigma_1, ..., \sigma_r; 1) = (-1)^r G(1 - \sigma_n, ..., 1 - \sigma_1; 1), \tag{1.82}$$

  since $G(a_1, ..., a_l; 0) = 0$ for $a_l \neq 0$.

- *Shuffle relations:*

$$G(\sigma_1, ..., \sigma_l; z) \cdot G(\sigma_{l+1}, ..., \sigma_{l+r}; z) = \sum_{\tau \in \Sigma(l,r)} G(\sigma_{\tau(1)}, ..., \sigma_{\tau(l+r)}; z). \tag{1.83}$$

  More abstractly (cf. appendix B.2.12): Let $X = (\sigma_i)_{i \in I} \subset \mathbb{C}$ be a finite set of distinct points which we take as an alphabet and form the set of words B over X. We can then think of $G(\cdot; z)$ as a map

$$G_z : B \to \mathbb{C}, \quad B \ni w = \sigma_1 \cdots \sigma_r \mapsto G_z(w) := G(\sigma_1, ..., \sigma_r; z). \tag{1.84}$$

  By the characteristic property of free vector spaces, this map G_z can be uniquely extended to a linear map on $\mathbb{C}\langle X\rangle$ (the free vector space of all formal $\mathbb{C}$-linear combinations of words). In this setting, the shuffle relations read as follows: $G_z : \mathbb{C}\langle X\rangle \to \mathbb{C}$ is an algebra homomorphism between the $\mathbb{C}$-algebra $(\mathbb{C}\langle X\rangle, ⧢)$ and the complex numbers, i.e. for all $w_1, w_2 \in \mathbb{C}\langle X\rangle$:

$$G_z(w_1 ⧢ w_2) = G_z(w_1) \cdot G_z(w_2). \tag{1.85}$$

– *Stuffle relations: Let* $X = ((m_i, \sigma_i))_{i \in I}$ *be a finite set of distinct elements of* $\mathbb{N}_0 \times \mathbb{C}$ *and* B *the set of words over* X*. Introduce additional structure on* X *in the form of the associative and commutative map*

$$\circ : X \times X \to X, \quad (m_1, \sigma_1) \circ (m_2, \sigma_2) := (m_1 + m_2, \sigma_1 \sigma_2). \tag{1.86}$$

Now define the stuffle product recursively through

$$\emptyset \mathbin{\widetilde{ш}} w := w \mathbin{\widetilde{ш}} \emptyset := w, \tag{1.87}$$

$$\begin{aligned}(x_1 \cdots x_k) \mathbin{\widetilde{ш}} (x_{k+1} \cdots x_r) := {} & x_1 \left[(x_2 \cdots x_k) \mathbin{\widetilde{ш}} (x_{k+1} \cdots x_r)\right] + \\ & + x_{k+1} \left[(x_1 \cdots x_k) \mathbin{\widetilde{ш}} (x_{k+2} \cdots x_r)\right] + \\ & + (x_1 \circ x_{k+1}) \left[(x_2 \cdots x_k) \mathbin{\widetilde{ш}} (x_{k+2} \cdots x_r)\right].\end{aligned} \tag{1.88}$$

One can show that $(\mathbb{C}\langle X \rangle, \widetilde{ш})$ *forms a* $\mathbb{C}$*-algebra called the stuffle-algebra. Analogous to above, we can think of* Li *as a linear map* $\mathrm{Li} : \mathbb{C}\langle X \rangle \to \mathbb{C}$ *uniquely defined by*

$$B \ni w = (m_1, z_1) \cdots (m_k, z_k) \mapsto \mathrm{Li}_{m_1,...,m_k}(z_1, ..., z_k). \tag{1.89}$$

The stuffle relations are characterised by the statement that Li *is again an algebra homomorphism between the stuffle algebra and the complex numbers so that for all* $w_1, w_2 \in \mathbb{C}\langle X \rangle$*:*

$$\mathrm{Li}(w_1 \mathbin{\widetilde{ш}} w_2) = \mathrm{Li}(w_1) \cdot \mathrm{Li}(w_2). \tag{1.90}$$

Shuffle- and stuffle-relations are in general independent. In union (using (ii)), they form the so called double-shuffle-relations.

Proof. (i) The here given analytic properties are mere observations and follow directly by spelling out the definition of MPLs.

(ii) First, the asserted convergence directly follows from the convergence of the geometric series:

$$\begin{aligned}\sum_{n_1 > ... > n_k > 0} \frac{|z_1^{n_1} \cdots z_k^{n_k}|}{n_1^{m_1} \cdots n_k^{m_k}} &= \sum_{n_1=1}^{\infty} \frac{|z_1|^{n_1}}{n_1^{m_1}} \sum_{n_2=1}^{n_1-1} \frac{|z_2|^{n_2}}{n_2^{m_2}} \cdots \sum_{n_k=1}^{n_{k-1}-1} \frac{|z_k|^{n_k}}{n_k^{m_k}} \leq \\ &\leq \sum_{n_1=1}^{\infty} \frac{|z_1|^{n_1}}{n_1^{m_1}} \sum_{n_2=1}^{n_1-1} \frac{|z_2|^{n_2}}{n_2^{m_2}} \cdots \sum_{n_{k-1}=1}^{n_{k-2}-1} \frac{|z_{k-1}|^{n_{k-1}}}{n_{k-1}^{m_{k-1}}} \frac{1}{1-|z_k|} \leq \\ &\leq \cdots \leq \prod_{i=1}^{k} \frac{1}{1-|z_i|} < \infty.\end{aligned} \tag{1.91}$$

As an aside, the condition for convergence can be relaxed to ([17], p.287):

$$(m_1, z_1) \neq (1, 1) \quad \text{and} \quad \forall j \in \{1, ..., k\} : \ |z_1 \cdots z_j| \leq 1. \tag{1.92}$$

The remainder of the proof also consists of exploiting the geometric series ([17], pp.735f.). First, note that

$$|a/b| < 1 \implies \frac{1}{a-b} = -\frac{1}{b} \cdot \frac{1}{1-a/b} = -\sum_{i=1}^{\infty} \frac{a^{i-1}}{b^i}. \tag{1.93}$$

Introduce the notations

$$a_j := \frac{1}{z_1 \cdots z_j} \quad \text{and} \quad \int_0^x \underbrace{\frac{\mathrm{d}z}{z} \circ \cdots \circ \frac{\mathrm{d}z}{z}}_{m} \circ \frac{\mathrm{d}z}{z-\sigma} =: \int_0^x \left[\frac{\mathrm{d}z}{z}\right]^m \frac{\mathrm{d}z}{z-\sigma} \tag{1.94}$$

for convenience and calculate first (for $|z_m/\sigma| < 1$):

$$\begin{aligned}
\int_0^x \left[\frac{\mathrm{d}z}{z}\right]^{m-1} \frac{\mathrm{d}z}{z-\sigma} &= \int_0^x \frac{\mathrm{d}z_1}{z_1} \int_0^{z_1} \frac{\mathrm{d}z_2}{z_2} \cdots \int_0^{z_{m-2}} \frac{\mathrm{d}z_{m-1}}{z_{m-1}} \int_0^{z_{m-1}} \frac{\mathrm{d}z_m}{z_m - \sigma} = \\
&= -\int_0^x \frac{\mathrm{d}z_1}{z_1} \int_0^{z_1} \frac{\mathrm{d}z_2}{z_2} \cdots \int_0^{z_{m-2}} \frac{\mathrm{d}z_{m-1}}{z_{m-1}} \int_0^{z_{m-1}} \mathrm{d}z_m \sum_{i=1}^{\infty} \frac{z_m^{i-1}}{\sigma^i} = \\
&= -\sum_{i=1}^{\infty} \int_0^x \frac{\mathrm{d}z_1}{z_1} \int_0^{z_1} \frac{\mathrm{d}z_2}{z_2} \cdots \int_0^{z_{m-2}} \frac{\mathrm{d}z_{m-1}}{z_{m-1}} \frac{1}{i} \frac{z_{m-1}^i}{\sigma^i} = \\
&= \cdots = -\sum_{i=1}^{\infty} \frac{1}{i^m} \frac{x^i}{\sigma^i}.
\end{aligned} \tag{1.95}$$

Repeating this calculation k times (i.e. successively integrating from right to left), we get

$$\begin{aligned}
(-1)^k G_{m_1,\ldots,m_k}(a_1,\ldots,a_k;1) &= (-1)^k \int_0^1 \left[\frac{\mathrm{d}z}{z}\right]^{m_1-1} \frac{\mathrm{d}z}{z-a_1} \circ \cdots \circ \left[\frac{\mathrm{d}z}{z}\right]^{m_k-1} \frac{\mathrm{d}z}{z-a_k} = \\
&= \sum_{i_1=1}^{\infty} \cdots \sum_{i_k=1}^{\infty} \frac{1}{(i_1+\cdots+i_k)^{m_1}} \frac{1}{a_1^{i_1}} \cdots \frac{1}{(i_{k-1}+i_k)^{m_{k-1}}} \frac{1}{a_{k-1}^{i_{k-1}}} \cdot \frac{1}{i_k^{m_k}} \frac{1}{a_k^{i_k}}.
\end{aligned} \tag{1.96}$$

Plugging in the definition of a_j and rearranging terms yields:

$$(-1)^k G_{m_1,\ldots,m_k}(a_1,\ldots,a_k;1) = \sum_{i_1=1}^{\infty} \cdots \sum_{i_k=1}^{\infty} \frac{z_1^{i_1+\cdots+i_k}}{(i_1+\cdots+i_k)^{m_1}} \cdots \frac{z_{k-1}^{i_{k-1}+i_k}}{(i_{k-1}+i_k)^{m_{k-1}}} \cdot \frac{z_k^{i_k}}{i_k^{m_k}}. \tag{1.97}$$

The change of order of summation described by $n_1 := i_1 + \cdots + i_k$, $n_2 := i_2 + \cdots + i_k$, ..., $n_k = i_k$ (allowed because of absolute convergence) finally leads to the assertion.

(iii) In order to obtain the total differential, we do the following three preparatory calculations. First,

$$\frac{\partial}{\partial x}\int\limits_0^x \frac{\mathrm{d}z}{z-\sigma_1}G(\sigma_2,...,\sigma_r;z)=\frac{1}{x-\sigma_1}G(\sigma_2,...,\sigma_r;x). \tag{1.98}$$

Then, for $1\leq k<r$ (using integration by parts, the fundamental theorem of calculus, partial fractioning and the definition of MPLs in this order):

$$\begin{aligned}
&\frac{\partial}{\partial\sigma_k}\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-2}}\frac{\mathrm{d}z_{k-1}}{z_{k-1}-\sigma_{k-1}}\int\limits_0^{z_{k-1}}\frac{\mathrm{d}z_k}{z_k-\sigma_k}G(\sigma_{k+1},...,\sigma_r;z_k)=\\
&=-\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-2}}\frac{\mathrm{d}z_{k-1}}{z_{k-1}-\sigma_{k-1}}\int\limits_0^{z_{k-1}}\mathrm{d}z_k\frac{\partial}{\partial z_k}\left(\frac{1}{z_k-\sigma_k}\right)G(\sigma_{k+1},...,\sigma_r;z_k)=\\
&=-\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-2}}\frac{\mathrm{d}z_{k-1}}{z_{k-1}-\sigma_{k-1}}\Bigg\{\left[\frac{1}{z_k-\sigma_k}G(\sigma_{k+1},...,\sigma_r;z_k)\right]_{z_k=0}^{z_{k-1}}-\\
&\qquad-\int\limits_0^{z_{k-1}}\frac{\mathrm{d}z_k}{z_k-\sigma_k}\frac{\partial}{\partial z_k}G(\sigma_{k+1},...,\sigma_r;z_k)\Bigg\}=\\
&=-\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-2}}\frac{\mathrm{d}z_{k-1}}{z_{k-1}-\sigma_{k-1}}\frac{1}{z_{k-1}-\sigma_k}G(\sigma_{k+1},...,\sigma_r;z_{k-1})+\\
&\qquad+\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-2}}\frac{\mathrm{d}z_{k-1}}{z_{k-1}-\sigma_{k-1}}\int\limits_0^{z_{k-1}}\frac{\mathrm{d}z_k}{z_k-\sigma_k}\frac{1}{z_k-\sigma_{k+1}}G(\sigma_{k+2},...,\sigma_r;z_k)=\\
&=-\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-2}}\mathrm{d}z_{k-1}\left(\frac{1}{z_{k-1}-\sigma_{k-1}}-\frac{1}{z_{k-1}-\sigma_k}\right)\frac{G(\sigma_{k+1},...,\sigma_r;z_{k-1})}{\sigma_{k-1}-\sigma_k}+\\
&\qquad+\int\limits_0^x\frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int\limits_0^{z_{k-1}}\mathrm{d}z_k\left(\frac{1}{z_k-\sigma_k}-\frac{1}{z_k-\sigma_{k+1}}\right)\frac{G(\sigma_{k+2},...,\sigma_r;z_k)}{\sigma_k-\sigma_{k+1}}=\\
&=-\frac{1}{\sigma_{k-1}-\sigma_k}G(\sigma_1,...,\hat{\sigma}_k,...,\sigma_r;x)+\frac{1}{\sigma_{k-1}-\sigma_k}G(\sigma_1,...,\hat{\sigma}_{k-1},...,\sigma_r;x)+\\
&\qquad+\frac{1}{\sigma_k-\sigma_{k+1}}G(\sigma_1,...,\hat{\sigma}_{k+1},...,\sigma_r;x)-\frac{1}{\sigma_k-\sigma_{k+1}}G(\sigma_1,...,\hat{\sigma}_k,...,\sigma_r;x).
\end{aligned}\tag{1.99}$$

The hat ˆ indicates the omission of the corresponding letter. Finally,

$$\begin{aligned}
&\frac{\partial}{\partial\sigma_r}\int_0^x \frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int_0^{z_{r-1}}\frac{\mathrm{d}z_r}{z_r-\sigma_r}= \\
&=\int_0^x \frac{\mathrm{d}z_1}{z_1-\sigma_1}\cdots\int_0^{z_{k-2}}\left(-\frac{1}{\sigma_r}-\frac{1}{z_{r-1}-\sigma_r}\right)\frac{1}{z_{r-1}-\sigma_{r-1}}\,\mathrm{d}z_{r-1}= \\
&=-\frac{1}{\sigma_r}G(\sigma_1,...,\hat{\sigma}_r;x)-\frac{1}{\sigma_r-\sigma_{r-1}}\left(G(\sigma_1,...,\hat{\sigma}_{r-1},\sigma_r;x)-G(\sigma_1,...,\hat{\sigma}_r;x)\right).
\end{aligned} \tag{1.100}$$

Now, knowing

$$\mathrm{d}(\log(\sigma_{k-1}-\sigma_k)-\log(\sigma_{k+1}-\sigma_k))=\frac{\mathrm{d}\sigma_{k-1}}{\sigma_{k-1}-\sigma_k}+\frac{\mathrm{d}\sigma_k}{\sigma_{k+1}-\sigma_k}-\frac{\mathrm{d}\sigma_k}{\sigma_{k-1}-\sigma_k}-\frac{\mathrm{d}\sigma_{k+1}}{\sigma_{k+1}-\sigma_k} \tag{1.101}$$

the desired result is just a matter of careful bookkeeping.

(iv) The scaling relation is apparent from the definition, whereas the Hölder convolution is derived in chapter 7 of [24] and will not be proven here. The shuffle relations are an immediate consequence of the general shuffle product formula for iterated integrals which has been proven in theorem 1.1.2 (iv). Of course, the underlying path of integration has to be the same for either of the factors (or must at least lie in the same homotopy class). The stuffle relation can be proven via induction.

- If $w_1=\emptyset$ or $w_2=\emptyset$, then the assertion is trivially clear. This sets up the base case.
- In order to see more clearly what is going on, we introduce some notation (similar to [25], p.28). Let $N\in\mathbb{N}_0\cup\{\infty\}$ and define

$$\mathrm{Li}_N(w):=\sum_{N>n_1>\cdots>n_k>0} f_{n_1}(m_1,z_1)\cdots f_{n_k}(m_k,z_k) \tag{1.102}$$

where

$$w=(m_1,z_1)\cdots(m_k,z_k)\quad\text{is a word and}\quad f_n(m,z)=\frac{z^n}{n^m}. \tag{1.103}$$

For the induction step, set $w_1=a_1w_1'$ and $w_2=a_2w_2'$ with lengths of a_1 and a_2

being 1. Then:

$$
\begin{aligned}
\mathrm{Li}(w_1)\mathrm{Li}(w_2) &= \left(\sum_{N_1>0} f_{N_1}(a_1)\mathrm{Li}_{N_1}(w_1')\right)\left(\sum_{N_2>0} f_{N_2}(a_2)\mathrm{Li}_{N_2}(w_2')\right) = \\
&= \left(\sum_{N_1>N_2>0} + \sum_{N_2>N_1>0} + \sum_{N_1=N_2>0}\right) f_{N_1}(a_1)\mathrm{Li}_{N_1}(w_1') f_{N_2}(a_2)\mathrm{Li}_{N_2}(w_2') = \\
&= \sum_{N_1>0} f_{N_1}(a_1)\mathrm{Li}_{N_1}(w_1')\mathrm{Li}_{N_1}(a_2 w_2') + \sum_{N_2>0} \mathrm{Li}_{N_2}(a_1 w_1') f_{N_2}(a_2)\mathrm{Li}_{N_2}(w_2') + \\
&\quad + \sum_{N_1>0} f_{N_1}(a_1) f_{N_1}(a_2)\mathrm{Li}_{N_1}(w_1')\mathrm{Li}_{N_1}(w_2') = \\
&= \sum_{N>0} f_N(a_1)\mathrm{Li}_N(w_1' \,\widetilde{\sqcup\!\sqcup}\, w_2) + \sum_{N>0} f_N(a_2)\mathrm{Li}_N(w_1 \,\widetilde{\sqcup\!\sqcup}\, w_2') + \\
&\quad + \sum_{N>0} f_N(a_1 \circ a_2)\mathrm{Li}_N(w_1' \,\widetilde{\sqcup\!\sqcup}\, w_2') = \\
&= \mathrm{Li}(a_1(w_1' \,\widetilde{\sqcup\!\sqcup}\, w_2)) + \mathrm{Li}(a_2(w_1 \,\widetilde{\sqcup\!\sqcup}\, w_2')) + \mathrm{Li}((a_1 \circ a_2)(w_1' \,\widetilde{\sqcup\!\sqcup}\, w_2')) = \\
&= \mathrm{Li}(w_1 \,\widetilde{\sqcup\!\sqcup}\, w_2).
\end{aligned}
\tag{1.104}
$$

The basic steps are: splitting the double sum into three pieces, using the definition of Li_N, using the induction step and

$$
f_n(m_1, z_1) f_n(m_2, z_2) = \frac{(z_1 z_2)^n}{n^{m_1+m_2}} = f_n((m_1, z_1) \circ (m_2, z_2)) \tag{1.105}
$$

and finally recalling the recursive definition of the stuffle product.

□

We will now discuss the regularization of multiple polylogarithms of the form

$$
G(\sigma_1, ..., \sigma_j, \underbrace{0, ..., 0}_{r}; z) = \int_\gamma [\omega_0]^r \omega_j \cdots \omega_1 \quad (\sigma_j \neq 0) \tag{1.106}
$$

and

$$
G(\underbrace{0, ..., 0}_{r}; z) = \int_\gamma [\omega_0]^r \tag{1.107}
$$

in some more detail and derive closed formulas; a comprehensive and mathematically fully rigorous treatment can be found e.g. in Erik Panzer's PhD-Thesis [21], chapter 3.

To this end, let $\epsilon > 0$ and start off with the shuffle relation (which motivates the name shuffle regularisation; the ansatz is similar to [17], p.293)

$$
\int_\epsilon^z \omega_0 \int_\epsilon^z [\omega_0]^{r-1} \omega_j \cdots \omega_1 = r \int_\epsilon^z [\omega_0]^r \omega_j \cdots \omega_1 + \int_\epsilon^z [\omega_0]^{r-1} \omega_j \left(\omega_0 \sqcup\!\sqcup\, \omega_{j-1} \cdots \omega_1\right). \tag{1.108}
$$

It is an important observation, that this equation can be rewritten as

$$\int_\epsilon^z [\omega_0]^r \omega_j \cdots \omega_1 = \frac{1}{r}\left[\int_\epsilon^z \omega_0 \int_\epsilon^z [\omega_0]^{r-1}\omega_j \cdots \omega_1 - \int_\epsilon^z [\omega_0]^{r-1}\omega_j \left(\omega_0 \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1\right)\right]. \quad (1.109)$$

Here, only $r-1$ problematic ω_0 forms appear inside the iterated integrals on the right hand side and one integral over ω_0 which is very easy to regularize has been factored out. Hence we can think of this equation as a recursion equation for the iterated integral we want to evaluate. Resolving the recursion by plugging this equation successively into itself yields

$$\begin{aligned}\int_\epsilon^z [\omega_0]^r \omega_j \cdots \omega_1 &= \frac{1}{r!}\sum_{k=0}^{r}(r-k)!(-1)^{r-k}\binom{r}{k}\left(\int_\epsilon^z \omega_0\right)^k \int_\epsilon^z \omega_j([\omega_0]^{r-k} \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1) = \\ &= \sum_{k=0}^{r}(-1)^{r-k}\frac{1}{k!}\log^k\left(\frac{z}{\epsilon}\right)\int_\epsilon^z \omega_j([\omega_0]^{r-k} \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1)\end{aligned} \quad (1.110)$$

We have used here that

$$(\omega_0 \sqcup\!\sqcup\, (\omega_0 \sqcup\!\sqcup\, (\cdots \sqcup\!\sqcup\, (\omega_0 \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1)))) = k![\omega_0]^k \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1. \quad (1.111)$$

which explains the factor $(r-k)!$. Noting that the iterated integral

$$\int_\epsilon^z \omega_j([\omega_0]^{r-k} \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1) \quad (1.112)$$

converges in the limit $\epsilon \to 0$, we deduce

$$\mathrm{Reg}_\epsilon \int_\gamma [\omega_0]^r \omega_j \cdots \omega_1 = \sum_{k=0}^{r}(-1)^{r-k}\frac{1}{k!}\log^k(z)\int_\gamma \omega_j([\omega_0]^{r-k} \sqcup\!\sqcup\, \omega_{j-1}\cdots\omega_1). \quad (1.113)$$

We give two examples:

(i) $r = j = 1$:

$$G^{\mathrm{reg}}(\sigma_1, 0; z) = -G(0,\sigma_1; z) + \log(z)G(\sigma_1; z). \quad (1.114)$$

(ii) $r = j = 2$:

$$\begin{aligned}G^{\mathrm{reg}}(\sigma_1,\sigma_2,0,0;z) &= G(0,0,\sigma_1,\sigma_2;z) + G(0,\sigma_1,0,\sigma_2;z) + G(\sigma_1,0,0,\sigma_2;z) - \\ &- \log(z)\left(G(\sigma_1,0,\sigma_2;z) + G(0,\sigma_1,\sigma_2;z)\right) + \frac{1}{2}\log^2(z)G(\sigma_1,\sigma_2;z).\end{aligned} \quad (1.115)$$

This shuffling procedure cannot be used for the case of $\int_\gamma [\omega_0]^r$. Instead, we observe:

$$\int_\epsilon^x [\omega_0]^r = \int_\epsilon^x \frac{\mathrm{d}z_1}{z_1} \int_\epsilon^{z_1} \frac{\mathrm{d}z_2}{z_2} \cdots \int_\epsilon^{z_{r-1}} \frac{\mathrm{d}z_r}{z_r} = \frac{1}{r!} \left(\int_\epsilon^x \frac{\mathrm{d}z}{z} \right)^r = \frac{1}{r!} \log^r \left(\frac{x}{\epsilon} \right) \tag{1.116}$$

Hence,

$$\mathrm{Reg}_\epsilon \int_\gamma [\omega_0]^r = \frac{1}{r!} \log^r(x). \tag{1.117}$$

We conclude this subsection with the definition of some special instances of multiple polylogarithms.

Definition 1.2.3. Special classes of MPLs ([22], pp.16f. and [21], p.99 and [1], p.4 and [26], p.3).

(i) Nielsen's generalized polylogarithms. They are given by

$$S_{n,p}(x) = (-1)^p G(\underbrace{0, ..., 0}_{n}, \underbrace{1, ..., 1}_{p}; x) = \mathrm{Li}_{(n+1),\, 1, \ldots, 1}(x, \underbrace{1, ..., 1}_{p-1}). \tag{1.118}$$

(ii) Harmonic polylogarithms (HPLs). These are MPLs whose vectors of singularities $(\sigma_1, ..., \sigma_r)$ consists of elements of $\Sigma = \{-1, 0, 1\}$. The alphabet of differential forms is thus given by

$$\{\mathrm{d}\log(x), \mathrm{d}\log(x-1), \mathrm{d}\log(x+1)\}. \tag{1.119}$$

For historical reasons

$$H(\sigma_1, ..., \sigma_r; x) = (-1)^p G(\sigma_1, ..., \sigma_r; x), \tag{1.120}$$

where p denotes the number of σ_i's equal to $+1$.

(iii) Two-dimensional harmonic polylogarithms (2dHPLs). Here, the first r entries are given by $\sigma_i \in \{0, 1, -z, 1-z\}$ for $z \in \mathbb{C}$ while the last entry will be denoted by y in this thesis. The alphabet of differential forms thus equals (z is taken to be constant here)

$$\{\mathrm{d}\log(y), \mathrm{d}\log(y-1), \mathrm{d}\log(y+z), \mathrm{d}\log(y+z-1)\}\,. \tag{1.121}$$

(iv) Cyclotomic harmonic polylogarithms (CHPLs). In this case, the vector of singularities consists of the k-th roots of unity together with 0:

$$\Sigma = \{0\} \cup \{\exp(2\pi i k/n) \mid 0 \leq k < n\}. \tag{1.122}$$

1.3 Hopf-Algebra Structure and the Symbol Map

For convenience, we will in this subsection mostly use the notation

$$I(a_0; a_1, ..., a_r; a_{r+1}) := \int_\gamma \omega_1 \cdots \omega_r \tag{1.123}$$

where

$$\omega_i = \frac{\mathrm{d}z}{z - a_i} \tag{1.124}$$

and γ is a path connecting a_0 with a_{r+1} in $\mathbb{C} \setminus \{a_1, ..., a_r\}$. These expressions (called multiple polylogarithms as well) are related to the G-functions via

$$I(0; \sigma_1, ..., \sigma_r; x) = G(\sigma_r, ..., \sigma_1; x). \tag{1.125}$$

Notice the reversal of letters.

We now want to introduce a Hopf algebra structure on the space of multiple polylogarithms, which will allow us to introduce the central object of this work: the symbol map. However, some technical difficulties arise here if one tries to do this directly at the level of the MPLs introduced analytically so far. In the mathematical literature (e.g. [5], [27], [28], [29]) one therefore goes over to algebraic objects called motivic multiple polylogarithms. From a technical point of view, this simplifies the discussion quite considerably and - after a conjecture - no essential information is lost; instead, various structures become clearer or apparent, such as the coproduct of MPLs (cf. [27], pp.4f. for a concretization of these claims). The concrete construction of motivic MPLs is rather involved and will therefore not be presented here. Instead, we introduce them as formal algebraic objects that satisfy certain computational rules. In fact, they shall possess all the relations discussed so far and only those. This approach is similar to that of [17] in Chapter 11; but this source introduces motivic MPLs according to Francis Brown's definition (see, for example, [28] for a relatively straightforward discussion), which fixes certain short-comings of the definition given by Alexander Goncharov (e.g. [27]): in Goncharov's version, for example, the motivic version of $\zeta(2)$ is necessarily zero, whereas in Brown's version it is not. Since for the purposes of this paper that flaw of Goncharov's theory does not matter and Brown's theory is conceptually somewhat more difficult (the latter requires (at least) the introduction of comodules and coactions, as done in [17], pp.374ff.), we always refer here to Goncharov's notion of motivic MPLs.

The following theorem summarizes the results of the theory we need in the remainder of this thesis. However, since it does not make use of the precise definitions of the objects, it should be taken with a grain of salt.

Theorem 1.3.1. *Motivic MPLs ([27], pp.2f.,10,18 and [30], pp.17f. and [31], pp.36ff.). Let $a_i, i \in \{0, .., r+1\}$, be elements of the field of algebraic numbers $\overline{\mathbb{Q}}$ thought of as embedded into $\mathbb{C}$ via some embedding (more generally - but with respect to the underlying theory even more abstractly - any number field will do). Then, there exists a graded commutative Hopf algebra $\mathcal{A}_\bullet(\overline{\mathbb{Q}})$ over $\mathbb{Q}$ and elements*

$$I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}) \in \mathcal{A}_r(\overline{\mathbb{Q}}) \tag{1.126}$$

such that all the relations discussed so far for the classical iterated integrals also hold for the motivic ones. I.e.,

(i) *For all* $a_0, a_1 \in \overline{\mathbb{Q}}$ *we have:* $I^{\mathcal{M}}(a_0; \emptyset; a_1) = \mathbf{1}$, *where* $\mathbf{1}$ *is the unit of* $\mathcal{A}_\bullet(\overline{\mathbb{Q}})$.

(ii) *The product is given by the shuffle product formula:*

$$I^{\mathcal{M}}(a; a_1, ..., a_l; b) \cdot I^{\mathcal{M}}(a; a_{l+1}, ..., a_{l+r}; b) = \sum_{\sigma \in \Sigma(l,r)} I^{\mathcal{M}}(a; a_{\sigma(1)}, ..., a_{\sigma(l+r)}; b). \tag{1.127}$$

(iii) *The path composition formula holds. For* $x \in \overline{\mathbb{Q}}$ *we have:*

$$I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}) = \sum_{k=0}^{r} I^{\mathcal{M}}(a_0; a_1, ..., a_k; x) \cdot I^{\mathcal{M}}(x; a_{k+1}, ..., a_r; a_{r+1}). \tag{1.128}$$

(iv) *We have* $I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_0) = 0$ *for* $r \geq 1$.

(v) *The path reversal formula holds:*

$$I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}) = (-1)^r I^{\mathcal{M}}(a_{r+1}; a_r, ..., a_1; a_0). \tag{1.129}$$

(vi) *The motivic logarithm which is related to the motivic MPL of weight one via*

$$I^{\mathcal{M}}(a_0; a_1; a_2) := \log^{\mathcal{M}}\left(\frac{a_2 - a_1}{a_0 - a_1}\right) \tag{1.130}$$

(with appropriate regularization as discussed below) fulfills the usual functional equation $\log^{\mathcal{M}}(a) + \log^{\mathcal{M}}(b) = \log^{\mathcal{M}}(ab)$. *This can be also regarded as a special case of the path composition formula for* $r = 1$*:*

$$\begin{aligned} I^{\mathcal{M}}(a; a_1, a_2) + I^{\mathcal{M}}(a_2; a_1; b) &= \log^{\mathcal{M}}\left(\frac{a_2 - a_1}{a - a_1}\right) + \log^{\mathcal{M}}\left(\frac{b - a_1}{a_2 - a_1}\right) = \\ &= \log^{\mathcal{M}}\left(\frac{b - a_1}{a - a_1}\right) = I^{\mathcal{M}}(a; a_1; b). \end{aligned} \tag{1.131}$$

Furthermore, all relations that hold on the motivic level also hold on the classical level (modulo integrals of lower weight). However, there might be some relations on the classical level that the motivic MPLs do not possess. That this is indeed not the case is still an open conjecture.

The $I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1})$ *are always associated with shuffle regularized iterated integrals* $I^{\text{reg}}(a_0; a_1, ..., a_r; a_{r+1})$ *(see below for a remark).*

The coproduct is given explicitly by

$$\begin{aligned} &\Delta I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}) = \\ &= \sum_{0 = i_0 < \cdots < i_{k+1} = r+1} I^{\mathcal{M}}(a_0; a_{i_1}, ..., a_{i_k}; a_{r+1}) \otimes \prod_{p=0}^{k} I^{\mathcal{M}}(a_{i_p}; a_{i_p + 1}, ..., a_{i_{p+1}-1}; a_{i_{p+1}}). \end{aligned} \tag{1.132}$$

Remark. (i) In practice (for example in [31]), one often identifies the algebraic object $I^{\mathcal{M}}$ with its analytic realization I. However, one has to be careful to use the properly shuffle regularized version of I, which we will denote by I^{reg}. On the contrary to what has been discussed in the last subsection, the shuffle regularization procedure has to be applied not only in the case when $a_1 = a_0$ discussed so far but also when $a_r = a_{r+1}$ ([31], p.39 and [27], pp.1f.). The basic idea is completely analogous to the case discussed above: suppose, we are given an expression $I(a_0; a_1, ..., a_r; a_{r+1})$ that is possibly divergent. Let $\gamma : [0, 1] \to \mathbb{C}\backslash\{a_1, ..., a_r\}$ again be a curve connecting a_0 with a_{r+1} and now consider a two-sided restricted path $\gamma|_{[\epsilon,1-\epsilon]}$ as well as the associated iterated integral, which converges. By applying the shuffle relations several times, we can isolate the expressions $\int_{a_0+\epsilon}^{a_{r+1}-\epsilon} \omega_0$ and $\int_{a_0+\epsilon}^{a_{r+1}-\epsilon} \omega_{r+1}$ completely analogous to above. For $a_0 \neq a_{r+1}$, a simple calculation of the regularized versions of these two expressions yields:

$$I^{\text{reg}}(a_0; a_0; a_{r+1}) = \log(a_{r+1} - a_0), \quad I^{\text{reg}}(a_0; a_{r+1}; a_{r+1}) = -\log(a_{r+1} - a_0). \tag{1.133}$$

For $a_0 = a_{r+1}$ we set $I^{\text{reg}}(a_0; a_0; a_0) = 0$. A closed formula for $I^{\text{reg}}(a_0; a_1, ..., a_r; a_{r+1})$, if one exists, will be quite messy - thus, let us directly calculate the regularization of the following iterated integral as an example ($a_i \neq a_j$ for $i \neq j$):

$$\begin{aligned} I^{\text{reg}}(a_0; a_0, a_1, a_2, a_2; a_2) &= I^{\text{reg}}(a_0; a_0; a_2) I^{\text{reg}}(a_0; a_1, a_2, a_2; a_2) - \\ &- I^{\text{reg}}(a_0; a_1, a_0, a_2, a_2; a_2) - I^{\text{reg}}(a_0; a_1, a_2, a_0, a_2; a_2) - \\ &- I^{\text{reg}}(a_0; a_1, a_2, a_2, a_0; a_2) = \\ &= \log(a_2 - a_0) I^{\text{reg}}(a_0; a_1, a_2, a_2; a_2) - I^{\text{reg}}(a_0; a_1, a_0, a_2, a_2; a_2) - \\ &- I^{\text{reg}}(a_0; a_1, a_2, a_0, a_2; a_2) - I(a_0; a_1, a_2, a_2, a_0; a_2). \end{aligned} \tag{1.134}$$

Now,

$$\begin{aligned} 2I^{\text{reg}}(a_0; a_1, a_2, a_2; a_2) &= I^{\text{reg}}(a_0; a_2; a_2) I^{\text{reg}}(a_0; a_1, a_2; a_2) - I^{\text{reg}}(a_0; a_2, a_1, a_2; a_2) = \\ &= -\log(a_2 - a_0) \left[I^{\text{reg}}(a_0; a_2; a_2) I^{\text{reg}}(a_0; a_1; a_2) - I^{\text{reg}}(a_0; a_2, a_1; a_2) \right] - \\ &- \left[I^{\text{reg}}(a_0; a_2, a_2) I^{\text{reg}}(a_0; a_2, a_1; a_2) - 2I^{\text{reg}}(a_0; a_2, a_2, a_1; a_2) \right] = \\ &= \log^2(a_2 - a_0) I(a_0; a_1; a_2) + \log(a_2 - a_0)[I(a_0; a_2, a_1; a_2) + I(a_0; a_2, a_1; a_2)] + \\ &+ 2I(a_0; a_2, a_2, a_1; a_2), \end{aligned} \tag{1.135}$$

similarly

$$\begin{aligned} I^{\text{reg}}(a_0; a_1, a_0, a_2, a_2; a_2) &= \frac{1}{2} \log^2(a_2 - a_0) I(a_0; a_1, a_0; a_2) + \\ &+ \log(a_2 - a_0)[I(a_0; a_2, a_1, a_0; a_2) + I(a_0; a_1, a_2, a_0; a_2)] + \\ &+ I(a_0; a_2, a_2, a_1, a_0; a_2) + I(a_0; a_1, a_2, a_2, a_0; a_2) + I(a_0; a_2, a_1, a_2, a_0; a_2), \end{aligned} \tag{1.136}$$

and

$$\begin{aligned}I^{\mathrm{reg}}(a_0; a_1, a_2, a_0, a_2; a_2) &= I^{\mathrm{reg}}(a_0; a_2; a_2) I^{\mathrm{reg}}(a_0; a_1, a_2, a_0; a_2) - \\ &- I^{\mathrm{reg}}(a_0; a_2, a_1, a_2, a_0; a_2) - 2I^{\mathrm{reg}}(a_0; a_1, a_2, a_2, a_0; a_2) = \\ &= -\log(a_2 - a_0) I(a_0; a_1, a_2, a_0; a_2) - I(a_0; a_2, a_1, a_2, a_0; a_2) - 2I(a_0; a_1, a_2, a_2, a_0; a_2).\end{aligned} \tag{1.137}$$

Putting everything together yields after a few cancellations:

$$\begin{aligned}I^{\mathrm{reg}}(a_0; a_0, a_1, a_2, a_2; a_2) &= \frac{1}{2}\log^3(a_2 - a_0) I(a_0; a_1; a_2) + \\ &+ \frac{1}{2}\log^2(a_2 - a_0)[I(a_0; a_2, a_1; a_2) + I(a_0; a_2, a_1; a_2) - I(a_0; a_1, a_0; a_2)] + \\ &+ \log(a_2 - a_0)[I(a_0; a_2, a_2, a_1; a_2) - I(a_0; a_2, a_1, a_0; a_2)] - \\ &- I(a_0; a_2, a_2, a_1, a_0; a_2) + I(a_0; a_1, a_2, a_2, a_0; a_2).\end{aligned} \tag{1.138}$$

(ii) The coproduct admits a nice graphical representation ([27], p.3), which we will introduce for the case $r = 3$ (it can be easily generalized). Associate to $I^{\mathcal{M}}(a_0; a_1, a_2, a_3; a_4)$ a diagram as in figure 1.1:

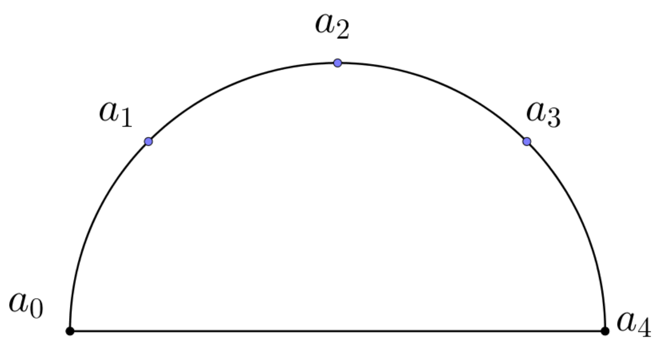

Figure 1.1: Diagram associated to $I^{\mathcal{M}}(a_0; a_1, a_2, a_3; a_4)$.

The terms in the coproduct are in a one-to-one correspondence with inscribed polygons as indicated in figure 1.2. From there, it is also quite easy to compute the total number of terms appearing in the coproduct:

$$\#(\mathrm{terms}) = \sum_{k=0}^{r} \binom{r}{k} = 2^r. \tag{1.139}$$

Proposition 1.3.2. *The coproduct defined above for motivic MPLs respects the weight in the sense of definition B.3.7 (ii), i.e.*

$$\Delta(\mathcal{A}_r(\overline{\mathbb{Q}})) \subseteq \bigoplus_{n+m=r} \mathcal{A}_n(\overline{\mathbb{Q}}) \otimes \mathcal{A}_m(\overline{\mathbb{Q}}). \tag{1.140}$$

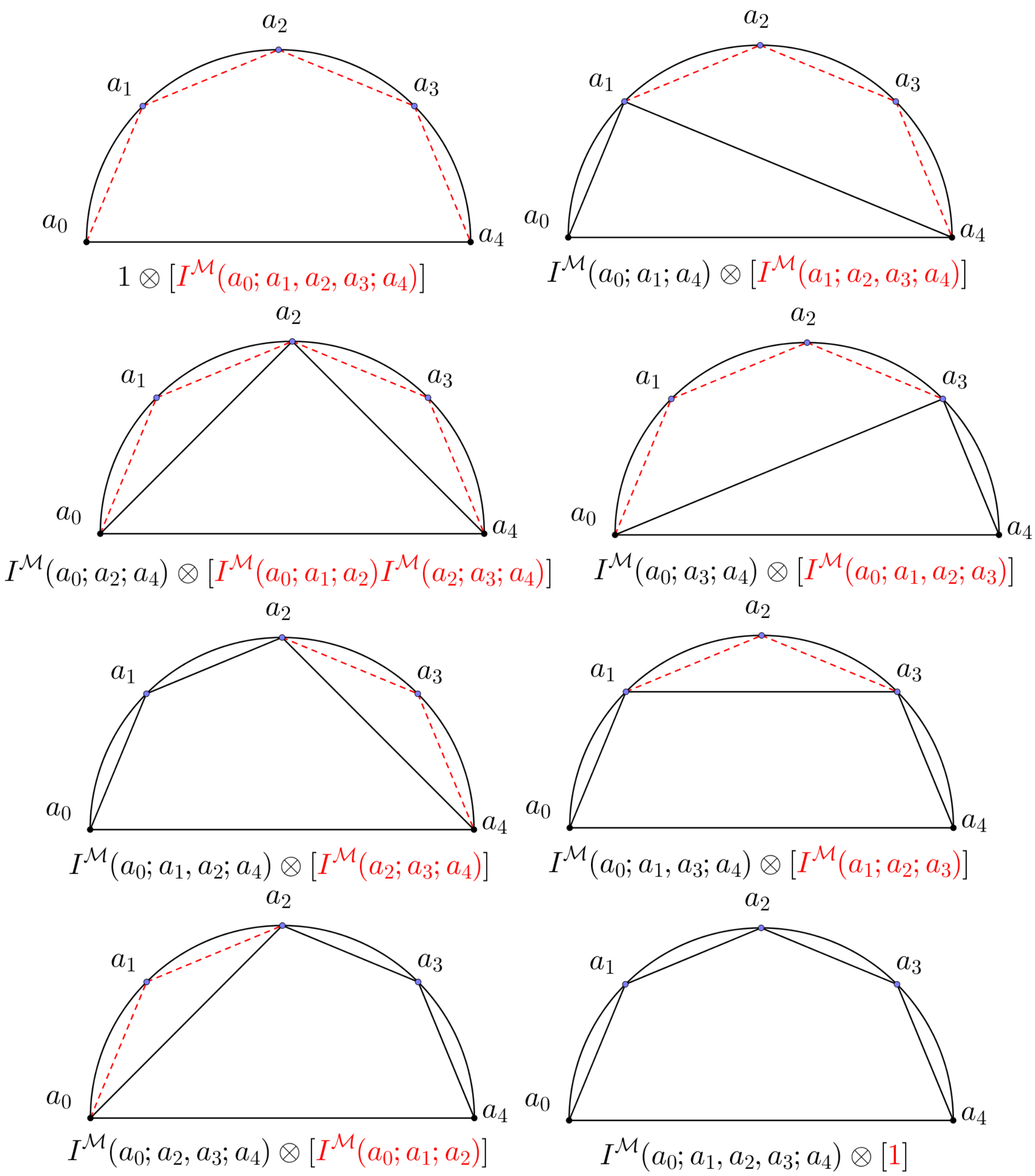

Figure 1.2: All terms appearing in the coproduct $\Delta I^{\mathcal{M}}(a_0; a_1, a_2, a_3; a_4)$.

Proof. This is immediately clear when looking at the graphical representation of the coproduct, as the semicircle is completely filled by the union of all complementary polygons. A little more formally: Let $k \in \{0, ..., r\}$ be arbitrary. Then, each term of the coproduct is of the form

$$I^{\mathcal{M}}(a_0; a_{i_1}, ..., a_{i_k}; a_{r+1}) \otimes \prod_{p=0}^{k} I^{\mathcal{M}}(a_{i_p}; a_{i_p+1}, ..., a_{i_{p+1}-1}; a_{i_{p+1}}). \tag{1.141}$$

The first factor of the tensor product has weight k. The second one has weight (telescope sum!)

$$\sum_{p=0}^{k}(i_{p+1} - 1) - (i_p) = i_{k+1} - i_0 - (k+1) = r + 1 - 0 - (k+1) = r - k. \tag{1.142}$$

Hence, the assertion follows. □

We now introduce the iterated coproduct, which will directly lead to the definition of the symbol map.

Definition 1.3.3. Iterated coproduct ([27], p.22 and [31], p.14). Let $H_\bullet = \bigoplus_{i>0} H_i$ be a positively graded Hopf algebra.

(i) Since the coproduct respects weight, the following map is well-defined. Let $n+m = r$ and introduce the projection

$$\pi_{n,m} : \bigoplus_{i+j=r} H_i \otimes H_j \to H_n \otimes H_m, \tag{1.143}$$

which selects from a given linear combination of tensor products in $\bigoplus_{i+j=r} H_i \otimes H_j$ exactly those terms whose first factor is in H_n and whose second factor is in H_m. Then define

$$\Delta_{n,m} := \pi_{n,m} \circ \Delta. \tag{1.144}$$

(ii) Define the iterated coproduct as the map

$$\Delta^{[r]} : H_r \to \bigotimes_{i=1}^{r} H_1 \tag{1.145}$$

given by the composition

$$H_r \xrightarrow{\Delta_{r-1,1}} H_{r-1} \otimes H_1 \xrightarrow{\Delta_{r-2,1}\otimes \mathrm{id}} H_{r-2} \otimes H_1 \otimes H_1 \xrightarrow{\Delta_{r-3,1}\otimes \mathrm{id}\otimes \mathrm{id}} \cdots \xrightarrow{\Delta_{1,1}\otimes \mathrm{id}^{\otimes(r-1)}} \bigotimes_{i=1}^{n} H_1.$$

Remark. The definition of the iterated coproduct above can be neatly summarized in the form of the following recursion

$$\Delta^{[r]} = (\Delta^{[r-1]} \otimes \mathrm{id}) \circ \Delta_{r-1,1} = (\mathrm{id} \otimes \Delta^{[r-1]}) \circ \Delta_{1,r-1} \text{ and } \Delta^{[1]} = \mathrm{id}, \tag{1.146}$$

where the second equality of the first equation is due to the coassociativity of Δ ([32], p.12).

Applying the iterated coproduct to the case of motivic MPLs leads to the definition of the symbol.

Definition 1.3.4. The symbol map ([27], p.23 and [31], p.20 and [30], p.111). Given $I(a_0; a_1, ..., a_r; a_{r+1})$, its symbol denoted by

$$\mathcal{S}(I(a_0; a_1, ..., a_r; a_{r+1})) \tag{1.147}$$

is an element of $\bigotimes_{i=1}^{r} \mathbb{Q}(a_1, ..., a_r)^*$ (the $\mathbb{Q}$-tensor algebra of invertible rational functions in the variables $a_1, ..., a_r$) constructed as follows:

(i) Lift $I(a_0; a_1, ..., a_r; a_{r+1})$ to its motivic counterpart $I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1})$ and calculate the iterated coproduct

$$\Delta^{[r]} I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}). \tag{1.148}$$

(ii) Associate to each $I^{\mathcal{M}}(a_0; a_k; a_{r+1})$ appearing in the iterated coproduct its regularized value (cf. equation 1.133):

$$I^{\mathrm{reg}}(a_0; a_k; a_{r+1}) = \begin{cases} \log\left(\frac{a_{r+1}-a_k}{a_0-a_k}\right) & \text{if} \quad a_0, a_k, a_{r+1} \text{ pairwise distinct,} \\ \log\left(\frac{1}{a_k-a_0}\right) & \text{if} \quad a_k \neq a_0 \text{ and } a_k = a_{r+1}, \\ \log\left(\frac{a_{r+1}-a_k}{1}\right) & \text{if} \quad a_k = a_0 \text{ and } a_k \neq a_{r+1}, \\ \log(1) & \text{if} \quad a_0 = a_k = a_{r+1}. \end{cases} \tag{1.149}$$

(iii) Replace each $\log(a)$ by a.

In the context of this construction, we can also formally allow that $a_i \in \mathbb{Q}(x_1, ..., x_s)$ for $i \in \{1, ..., r\}$ (imagine the rational functions a_i then evaluated at arbitrary points), so that

$$\mathcal{S}(I(a_0; a_1, ..., a_r; a_{r+1})) \in \bigotimes_{i=1}^{r} \mathbb{Q}(x_1, ..., x_s)^*. \tag{1.150}$$

The symbol map is extended by linearity to define it for rational linear combinations of MPLs.

The following proposition provides some computational rules for dealing with symbols.

Proposition 1.3.5. *Symbol Calculus ([1], pp.10f.). Let A, B be fixed elementary tensors and f, g rational functions, such that*

$$A \otimes (f \cdot g) \otimes B \tag{1.151}$$

lies in the range of the symbol map.

(i) Linearity.

$$A \otimes (f \cdot g) \otimes B = A \otimes f \otimes B + A \otimes g \otimes B. \tag{1.152}$$

In particular, if ρ_n denotes the n-th root of unit, we have $A \otimes \rho_n \otimes B = 0$.

(ii) *Shuffle Product.*

$$\begin{aligned}&\mathcal{S}(I(a;a_1,...,a_l;b)\cdot I(a;a_{l+1},...,a_{l+r};b)) = \\ &\qquad = \mathcal{S}(I(a;a_1,...,a_l;b)) \sqcup\!\sqcup\, \mathcal{S}(I(a;a_{l+1},...,a_{l+r};b)).\end{aligned} \tag{1.153}$$

(iii) *The constants $i\pi$ and ζ_n $(n \geq 2)$ lie in the kernel of the symbol map.*

Proof. (i) The first property follows directly from the multilinearity of the tensor product and the properties of the logarithm. The fact that $A \otimes (f \cdot g) \otimes B$ lies in the range of the symbol map means that this expression comes from

$$\tilde{A}\otimes\log(f\cdot g)\otimes\tilde{B} = \tilde{A}\otimes(\log(f)+\log(g))\otimes\tilde{B} = \tilde{A}\otimes\log(f)\otimes\tilde{B}+\tilde{A}\otimes\log(g)\otimes\tilde{B} \tag{1.154}$$

and should thus be equal to $A \otimes f \otimes B + A \otimes g \otimes B$. The statement about the n-th root of unity follows from

$$A \otimes 1 \otimes B = A \otimes \rho_n^n \otimes B = n(A \otimes \rho_n \otimes B) \tag{1.155}$$

and

$$A \otimes 1 \otimes B = A \otimes 1^2 \otimes B = 2(A \otimes 1 \otimes B) \implies A \otimes 1 \otimes B = 0. \tag{1.156}$$

(ii) The second property is not trivial and we follow [32], pp.12f. for the proof by induction on weight. It is sufficient to prove that

$$\begin{aligned}&\Delta^{[l+r]}(I^{\mathcal{M}}(a;a_1,...,a_l;b)\cdot I^{\mathcal{M}}(a;a_{l+1},...,a_{l+r};b)) = \\ &\qquad = \Delta^{[l]}(I^{\mathcal{M}}(a;a_1,...,a_l;b)) \sqcup\!\sqcup\, \Delta^{[r]}(I^{\mathcal{M}}(a;a_{l+1},...,a_{l+r};b)).\end{aligned} \tag{1.157}$$

– Base case. The case of one weight being zero is trivial. To show some more details, we discuss the case of both weights being one where the assertion can be easily verified by direct computation (using the path composition formula):

$$\begin{aligned}\Delta^{[2]}&(I^{\mathcal{M}}(a;a_1;b)I^{\mathcal{M}}(a;a_2;b)) = \Delta^{[2]}(I^{\mathcal{M}}(a;a_1,a_2;b)) + \Delta^{[2]}(I^{\mathcal{M}}(a;a_2,a_1;b)) = \\ &= I^{\mathcal{M}}(a;a_1;b)\otimes[I^{\mathcal{M}}(a_1;a_2;b)+I^{\mathcal{M}}(a;a_2;a_1)]+ \\ &\quad + I^{\mathcal{M}}(a;a_2;b)\otimes[I^{\mathcal{M}}(a;a_1;a_2)+I^{\mathcal{M}}(a_2;a_1;b)] = \\ &= I^{\mathcal{M}}(a;a_1;b)\otimes I^{\mathcal{M}}(a;a_2;b)+I^{\mathcal{M}}(a;a_2;b)\otimes I^{\mathcal{M}}(a;a_1;b) = \\ &= \Delta^{[1]}(I^{\mathcal{M}}(a;a_1;b)) \sqcup\!\sqcup\, \Delta^{[1]}(I^{\mathcal{M}}(a;a_2;b)).\end{aligned} \tag{1.158}$$

– Induction step. In order to make the notation a little more transparent, we associate to $I^{\mathcal{M}}(a;a_1,...,a_l;b)$ the word $w = a_1\cdots a_l$ with length l and to $I^{\mathcal{M}}(a;a_{l+1},...,a_{l+r};b)$ the word $v = a_{l+1}\cdots a_{l+r}$ with length r (the symbol wv is associated with the product of the corresponding motivic MPLs). Then there are words ω_i, ν_i of length 1 and w_i, v_i of lengths $l-1$ and $r-1$, respectively, such that

$$\Delta_{1,l-1}(w) = \sum_i \omega_i \otimes w_i \quad \text{and} \quad \Delta_{1,r-1}(v) = \sum_j \nu_j \otimes v_j. \tag{1.159}$$

Using the recursive definition of the iterated coproduct we obtain:

$$\Delta^{[l]}(w) = \sum_i \omega_i \otimes \Delta^{[l-1]}(w_i) \quad \text{and} \quad \Delta^{[r]}(v) = \sum_j \nu_j \otimes \Delta^{[r-1]}(v_j) \tag{1.160}$$

Now, we use the property that Δ needs to be an algebra homomorphism (see appendix; μ denotes the product)

$$\Delta \circ \mu = \mu_\otimes \circ (\Delta \otimes \Delta) \tag{1.161}$$

to deduce for any elements w, v of the Hopf algebra whose coproducts are given by

$$\Delta(w) = \sum_i w_i^{(1)} \otimes w_i^{(2)} \quad \text{and} \quad \Delta(v) = \sum_j v_j^{(1)} \otimes v_j^{(2)} \tag{1.162}$$

the equation:

$$\begin{aligned}\Delta(\mu(w \otimes v)) &= \mu_\otimes\big((\Delta \otimes \Delta)(w \otimes v)\big) = \mu_\otimes\big(\Delta(w) \otimes \Delta(v)\big) = \\ &= \sum_i \sum_j \mu_\otimes\big((w_i^{(1)} \otimes w_i^{(2)}) \otimes (v_j^{(1)} \otimes v_j^{(2)})\big) = \\ &= \sum_i \sum_j \mu(w_i^{(1)} \otimes v_j^{(1)}) \otimes \mu(w_i^{(2)} \otimes v_j^{(2)}).\end{aligned} \tag{1.163}$$

Since the product respects the grading (given explicitly by the map deg which associates elements of the graded Hopf algebra with their respective weights), we can conclude:

$$\begin{aligned}&\deg(\mu(w_i^{(1)} \otimes v_j^{(1)})) = 1 \iff \\ &\big(\deg(w_i^{(1)}) = 1 \wedge \deg(v_j^{(1)}) = 0\big) \vee \big(\deg(w_i^{(1)}) = 0 \wedge \deg(v_j^{(1)}) = 1\big).\end{aligned} \tag{1.164}$$

Furthermore, since the coproduct respects the grading as well, we get

$$\deg(w_i^{(1)}) = x \iff \deg(w_i^{(2)}) = l - x, \quad \deg(v_j^{(1)}) = y \iff \deg(v_j^{(2)}) = r - y \tag{1.165}$$

for all $x \in \{0, 1, ..., l\}, y \in \{0, 1, ..., r\}$. This proves

$$\begin{aligned}\Delta_{1,l+r-1}(wv) &= \sum_i \mu(\omega_i \otimes 1) \otimes \mu(w_i \otimes v) + \sum_j \mu(1 \otimes \nu_j) \otimes \mu(w \otimes v_j) = \\ &= \sum_i \omega_i \otimes (w_i v) + \sum_j \nu_j \otimes (w v_j).\end{aligned} \tag{1.166}$$

Using these results we obtain (also by inserting the induction hypothesis for the third equality):

$$\begin{aligned}\Delta^{[l+r]}(wv) &= (\mathrm{id} \otimes \Delta^{[l+r-1]}) \circ \Delta_{1,l+r-1}(wv) = \\ &= \sum_i \omega_i \otimes \Delta^{[l+r-1]}(w_i v) + \sum_j \nu_j \otimes \Delta^{[l+r-1]}(w v_j) = \\ &= \sum_i \omega_i \otimes (\Delta^{[l-1]}(w_i) \sqcup\!\sqcup \Delta^{[r]}(v)) + \sum_j \nu_j \otimes (\Delta^{[l]}(w) \sqcup\!\sqcup \Delta^{[r-1]}(v_j)).\end{aligned} \tag{1.167}$$

On the other hand, recalling the recursive definition of shuffles, one can also write:

$$
\begin{aligned}
\Delta^{[l]}(w) \sqcup\!\sqcup \Delta^{[r]}(v) &= \left(\sum_i \omega_i \otimes \Delta^{[l-1]}(w_i)\right) \sqcup\!\sqcup \left(\sum_j \nu_j \otimes \Delta^{[r-1]}(v_j)\right) = \\
&= \sum_{i,j} (\omega_i \otimes \Delta^{[l-1]}(w_i)) \sqcup\!\sqcup (\nu_j \otimes \Delta^{[r-1]}(v_j)) = \\
&= \sum_{i,j} \omega_i \otimes \big(\Delta^{[l-1]}(w_i) \sqcup\!\sqcup (\nu_j \otimes \Delta^{[r-1]}(v_j))\big) + \\
&\qquad + \nu_j \otimes \big((\omega_i \otimes \Delta^{[l-1]}(w_i)) \sqcup\!\sqcup \Delta^{[r-1]}(v_j)\big) = \\
&= \sum_i \omega_i \otimes \left(\Delta^{[l-1]}(w_i) \sqcup\!\sqcup \left(\sum_j \nu_j \otimes \Delta^{[r-1]}(v_j)\right)\right) + \\
&\qquad + \sum_j \nu_j \otimes \left(\left(\sum_i \omega_i \otimes \Delta^{[l-1]}(w_i)\right) \sqcup\!\sqcup \Delta^{[r-1]}(v_j)\right) = \\
&= \sum_i \omega_i \otimes (\Delta^{[l-1]}(w_i) \sqcup\!\sqcup \Delta^{[r]}(v)) + \sum_j \nu_j \otimes (\Delta^{[l]}(w) \sqcup\!\sqcup \Delta^{[r-1]}(v_j)).
\end{aligned} \tag{1.168}
$$

(iii) First, notice that

$$\mathcal{S}(i\pi) = \mathcal{S}(\log(-1)) = \otimes(-1) = 0, \tag{1.169}$$

since -1 is a root of unity. For the second assertion, one quickly realises that for

$$-\zeta_n = -\mathrm{Li}_n(1) = I(0; 1, \underbrace{0, ..., 0}_{n-1}; 1) \tag{1.170}$$

all terms must vanish. This is, because in the iterated coproduct only the following terms can appear, which all lead to the vanishing of the symbol due to (i):

$$I^{\mathcal{M}}(0;0;0), I^{\mathcal{M}}(0;0;1), I^{\mathcal{M}}(0;1;0), I^{\mathcal{M}}(1;0;0), I^{\mathcal{M}}(0;1;1), I^{\mathcal{M}}(1;0;1). \tag{1.171}$$

□

Example 1.3.6. Examples of symbols.

(i) The symbol of $I(0; 1-z, -z, -z; y)$. First:

$$
\begin{aligned}
\Delta_{3-1,1} I^{\mathcal{M}}(0; 1-z, -z, -z; y) &= \pi_{2,1}\big(I^{\mathcal{M}}(0; 1-z; y) \otimes I^{\mathcal{M}}(1-z; -z, -z; y) + \\
&+ I^{\mathcal{M}}(0; -z; y) \otimes [I^{\mathcal{M}}(0; 1-z; -z) I^{\mathcal{M}}(-z; -z; y)] + \\
&+ I^{\mathcal{M}}(0; -z; y) \otimes I^{\mathcal{M}}(0; 1-z, -z; z) + I^{\mathcal{M}}(0; 1-z, -z; y) \otimes I^{\mathcal{M}}(-z; -z; y) + \\
&+ I^{\mathcal{M}}(0; 1-z, -z; y) \otimes I^{\mathcal{M}}(1-z; -z; -z) + I^{\mathcal{M}}(0; -z, -z; y) \otimes I^{\mathcal{M}}(0; 1-z; -z) + \\
&+ 1 \otimes I^{\mathcal{M}}(0; 1-z, -z, -z; y) + I^{\mathcal{M}}(0; 1-z, -z, -z; y) \otimes 1\big) = \\
&= I^{\mathcal{M}}(0; 1-z, -z; y) \otimes I^{\mathcal{M}}(-z; -z; y) + I^{\mathcal{M}}(0; 1-z, -z; y) \otimes I^{\mathcal{M}}(1-z; -z; -z) + \\
&+ I^{\mathcal{M}}(0; -z, -z; y) \otimes I^{\mathcal{M}}(0; 1-z; -z).
\end{aligned} \tag{1.172}
$$

Now,

$$\begin{aligned}\Delta_{1,1}(I^{\mathcal{M}}(0;1-z,-z;y)) = I^{\mathcal{M}}(0;1-z;y)\otimes I^{\mathcal{M}}(1-z;-z;y)+\\ +I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(0;1-z;-z),\end{aligned} \tag{1.173}$$

$$\begin{aligned}\Delta_{1,1}(I^{\mathcal{M}}(0;-z,-z;y)) = I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(-z;-z;y)+\\ +I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(0;-z;-z).\end{aligned} \tag{1.174}$$

Thus:

$$\begin{aligned}\Delta^{[3]}I^{\mathcal{M}}(0;1-z,-z,-z;y) &= I^{\mathcal{M}}(0;1-z;y)\otimes I^{\mathcal{M}}(1-z;-z;y)\otimes I^{\mathcal{M}}(-z;-z;y)+\\ &+I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(0;1-z;-z)\otimes I^{\mathcal{M}}(-z;-z;y)+\\ &+I^{\mathcal{M}}(0;1-z;y)\otimes I^{\mathcal{M}}(1-z;-z;y)\otimes I^{\mathcal{M}}(1-z;-z;-z)+\\ &+I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(0;1-z;-z)\otimes I^{\mathcal{M}}(1-z;-z;-z)+\\ &+I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(-z;-z;y)\otimes I^{\mathcal{M}}(0;1-z;-z)+\\ &+I^{\mathcal{M}}(0;-z;y)\otimes I^{\mathcal{M}}(0;-z;-z)\otimes I^{\mathcal{M}}(0;1-z;-z).\end{aligned} \tag{1.175}$$

From there, it is easy to read off the symbol. Subsequent simplifications using the symbol calculus lead to:

$$\begin{aligned}\mathcal{S}(I(0;1-z,-z,-z;y)) &= \left(\frac{y-1+z}{-1+z}\right)\otimes\left(\frac{y+z}{1}\right)\otimes\left(\frac{y+z}{1}\right)+\\ &+\left(\frac{y+z}{z}\right)\otimes\left(\frac{-1}{-1+z}\right)\otimes\left(\frac{y+z}{1}\right)+\left(\frac{y-1+z}{-1+z}\right)\otimes\left(\frac{y+z}{1}\right)\otimes\left(\frac{1}{-1}\right)+\\ &+\left(\frac{y+z}{z}\right)\otimes\left(\frac{-1}{-1+z}\right)\otimes\left(\frac{1}{-1}\right)+\left(\frac{y+z}{z}\right)\otimes\left(\frac{y+z}{1}\right)\otimes\left(\frac{-1}{-1+z}\right)+\\ &+\left(\frac{y+z}{z}\right)\otimes\left(\frac{1}{-z}\right)\otimes\left(\frac{-1}{-1+z}\right)=\\ &=(y-1+z)\otimes(y+z)\otimes(y+z)-(-1+z)\otimes(y+z)\otimes(y+z)-\\ &-(y+z)\otimes(-1+z)\otimes(y+z)+(z)\otimes(-1+z)\otimes(y+z)-\\ &-(y+z)\otimes(y+z)\otimes(-1+z)+(z)\otimes(y+z)\otimes(-1+z)+\\ &+(y+z)\otimes(z)\otimes(-1+z)-(z)\otimes(z)\otimes(-1+z).\end{aligned} \tag{1.176}$$

(ii) The symbol of $\mathrm{Li}_n(x) = -I(0;1,\underbrace{0,...,0}_{n-1};x)$. We will prove that

$$\mathcal{S}(\mathrm{Li}_n(x)) = -(1-x)\otimes\underbrace{(x)\otimes\cdots\otimes(x)}_{n-1}. \tag{1.177}$$

The associated diagram to $\mathrm{Li}_n(x)$ is shown in figure 1.3. Also shown is the single term that contributes to the $\Delta_{n-1,1}$ component of the coproduct. This is because all

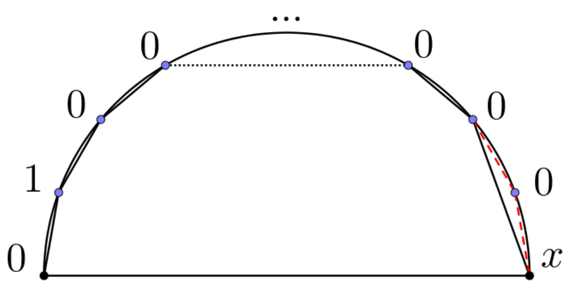

Figure 1.3: Diagram associated to $\mathrm{Li}_n(x)$ with the only term contributing to $\Delta_{n-1,1}(\mathrm{Li}_n(x))$.

other terms vanish due to the fact that $I^{\mathcal{M}}(0;1;0), I^{\mathcal{M}}(1;0;0), I^{\mathcal{M}}(0;0;0)$ all yield zero. Therefore,

$$\Delta_{n-1,1}(I^{\mathcal{M}}(0;1,\underbrace{0,...,0}_{n-1};x)) = I^{\mathcal{M}}(0;1,\underbrace{0,...,0}_{n-2};x) \otimes I^{\mathcal{M}}(0;0;x). \tag{1.178}$$

Using the recursive definition of the iterated coproduct we obtain

$$\Delta^{[n]}(I^{\mathcal{M}}(0;1,\underbrace{0,...,0}_{n-1};x)) = I^{\mathcal{M}}(0;1;x) \otimes \underbrace{I^{\mathcal{M}}(0;0;x) \otimes \cdots \otimes I^{\mathcal{M}}(0;0;x)}_{n-1}. \tag{1.179}$$

This leads to the above mentioned symbol. Note also that from this, for example, the symbol of $\mathrm{Li}_4(3)$ can also be deduced to be $2 \otimes 3 \otimes 3 \otimes 3$.

The following theorem provides an alternative way of obtaining the symbol of an MPL.

Theorem 1.3.7. *Alternative definition of the symbol ([33], p.2 and [1], p.13 and [30], p.113). In analogy to the differential equation 1.79*

$$\mathrm{d}I(a_0;a_1,...,a_r;a_{r+1}) = \sum_{j=1}^{r} I(a_0;a_1,...,\hat{a}_j,...,a_r;a_{r+1})[\mathrm{d}\log(a_{j+1}-a_j) - \mathrm{d}\log(a_{j-1}-a_j)] \tag{1.180}$$

(where $\mathrm{d}\log(0) := 0$ *and the hat indicates a missing element) the symbol of* $I(a_0;a_1,...,a_r;a_{r+1})$ *can be defined recursively via*

$$\begin{aligned}\mathcal{S}(I(a_0;a_1,...,a_r;a_{r+1})) = \sum_{j=1}^{r} &\mathcal{S}(I(a_0;a_1,...,\hat{a}_j,...,a_r;a_{r+1})) \otimes (a_{j+1}-a_j) - \\ &- \mathcal{S}(I(a_0;a_1,...,\hat{a}_j,...,a_r;a_{r+1})) \otimes (a_{j-1}-a_j).\end{aligned} \tag{1.181}$$

The recursion starts with

$$\mathcal{S}(I(a_0;a_1;a_2)) := \otimes(a_2-a_1) - \otimes(a_0-a_1), \tag{1.182}$$

where the leading $\otimes$ *indicates that the expression is to be interpreted as an element of the tensor product space in which the symbol takes its values. Here,* $a_1,...,a_r$ *can again be rational functions of several variables.*

Proof. Since the recursion 1.181 together with the initial condition 1.182 defines the symbol of an MPL uniquely and the symbol as defined via the iterated coproduct satisfies 1.182, one only has to verify that the original definition satisfies the recursion relation 1.181. It suffices to show that

$$\Delta^{[r]} I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}) = \sum_{j=1}^{r} \Delta^{[r-1]} I^{\mathcal{M}}(a_0; a_1, ..., \hat{a}_j, ..., a_r; a_{r+1}) \otimes I^{\mathcal{M}}(a_{j-1}; a_j; a_{j+1}). \tag{1.183}$$

But recalling the recursive relation

$$\Delta^{[r]} = (\Delta^{[r-1]} \otimes \mathrm{id}) \circ \Delta_{r-1,1} \tag{1.184}$$

from equation 1.146 this is quite simple, since it can be quickly seen from the pictorial representation of the coproduct that

$$\Delta_{r-1,1} I^{\mathcal{M}}(a_0; a_1, ..., a_r; a_{r+1}) = \sum_{j=1}^{r} I^{\mathcal{M}}(a_0, a_1, ..., \hat{a}_j, ..., a_r; a_{r+1}) \otimes I^{\mathcal{M}}(a_{j-1}; a_j; a_{j+1}). \tag{1.185}$$

□

Remark. From this theorem, a connection can be made to the original definition of the symbol in [33] ([34] for the mathematical background). Note that equation 1.180 comes precisely from the special form of the iterated integral (recall the proof of this differential equation):

$$I(a_0; a_1, ..., a_r; a_{r+1}) = \int_{a_0}^{a_{r+1}} \mathrm{d}\log(a_1) \circ \cdots \mathrm{d}\log(a_r). \tag{1.186}$$

In [33], p.2, the symbol $a_1 \otimes \cdots \otimes a_r$ is assigned to such an iterated integral.

A little more generally ([31], p.5): Whenever the total differential of a function $f_w : (x_1, ..., x_n) \mapsto \mathbb{C}$ (where w denotes some kind of weight) can be expressed as

$$\mathrm{d}f_w = \sum_i f_{w-1}^{(i)} \, \mathrm{d}\log(R_i), \tag{1.187}$$

where $f_{w-1}^{(i)}$ are functions of weight $w-1$ and R_i are rational functions in the variables $x_1, ..., x_n$, then the symbol may be defined recursively by

$$\mathcal{S}(f_w) = \sum_i \mathcal{S}(f_{w-1}^{(i)}) \otimes R_i. \tag{1.188}$$

It will be important to know the kernel of the symbol map well. The subsequent theorem summarizes a few results regarding this problem.

Theorem 1.3.8. *Multiple zeta values and elements of the kernel of the symbol map ([35] and [1], p.29). Whenever convergent, define the colored multiple zeta values (cMZVs) by*

$$\zeta(m_1, ..., m_k; s_1, ..., s_k) := \sum_{0<n_1<\cdots<n_k} \frac{s_1^{n_1} \cdots s_k^{n_k}}{n_1^{m_1} \cdots n_k^{m_k}} \tag{1.189}$$

where $m_i \in \mathbb{N}$ *and* $s_i \in \{-1, +1\}$. *The numbers* $\zeta(m_1, ..., m_k; 1, ..., 1) =: \zeta(m_1, ..., m_k)$ *are called multiple zeta values (MZVs) and can be expressed as*

$$\zeta(m_1, ..., m_k) = \mathrm{Li}_{m_1,...,m_k}(1, ..., 1). \tag{1.190}$$

As a remark: by using the regularization techniques discussed so far, one can introduce regularized MZVs as well.

We give some elements of the kernel of the symbol map.

(i) All MZVs fulfill
$$\mathcal{S}(\zeta(m_1, ..., m_k)) = 0. \tag{1.191}$$

(ii) If there is at least one m_i *such that* $m_i \neq \pm 1$ *and* $(m_1, s_1) \neq (1, 1)$, *then*

$$\mathcal{S}(\zeta(m_1, ..., m_k; s_1, ..., s_k)) = 0. \tag{1.192}$$

(iii) Finally,
$$\mathcal{S}\left(\zeta(\underbrace{1, ..., 1}_{k}; -1, s_2, ..., s_k) - \frac{1}{k!}\log^k\left(\frac{1}{2}\right)\right) = 0. \tag{1.193}$$

Chapter 2

Integration of Symbols

2.1 Statement and Relevance of the Problem

As we have seen in the previous chapter, for example with the shuffle and stuffle relations, multiple polylogarithms fulfill a plethora of functional equations. In addition, with the symbol map we have introduced a tool that allows us to assign an algebraic object on a tensor product space of rational functions to the complicated analytic objects of the MPLs. Of central importance is the following observation: A necessary condition for the existence of a relation of the form $A = B$ between MPLs is that $\mathcal{S}(A - B) = 0$. This means that we can act at the level of the computationally much simpler tensors in order to search for functional equations of the complicated MPLs. This is explored in this chapter in a structured way following a paper by C. Duhr, H. Gangl and J. Rhodes [1]. More specifically, we consider the following problem in an algorithmic way:

Input: Some tensor of mixed weight

$$S = \sum_{k=1}^{w_{\max}} \sum_{i_1,\ldots,i_k} c^{(k)}_{i_1,\ldots,i_k} \left(R^{(k)}_{i_1} \otimes \cdots \otimes R^{(k)}_{i_k} \right), \tag{2.1}$$

where the coefficients $c^{(k)}_{i_1,\ldots,i_k}$ are rational numbers, $R^{(k)}_{i_1}, \ldots, R^{(k)}_{i_k}$ are rational functions in the variables $x_1, \ldots, x_n$ and all sums are finite.

Output: A function F which is a linear combination of MPLs and whose symbol coincides with S: $\mathcal{S}(F) = S$. In order for such a function to exist it is necessary and sufficient that ([1], p.12)

$$\sum_{i_1,\ldots,i_k} c^{(k)}_{i_1,\ldots,i_k} \left(\mathrm{d}\log(R^{(k)}_{i_j}) \wedge \mathrm{d}\log(R^{(k)}_{i_{j+1}}) \right) R^{(k)}_{i_1} \otimes \cdots \otimes \hat{R}^{(k)}_{i_j} \otimes \hat{R}^{(k)}_{i_{j+1}} \otimes R^{(k)}_{i_k} = 0 \tag{2.2}$$

for all $j \in \{1, \ldots, k\}$ and $k \in \{1, 2, \ldots, w_{\max}\}$, where the hat $\hat{\cdot}$ indicates missing factors as usual. A tensor product fulfilling this condition is called integrable.

Remark. Note that this is - except for small notational differences - just the condition for integrability from Theorem 1.1.5, since all of the differential forms $\mathrm{d}\log(R_i^{(k)})$ are closed due to $\mathrm{d}\circ\mathrm{d} = 0$. Moreover, if we recall the discussion around equation 1.186, we see that the integrability of the symbol is a necessary condition for the iterated integral associated with this symbol (i.e., F) to be a homotopy functional and thus well-defined. In other words: if the symbol were not integrable, there would be no homotopy functional F with that symbol and therefore, since MPLs are homotopy functionals, there would be no expression consisting of MPLs with that symbol, rendering the problem unsolvable.

Solving this problem is called integration of symbols. A related problem is the following: Given a special class of MPLs, is it possible to find a minimal spanning set of functions as simple as possible, so that all instances of this special class can be expressed by those basic functions?

Both problems as well as their implementation in Mathematica will be treated in this chapter and examples will be provided: a minimal spanning set of 2dHPLs in the region $0 \leq y, z \leq 1$ and $y+z \leq 1$ will be constructed and the integration algorithm will be applied to simplify the one- and two-loop helicity amplitudes for the processes $H \to ggg$ given in [36] as well as to the amplitudes describing the interference of the processes $gg \to Z\gamma$ and $gg \to H \to Z\gamma$. As a motivating example of what simplifications are possible using the algorithm, consider the following equation for weight two found by it:

$$\begin{aligned}
&- G(0;z)G(1;y) + G(1;y)G(-y;z) + G(0,1;y) - G(0,1-y;z) - G(1-y,0;z)+ \\
&\qquad + G(-y,1-y;z) = \\
&= -\mathrm{Li}_2(y+z) - \log(1-y-z)\log(z).
\end{aligned} \tag{2.3}$$

From a more general perspective, the algorithm for the integration of symbols plays an even more important role than that of simplifying already existing expressions: it is particularly important in the bootstrap method for the analytical representation of, for example, Feynman integrals. Here, using various physical constraints, one constructs an ansatz for the symbol of the quantity to be calculated, which one expects to be expressed as a linear combination of MPLs. The method of integration of symbols is then used to find the complete analytical expression. Examples of this method can be found in [17], pp.392ff., and in the references therein.

2.2 Algorithmic Approach and Implementation in Mathematica

In order to allow for easier interoperability with the popular Mathematica package PolyLogTools [37] by C. Duhr and F. Dulat, the algorithm is implemented in Mathematica as well (version 13.1). The source code itself is mostly independent of PolyLogTools; only for the numerical evaluation of polylogarithmic expressions the `Ginsh[]` function of PolyLogTools and thus ultimately the well-established GiNaC library `https://www.ginac.de/` is used. The source code developed for this thesis can be found at `https://github.com/maxlouda/IntegrationOfSymbols`.

In the following we will discuss the algorithm from [1] step by step and go into some details of the implementation.

Framework, syntax and basic functions

In order to benefit as much as possible from Mathematica's built-in functions, there are three different ways of representing symbols:

(i) As a "readable expression", which is just the mathematical standard form with the usual tensor product $\otimes$ as well as addition $+$ and scalar multiplication $\cdot$ on the tensor product space. All outputs should be converted to this form.

(ii) As a "symbolic expression", which aims to separate the addition and multiplication on the level of rational functions from the addition and scalar multiplication on the level of the tensor product space. To this end, addition, scalar multiplication and tensor products are replaced with `SymbPlus[]`, `SymbScalar[]` and `Symb[]` while addition and multiplication on the level of rational functions remain in standard notation.

(iii) In list form. Here, symbols are represented as nested lists in order to benefit from the multitude of list algorithms Mathematica provides. This list representation only works for fully flattened symbols (i.e., where the distributive law has been maximally iterated).

The functions `SymbolicExpressionToReadable[]`, `ReadableToSymbolicExpression[]`, `SymbolicExpressionToList[]` and `ListToSymbolicExpression[]` allow for transitions between those representation.

Example 2.2.1. Let us consider the symbol

$$2[(-1+y)\otimes(-1+y)\otimes(-1+y)]-(-1+y)\otimes(-1+y)\otimes z+z\otimes(-1+y)\otimes(-1+y)$$

in its "readable" form. The associated symbolic expression is given by

```
SymbPlus[SymbScalar[2, Symb[-1+y, -1+y, -1+y]],
    SymbScalar[-1, Symb[-1+y, -1+y, z]],
    SymbScalar[1, Symb[z, -1+y, -1+y]]]
```

and the associated list form is given by

```
{{2, {-1+y, -1+y, -1+y}}, {-1, {-1+y, -1+y, z}}, {1,{z, -1+y, -1+y}}}
```

with the levels of the nested list corresponding to the operations of addition, scalar multiplication and taking the tensor product.

In order to avoid name clashes with PolyLogTools, multiple polylogarithms are implemented as `G2[]`. The following functions are used to work with the objects defined above and are all implemented in the package `Symbols2.wl`:

- `FlattenSymbolicExpression[]`. This function takes a (deeply nested) symbolic expression as input and applies the distributive law as often as possible. It is called automatically, when using `SymbolicExpressionToList[]`. Example: if one calls this function on the symbolic expression

  ```
  SymbPlus[SymbScalar[1/2, Symb[a, b]], SymbScalar[-1,
      SymbPlus[SymbScalar[2, Symb[c, d]], SymbScalar[-2, Symb[a, d]]]]]
  ```

  one gets

  ```
  SymbPlus[SymbScalar[1/2, Symb[a, b]], SymbScalar[-2, Symb[c, d]],
      SymbScalar[2, Symb[a, d]]]
  ```

  as expected.

- `SymbolExpandSymb[]`. This function takes a symbolic expression as input and outputs the fully expanded version using symbol calculus. To do this, the symbolic expression is internally converted to list form and factorization functions are called on the elements. Example: The symbol

  ```
  SymbPlus[SymbScalar[2, Symb[(x^2-1)/(x+1), x/(x+1)]],
      SymbScalar[-1, Symb[1/(x-1), (x+1)/(x-1) + 1]]]
  ```

  is simplified to

  ```
  SymbPlus[SymbScalar[1, Symb[-1+x, 2]], SymbScalar[1, Symb[-1+x, x]],
      SymbScalar[-1, Symb[-1+x, -1+x]], SymbScalar[2, Symb[-1+x, x]],
      SymbScalar[-2, Symb[-1+x, 1+x]]]
  ```

  using this function.

- `SymbGSymb[]` and `SymbGFast[]`. Both functions compute the symbol of an MPL `G2[a1, ..., an, x]`. However, `SymbGFast[]` makes use of precomputed symbols of generic MPLs up to and including weight six, whereas `SymbGSymb[]` computes the symbol from scratch using the alternative recursive definition of the symbol introduced in theorem 1.3.7. Example: the symbol of `G2[0, 1-y, 0, z]` is computed to be

  ```
  SymbPlus[SymbScalar[-2, Symb[-1+y+z, -1+y, -1+y]],
      SymbScalar[-1, Symb[-1+y, -1+y, z]],
      SymbScalar[-1, Symb[-1+y, z, -1+y]],
      SymbScalar[-1, Symb[z, -1+y, z]],
      SymbScalar[-1, Symb[z, -1+y+z, -1+y]],
      SymbScalar[1, Symb[z, -1+y, -1+y]],
      SymbScalar[1, Symb[z, -1+y+z, z]],
      SymbScalar[1, Symb[-1+y+z, -1+y, z]],
      SymbScalar[1, Symb[-1+y+z, z, -1+y]],
      SymbScalar[2, Symb[-1+y, -1+y, -1+y]]]
  ```

  by both functions.

- `ShuffleSymb[]`. This function takes a list of symbolic expressions `{s1, s2, ..., sn}` and returns `s1` ⧢ `s2` ⧢ ⋯ ⧢ `sn`. It respects the linearity of the shuffle operation and is implemented using the recursive definition. Example: The shuffle of

  ```
  {Symb[a, b], SymbPlus[SymbScalar[2, Symb[b, c]], SymbScalar[-1, Symb[a, c]]]}
  ```

  turns out to be

  ```
  SymbPlus[SymbScalar[-2, Symb[a, a, b, c]],
      SymbScalar[-2, Symb[a, a, c, b]], SymbScalar[-1, Symb[a, b, a, c]],
      SymbScalar[-1, Symb[a, c, a, b]], SymbScalar[2, Symb[a, b, c, b]],
      SymbScalar[2, Symb[b, a, b, c]], SymbScalar[2, Symb[b, a, c, b]],
      SymbScalar[2, Symb[b, c, a, b]], SymbScalar[4, Symb[a, b, b, c]]]
  ```

  after applying `ShuffleSymb[]`.

- `SymbGExp[]`. This function takes as input a rational linear combination of MPLs and returns its fully simplified symbol. Since the implementation uses `SymbGFast[]` by default, it only works up to and including weight six. Example: Consider

  ```
  1/2 (-G2[0, 1, y] - G2[1, 0, y]) - G2[1, 0, z] +
      1/2 (G2[0, y] (G2[0, z] + G2[1 - y, z]) +
      G2[1, y] (G2[0, z] + G2[1 - y, z]) + G2[0, 0, y] + G2[0, 0, z] +
      G2[0, 1 - y, z] + G2[1, 1, y] + G2[1 - y, 0, z] +
      G2[1 - y, 1 - y, z]) - G2[-y, 1 - y, z]
  ```

  as a typical linear expression consisting of linear combinations and products of MPLs. Its symbol can be computed to be

  $$\begin{aligned}&-[(-1+y)\otimes y]+(-1+y)\otimes(y+z)-2[y\otimes(-1+y)]+\frac{1}{2}[y\otimes y]+\frac{1}{2}[y\otimes z]+\\&+\frac{1}{2}[y\otimes(-1+y+z)]+\frac{1}{2}[z\otimes y]-z\otimes(-1+z)+\frac{1}{2}[z\otimes z]+\\&+\frac{1}{2}[z\otimes(-1+y+z)]+\frac{1}{2}[(-1+y+z)\otimes y]+\frac{1}{2}[(-1+y+z)\otimes z]+\\&+\frac{1}{2}[(-1+y+z)\otimes(-1+y+z)]-[(-1+y+z)\otimes(y+z)+(y+z)\otimes(-1+y)]\end{aligned}$$

  using this function.

Construction of irreducible polynomials.
As a first preparatory step the tensor S of mixed weight from 2.1 has to be split into terms of pure weight: $S = S^{(1)} + \cdots + S^{(w_{\max})}$, i.e. one has to group together all terms in 2.1 with the same number of factors in the tensor product. The following steps are to be applied to each $S^{(j)}, 1 \le j \le w_{\max}$ separately. Therefore, the superscript (j) will be omitted in the future.

The actual algorithm starts with the construction of a set of irreducible polynomials which serve as the fundamental building blocks for the task of finding possible arguments. More precisely, return to equation 2.1 and factorize each rational function

$R_i \in \mathbb{Q}(x_1, ..., x_n)$ into irreducible polynomials over $\mathbb{Q}$. To do this, let $R_i = f_i/g_i$ with all common divisors already cancelled out and $f_i, g_i \in \mathbb{Q}[x_1, ..., x_n]$. Now factorize f_i and g_i into irreducible polynomials over $\mathbb{Q}$ and denote their factors by

$$\pi_1^{(f)}, ..., \pi_a^{(f)}, \pi_1^{(g)}, ..., \pi_b^{(g)} \in \mathbb{Q}[x_1, ..., x_n]. \tag{2.4}$$

The package ArgumentSearch.wl contains the function `GetPIsFromRs[]` to do this task. It takes a list of rational functions as input and outputs a list of all irreducible factors. Plugging the obtained factorizations into equation 2.1 and using the symbol calculus one can write S as follows:

$$S = \sum_{j_1,...,j_w} \tilde{c}_{j_1,...,j_w} \pi_{j_1} \otimes \cdots \otimes \pi_{j_w}. \tag{2.5}$$

This sum is finite. If the set of all irreducible polynomials is denoted by $P_S := \{\pi_1, ..., \pi_K\}$ with $K \in \mathbb{N}$, the (not necessarily fully flattened out) symbol may be viewed as an element

$$S \in \left\langle \pm \prod_{j=1}^{K} \pi_j^{n_j} \mid n_j \in \mathbb{Z} \right\rangle^{\otimes w}, \tag{2.6}$$

where we only consider rational linear combinations of pure tensors. Technical remark: the underlying set $\left\{ \pm \prod_{j=1}^{K} \pi_j^{n_j} \mid n_j \in \mathbb{Z} \right\}$ together with the usual multiplication is an abelian group (and can thus be identified with unitary $\mathbb{Z}$-module); it is however no vector space. The appropriate mathematical language to use here is therefore that of tensor products of modules, but we will not introduce it since it is not really relevant to the problem at hand. Here and in the following we will therefore use the symbol $\otimes$ only formally and associate it mainly with the underlying rules of symbol calculus rather than with the underlying space.

Example 2.2.2. Often, the symbol under consideration comes from only one special class of MPLs, which also limits the set of all irreducible polynomials that can occur to a few. These can be quickly read off from the defining alphabet (cf. definition 1.2.3), as the following two examples show.

(i) Harmonic Polylogarithms. Here, the entries σ_i in $G(\sigma_1, ..., \sigma_r; x)$ are elements of $\Sigma_{\text{HPL}} = \{-1, 0, 1\}$. Thus, only the following polynomials can occur (overall minus signs do not matter because of symbol calculus):

$$P_S^{(\text{HPL})} = \{x, 1 + x, 1 - x, 2\}. \tag{2.7}$$

(ii) 2d Harmonic Polylogarithms. In this case we have $\Sigma_{\text{2dHPL}} = \{0, 1, -z, 1 - z\}$ and the last entry is called y. Thus:

$$P_S^{(\text{2dHPL})} = \{y, z, 1 - y, 1 - z, 1 - y - z, y + z, 1 + z\}. \tag{2.8}$$

These are exactly all the pairwise differences of elements in $\Sigma_{\text{HPL}} \cup \{x\}$ or $\Sigma_{\text{2dHPL}} \cup \{z\}$ without $0, 1, -1$ and after identifying an expression with its negative. That these are the only terms that can appear in the (fully flattened out symbol) becomes clear when one considers the construction of the symbol and, in particular, equation 1.149.

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

Table 2.1: Indecomposable function types. Up to weight 6 see [1], p.20.

The next step is to form P'_S as the set of all irreducible polynomials appearing as factors in $\pi_i \pm \pi_j$ and $1 \pm \pi_i$ (again after identifying an expression with its negative and discarding $0, 1, -1$). The final set of irreducible polynomials one considers in this algorithm is given by $\overline{P_S} := P_S \cup P'_S$ and its elements are denoted by $\bar{\pi}_j,\ 1 \leq j \leq \bar{K}$. The package Argument-Search.wl contains a function `GetPIBarsFromPIs[]` which constructs $\overline{P_S}$ given the list P_S as input.

Example 2.2.3. (i) Harmonic Polylogarithms. One gets:

$$\overline{P_S}^{(\mathrm{HPL})} = \{x, 1 \pm x, 2, 3, 1 \pm 2x, x \pm 2, x \pm 3\}. \tag{2.9}$$

(ii) The result for 2d HPLs is given by

$$\begin{aligned}\overline{P_S}^{(\mathrm{2dHPL})} = \{&2, y, z, 1 \pm y, 1 \pm z, y \pm z, 1 \pm 2z, -1 + 2y, z \pm 2, y - 2,\\ &\pm 1 + y - z, \pm 1 + y + z, \pm 1 + y + 2z, -2 + y \pm z,\\ &-2 + 2y + z, 2y + z, -2 + y + 2z, -1 + y + 2z, y + 2z, -1 + 2y + 2z\}.\end{aligned} \tag{2.10}$$

Selection of function types.
In a next step the types of functions that shall appear in F (the function we seek to construct such that $\mathcal{S}(F) = S$) have to be chosen. Here, we are only interested in multiple polylogarithms $\mathrm{Li}_{m_1,\dots,m_k}(x_1, \dots, x_k)$ that are simplest in the following sense: a product of lower weight function types is simpler than function types of pure weight. In other words: we are interested only in those MPLs that cannot be reduced to (linear combinations) of products of lower weight functions.

Up to weight 6 the simplest such MPLs are given in the following table 2.1. In order to illustrate the arguments leading to the results displayed in the table, we will discuss how to come up with the four function types at weight 6.

(i) According to a conjecture ([1], p.20), MPLs $\mathrm{Li}_{m_1,\dots,m_k}(x_1, \dots, x_k)$ where at least one index m_j equals 1 are decomposable as a sum of products of MPLs where no index equals 1. Thus, e.g. $\mathrm{Li}_{1,5}(x,y)$ or $\mathrm{Li}_{1,2,3}(x,y,z)$ do not appear. Also, the maximal depth is therefore equal to three.

(ii) Because of the stuffle relation

$$\mathrm{Li}_{m_1}(x)\mathrm{Li}_{m_2}(y) = \mathrm{Li}_{m_1,m_2}(x,y) + \mathrm{Li}_{m_2,m_1}(x,y) + \mathrm{Li}_{m_1+m_2}(xy) \tag{2.11}$$

we can restrict to $\mathrm{Li}_{m_1,m_2}(x,y)$ with $m_1 \leq m_2$. For example, the function type $\mathrm{Li}_{4,2}$ can be related to $\mathrm{Li}_{2,4}$ and Li_6 (which are already in the table above) and is hence redundant.

(iii) Finally, $\mathrm{Li}_{2,2,2}(x,y,z)$ is the only depth three MPL of weight six that satisfies (i).

In the implementation, the function types have to be defined manually in the integration notebooks.

Construction of arguments.

In the next step, we use the irreducible polynomials in $\overline{P_S}$ as basic building blocks to construct the set of possible arguments. To make things more transparent, we further subdivide this task.

(i) Definition of a pool of possible arguments. Set

$$\mathcal{R}_S := \bigcup_{N\in\mathbb{N}_0} \mathcal{R}_S^{(N)} \quad \text{with} \quad \mathcal{R}_S^{(N)} := \{\pm\bar{\pi}_1^{n_1}\cdots\bar{\pi}_{\bar{K}}^{n_{\bar{K}}} \mid n_1,...,n_{\bar{K}} \in \mathbb{Z},\ |n_1|+\cdots+|n_{\bar{K}}| = N\}. \tag{2.12}$$

Then $(\mathcal{R}_S, \cdot)$ possesses the structure of an abelian group. In practice, it is impossible to work with this infinite set. One must work up to an upper bound $N_{\max}$, and in the tests performed so far this is indeed sufficient for the rest of the algorithm to work. In fact, empirically, the condition imposed on the arguments in (ii) below seems to naturally introduce a cutoff integer in the sense that there seems to be an $N^* \in \mathbb{N}_0$ such that no $f \in \mathcal{R}_S^{(n)}$ satisfies this condition for $n > N^*$. Note, however, that this cutoff integer destroys the group properties of $\mathcal{R}_S$ as the product of two elements may lie outside the set under consideration.

(ii) Restriction to suitable arguments for depth one. Recall that all depth one function types relevant to this algorithm are of the form Li_n where $n \in \mathbb{N}$. As was calculated in example 1.3.6 (ii), this leads to symbols

$$\mathcal{S}(\mathrm{Li}_n(R)) = -(1-R) \otimes \underbrace{R \otimes \cdots \otimes R}_{n-1}. \tag{2.13}$$

The goal is to construct a set of rational functions (constituting the arguments) in such a way that the symbol of all occurring functions (i.e. function types with arguments inserted) can be expressed as a tensor with factors in that same set. In particular we have to restrict the set $\mathcal{R}_S$ to

$$\mathcal{R}_S^{(1)} := \{R \in \mathcal{R}_S \mid 1 - R \in \mathcal{R}_S\}. \tag{2.14}$$

In the implementation, we use two useful facts pointed out in [1]:

- One can define a group action of S_3 (the symmetric group of order 3) on the set $\mathcal{R}_S^{(1)}$ as follows:

$$\begin{aligned} &\sigma_1(R) := R,\ \sigma_2(R) := 1-R,\ \sigma_3(R) := \frac{1}{R},\ \sigma_4(R) := \frac{1}{1-R}, \\ &\sigma_5(R) := 1-\frac{1}{R},\ \sigma_6(R) := \frac{R}{R-1}. \end{aligned} \tag{2.15}$$

  Then $(\{\sigma_1, ..., \sigma_6\}, \circ) \cong S_3$ and $\mathcal{R}_S^{(1)}$ is closed under this group action as one can easily prove. This can be used to traverse $\mathcal{R}_S^{(1)}$ much faster.

- Verifying that $1-R \in \mathcal{R}_S$ requires a factorization of polynomials and is thus computationally expensive. Consider instead ($s \in \{-1,+1\}$ and $n_i \in \mathbb{N}$):

$$R = s\frac{\bar{\pi}_1^{n_1}\cdots\bar{\pi}_l^{n_l}}{\bar{\pi}_{l+1}^{n_{l+1}}\cdots\bar{\pi}_k^{n_k}} \implies 1-R = \frac{\bar{\pi}_{l+1}^{n_{l+1}}\cdot\bar{\pi}_k^{n_k} - s\bar{\pi}_1^{n_1}\cdots\bar{\pi}_l^{n_l}}{\bar{\pi}_{l+1}^{n_{l+1}}\cdots\bar{\pi}_k^{n_k}} =: \frac{\Pi}{\bar{\pi}_{l+1}^{n_{l+1}}\cdots\bar{\pi}_k^{n_k}}. \tag{2.16}$$

  Given $\overline{P_S}$, construct prime numbers $p_1, ..., p_n$ such that $\bar{\pi}_i(p_1, ..., p_n) \neq \bar{\pi}_j(p_1, ..., p_n)$ whenever $i \neq j$. A necessary condition for $R \in \mathcal{R}_S^{(1)}$ is then given by

$$\bar{\pi}_i(p_1, ..., p_n)|\Pi(p_1, ..., p_n) \tag{2.17}$$

  for at least one $i \in \{1, ..., \bar{K}\}$, where $|$ means "divides". In fact, in the implementation three distinct sets of primes are constructed and the condition 2.17 is checked for each of them making it much stronger and reducing the number of false positives greatly.

(iii) Restriction to suitable arguments for higher depths. At this point I deviate from the presentation in [1]. There (on pages 22f.) a condition for the different function type $G_{m_1,...,m_k}$ with

$$G_{m_1,...,m_k}(x_1, ..., x_k) := G(\underbrace{0, ..., 0}_{m_1-1}, x_1, ..., \underbrace{0, ..., 0}_{m_k-1}, x_k; 1) \tag{2.18}$$

is derived, which in general is *not* equivalent to the condition for the $\mathrm{Li}_{m_1,...,m_k}$ function type, as we will see. It is important for the success of the algorithm that one always sticks to the function type chosen at the beginning, even if another one spans the same space of functions.

Similarly to above, we consider the symbol

$$\mathcal{S}(\mathrm{Li}_{m_1,...,m_k}(R_1, ..., R_k)) = (-1)^k\mathcal{S}\left(G_{m_1,...,m_k}\left(\frac{1}{R_1}, \frac{1}{R_1R_2}, ..., \frac{1}{R_1\cdots R_k}\right)\right). \tag{2.19}$$

The following proposition is of key importance.

Proposition 2.2.4. *(i) The only expressions appearing as factors in the fully flattened out symbol of $G_{m_1,...,m_k}(R_1, ..., R_k)$ are $1-R_i$ for $i \in \{1, ..., k\}$ and $R_i - R_j$ for $1 \leq i < j \leq k$ (again, overall minus signs do not matter).*

(ii) The only expressions appearing as factors in the fully flattened out symbol of $\mathrm{Li}_{m_1,...,m_k}(R_1, ..., R_k)$ *are* $1 - \prod_{i=k_1+1}^{k_2} R_i$ *with* $0 \leq k_1 < k_2 \leq k$.

Proof. (i) is a simple observation that follows immediately from the definition of the symbol map and in particular, equation 1.149. (ii) follows from (i) using the relation

$$\mathrm{Li}_{m_1,...,m_k}(R_1, ..., R_k) = (-1)^k G_{m_1,...,m_k}\left(\frac{1}{R_1}, \frac{1}{R_1 R_2}, ..., \frac{1}{R_1 \cdots R_k}\right). \tag{2.20}$$

This is, because ($0 \leq k_1 < k_2 \leq k$ with an empty product being equal to 1):

$$\frac{1}{\prod_{i=1}^{k_1} R_i} - \frac{1}{\prod_{j=1}^{k_2} R_j} = -\frac{1 - \prod_{i=k_1+1}^{k_2} R_i}{\prod_{j=1}^{k_2} R_j} \tag{2.21}$$

and the rules of symbol calculus apply. □

If one still wants that the polynomials from $\overline{P_S}$ are the fundamental building blocks for the arguments and that all symbols can be expressed as tensor products of only these, one must therefore impose the following condition on k-tuples of elements from $\mathcal{R}_S$ so that they are admissible arguments of depth k polylogarithms:

$$\mathcal{R}_S^{(k)} = \left\{ (R_1, ..., R_k) \in \mathcal{R}_S \times \cdots \times \mathcal{R}_S \;\middle|\; \forall 0 \leq k_1 < k_2 \leq k: \; 1 - \prod_{i=k_1+1}^{k_2} R_i \in \mathcal{R}_S \right\}. \tag{2.22}$$

Or, equivalently:

$$\mathcal{R}_S^{(k)} = \left\{ (R_1, ..., R_k) \in \mathcal{R}_S^{(1)} \times \cdots \times \mathcal{R}_S^{(1)} \;\middle|\; \forall 1 \leq k_1 < k_2 \leq k: \; 1 - \prod_{i=k_1}^{k_2} R_i \in \mathcal{R}_S \right\}. \tag{2.23}$$

In the implementation, the condition $1 - \prod_{i=k_1}^{k_2} R_i \in \mathcal{R}_S$ is checked numerically with the aid of suitably selected primes exactly as in (ii) before. Also, the set is closed under the following group action of S^k

$$(R_1, ..., R_k) \mapsto (R_{\rho(1)}, ..., R_{\rho(k)}), \quad \rho \in S^k, \tag{2.24}$$

which, again, allows for a faster traversal of $\mathcal{R}_S^{(k)}$.

Remark. A few remarks are in order.

- It becomes increasingly clear that the success of the algorithm depends largely on the choice of the set of irreducible polynomials. If the set is too small, not enough arguments are generated and the integration step described in the next subsection fails. If the set is too large, the rapidly growing combinatorics cause the algorithm to become unusable. In which way the set of polynomials can be chosen algorithmically optimal is an open problem to the author's knowledge. It is only clear that this set must include the set P_S of all pairwise differences of letters of the underlying class of polylogarithms, because otherwise not even all symbols for this special class can be written as tensor products of the polynomials. Moreover, in the tests performed for HPLs and 2dHPLs up to weight 4, the set of all polynomials actually needed is always a subset of $\overline{P_S}$:

$$P^{\text{HPL}} = \{2, x, 1-x, 1+x\}, \tag{2.25}$$

$$P^{\text{2dHPL}} = \{y, z, 1-y, 1-z, 1-y-z, y+z, 1+z, -1+y+2z, -1+2y+z\}. \tag{2.26}$$

Determining those polynomials, however, that must be added from P'_S to P_S for the algorithm to work is tedious.

– If instead of $\text{Li}_{m_1,...,m_k}$ one decides to use the function type $G_{m_1,...,m_k}$, the set of admissible arguments for depth k reads according to the proposition above (see also [1], p.23):

$$\mathcal{R}_S^{(k)} = \{(R_1, ..., R_k) \in \mathcal{R}_S^{(1)} \times \cdots \times \mathcal{R}_S^{(1)} \mid \forall 1 \leq i < j \leq k : \; R_i - R_j \in \mathcal{R}_S\}. \tag{2.27}$$

In this case, the action of a product group isomorphic to $S_3 \times S_k$ under which $\mathcal{R}_S^{(k)}$ is closed can be introduced as well (the S_3 component is the same as for the $\mathcal{R}_S^{(1)}$ case):

$$S_3 \times S_k : \mathcal{R}_S^{(k)} \to \mathcal{R}_S^{(k)}, \quad (\sigma, \rho) : (R_1, ..., R_k) \mapsto (\sigma(R_{\rho(1)}), ..., \sigma(R_{\rho(k)})). \tag{2.28}$$

(iv) Implementation. The following functions have been implemented to help constructing the arguments.

– `GenerateRS1[]`. This function takes two quantities as input. First, the cutoff integer $N_{\max}$ introduced in (i). For HPLs and 2dHPLs, $N_{\max} = 5$ is a choice that works well. Second, the list of irreducible polynomials one has chosen to use. It outputs a list of all admissible depth one arguments.

– `GenerateRSn[]`. This function takes the list of arguments for functions of depth one, the desired depth as well as the list of irreducible polynomials as input. A list of all admissible arguments for the functions of the desired depth is its output.

– `GenerateRSn2[]`. This function fulfills the same purpose as `GenerateRSn[]` but relies on the $G_{m_1,...,m_k}$- rather than the $\text{Li}_{m_1,...,m_k}$-function type.

Integration of symbols.

The above steps have lead to the enumeration of all possible function types for a given weight as well as arguments for a given depth. Now, appropriately combine those two results to form a finite set of functions Φ and partition Φ with respect to weight w into subsets $\Phi^{(w)} = \{b_i^{(w)}\}_i$. We now make the ansatz:

$$S = \sum_i c_i \mathcal{S}(b_i^{(w)}) + \sum_{i_1,i_2,w_1+w_2=w} c_{i_1,i_2} \mathcal{S}(b_{i_1}^{w_1} b_{i_2}^{w_2}) + \cdots + \sum_{i_1,...,i_w} c_{i_1,...,i_w} \mathcal{S}(b_{i_1}^{(1)} \cdots b_{i_w}^{(1)}). \tag{2.29}$$

The rational coefficients appearing above are to be calculated, which is essentially a linear algebra problem. To do this in a clever and not too computationally expensive way, we make use of the inductive approach described in [1].

(i) First, some general concepts have to be introduced. Define a set of linear maps Π_w, $w \in \mathbb{N}$, recursively by

$$\Pi_1 := \mathrm{id}, \tag{2.30}$$

$$\Pi_w(a_1 \otimes \cdots \otimes a_w) := \frac{w-1}{w}\left[\Pi_{w-1}(a_1 \otimes \cdots \otimes a_{w-1}) \otimes a_w - \Pi_{w-1}(a_2 \otimes \cdots \otimes a_w) \otimes a_1\right] \tag{2.31}$$

and extend by linearity. These maps possess the following properties.

Proposition 2.2.5. *Properties of* Π_w *([1], p.25).*

(i) $\Pi_w(\xi) = 0$ *if and only if* ξ *can be expressed as a linear combination of shuffle products.*

(ii) $\Pi_w \circ \Pi_w = \Pi_w$*, i.e.* Π_w *are projectors.*

In the algorithm, we only need property (i) which holds true also without the normalization constant $(w-1)/w$ appearing in the recursive definition. Thus, the package Symbols2.wl contains only the implementation of the function $\rho_w := w\Pi_w$ with the name `Proj[]`. This function takes as input a symbolic expression and outputs the result as a symbolic expression as well.

Now, let $\lambda = (\lambda_1, ..., \lambda_r)$ denote an integer partition of the weight $w \in \mathbb{N}$ with length $\ell(\lambda) = r$, i.e. $\lambda_1, ..., \lambda_r \in \mathbb{N}$ and $\sum_{i=1}^{r} \lambda_i = w$. Define the following concepts:

- λ-shuffle. It is defined by

$$\begin{aligned}\sqcup\!\sqcup_\lambda(a_1 \otimes \cdots \otimes a_w) := (a_1 \otimes \cdots \otimes a_{\lambda_1}) \sqcup\!\sqcup (a_{\lambda_1+1} \otimes \cdots \otimes a_{\lambda_1+\lambda_2}) \sqcup\!\sqcup \cdots \\ \sqcup\!\sqcup (a_{\lambda_1+\cdots+\lambda_{r-1}+1} \otimes \cdots \otimes a_w).\end{aligned} \tag{2.32}$$

  Note that the λ-shuffle can be easily implemented with the `ShuffleSymb[]` function already introduced.

- λ-projector. For $\lambda' = (\lambda'_1, ..., \lambda'_s)$ the λ'-projector is defined by

$$\Pi_{\lambda'} := \Pi_{\lambda'_1} \otimes \Pi_{\lambda'_2} \otimes \cdots \otimes \Pi_{\lambda'_s}, \tag{2.33}$$

  where the right hand side is just the usual tensor product of linear maps. In particular, it follows for $\lambda' = (w)$ that $\Pi_{\lambda'} \equiv \Pi_w$. The λ'-projector is implemented in the package Symbols2.wl under the name of `ProjLambda[]`, which takes first a symbolic expression and then a list of integers defining the desired partition as input.

An important result that is heavily used in the implementation is the following:

Proposition 2.2.6. *Properties of* Π_λ *([1], p.27). Let* λ, λ' *be non-increasing integer partitions of* $w \in \mathbb{N}$ *with lengths* $\ell(\lambda), \ell(\lambda')$*. Then it holds:*

$$\ell(\lambda') \le \ell(\lambda) \implies \Pi_{\lambda'}(\sqcup\!\sqcup_\lambda(a_1 \otimes \cdots \otimes a_w)) = 0. \tag{2.34}$$

Note that this proposition contains the last one as a special case. We make use of this fact in the following way. First, equip the set of integer partitions for a given weight with an (arbitrary) ordering $\succ$ such that the condition

$$\ell(\lambda') < \ell(\lambda) \implies \lambda' \succ \lambda \tag{2.35}$$

is met. An example of this ordering can be constructed by first sorting by length and then introducing lexicographic ordering within groups of equal length. We call this the pseudo-lexicographic ordering and denote by $\mathrm{succ}(\lambda)$ the successor of λ in this ordering. For example,

$$\begin{aligned}(6) \succ (5,1) \succ (4,2) \succ (3,3) \succ (4,1,1) \succ (3,2,1) \succ (2,2,2) \succ (3,1,1,1) \succ \\ \succ (2,2,1,1) \succ (2,1,1,1,1) \succ (1,1,1,1,1,1)\end{aligned} \tag{2.36}$$

and $\mathrm{succ}((4,2)) = (5,1)$ in this pseudo-lexicographic ordering. Up to and including weight five, the pseudo-lexicographic ordering coincides with the usual lexicographic ordering. Starting at weight six, however, they differ as can be seen from $(4,1,1) \succ_l (3,3)$ in lexicographic ordering $\succ_l$. Now, use this ordering to define a filtration of the underlying tensor product space $V^{\otimes w}$ of w-th grading: set

$$\mathcal{F}_\lambda := \langle \{\mu\text{-shuffles} \mid \lambda \succeq \mu\} \rangle_{\mathbb{Q}} \subseteq V^{\otimes w} \tag{2.37}$$

with $\langle \cdot \rangle_{\mathbb{Q}}$ denoting the linear span with rational coefficients. Clearly, these subspaces form a filtration, e.g. for $w = 6$:

$$V^{\otimes w} = \mathcal{F}_{(6)} \supseteq \mathcal{F}_{(5,1)} \supseteq \mathcal{F}_{(4,2)} \supseteq \cdots \supseteq \mathcal{F}_{(1,1,1,1,1,1)}. \tag{2.38}$$

Notice that $\mathcal{F}_\lambda \subseteq \mathrm{Kern}(\Pi_{\mathrm{succ}(\lambda)})$ for $\lambda \neq (w)$: this is because $\ell(\mathrm{succ}(\lambda)) \leq \ell(\lambda)$ and thus proposition 2.2.6 can be applied. This onion-like structure provided by the filtration and $\mathcal{F}_\lambda \subseteq \mathrm{Kern}(\Pi_{\mathrm{succ}(\lambda)})$ can be used to solve the problem of determining the rational coefficients in equation 2.29 in a efficient step-by-step manner, as is indicated in figure 2.1.

(ii) After those preparations, we finally turn to the actual integration steps. As mentioned before we use an inductive approach which starts at $\lambda = (w)$. Using proposition 2.2.6 we conclude:

$$\Pi_w(S) = \sum_i c_i \Pi_w(\mathcal{S}(b_i^{(w)})). \tag{2.39}$$

By evaluating the symbol map $\mathcal{S}$ as well as the projector Π_w and comparing the coefficients in front of the elementary tensors (i.e. solving a linear system) we can immediately deduce the coefficients c_i. This yields the first approximation $S_{\lambda=(w)} = \sum_i c_i \mathcal{S}(b_i^{(w)})$.

Induction step. Given some integer partition λ of w, assume that we have found an approximation S_λ to the true symbol S, such that $\Pi_\lambda(S - S_\lambda) = 0$. Our goal now is

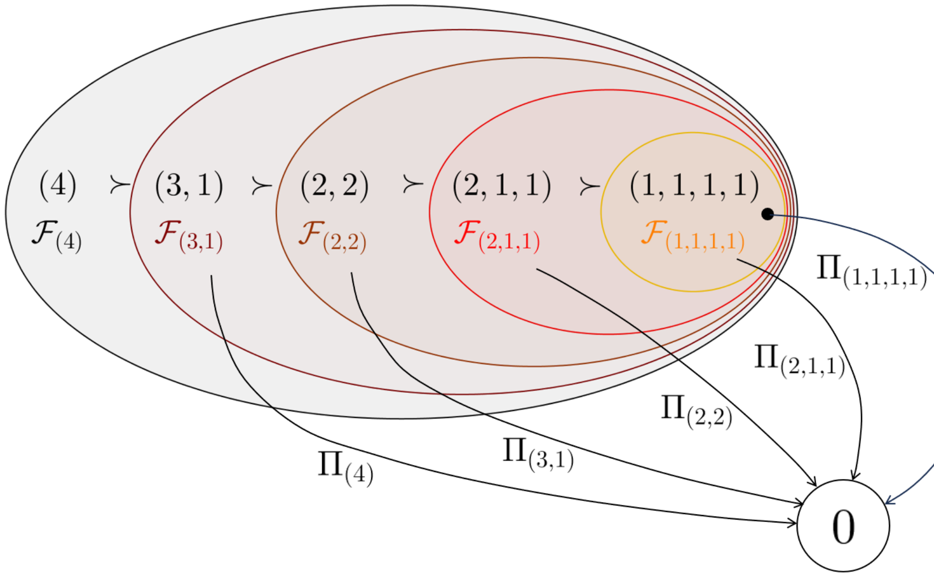

Figure 2.1: The filtration and $\mathcal{F}_\lambda \subseteq \mathrm{Kern}(\Pi_{\mathrm{succ}(\lambda)})$ are shown for $w = 4$.

to find $S_{\mathrm{pred}(\lambda)} = S_\lambda + T_{\mathrm{pred}(\lambda)}$ such that $\Pi_{\mathrm{pred}(\lambda)}(S - S_{\mathrm{pred}(\lambda)}) = 0$. Here, $\mathrm{pred}(\lambda)$ denotes the predecessor of λ. This leads to the following equation:

$$\Pi_{\mathrm{pred}(\lambda)}(S - S_\lambda) = \Pi_{\mathrm{pred}(\lambda)}(T_{\mathrm{pred}(\lambda)}) = \sum_{i_1,\ldots,i_l} c_{i_1,\ldots,i_l} \Pi_{\mathrm{pred}(\lambda)}\big(\mathcal{S}(b_{i_1}^{(\mathrm{pred}(\lambda)_1)} \cdots b_{i_l}^{(\mathrm{pred}(\lambda)_l)})\big) \tag{2.40}$$

By solving the resulting linear system, we get the coefficients and hence $S_{\mathrm{pred}(\lambda)} = S_\lambda + \sum_{i_1,\ldots,i_l} c_{i_1,\ldots,i_l} \mathcal{S}(b_{i_1}^{(\mathrm{pred}(\lambda)_1)} \cdots b_{i_l}^{(\mathrm{pred}(\lambda)_l)}))$ as our new and better approximation to the true symbol. Iterating this and assuming that each linear system has a solution (otherwise the set of functions Φ we have constructed above is too small), we get a tensor $S_{(1,\ldots,1)}$ such that $S - S_{(1,\ldots,1)} = 0$.

This inductive reconstruction of the symbol is carried out in the notebooks Integration-Weight2.nb, IntegrationWeight3.nb and IntegrationWeight4.nb. The code can be easily adapted to account for higher weights. As an example, we discuss the code for constructing $S_{(2,1)}$ given $S_{(3)}$ from IntegrationWeight3.nb in detail.

First step: Calculate $\Pi_{(2,1)}(S - S_{(3)})$. This is the left hand side of equation 2.40. If the result is already zero, one can skip this block of calculating $S_{(2,1)}$ since $S_{(3)} = S_{(2,1)}$ in this case.

```
Print["{2,1} - Computing symbols of left and right hand side."];
LHS21 = SymbolicExpressionToReadable[
   ProjLambda[ReadableToSymbolicExpression[result3], {2, 1}]];
If[LHS21 === 0, result21 = result3; functions21 = {0};
 solutions21 = {0}; indicesNotZero21 = {1};
 Print["{2,1} - No work to be done here."],
```

The next step is to collect all symbols that appear in `LHS21`. Only those functions whose symbols contain a subset of those letters from `LHS21` are considered for the next step. This increases efficiency in many cases by a significant amount, but it is not guaranteed that this procedure always works: for example, if `LHS21` already contains all letters that can occur, this step does not lead to a speedup. Second, it is also not clear that the above condition is not too strong: it may well be that functions with symbols outside the alphabet determined from `LHS21` are needed. In the tests with HPLs and 2dHPLs up to and including weight 4, this did happen on very rare occasions. For example, consider the 2dHPLs $G(1,0,-z;y)$ and $G(1,1-z,-z;y)$. While the algorithm is capable of integrating these functions individually, it fails when applied to $G(1,0,-z;y)+G(1,1-z,-z;y)$. The reason is that the symbols of these 2dHPLs contain, among others, the letter $1+z$, but the linear combination above does not, due to unfortunate term cancellations. This leads to the fact that the algorithm in its present form excludes too many functions and the subsequently introduced linear equation system has no solution. This fault can be easily fixed by commenting out the appropriate lines in the code as needed. Finally, all variables that are not needed any more, are cleared.

```
input21 =
 ReadableToSymbolicExpression[
   LHS21] /. {Symb[args__] :> List @@ (Symb /@ {args})};
goodSymbols21 = DeleteDuplicates@Cases[input21, _Symb, Infinity];
ToBeFiltered21§2 = SymbGExp2 /@ FunctionsW2D1Real;
ToBeFiltered21§1 = SymbGExp2 /@ FunctionsW1D1Real;
symbs21§2 =
 Join @@@ (Map[Cases[#, _Symb, Infinity] &,
     ToBeFiltered21§2] /. {Symb[args__] :>
      List @@ (Symb /@ {args})});
symbs21§1 =
 Join @@@ (Map[Cases[#, _Symb, Infinity] &,
     ToBeFiltered21§1] /. {Symb[args__] :>
      List @@ (Symb /@ {args})});
filteredIndices21§2 =
 Flatten[Position[Map[SubsetQ[goodSymbols21, #] &, symbs21§2],
   True]];
filteredIndices21§1 =
 Flatten[Position[Map[SubsetQ[goodSymbols21, #] &, symbs21§1],
   True]];
FunctionsW2D1Filtered = FunctionsW2D1Real[[filteredIndices21§2]];
FunctionsW1D1Filtered = FunctionsW1D1Real[[filteredIndices21§1]];
FunctionsW2D1FilteredSymbs = ToBeFiltered21§2[[filteredIndices21§2]];
FunctionsW1D1FilteredSymbs = ToBeFiltered21§1[[filteredIndices21§1]];
Clear[input21, goodSymbols21, ToBeFiltered21§1, ToBeFiltered21§2,
 symbs21§2, symbs21§1, filteredIndices21§1, filteredIndices21§2];
```

Now, compute the right hand side of equation 2.40.

```
RHS21 = Expand[
   Sum[Indexed[c, {k, l}]*
     SymbolicExpressionToReadable[
      ProjLambda[
       ShuffleSymb[{FunctionsW2D1FilteredSymbs[[k]],
          FunctionsW1D1FilteredSymbs[[l]]}] /. {SymbPlus[args__] :>
          SymbPlus @@ (Replace[{args},
             a_ /; Head[a] =!= SymbScalar :>
              SymbScalar[1, a], {1}])}, {2, 1}]],
     {k, 1, Length[FunctionsW2D1Filtered]},
     {l, 1, Length[FunctionsW1D1Filtered]}]];
```

As a next step, we extract the set of linear equations for the coefficients by comparing the coefficients of the symbols appearing in `LHS21` and `RHS21`. Furthermore, we exclude those equations that are obviously linearly dependent on already existing ones.

```
Print["{2,1} - Setting up equations."];
vars21 =
  Flatten[Table[
    Indexed[c, {k, l}], {k, 1, Length[FunctionsW2D1Filtered]}, {l, 1,
     Length[FunctionsW1D1Filtered]}]];
res21 = GroupBy[SymbolicExpressionToList[RHS21 - LHS21], Extract[{2}]];
Clear[RHS21, LHS21];
res21 = KeyValueMap[
   Function[{key, value}, {Total[value[[All, 1]]], key}], res21];
res21 = DeleteDuplicates[res21,
   Or[First[#1] === First[#2], First[#1] === -First[#2]] &];
eqns21 = res21[[All, 1]];
```

Now, this system of linear equations is solved using `LinearSolve[]`. If there is an error, the algorithm aborts.

```
Print["{2,1} - Solving equations."];
mat21 = Normal@CoefficientArrays[eqns21, vars21][[2]];
b21 = -Map[
    Function[{elem},
     Total[Select[If[Head[elem] === Plus, List @@ elem, {elem}],
       FreeQ[#, _Indexed | _Plus] &]]], eqns21];
solutions21 = Check[LinearSolve[mat21, b21], $Failed];
If[solutions21 === $Failed,
  Print["{2,1} - Linear system encountered that has no solution."];
  Clear[res21, eqns21, mat21, b21, vars21,
   FunctionsW2D1FilteredSymbs, FunctionsW1D1FilteredSymbs];
  Return[];];
Clear[res21, eqns21, mat21, b21, vars21, FunctionsW2D1FilteredSymbs,
  FunctionsW1D1FilteredSymbs];
```

In a last step the new symbol $S_{(2,1)}$ is constructed and it is tested whether or not the constructed symbol matches $\Pi_{(2,1)}(S - S_{(3)})$. If the test yields a positive result, $S - S_{(3)} - S_{(2,1)}$ (called `result21`) is formed for a new iteration.

```
Print["{2,1} - Extracting functions and checking result."];
  indicesNotZero21 = Flatten[Position[solutions21, x_ /; x != 0]];
  functions21 =
    Flatten[Table[
       GProduct[FunctionsW2D1Filtered[[k]],
        FunctionsW1D1Filtered[[l]]], {k, 1,
        Length[FunctionsW2D1Filtered]}, {l, 1,
        Length[FunctionsW1D1Filtered]}], 1][[indicesNotZero21]];
  symb21 =
    Simplify[
     Sum[solutions21[[indicesNotZero21]][[i]]*
       SymbolicExpressionToReadable[SymbGExp[functions21[[i]]]], {i,
       1, Length[indicesNotZero21]}]];
  checkSymb21 = ProjLambda[symb21, {2, 1}];
  If[Simplify[
      SymbolicExpressionToReadable[checkSymb21] -
       SymbolicExpressionToReadable[ProjLambda[result3, {2, 1}]]] === 0,
     Print["{2,1} - Constructed symbol matches given symbol."],
    Print["{2,1} - Constructed symbol does not match given symbol."]];
  result21 = Simplify[result3 - symb21];
  Clear[checkSymb21, symb21, FunctionsW2D1Filtered,
    FunctionsW1D1Filtered];];
```

Reconstruction of elements of the symbol-kernel.
At first, one might think that the task of integration of symbols would be solved after one has successfully reconstructed $S_{(1,\dots,1)} = S$ and that

$$F = \sum_i c_i b_i^{(w)} + \sum_{i_1,i_2,w_1+w_2=w} c_{i_1,i_2} b_{i_1}^{w_1} b_{i_2}^{w_2} + \cdots + \sum_{i_1,\dots,i_w} c_{i_1,\dots,i_w} b_{i_1}^{(1)} \cdots b_{i_w}^{(1)}. \tag{2.41}$$

with the now known rational coefficients can be set. However, due to non-trivial elements in the kernel of the symbol-map this is generally wrong. So one has to find a way to reconstruct these elements. For the remainder of this section, denote the result 2.41 of fitting functions to the known symbol by F_0.

To this end and further following the ideas presented in [1], I have implemented two different methods in the IntegrationWeight2-4.nb notebooks. Both methods need that the values of the function F one tries to construct are known at least for some specific instances of the variables. In the case of the applications considered here (see next chapter), it is even known everywhere on its domain.

The first one relies on the Mathematica implementation `FindIntegerNullVector[{x1, ..., xn}, d]` ($x_i \in \mathbb{R}$) of the celebrated PSLQ-algorithm [38] which allows one to find $a_1, ..., a_n \in \mathbb{Z}$ such that

$$\sum_{i=1}^{n} a_i x_i = 0 \quad \text{and} \quad \sum_{i=1}^{n} a_i^2 < d^2. \tag{2.42}$$

More specifically, an ansatz of possible functions of fixed weight in the kernel of the symbol is generated relying on the results of theorem 1.3.8 (ζ_n is ascribed the weight n). Then, using `Ginsh[]` from PolyLogTools, the difference $F - F_0$ as well as all candidate functions from the ansatz are evaluated at some random point and the PSLQ-algorithm is used to find an integer relation between those real numbers and thus find the fully reconstructed function. As the PSLQ-algorithm may fail for some instances of random points, a while-loop is used to eventually produce a valid list of integers. At the end it is numerically checked with high precision whether our result evaluated at some new random points is different from the input function evaluated at the same points or not. If not, the integration algorithm was successful. The code (for weight 4) is shown below:

```
CandidatesW4 =
  DeleteDuplicates[
   Join[Flatten[
     Outer[Times, SymbolKernelW2,
      Join[SpanningSetW2D1HPL2d /. {G2 -> G},
       Times @@@ Tuples[SpanningSetW1D1HPL2d /. {G2 -> G}, {2}]]]],
    Flatten[Outer[Times, SymbolKernelW3,
      SpanningSetW1D1HPL2d /. {G2 -> G}]], SymbolKernelW4]];
Region2D = Triangle[{{0, 0}, {0, 1}, {1, 0}}];
boolean = True; idx = 1; resIntegers = {}; cutoff = 20;
While[And[boolean, idx < cutoff],
 TestYZs = RandomPoint[Region2D, idx];
 GinshCandidatesW42d =
  Table[Ginsh[#, {y -> TestYZs[[k, 1]], z -> TestYZs[[k, 2]]},
      PrecisionGoal -> 100] & /@ CandidatesW4, {k, 1,
    Length[TestYZs]}];
 ToFindW42d =
  Table[Ginsh[
    FGivenInGinshForm - resfinalInGinshForm, {y -> TestYZs[[k, 1]],
     z -> TestYZs[[k, 2]]}, PrecisionGoal -> 100], {k, 1,
    Length[TestYZs]}];
 Do[resIntegers =
   Join[resIntegers, {Quiet[
      Check[FindIntegerNullVector[
        Join[GinshCandidatesW42d[[i]], {-ToFindW42d[[i]]}], 5000,
        WorkingPrecision -> 80], $Failed]]}], {i, 1, idx}];
 If[Complement[resIntegers, Table[$Failed, {i, 1, idx}]] === {}, idx++,
   boolean = False]]
If[idx == cutoff,
```

```
 Print["PSLQ failed."]; Abort[], Print["PSLQ succeeded."]]
resIntegers = FirstCase[resIntegers, _List];
resIntegers = Delete[1/resIntegers[[-1]]*resIntegers, -1];
FinalFunction = resfinalInGinshForm + resIntegers . CandidatesW4
TestYZs2 = RandomPoint[Region2D, 5];
If[Abs[Total[
    Table[Ginsh[#, {y -> TestYZs2[[k, 1]], z -> TestYZs2[[k, 2]]},
        PrecisionGoal -> 100] & /@ (FGivenInGinshForm -
        FinalFunction), {k, 1, Length[TestYZs2]}]]] < 10^(-90),
 Print["Integration suceeded."], Print["Integration failed."]]
Clear[CandidatesW4, Region2D, boolean, idx, resIntegers, TestYZs,
 GinshCandidatesW42d, ToFindW42d, cutoff]
```

The second method relies on the built-in functions `LinearSolve[]`, `Rationalize[]` and `LatticeReduce[]`, is typically slower than the first one and is included only for legacy reasons (the construction of the minimal spanning set has been done with this second method) and for the case that the first method fails. We will not discuss it any further.

Chapter 3

Applications

3.1 A Minimal Spanning Set for HPLs and 2dHPLs

As a first step, we construct minimal spanning sets for HPLs and 2dHPLs up to and including weight 4 consisting of relatively simple functions: classical polylogarithms Li_n and the single MPL $\mathrm{Li}_{2,2}$. The HPL-case has already been carried out in [1] and we aim to reproduce this result, the 2dHPL-case has not been covered yet using this method of integration of symbols (however, related results exist, e.g. in [2] and [3]). The basic procedure of obtaining such a minimal spanning set of a special class of MPLs is as follows:

(i) Collect all instances of the special class under consideration up to the desired weight that we want to express through the minimal spanning set. The following two tables show those for the case of HPLs (table 3.1) and 2dHPLs (table 3.2).

(ii) Define the set of functions Φ that is used for the integration algorithm (see last chapter). One can at least indirectly specify preferences which functions Mathematica should select in the probable case that the linear system appearing in the integration step is underdetermined: For example, preference should be given to arguments that are, in some sense, as simple as possible, so one sorts the functions from Φ in such a way that those with the simplest arguments are at the top of the corresponding list. As I have found out by testing, this leads to the effect that when solving an underdetermined system of equations (whose solution is not unique), Mathematica preferably selects the functions that have the simplest possible arguments. For numerical reasons, it is also advantageous if the arguments take values in the interval

Weight 1	$H(0;x)$, $H(1;x)$, $H(-1;x)$
Weight 2	$H(0,1;x)$, $H(0,-1;x)$, $H(-1,1;x)$
Weight 3	$H(-1,1,-1;x)$, $H(-1,1,1;x)$, $H(0,-1,-1;x)$, $H(0,-1,1;x)$, $H(0,0,-1;x)$, $H(0,0,1;x)$, $H(0,1,-1;x)$
Weight 4	$H(-1,1,-1,-1;x)$, $H(-1,1,-1,1;x)$, $H(0,-1,-1,-1;x)$, $H(0,-1,-1,1;x)$, $H(0,-1,1,-1;x)$, $H(0,-1,1,1;x)$, $H(0,0,-1,-1;x)$, $H(0,0,-1,1;x)$, $H(0,0,0,-1;x)$, $H(0,0,0,1;x)$, $H(0,0,1,-1;x)$, $H(0,1,-1,-1;x)$, $H(0,1,-1,1;x)$, $H(0,1,0,-1;x)$, $H(0,1,0,1;x)$, $H(0,1,1,-1;x)$, $H(0,1,1,1;x)$

Table 3.1: HPLs up to and including weight 4 ([1], p.63ff.) Only a subset of all possible HPLs is shown; the rest can be obtained via shuffle relations.

Weight 1	$G(0;y)$, $G(1;y)$, $G(1-z;y)$, $G(-z;y)$
Weight 2	$G(0,1;y)$, $G(0,1-z;y)$, $G(0,-z;y)$, $G(1-z,1;y)$, $G(-z,1;y)$, $G(-z,1-z;y)$
Weight 3	$G(0,0,1;y)$, $G(0,1,1;y)$, $G(0,0,1-z;y)$, $G(0,1-z,1-z;y)$, $G(0,0,-z;y)$, $G(0,-z,-z;y)$, $G(0,1-z,1;y)$, $G(1-z,0,1;y)$, $G(1-z,1,1;y)$, $G(1-z,1-z,1;y)$, $G(0,-z,1;y)$, $G(-z,0,1;y)$, $G(-z,1,1;y)$, $G(-z,-z,1;y)$, $G(0,-z,1;y)$, $G(-z,0,1;y)$, $G(-z,1,1;y)$, $G(-z,-z,1;y)$, $G(1-z,-z,1;y)$, $G(-z,1-z,1;y)$
Weight 4	$G(0,0,0,1;y)$, $G(0,0,1,1;y)$, $G(0,1,1,1;y)$, $G(0,0,0,1-z;y)$ $G(0,0,1-z,1-z;y)$, $G(0,1-z,1-z,1-z;y)$, $G(0,0,0,-z;y)$ $G(0,0,-z,-z;y)$, $G(0,-z,-z,-z;y)$, $G(0,0,1-z,1;y)$, $G(0,1,1-z,1;y)$, $G(0,1-z,0,1;y)$, $G(0,1-z,1,1;y)$, $G(0,1-z,1-z,1;y)$, $G(1-z,0,0,1;y)$, $G(1-z,0,1,1;y)$, $G(1-z,0,1-z,1;y)$, $G(1-z,1,1,1;y)$, $G(1-z,1-z,0,1;y)$, $G(1-z,1-z,1,1;y)$, $G(1-z,1-z,1-z,1;y)$, $G(0,0,-z,1;y)$, $G(0,1,-z,1;y)$, $G(0,-z,0,1;y)$, $G(0,-z,1,1;y)$, $G(0,-z,-z,1;y)$, $G(-z,0,0,1;y)$, $G(-z,0,1,1;y)$, $G(-z,0,-z,1;y)$, $G(-z,1,1,1;y)$, $G(-z,-z,0,1;y)$, $G(-z,-z,1,1;y)$, $G(-z,-z,-z,1;y)$, $G(0,0,-z,1-z;y)$, $G(0,1-z,-z,1-z;y)$, $G(0,-z,0,1-z;y)$, $G(0,-z,1-z,1-z;y)$, $G(0,-z,-z,1-z;y)$, $G(-z,0,0,1-z;y)$, $G(-z,0,1-z,1-z;y)$, $G(-z,0,-z,1-z;y)$, $G(-z,1-z,1-z,1-z;y)$, $G(-z,-z,0,1-z;y)$, $G(-z,-z,1-z,1-z;y)$, $G(-z,-z,-z,1-z;y)$, $G(0,1-z,-z,1;y)$, $G(0,-z,1-z,1;y)$, $G(1-z,0,-z,1;y)$, $G(1-z,1-z,-z,1;y)$, $G(1-z,-z,0,1;y)$, $G(1-z,-z,1,1;y)$, $G(1-z,-z,1-z,1;y)$, $G(1-z,-z,-z,1;y)$, $G(-z,0,1-z,1;y)$, $G(-z,0,-z,1;y)$, $G(-z,1,1-z,1;y)$, $G(-z,1-z,0,1;y)$, $G(-z,1-z,1,1;y)$, $G(-z,1-z,1-z,1;y)$, $G(-z,1-z,-z,1;y)$, $G(-z,-z,1-z,1;y)$

Table 3.2: 2dHPLs up to and including weight 4 ([26], p.6). Again, not all 2dHPLs are shown but only those that cannot be reduced by so-called integration by parts identities.

$(-1,1)$. Finally, if the function one wants to reconstruct is real-valued on the domain under consideration, it is a good heuristic to use only the real-valued functions from Φ.

(iii) Now, for all elements of the considered special class of MPLs (see tables 3.1 and 3.2), starting with the smallest weight (typically $w=2$, since $w=1$ is trivial), one runs the integration algorithm. In the process, all occurring functions needed for the integration are collected. If one advances to the next weight $w+1$, it is advisable for performance reasons and does not lead to errors in the performed tests, that one replaces the functions from Φ with the weight w by the just constructed basis functions of the same weight. In this way one can generate a spanning set step by step. Note that the spanning set is not unique.

(iv) Finally, we have to make sure that the found spanning set (including the appropriate elements of the kernel of the symbol-map) denoted by

$$\mathcal{B} = \bigcup_{w} \mathcal{B}_{(w)} \tag{3.1}$$

is indeed a minimal spanning set and, if necessary, reduce the found spanning set as much as possible. By minimal, we mean here that for each weight w, the set of functions

$$\mathcal{C}_{(w)} := \bigcup_{l\geq 1} \bigcup_{w_1,\ldots,w_l \geq 1} \mathcal{B}_{(w_1)} \odot \cdots \odot \mathcal{B}_{(w_l)} \delta_{w,w_1+\cdots+w_l} \tag{3.2}$$

is linearly independent over $\mathbb{Q}$ (where $\mathcal{A} \odot \mathcal{B} := \{ab \mid a \in \mathcal{A},\ b \in \mathcal{B}\}$). For very low weights ($w = 2$ and maybe $w = 3$) this can be explicitly checked by numerical evaluation at random points and using the PSLQ-algorithm. However, the cardinality of $\mathcal{C}_{(w)}$ grows extremely fast and this notion of minimality cannot be checked explicitly anymore.

However, under the well-motivated assumption that the algorithm works as it should, we can use it itself to check for minimality. For this, take an $f \in \mathcal{B}$ with weight w, set $\Phi = \mathcal{B} \setminus \{f\}$ and try to apply the integration algorithm to f. Under the above assumption, the algorithm succeeds if and only if $\mathcal{C}_{(w)}$ is linearly dependent because in the case of success, f can be written as a nontrivial linear combination of elements from $\mathcal{C}_{(w)} \setminus \{f\}$. In order to reduce the spanning set to a minimal one, one has to iterate over $\mathcal{B}$, apply the algorithm, check for success, update $\mathcal{B} \leftarrow \mathcal{B} \setminus \{f\}$ in case f could be integrated using functions from $\mathcal{B} \setminus \{f\}$ and repeat. The minimal spanning set is not unique, either (its cardinality, however, is).

Performing the algorithm just discussed for HPLs results in the minimal spanning set shown in table 3.3. Here, the first iteration of the algorithm additionally returned the function $\mathrm{Li}_4\left(\frac{(-1+x)^2}{(1+x)^2}\right)$. However, since this function satisfies for $x \in [0, 1]$ the equation

$$\mathrm{Li}_4\left(\frac{(-1+x)^2}{(1+x)^2}\right) = 8\mathrm{Li}_4\left(\frac{1-x}{1+x}\right) + 8\mathrm{Li}_4\left(\frac{-1+x}{1+x}\right) \tag{3.3}$$

it can be excluded from the spanning set. There are no more relations found by the algorithm, so we get the minimal spanning set. Comparing this with the already known result from [1], pp.31ff., two things stand out: first, some of the basis functions differ, which underlines that the minimal spanning set is not unique. Second, the cardinalities of $\mathcal{B}_{(w)}$ for all $w \in \{1, 2, 3, 4\}$ coincide with those of [1], as was to be expected.

A completely analogous procedure leads to the minimal spanning set for the two-dimensional harmonic polylogarithms shown in Table 3.4. Both the spanning set for the HPLs and that for the 2dHPLs are contained in the Mathematica notebook Integration-Weight4.nb.

3.2 Simplification of Helicity Amplitudes for $H \to ggg$.

As a further application, let us now simplify those parts of the one- and two-loop helicity amplitudes of the decay of the Higgs boson into three gluons $H \to ggg$ where MPLs oc-

$w=1$	$\log(x)$, $\log(1-x)$, $\log(1+x)$, $\log(2)$
$w=2$	$\mathrm{Li}_2(x)$, $\mathrm{Li}_2(-x)$, $\mathrm{Li}_2\left(\frac{1-x}{2}\right)$
$w=3$	$\mathrm{Li}_3(x)$, $\mathrm{Li}_3(-x)$, $\mathrm{Li}_3(1-x)$, $\mathrm{Li}_3(1-x^2)$, $\mathrm{Li}_3\left(\frac{1-x}{2}\right)$, $\mathrm{Li}_3\left(\frac{1+x}{2}\right)$, $\mathrm{Li}_3\left(\frac{1}{1+x}\right)$, $\mathrm{Li}_3\left(\frac{-1+x}{2x}\right)$
$w=4$	$\mathrm{Li}_4(x)$, $\mathrm{Li}_4(-x)$, $\mathrm{Li}_4(1-x)$, $\mathrm{Li}_4(1-x^2)$, $\mathrm{Li}_4\left(\frac{1+x}{2}\right)$, $\mathrm{Li}_4\left(\frac{1-x}{2}\right)$, $\mathrm{Li}_4\left(\frac{1}{1+x}\right)$, $\mathrm{Li}_4\left(\frac{x}{1+x}\right)$, $\mathrm{Li}_4\left(\frac{-1+x}{x}\right)$, $\mathrm{Li}_4\left(\frac{-1+x}{1+x}\right)$, $\mathrm{Li}_4\left(\frac{1-x}{1+x}\right)$, $\mathrm{Li}_4\left(\frac{-1+x}{2x}\right)$, $\mathrm{Li}_4\left(1-\frac{1}{x^2}\right)$, $\mathrm{Li}_4\left(\frac{4x}{(1+x)^2}\right)$, $\mathrm{Li}_4\left(-\frac{(-1+x)^2}{4x}\right)$, $\mathrm{Li}_{2,2}(-1,x)$, $\mathrm{Li}_{2,2}\left(2,\frac{-1+x}{2x}\right)$, $\mathrm{Li}_{2,2}\left(\frac{-1+x}{1+x},\frac{1-x}{1+x}\right)$

Table 3.3: A minimal spanning set for HPLs up to and including weight 4.

cur. These form factors have been derived in [36] within an effective theory with infinite top quark mass. The calculations from this paper show that all appearing MPLs belong to the special class of 2dHPLs. Thus, we can use the minimal spanning set derived in the last section. In [31] it was shown with the help of the coproduct that the classical polylogarithms suffice here. We want to reproduce this result with the help of the integration of symbols algorithm. As a starting point, we use the expressions contained in the files `FiniteRemainder/Hggg/alpha.m` and `FiniteRemainder/Hggg/beta.m` which can be found in the supplementary material to [36]. That part of the amplitudes which is to be studied here consists of a linear combination of two-dimensional harmonic polylogarithms of mixed weight, where the coefficients may be rational functions in the variables y, z. As a first step towards simplification, those rational functions must be put into a standard form consisting of a common set of irreducible rational functions. In this way, one can ensure that no relations between MPLs, which can be used to simplify the amplitudes, are obscured by an unfavorable form of the coefficients. As a simple but instructive example, consider the following expression:

$$\frac{3y-2y^2+z-2yz}{(1-y-z)(y+z)}G(0,-z;y)+\frac{2y}{y+z}G(-z,0;y). \tag{3.4}$$

It can lead to suboptimal results if one directly applies the integration algorithm to $G(0,-z;y)$ and $G(-z,0;y)$ as this results in

$$\frac{3y-2y^2+z-2yz}{(1-y-z)(y+z)}\mathrm{Li}_2\left(-\frac{y}{z}\right)+\frac{2y}{y+z}\left(\mathrm{Li}_2\left(-\frac{y}{z}\right)-\log(y)\log(z)+\log(y)\log(y+z)\right). \tag{3.5}$$

If instead we first apply the function `MultivariateApart[]` of the Mathematica package MultivariateApart by M. Heller and A. von Manteuffel [39] to the rational functions, we

$w=1$	$\log(y)$, $\log(1-y)$, $\log(z)$, $\log(1-z)$, $\log(1+z)$, $\log(y+z)$, $\log(1-y-z)$
$w=2$	$\mathrm{Li}_2(y)$, $\mathrm{Li}_2(z)$, $\mathrm{Li}_2(-z)$, $\mathrm{Li}_2(y+z)$, $\mathrm{Li}_2\left(-\frac{y}{z}\right)$, $\mathrm{Li}_2\left(\frac{1-y}{1+z}\right)$, $\mathrm{Li}_2\left(\frac{-1+y+z}{y}\right)$, $\mathrm{Li}_2\left(\frac{-1+y+z}{z}\right)$
$w=3$	$\mathrm{Li}_3(y)$, $\mathrm{Li}_3(z)$, $\mathrm{Li}_3(-z)$, $\mathrm{Li}_3(1-y)$, $\mathrm{Li}_3(1-z)$, $\mathrm{Li}_3(y+z)$, $\mathrm{Li}_3(1-y-z)$, $\mathrm{Li}_3(1-z^2)$, $\mathrm{Li}_3\left(\frac{y}{1-z}\right)$, $\mathrm{Li}_3\left(\frac{z}{1-y}\right)$, $\mathrm{Li}_3\left(\frac{-1+y+z}{y}\right)$, $\mathrm{Li}_3\left(\frac{-1+y+z}{z}\right)$, $\mathrm{Li}_3\left(-\frac{y}{z}\right)$, $\mathrm{Li}_3\left(\frac{y}{y+z}\right)$, $\mathrm{Li}_3\left(\frac{1}{1+z}\right)$, $\mathrm{Li}_3\left(\frac{1-y}{1+z}\right)$, $\mathrm{Li}_3\left(\frac{-1+y}{y+z}\right)$, $\mathrm{Li}_3\left(\frac{yz}{(1-y)(1-z)}\right)$, $\mathrm{Li}_3\left(\frac{-1+y+z}{yz}\right)$, $\mathrm{Li}_3\left(\frac{(-1+y)z}{y(1+z)}\right)$, $\mathrm{Li}_3\left(\frac{y(1+z)}{y+z}\right)$, $\mathrm{Li}_3\left(\frac{z(-1+y+z)}{y}\right)$, $\mathrm{Li}_3\left(\frac{y}{(1-z)(y+z)}\right)$, $\mathrm{Li}_3\left(\frac{(1+z)(1-y-z)}{1-y}\right)$, $\mathrm{Li}_3\left(\frac{(1+z)(-1+y+z)}{z(y+z)}\right)$
$w=4$	$\mathrm{Li}_4(y)$, $\mathrm{Li}_4(z)$, $\mathrm{Li}_4(-z)$, $\mathrm{Li}_4(1-y)$, $\mathrm{Li}_4(1-z)$, $\mathrm{Li}_4(1-y-z)$, $\mathrm{Li}_4(y+z)$, $\mathrm{Li}_4(1-z^2)$, $\mathrm{Li}_4\left(\frac{1}{1+z}\right)$, $\mathrm{Li}_4\left(\frac{-1+y}{y}\right)$, $\mathrm{Li}_4\left(\frac{1-y}{1+z}\right)$, $\mathrm{Li}_4\left(\frac{y}{1-z}\right)$, $\mathrm{Li}_4\left(\frac{-1+z}{z}\right)$, $\mathrm{Li}_4\left(\frac{y}{y+z}\right)$, $\mathrm{Li}_4\left(\frac{z}{y+z}\right)$, $\mathrm{Li}_4\left(\frac{z}{1+z}\right)$, $\mathrm{Li}_4\left(\frac{-1+y}{y+z}\right)$, $\mathrm{Li}_4\left(\frac{z}{1-y}\right)$, $\mathrm{Li}_4\left(\frac{z(-1+y)}{y(1+z)}\right)$, $\mathrm{Li}_4\left(\frac{yz}{(1-y)(1-z)}\right)$, $\mathrm{Li}_4\left(\frac{1-y-z}{1-y}\right)$, $\mathrm{Li}_4\left(\frac{y+z}{1+z}\right)$, $\mathrm{Li}_4\left(\frac{-1+y+z}{y}\right)$, $\mathrm{Li}_4\left(\frac{z(1-y)}{y+z}\right)$, $\mathrm{Li}_4\left(\frac{1-y-z}{1-z}\right)$, $\mathrm{Li}_4\left(\frac{-1+y+z}{y+z}\right)$, $\mathrm{Li}_4\left(\frac{1-y-z}{(1-y)(1-z)}\right)$, $\mathrm{Li}_4\left(\frac{-1+y+z}{z}\right)$, $\mathrm{Li}_4\left(\frac{-1+y+z}{yz}\right)$, $\mathrm{Li}_4\left(-\frac{y}{z}\right)$, $\mathrm{Li}_4\left(\frac{y(1+z)}{y+z}\right)$, $\mathrm{Li}_4\left(\frac{z(-1+y+z)}{y}\right)$, $\mathrm{Li}_4\left(\frac{y}{(1-z)(y+z)}\right)$, $\mathrm{Li}_4\left(\frac{z(1-y-z)}{(1-z)(y+z)}\right)$, $\mathrm{Li}_4\left(1-\frac{1}{z^2}\right)$, $\mathrm{Li}_4\left(\frac{y(-1+y+z)}{z}\right)$, $\mathrm{Li}_4\left(\frac{z}{(1-y)(y+z)}\right)$, $\mathrm{Li}_4\left(\frac{y(1-y-z)}{(1-y)(y+z)}\right)$, $\mathrm{Li}_4\left(\frac{z(y+z)}{1-y}\right)$, $\mathrm{Li}_4\left(\frac{(1+z)(1-y-z)}{1-y}\right)$, $\mathrm{Li}_4\left(\frac{(1+z)(-1+y+z)}{z(y+z)}\right)$, $\mathrm{Li}_{2,2}\left(y, \frac{z}{-1+y+z}\right)$, $\mathrm{Li}_{2,2}\left(y, -\frac{1}{z}\right)$, $\mathrm{Li}_{2,2}\left(y, -\frac{z}{y}\right)$, $\mathrm{Li}_{2,2}\left(y, \frac{-1+y+z}{z}\right)$, $\mathrm{Li}_{2,2}\left(z, \frac{y}{z(-1+y+z)}\right)$, $\mathrm{Li}_{2,2}\left(z, \frac{-1+y+z}{y}\right)$, $\mathrm{Li}_{2,2}\left(-z, \frac{-1+y+z}{z}\right)$, $\mathrm{Li}_{2,2}\left(-z, \frac{y+z}{-1+y}\right)$ $\mathrm{Li}_{2,2}\left(1-y, \frac{1}{1+z}\right)$, $\mathrm{Li}_{2,2}\left(1-y, \frac{z}{1-y}\right)$, $\mathrm{Li}_{2,2}\left(1-y, \frac{z}{y+z}\right)$, $\mathrm{Li}_{2,2}\left(1-z, \frac{y}{(1-z)(y+z)}\right)$, $\mathrm{Li}_{2,2}\left(1+z, \frac{1-y-z}{1-y}\right)$, $\mathrm{Li}_{2,2}\left(1-z^2, \frac{y}{(1-z)(y+z)}\right)$, $\mathrm{Li}_{2,2}\left(1-z^2, \frac{1-y-z}{(1-y)(1-z)}\right)$, $\mathrm{Li}_{2,2}\left(\frac{1-z}{y}, y\right)$, $\mathrm{Li}_{2,2}\left(\frac{y+z}{y(1+z)}, y\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1-z}, y\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{y+z}, y\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1-y}, z\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{y+z}, z\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1-z^2}, 1-z\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1+z}, y+z\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1-z}, 1-y-z\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1-y}, 1-y-z\right)$, $\mathrm{Li}_{2,2}\left(-\frac{1}{z}, 1-y-z\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{z}, z^2\right)$, $\mathrm{Li}_{2,2}\left(\frac{y}{-1+y}, \frac{z}{-1+z}\right)$, $\mathrm{Li}_{2,2}\left(\frac{-1+y}{y}, \frac{z}{1+z}\right)$, $\mathrm{Li}_{2,2}\left(\frac{z}{-1+z}, \frac{-1+y+z}{y+z}\right)$, $\mathrm{Li}_{2,2}\left(\frac{1}{1-y}, \frac{z}{y+z}\right)$, $\mathrm{Li}_{2,2}\left(\frac{y}{-1+y}, \frac{-1+y+z}{y+z}\right)$, $\mathrm{Li}_{2,2}\left(1-\frac{1}{z^2}, \frac{z(1-y-z)}{(1-z)(y+z)}\right)$, $\mathrm{Li}_{2,2}\left(\frac{1+z}{z}, \frac{-1+y+z}{y+z}\right)$

Table 3.4: A minimal spanning set for 2dHPLs up to and including weight 4.

obtain the following manifestly simpler result:

$$
\begin{aligned}
&\left(\frac{2y}{y+z}+\frac{1}{1-y-z}\right)G(0,-z;y)+\frac{2y}{y+z}G(-z,0;y)= \\
&\quad=\frac{2y}{y+z}(G(0,-z;y)+G(-z,0;y))+\frac{1}{1-y-z}G(0,-z;y)= \\
&\quad=\frac{2y}{y+z}(\log(y)\log(y+z)-\log(y)\log(z))+\frac{1}{1-y-z}\mathrm{Li}_2\left(-\frac{y}{z}\right).
\end{aligned}
\tag{3.6}
$$

For more complicated expressions, one should be careful to always use the same list of irreducible denominator factors for each rational function one applies this method of partial fractioning to. Details on how to do this within the package MultivaluedApart are given in [39] in chapter 4.2.

Since the algorithm as developed in the last chapter can only be applied to fixed weight terms, the expression for amplitude must be further prepared accordingly. The Mathematica notebook Preparations.nb contains a useful routine for this making use of the PolyLogTools function `GetWeightTerms[]`: the routine takes as input any linear combination of MPLs with rational functions or numbers as coefficients (possibly multiplied by transcendental constants and ideally already rewritten using `MultivaluedApart[]`) and produces a list of the form `{{`r_1`, `$g_1^{(1)}$`}, {`r_1`, `$g_1^{(2)}$`}, ..., {`r_k`, `$g_k^{(n)}$`}}` with rational functions r_i (multiplied by transcendental constants) and linear combinations of MPLs $g_i^{(w)}$ with coefficients in $\mathbb{Q}$ (no rational functions here) and fixed weight w.

Now, the integration of symbols algorithm can be applied to each $g_i^{(w)}$ separately. This step can be easily parallelized if necessary.

That method was finally applied to rewrite the two-loop helicity amplitude for the Higgs decay $H \to ggg$ calculated in [36] using functions from the minimal spanning set for 2dHPLs as constructed in the last section. Here, the already known result mentioned above was confirmed that no $\mathrm{Li}_{2,2}$-MPLs appear and the classical (poly)logarithms $\log, \mathrm{Li}_2, \mathrm{Li}_3$ and Li_4 suffice. That this is not always the case was shown by a second two-loop amplitude representing the interference of $gg \to Z\gamma$ and $gg \to H \to Z\gamma$ provided to me by Lorenzo Tancredi. The results can be found in the files HgggAlpha.wl, HgggBeta.wl and Int.wl and were checked numerically using the PolyLogTools function `Ginsh[]`. In fact, speedups in computation time ranging from a factor of two to a factor of ten were observed, thus indicating the achievement of the simplification objective.

Conclusion

This thesis has focused on the special class of functions of multiple polylogarithms, covering three major topics. First, the mathematical foundations for dealing with multiple polylogarithms have been established in detail and in a self-contained manner. Essential properties such as the shuffle and stuffle relations were proved, the Hopf algebra structure of (motivic) multiple polylogarithms was introduced, and the symbol map was defined. Second, a very powerful and general algorithm exploiting those algebraic properties of multiple polylogarithms, the Duhr-Gangl-Rhodes integration of symbols algorithm, was discussed in detail. Its implementation is available to the public at `https://github.com/maxlouda/IntegrationOfSymbols`. So far, it has been fully implemented only up to and including weight four, but it is in principle straightforward to expand the code and handle higher weights, for example, up to and including weight six. Finally, this algorithm was used for finding bases of the function spaces of the one- and two-dimensional harmonic polylogarithms up to and including weight four, and helicity amplitudes for the processes $H \to ggg$ and the interference of $gg \to Z\gamma$ with $gg \to H \to Z\gamma$ were rewritten using the simplest possible functions. Results which had already been known from the literature were confirmed and the correctness of the reformulated amplitudes was numerically verified.

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Appendix A

Review of Differential Geometry

Differential forms are of fundamental importance for this work and will therefore be briefly introduced in this chapter of the appendix. As an underlying mathematical structure, the concept of a differentiable manifold must be clarified first.

A.1 Manifolds

Roughly speaking, differentiable manifolds are topological spaces that firstly look locally like a Euclidean space and secondly carry additional structure that allows analysis to be performed. The following definition serves to introduce two terms from complex analysis.

Definition A.1.1. Holomorphic functions and maps.

(i) Multivariate holomorphic functions ([40], p.2). Let $D \subseteq \mathbb{C}^n$ be a domain and $f : D \to \mathbb{C}$ be a continuous function. f is called holomorphic if for all $j \in \{1, ..., n\}$ the functions

$$f(z_1, ..., z_{k-1}, \cdot, z_{k+1}, ..., z_n) : z_k \mapsto f(z_1, ..., z_k, ..., z_n) \tag{A.1}$$

are holomorphic in the sense of the complex analysis of one variable.

(ii) Multidimensional holomorphic maps ([40], p.24). Let $D \subseteq \mathbb{C}^n$ be a domain and $f : D \to f(D) \subseteq \mathbb{C}^m,\ (z_1, ..., z_n) \mapsto (f_1(z_1, ..., z_n), ..., f_m(z_1, ..., z_n))$ be a mapping. f is called holomorphic if every component function $f_j,\ j \in \{1, ..., m\}$ is holomorphic in the sense of (i). f is called biholomorphic if $n = m$, f is bijective and both f and f^{-1} are holomorphic.

It should be noted that many results of one-dimensional complex analysis, such as Cauchy's integral theorem, results for analytical continuation or existence of power series expansions, can also be transferred to the multidimensional case touched on here (cf. first chapter from [40]).

The following definition introduces the differential geometric concept of a manifold. Some basic concepts from topology are assumed; compare for example chapter 2 of [41] for a compact introduction.

Definition A.1.2. Toplogical Manifolds and Differentiable Manifolds. Real and complex case.

(i) Topological manifolds ([42], pp.2ff.). Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ and M be a topological space which is also a Hausdorff space and second countable. One calls M a topological n-manifold if for every point $p \in M$ there is a tuple (U, φ) such that $U \subseteq M$ is open and contains p and $\varphi : U \to \varphi(U) \subseteq \mathbb{K}^n$ is a homeomorphism. The tuple (U, φ) is called a chart, U is called a coordinate domain and φ is called a coordinate mapping. Of central importance is the notion of local coordinates - by these we mean the component mappings $(x^1, ..., x^n) : U \to \varphi(U)$ which are given by the condition

$$\forall p \in U : \quad \varphi(p) = (x^1(p), ..., x^n(p)). \tag{A.2}$$

(ii) Differentiable real manifolds ([42], pp.11ff.). Let $\mathbb{K} = \mathbb{R}$ and M be a topological manifold. A smooth atlas $\mathcal{A} = (U_i, \varphi_i)_{i \in I}$ is characterized by the fact that first, the coordinate domains form an open cover of M

$$\bigcup_{i \in I} \varphi_i(U_i) = M, \tag{A.3}$$

and second, the coordinate mappings are smoothly compatible, i.e. for all $i, j \in I$ we have that $U_i \cap U_j = \emptyset$ or that

$$\varphi_j \circ \varphi_i^{-1} : \varphi_i(U_i \cap U_j) \subseteq \mathbb{R}^n \to \varphi_j(U_i \cap U_j) \subseteq \mathbb{R}^n \tag{A.4}$$

are diffeomorphisms. A maximal smooth atlas $\mathcal{A} = (U_i, \varphi_i)_{i \in I}$ is characterized by the fact that each additional map $(V, \psi) \notin \mathcal{A}$ is not smoothly compatible with all (U_i, φ_i). The tuple $(M, \mathcal{A})$ consisting of a topological manifold M and a maximal smooth atlas is called a real differentiable manifold.

(iii) Differentiable complex manifolds ([40], pp.28f.). Let $\mathbb{K} = \mathbb{C}$ and M be a connected topological manifold. A holomorphic atlas $\mathcal{A} = (U_i, \varphi_i)_{i \in I}$ is characterized similarly to the real case also by

$$\bigcup_{i \in I} \varphi_i(U_i) = M \tag{A.5}$$

whereas for the transition maps it must be required that for all $i, j \in I$ in the case $U_i \cap U_j \neq \emptyset$ the mapping

$$\varphi_j \circ \varphi_i^{-1} : \varphi_i(U_i \cap U_j) \subseteq \mathbb{C}^n \to \varphi_j(U_i \cap U_j) \subseteq \mathbb{C}^n \tag{A.6}$$

is biholomorphic. For technical reasons, we also require the maximality of $\mathcal{A}$ here, so that $(M, \mathcal{A})$ forms a complex differentiable manifold.

Remark. Given an atlas, one can always construct a maximal atlas by adding compatible maps. This maximal atlas is unique according to Zorn's lemma.

Examples include the n-spheres as well as the real and complex projective spaces (see [42], pp.6f.,21 and [40], pp.29f. and [43] for a full discussion). It is also useful to know that any open subset U of a manifold M can be conceived as a manifold ([42], p.19) and that for real or complex differentiable manifolds $M_1, ..., M_n$ of dimensions $d_1, ..., d_n$ the Cartesian product $M_1 \times \cdots \times M_n$ can be made into a $d_1 + \cdots + d_n$ dimensional real or complex manifold (cf. [42], p.21). The charts here have the structure $(U_1 \times \cdots \times U_n, \varphi_1 \times \cdots \times \varphi_n)$.

Finally, each complex manifold $(M, (U_i, \varphi_i = (z_i^j)_{j\in\{1,...,n\}})_{i\in I})$ of dimension n has a canonical underlying real manifold $\Sigma = (M, (U_i, \psi_i = (x_i^j)_{j\in\{1,...,2n\}})_{i\in I})$ of dimension $2n$: by splitting up the local coordinates $(z_i^1, ..., z_i^n) : U_i \to \varphi_i(U_i) \subseteq \mathbb{C}^n$ into their real and imaginary parts $z_i^j = x_i^{2j-1} + ix_i^{2j}$ one obtains local coordinate systems

$$\psi_i = (x_i^1, ..., x_i^{2n}) : U_i \to \psi_i(U_i) \subseteq \mathbb{R}^{2n}, \tag{A.7}$$

which fulfill (ii) of the above definition ([40], p.38).

The next definition explains what is meant by holomorphic mappings between two manifolds.

Definition A.1.3. Differentiable and holomorphic maps between manifolds ([40], p.31 and [42], p.34). Let $(M, \mathcal{A}_M), (N, \mathcal{A}_N)$ be real or complex differentiable manifolds of dimensions m and n and $f : D \subseteq M \to N$ be a continuous mapping. f is called differentiable of class C^k or holomorphic if for all $p \in D$ there exists a map $(U, \varphi) \in \mathcal{A}_M$ with $p \in U$ as well as a map $(V, \psi) \in \mathcal{A}_N$ with $f(U) \subseteq V$ such that

$$\psi \circ f \circ \varphi^{-1} : \varphi(U) \to \psi(V) \tag{A.8}$$

as a mapping $\mathbb{K}^m \to \mathbb{K}^n$ is differentiable of class C^k or holomorphic. The following commutative diagram illustrates the situation for fixed $p \in D$:

$$\begin{array}{ccc}
p \in U \subseteq M & \xrightarrow{f} & f(p) \in V \subseteq N \\
\Big\downarrow \varphi & & \Big\downarrow \psi \\
\varphi(U) \subseteq \mathbb{K}^n & \xrightarrow{\psi\circ f\circ\varphi^{-1}} & \psi(V) \subseteq \mathbb{K}^m
\end{array}$$

We call $\hat{f} := \psi \circ f \circ \varphi^{-1}$ the coordinate representation of f with respect to (U, φ) and (V, ψ).

For the next few definitions we will turn to the real case.

Definition A.1.4. Tangent vectors ([42], p.54.) Let M be a real differentiable manifold. Define the set of derivations at $p \in M$

$$\mathcal{D}_p := \{v : C^\infty(M) \text{ linear} \mid \forall f, g \in C^\infty(M) : \ v(fg) = v(f)g(p) + f(p)v(g)\}. \tag{A.9}$$

A tangent vector to M at p is a derivation at p. The set of all derivations at p with the obvious vector space structure makes up the tangent space T_pM.

Example A.1.5. $M = \mathbb{R}^n$ ([42], pp.51ff.). To $v = v^i e_i|_p \in \mathbb{R}^n_p$ (thought of as a vector with basepoint p) and $p \in \mathbb{R}^n$ (thought of as a point) we can associate the differential operator

$$D_v|_p : C^\infty(\mathbb{R}^n) \to \mathbb{R}, \quad f \mapsto D_v|_p f := \frac{\mathrm{d}}{\mathrm{d}t} f(a + tv)|_{t=0} = v^i \frac{\partial}{\partial x^i} f(p). \tag{A.10}$$

This differential operator clearly is a derivation at p, so $D_v|_p$ is a tangent vector to $\mathbb{R}^n$ at p. The tangent space $T_p\mathbb{R}^n$ can be shown to be equal to $\{D_v|_p \mid v \in \mathbb{R}^n_p\}$. One can further prove that for any $p \in \mathbb{R}^n$, the n derivations

$$\frac{\partial}{\partial x^1}\Big|_p, ..., \frac{\partial}{\partial x^n}\Big|_p \tag{A.11}$$

defined by the obvious prescription $\frac{\partial}{\partial x^i}\big|_p f := \frac{\partial f}{\partial x^i}(p)$ form a basis for $T_p\mathbb{R}^n$.

Definition A.1.6. Differentials of smooth maps ([42], p.55). Let M, N be real differentiable manifolds and $f : M \to N$ a differentiable map. The differential $\mathrm{d}f_p : T_pM \to T_{f(p)}N$ is the linear map defined through

$$\forall v \in T_pM\ \forall n \in C^\infty(N):\ \mathrm{d}f_p(v)(n) := v(n \circ f). \tag{A.12}$$

Using $(n_1 n_2) \circ f = (n_1 \circ f)(n_2 \circ f)$ as well as the properties of v, one can easily show that $\mathrm{d}f_p(v)$ is in fact a derivation on N at $f(p)$.

Proposition A.1.7. *Properties of differentials ([42], p.55). Let M, N, Q be real differentiable manifolds and $f : M \to N$, $g : N \to Q$ be differentiable maps.*

(i) The chain rule holds:

$$\mathrm{d}(g \circ f)_p = \mathrm{d}g_{f(p)} \circ \mathrm{d}f_p : T_pM \to T_{(g\circ f)(p)}Q. \tag{A.13}$$

(ii) If f is a diffeomorphism, then $\mathrm{d}f_p$ is a vector space isomorphism and

$$(\mathrm{d}f_p)^{-1} = \mathrm{d}(f^{-1})_{f(p)}. \tag{A.14}$$

Theorem A.1.8. *Basis of the tangent space ([44], pp.40f. and [42], pp.54ff.) Let (U, φ) be a chart of M such that $p \in U$. Define derivations on M at p by*

$$\partial_i|_p := \frac{\partial}{\partial x^i}\Big|_p = (\mathrm{d}\varphi_p)^{-1}\left(\frac{\partial}{\partial x^i}\Big|_{\varphi(p)}\right), \tag{A.15}$$

where

$$\frac{\partial}{\partial x^1}\Big|_{\varphi(p)}, ..., \frac{\partial}{\partial x^n}\Big|_{\varphi(p)} \tag{A.16}$$

is the basis of $T_{\varphi(p)}\mathbb{R}^n$ as discussed earlier. Then $\{\partial_1|_p, ..., \partial_n|_p\}$ is linearly independent and $T_pM \cong \mathrm{span}(\partial_1|_p, ..., \partial_n|_p)$; in particular $\dim(T_pM) = \dim(M)$.

To make the previous explanations a little more concrete, we will now discuss computations in local coordinates using selected examples ([42], pp.60ff.).

(i) Partial derivative of a function $f : M \to \mathbb{R}$ at $p \in M$. Calculate:

$$\begin{aligned}\partial_i|_p f &= (\mathrm{d}\varphi_p)^{-1}\left(\frac{\partial}{\partial x^i}\Big|_{\varphi(p)}\right)(f) = \mathrm{d}(\varphi^{-1})_{\varphi(p)}\left(\frac{\partial}{\partial x^i}\Big|_{\varphi(p)}\right)(f) = \\ &= \frac{\partial}{\partial x^i}\Big|_{\varphi(p)}(f \circ \varphi^{-1}) = \frac{\partial \hat{f}}{\partial x^i}(\varphi(p)).\end{aligned} \tag{A.17}$$

Here, $\hat{f} = \mathrm{id}_\mathbb{R} \circ f \circ \varphi^{-1}$ is the coordinate representation of f with respect to (U, φ) and $(\mathbb{R}, \mathrm{id}_\mathbb{R})$.

(ii) Differential of a function $f : M \to N$. Let

- (U, φ) be a chart for M with $p \in U$ and coordinate functions x^i,
- (V, ψ) be a chart for N with $f(p) \in V$ and coordinate functions y^j.

Then we get for any differentiable function $h : f(U) \cap V \to \mathbb{R}$:

$$\begin{aligned}
\mathrm{d}f_p(\partial_i|_p)(h) &= \partial_i|_p(h \circ f) = \partial_i|_p(h \circ \psi^{-1} \circ \psi \circ f \circ \varphi^{-1} \circ \varphi) = \partial_i|_p(\hat{h} \circ \hat{f} \circ \varphi) = \\
&= \frac{\partial}{\partial x^i}\Big|_{\varphi(p)}(\hat{h} \circ \hat{f} \circ \varphi \circ \varphi^{-1}) = \sum_{j=1}^{\dim(N)} \frac{\partial \hat{f}^j}{\partial x^i}\Big|_{\varphi(p)} \frac{\partial \hat{h}}{\partial y^j}\Big|_{\hat{f}(\varphi(p))} = \\
&= \left(\sum_{j=1}^{\dim(N)} \frac{\partial f^j}{\partial x^i}\Big|_p \frac{\partial}{\partial y^j}\Big|_{f(p)} \right) h.
\end{aligned} \tag{A.18}$$

So $\mathrm{d}f_p(\partial_i|_p)$ is a tangent vector to N at $f(p)$ with components given by the Jacobi-Matrix. Here, we have used the definition of the differential as well as the usual chain rule for differentiable functions from $\mathbb{R}^{\dim(M)}$ to $\mathbb{R}^{\dim(N)}$. In particular, consider $f = x^k : M \to N = \mathbb{R}$. Then

$$\hat{f}(a_1, ..., a_k, ..., a_n) = (x^k \circ \varphi^{-1})(a_1, ..., a_k, ..., a_n) = a_k \tag{A.19}$$

for any $(a_1, ..., a_n) \in \varphi(U)$ and hence

$$\mathrm{d}x_p^k(\partial_i|_p) = \delta_i^k \frac{\mathrm{d}}{\mathrm{d}y}|_{a_k} \equiv \delta_i^k \tag{A.20}$$

where we have used the canonical identification of $T_q\mathbb{R}$ with $\mathbb{R}$ for any $q \in \mathbb{R}$. From Linear Algebra it follows that the cotangent space (i.e. the dual of T_pM) is thus spanned by those differentials of the coordinate functions: $T_p^*M = \mathrm{span}(\mathrm{d}x_p^1, ..., \mathrm{d}x_p^n)$.

(iii) Change of coordinates. Let (U, φ) and (V, ψ) be charts on M with $W := \varphi(U) \cap \psi(V) \neq \emptyset$ and $p \in W$. Consider the transition map

$$\psi \circ \varphi^{-1} : \varphi(W) \to \psi(W), \quad x \mapsto (\tilde{x}^1(x), ..., \tilde{x}^n(x)). \tag{A.21}$$

Then (using (ii) to evaluate $\mathrm{d}(\psi \circ \varphi^{-1})_{\varphi(p)}$):

$$\begin{aligned}
\frac{\partial}{\partial x^i}\Big|_p &= \mathrm{d}(\varphi^{-1})_{\varphi(p)} \left(\frac{\partial}{\partial x^i}\Big|_{\varphi(p)} \right) = \mathrm{d}(\psi^{-1} \circ \psi \circ \varphi^{-1})_{\varphi(p)} \left(\frac{\partial}{\partial x^i}\Big|_{\varphi(p)} \right) = \\
&= \mathrm{d}(\psi^{-1})_{\psi(p)} \circ \mathrm{d}(\psi \circ \varphi^{-1})_{\varphi(p)} \left(\frac{\partial}{\partial x^i}\Big|_{\varphi(p)} \right) = \\
&= \mathrm{d}(\psi^{-1})_{\psi(p)} \left(\frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p)) \frac{\partial}{\partial \tilde{x}^j}\Big|_{\psi(p)} \right) = \\
&= \frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p)) \mathrm{d}(\psi^{-1})_{\psi(p)} \left(\frac{\partial}{\partial \tilde{x}^j}\Big|_{\psi(p)} \right) = \frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p)) \frac{\partial}{\partial \tilde{x}^j}\Big|_p .
\end{aligned} \tag{A.22}$$

This is the covariant transformation law of basis vectors. Let $v \in T_pM$. Because of $v = v^i\partial_i|_p = \tilde{v}^j\tilde{\partial}_j|_p$ (v is a geometric object and does not depend on the choice of local coordinates), this implies the contravariant transformation law of vector components

$$\tilde{v}^j = \frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p))v^i. \tag{A.23}$$

Analogously, let $\omega = \omega_i \, \mathrm{d}x_p^i \in T_p^*M$. Here,

$$\omega(\partial_j|_p) = \omega_i \, \mathrm{d}x_p^i(\partial_j|_p) = \omega_i\delta_j^i = \omega_j \tag{A.24}$$

and therefore we get the covariant transformation law of covector components

$$\omega_i = \omega(\partial_i|_p) = \frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p))\omega(\tilde{\partial}_j|_p) = \frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p))\tilde{\omega}_j. \tag{A.25}$$

Similarly to above, the equality $\omega = \omega_i \, \mathrm{d}x_p^i = \tilde{\omega}_j \, \mathrm{d}x_p^j$ leads to the contravariant transformation law of basis covectors:

$$\mathrm{d}\tilde{x}_p^j = \frac{\partial \tilde{x}^j}{\partial x^i}(\varphi(p)) \, \mathrm{d}x_p^i. \tag{A.26}$$

Definition A.1.9. Tangent and cotangent bundles, vector and covector fields ([42], pp.65,174f.,276ff. and [44], pp.41f.).

(i) The underlying set of the tangent bundle is given by

$$TM := \coprod_{p\in M} T_pM, \tag{A.27}$$

where $\coprod$ denotes the disjoint union. Elements of TM are written in the form (p, v_p) with $p \in M$ and $v_p \in T_pM$. If M is a n-dimensional differentiable manifold, it can be equipped with the structure of a $2n$-dimensional differentiable manifold. Vector fields are maps $X : M \to TM, p \mapsto X_p \in T_pM$. If $(U, \varphi = (x^i))$ is a chart of M, one can write

$$\forall p \in U: \quad X_p = X^i(p)\partial_i|_p \tag{A.28}$$

defining functions $X^i : U \to \mathbb{R}$. Vector fields are differentiable maps iff X^i are differentiable for any chart (U, φ).

(ii) Similarly one defines

$$T^*M := \coprod_{p\in M} T_p^*M \tag{A.29}$$

for the cotangent bundle (which can be made into a $2n$-dimensional differentiable manifold as well). Covector fields or 1-forms are maps $\omega : M \to T^*M, p \mapsto \omega_p \in T_p^*M$ and can be locally represented (in a chart $(U, (x^i))$) by $\omega_p = \omega_i(p) \, \mathrm{d}x_p^i$. They are differentiable iff $\omega_i : M \to \mathbb{R}$ are differentiable for any chart or, equivalently, the map $\omega(X) : M \to \mathbb{R}, p \mapsto \omega_p(X_p)$ is differentiable for any differentiable vector field X.

An important example of a covector field is given by the differential of a real valued function $f : M \to \mathbb{R}$ (which is just the differential of a function between two manifolds in the sense of definition A.1.6 after the canoncial identification $\mathbb{R} \cong T_q\mathbb{R}$ for all $q \in \mathbb{R}$) defined by ([42], p.281)

$$\forall v \in T_pM: \ \mathrm{d}f_p(v) = vf. \tag{A.30}$$

A.2 Differential Forms

Definition A.2.1. Exterior forms and the wedge product ([42], pp.350ff. and [44], pp.3ff.). Given a K-vector space V (K is the field of real or complex numbers), an ℓ-exterior form ω is an ℓ-multilinear map $\omega : V^\ell \to K$ which is alternating, i.e.

$$\forall v_1, ..., v_\ell \in V \ \forall i, j \in \{1, ..., \ell\} : \ \omega(v_1, ..., v_i, ..., v_j, ..., v_\ell) = -\omega(v_1, ..., v_j, ..., v_i, ..., v_\ell). \tag{A.31}$$

The K-vector space of all ℓ-exterior forms is denoted by $\Lambda^\ell(V^*)$. In particular, $\Lambda^0(V^*) := K$, $\Lambda^1(V^*) = V^*$ and $\Lambda^k(V^*) = \{0\}$ for $k \geq \dim(V)$. On $\Lambda^k(V^*)$ one can introduce a product, called the wedge product. To do this, we proceed in three steps.

(i) Wedge product of covectors. Let $\omega_1, ..., \omega_\ell \in V^*$. Then one defines $\omega_1 \wedge \cdots \wedge \omega_\ell \in \Lambda^\ell(V^*)$ via

$$(\omega_1 \wedge \cdots \wedge \omega_\ell)(v_1, ..., v_\ell) := \det\left(\left(\omega_i(v_j)\right)_{i,j\in\{1,...,\ell\}}\right). \tag{A.32}$$

(ii) Basis for $\Lambda^\ell(V^*)$. Let $\{\varepsilon^i\}_{i\in\{1,...,n\}}$ be a basis of V^*. Then

$$\mathcal{E} := \left\{\varepsilon^{i_1} \wedge \cdots \wedge \varepsilon^{i_\ell} \mid 1 \leq i_1 < \cdots < i_\ell \leq n\right\} \tag{A.33}$$

is a basis for $\Lambda^\ell(V^*)$. It follows: $\dim(\Lambda^\ell(V^*)) = \binom{n}{\ell}$. We write $\varepsilon^I := \varepsilon^{i_1} \wedge \cdots \wedge \varepsilon^{i_\ell}$ for any multiindex $I = (i_1, ..., i_\ell)$ and define $\varepsilon^I \wedge \varepsilon^J := \varepsilon^{IJ}$ where IJ is the concatenation of arbitrary multiindices I with J.

(iii) Wedge product of arbitrary exterior forms. Let

$$\omega := \sum_{I \text{ inc.}} a_I \varepsilon^I = \sum_{1\leq i_1<\cdots<i_\ell\leq n} a_{i_1,...,i_\ell} \varepsilon^{i_1} \wedge \cdots \wedge \varepsilon^{i_\ell} \in \Lambda^\ell(V^*), \tag{A.34}$$

$$\sigma := \sum_{J \text{ inc.}} b_J \varepsilon^J = \sum_{1\leq j_1<\cdots<j_k\leq n} b_{j_1,...,j_\ell} \varepsilon^{j_1} \wedge \cdots \wedge \varepsilon^{j_k} \in \Lambda^k(V^*) \tag{A.35}$$

be arbitrary exterior forms (inc. indicates summation over increasing multiindices). The wedge product of ω with σ is then defined by

$$\omega \wedge \sigma := \sum_{I \text{ inc.}} \sum_{J \text{ inc.}} a_I b_J \varepsilon^I \wedge \varepsilon^J \equiv \sum_{IJ \text{ inc.}} a_I b_J \varepsilon^{IJ}. \tag{A.36}$$

Proposition A.2.2. *Properties of wedge products ([42], p.356). Let ω be a ℓ-exterior form, φ a k-exterior form and θ a s-exterior form. Then:*

(i) The wedge product is associative: $\omega \wedge (\varphi \wedge \theta) = (\omega \wedge \varphi) \wedge \theta$.

(ii) The wedge product is bilinear: For all $\lambda_1, \lambda_2 \in K$ we have

$$(\lambda_1\omega + \lambda_2\varphi) \wedge \theta = \lambda_1(\omega \wedge \theta) + \lambda_2(\varphi \wedge \theta), \tag{A.37}$$

$$\omega \wedge (\lambda_1\varphi + \lambda_2\theta) = \lambda_1(\omega \wedge \varphi) + \lambda_2(\omega \wedge \theta). \tag{A.38}$$

(iii) The wedge product is graded anticommutative: $\omega \wedge \varphi = (-1)^{\ell k} \varphi \wedge \omega$.

Definition A.2.3. Real differential forms ([42], pp.359f.) Let M be a real differentiable manifold of dimension n and set

$$\Lambda^\ell T^* M := \coprod_{p \in M} \Lambda^\ell (T_p^* M). \tag{A.39}$$

A differential ℓ-form is a map $\omega : M \to \Lambda^\ell T^* M,\ p \mapsto \omega_p \in \Lambda^\ell (T_p^* M)$ such that for any local representation in a chart $(U, (x^i))$

$$\omega = \sum_{I \text{ inc.}} \omega_I \, \mathrm{d}x^I \tag{A.40}$$

the functions $\omega_I : M \to \mathbb{R}$ are differentiable. One can show:

$$\omega_{i_1, \ldots, i_\ell} = \omega \left(\partial_{i_1}, \ldots, \partial_{i_\ell} \right), \tag{A.41}$$

where ∂_i is the vector field $p \mapsto \partial_i|_p$.

The real vector space of all differential ℓ-forms is denoted by $\Omega^\ell(M)$. The graded vector space $\Omega^*(M) := \bigoplus_{\ell=0}^n \Omega^\ell(M)$ can be equipped with the wedge product by setting $(\omega \wedge \sigma)_p := \omega_p \wedge \sigma_p$ for all $p \in M$, $\omega \in \Omega^\ell(M)$ and $\sigma \in \Omega^k(M)$ and thus constitutes an anticommutative graded algebra (see next chapter in the appendix).

Two special cases have to be clarified: First, $\Omega^0(M)$ consists of all differentiable functions $M \to \mathbb{R}$. Second, the wedge product between a differentiable function f and an arbitrary differential form ω is defined as the ordinary, pointwise product $(f \wedge \omega)_p := (f\omega)_p = f(p)\omega_p$.

Definition A.2.4. Pullback of differential forms ([42], p.360). Let $f : M \to N$ be a differentiable map between to real differentiable manifolds M, N and $\omega \in \Omega^\ell(N)$. The pullback $f^*\omega$ of ω under f is the differential ℓ-form on M defined by

$$(f^*\omega)_p(v_1, \ldots, v_\ell) := \omega_{f(p)}(\mathrm{d}f_p(v_1), \ldots, \mathrm{d}f_p(v_\ell)) \tag{A.42}$$

for all $p \in M$ and $v_1, \ldots, v_\ell \in T_p M$.

Proposition A.2.5. *Properties of the pullback ([42], pp.285,361 and [44], p.8). Let* $f : M \to N$ *and* $g : N \to P$ *be differentiable maps as above and* ω, σ *differential forms. Then*

(i) $f^* : \Omega^\ell(N) \to \Omega^\ell(M)$ *is* $\mathbb{R}$*-linear.*

(ii) The pullback is compatible with the wedge product: $f^*(\omega \wedge \sigma) = (f^*\omega) \wedge (f^*\sigma)$.

(iii) In any chart $(V, (y^i))$ *of* N *we have*

$$f^* \left(\sum_{I \text{ inc.}} \omega_I \, \mathrm{d}y^I \right) = \sum_{I \text{ inc.}} (\omega_I \circ f) \mathrm{d}(y^{i_1} \circ f) \wedge \cdots \wedge \mathrm{d}(y^{i_\ell} \circ f). \tag{A.43}$$

(iv) $f^*(g^*(\omega)) = (g \circ f)^* \omega$.

(v) Specialising to one-forms $\omega \in \Omega^1(N)$ one finds for any differentiable real-valued function $u : N \to \mathbb{R}$:

$$f^*(u\omega) = (u \circ f) f^*(\omega) \quad \text{and} \quad f^*(\mathrm{d}u) = \mathrm{d}(u \circ f). \tag{A.44}$$

Theorem A.2.6. *Definition and properties of the exterior derivative ([42], pp.363ff.). The exterior derivative is introduced in two stages.*

(i) Differential forms on $U \subseteq \mathbb{R}^n$ open. Let $\omega = \sum_{I \text{ inc.}} \omega_J \, \mathrm{d}x^J \in \Omega^\ell(U)$. The exterior derivative of ω is a $(\ell+1)$-form defined by

$$\mathrm{d}\left(\sum_{I \text{ inc.}} \omega_I \, \mathrm{d}x^I\right) := \sum_{I \text{ inc.}} \mathrm{d}\omega_I \wedge \omega^I = \sum_{I \text{ inc.}} \sum_j \frac{\partial \omega_I}{\partial x^j} \, \mathrm{d}x^j \wedge \mathrm{d}x^{i_1} \wedge \cdots \wedge \mathrm{d}x^{i_\ell}. \tag{A.45}$$

It has the subsequent properties:

- $\mathrm{d} : \Omega^\ell(U) \to \Omega^{\ell+1}(U)$ *is $\mathbb{R}$-linear.*
- *If $\omega \in \Omega^k(U)$ and $\sigma \in \Omega^\ell(U)$, then*
$$\mathrm{d}(\omega \wedge \sigma) = (\mathrm{d}\omega) \wedge \sigma + (-1)^k \omega \wedge (\mathrm{d}\sigma). \tag{A.46}$$
- $\mathrm{d} \circ \mathrm{d} = 0.$
- *Let $f : U \subseteq \mathbb{R}^n \to V \subseteq \mathbb{R}^m$ be differentiable and $\omega \in \Omega^k(V)$. Then $f^*(\mathrm{d}\omega) = \mathrm{d}(f^*\omega)$.*

(ii) Differential forms on manifolds. Define for each chart (U, φ) of M:

$$\mathrm{d} : \Omega^\ell(M) \to \Omega^{\ell+1}(M), \quad \mathrm{d}\omega := \varphi^* \mathrm{d}((\varphi^{-1})^* \omega). \tag{A.47}$$

This prescription is well-defined, has the same properties as in (i) and is in fact uniquely determined by the first three properties together with $\mathrm{d}f(X) = Xf$ for an arbitrary vector field X and $f \in \Omega^0(M)$. In local coordinates, the exterior derivative can be computed with the exact same formula as in equation A.45.

We will now discuss the complex case in an ad hoc way following Kodaira [40]. A more modern, conceptual approach can be found in [45], for example.

Definition A.2.7. Complex differential forms ([40], pp.76ff.). Let $(M, (U_i, \varphi_i = (z_i^j)_{j \in \{1,\dots,n\}})_{i \in I})$ be a complex differentiable manifold of dimension n and denote by $\Sigma = (M, (U_i, \psi_i = (x_i^j)_{j \in \{1,\dots,2n\}})_{i \in I})$ its underlying real differentiable manifold of dimension $2n$ (cf. equation A.7).

(i) General form. A complex differential r-form on M is in general on a chart $(U, \psi = (x^j))$ represented locally by

$$\omega = \sum_{1 \le j_1 < \cdots < j_r \le 2n} \omega_{j_1,\dots,j_r} \, \mathrm{d}x^{j_1} \wedge \cdots \wedge \mathrm{d}x^{j_r}, \tag{A.48}$$

where $\omega_{j_1,\dots,j_r} : U \to \mathbb{C}$ are complex valued (in general only continuous) functions. The space of all such complex differential r-forms on M is denoted by $\Omega^r(M; \mathbb{C})$.

(ii) Canonical form. Using

$$x^{2j-1} = \frac{1}{2}(z^j + \bar{z}^j) \quad \text{and} \quad x^{2j} = \frac{1}{2i}(z^j - \bar{z}^j) \tag{A.49}$$

we find

$$\mathrm{d}x^{2j-1} = \frac{1}{2}(\mathrm{d}z^j + \mathrm{d}\bar{z}^j) \quad \text{and} \quad \mathrm{d}x^{2j} = \frac{1}{2i}(\mathrm{d}z^j - \mathrm{d}\bar{z}^j) \tag{A.50}$$

which leads to

$$\omega = \sum_{p+q=r} \sum_{|I|=p \text{ inc.}} \sum_{|J|=q \text{ inc.}} \omega_{IJ}\, \mathrm{d}z^I \wedge \mathrm{d}\bar{z}^J. \tag{A.51}$$

A differential form that can be written as

$$\omega = \sum_{|I|=p \text{ inc.}} \sum_{|J|=q \text{ inc.}} \omega_{IJ}\, \mathrm{d}z^I \wedge \mathrm{d}\bar{z}^J \tag{A.52}$$

is called a (p,q)-form. The space of such (p,q)-forms on M is denoted by $\Omega^{p,q}(M)$. We have $\Omega^r(M;\mathbb{C}) = \bigoplus_{p+q=r} \Omega^{p,q}(M)$.

(iii) Exterior derivative and Dolbeault operators. Let $\omega \in \Omega^{p,q}(M)$ and compute

$$\begin{aligned}\mathrm{d}\omega &= \sum_{|I|=p \text{ inc.}} \sum_{|J|=q \text{ inc.}} \sum_{j=1}^{n} \left(\frac{\partial}{\partial x^{2j-1}}(\omega_{IJ})\, \mathrm{d}x^{2j-1} + \frac{\partial}{\partial x^{2j}}(\omega_{IJ})\, \mathrm{d}x^{2j} \right) \wedge \mathrm{d}z^I \wedge \mathrm{d}\bar{z}^J = \\ &= \sum_{|I|=p \text{ inc.}} \sum_{|J|=q \text{ inc.}} \sum_{j=1}^{n} \left(\frac{\partial}{\partial z^j}(\omega_{IJ})\, \mathrm{d}z^j + \frac{\partial}{\partial \bar{z}^j}(\omega_{IJ}) \mathrm{d}\bar{z}^j \right) \wedge \mathrm{d}z^I \wedge \mathrm{d}\bar{z}^J.\end{aligned} \tag{A.53}$$

One sets

$$\partial\omega := \sum_{|I|=p \text{ inc.}} \sum_{|J|=q \text{ inc.}} \sum_{j=1}^{n} \frac{\partial}{\partial z^j}(\omega_{IJ})\, \mathrm{d}z^j \wedge \mathrm{d}z^I \wedge \mathrm{d}\bar{z}^J \in \Omega^{p+1,q}(M), \tag{A.54}$$

$$\bar{\partial}\omega := \sum_{|I|=p \text{ inc.}} \sum_{|J|=q \text{ inc.}} \sum_{j=1}^{n} \frac{\partial}{\partial \bar{z}^j}(\omega_{IJ}) \mathrm{d}\bar{z}^j \wedge \mathrm{d}z^I \wedge \mathrm{d}\bar{z}^J \in \Omega^{p,q+1}(M). \tag{A.55}$$

This defines the Dolbeault operators. They satisfy

$$\mathrm{d} = \partial + \bar{\partial},\ \partial^2 = 0,\ \bar{\partial}^2 = 0,\ \partial\bar{\partial} = -\bar{\partial}\partial \tag{A.56}$$

as well as the graded Leibniz rules ($\omega \in \Omega^\ell(M;\mathbb{C})$)

$$\partial(\omega \wedge \sigma) = (\partial\omega) \wedge \sigma + (-1)^\ell \omega \wedge (\partial\sigma), \tag{A.57}$$

$$\bar{\partial}(\omega \wedge \sigma) = (\bar{\partial}\omega) \wedge \sigma + (-1)^\ell \omega \wedge (\bar{\partial}\sigma). \tag{A.58}$$

(iv) Holomorphic and meromorphic forms. Let

$$\omega = \sum_{|I|=p \text{ inc.}} \omega_I \,\mathrm{d}z^I \in \Omega^{p,0}(M). \tag{A.59}$$

It is called holomorphic (meromorphic), if all $\omega_I : U \to \mathbb{C}$ are holomorphic (meromorphic). Furthermore, ω is holomorphic iff $\bar{\partial}\omega = 0$.

We now briefly discuss the integration of differential forms. First, we turn to the definition of the real and complex line integral.

Definition A.2.8. Line integrals ([42], pp.288f. and [46], p.21). Let M be a real or complex differentiable manifold, $\gamma : [a,b] \to M$ a piecewise smooth curve with subintervals $[a_{i_1}, a_i],\ i \in \{1, ..., k\},\ a_0 = a,\ a_k = b$ on which γ is smooth.

(i) Real case. Let $\omega \in \Omega^1(M)$. Then one defines

$$\int_\gamma \omega := \sum_{i=1}^{k} \int_{[a_{i-1}, a_i]} \gamma^*\omega, \tag{A.60}$$

where the right hand side is an integral over an $\mathbb{R}$-valued one-dimensional function.

(ii) Complex case. Here, we only need the special case $M \subseteq \mathbb{C}$. Let $\omega = f(z)\,\mathrm{d}z$ be a meromorphic complex differential form on M. Then:

$$\int_\gamma \omega := \sum_{i=1}^{k} \int_{[a_{i-1}, a_i]} \gamma^*\omega \equiv \sum_{i=1}^{k} \int_{[a_{i-1}, a_i]} f(\gamma(t))\gamma'(t)\,\mathrm{d}t. \tag{A.61}$$

Proposition A.2.9. *Properties of line integrals ([42], pp.289f and [46], p.22). Let $\omega, \omega_1, \omega_2$ be $\mathbb{K}$-valued differential forms as above. In both the complex and real case the line integral has the following properties:*

(i) Linearity. For all $\lambda_1, \lambda_2 \in \mathbb{K}$:

$$\int_\gamma (\lambda_1\omega_1 + \lambda_2\omega_2) = \lambda_1 \int_\gamma \omega_1 + \lambda_2 \int_\gamma \omega_2. \tag{A.62}$$

(ii) Diffeomorphism invariance. Let $\phi : [c,d] \to [a,b]$ be an increasing diffeomorphism. Then

$$\int_{\gamma\circ\phi} \omega = \int_\gamma \omega. \tag{A.63}$$

Differential forms of higher order can be integrated as well. We will only discuss the real case as this thesis does not make use of the integration theory over complex manifolds.

Definition A.2.10. Orientability of manifolds ([44], p.50 and [40], pp.85f. and [42], pp.381f.). Let M be a real differentiable manifold with atlas $(U_i, \varphi_i)_{i\in I}$. M is called orientable if for all $a, b \in I$ with $U_a \cap U_b \neq \emptyset$ the Jacobian of $\varphi_b \circ \varphi_a^{-1}$ has positive determinant. A chart $(U, \varphi = (x^i))$ is called positively oriented if the ordered basis $(\partial_1|_p, ..., \partial_n|_p)$ of T_pM is right-handed for all $p \in U$. If M is orientable, it is possible to choose the atlas such that each chart is positively oriented.

Proposition A.2.11. *Existence of a partition of unity ([42], p.43). Let M be a real differentiable manifold and $\mathcal{U} := (U_i)_{i\in I}$ an arbitrary open cover of M. Then there exists a set of differentiable functions $(\psi_i : M \to \mathbb{R})_{i\in I}$ called smooth partition of unity subordinate to $\mathcal{U}$ such that*

(i) $0 \leq \psi_i(p) \leq 1$ *for all* $p \in M$ *and* $i \in I$.

(ii) $\mathrm{supp}(\psi_i) \subseteq U_i$ *for all* $i \in I$.

(iii) $(\mathrm{supp}(\psi_i))_{i\in I}$ *has the property that every* $p \in M$ *has a neighborhood* V *such that* $V \cap \mathrm{supp}(\psi_i) \neq \emptyset$ *only for finitely many* $i \in I$ *(it is locally finite).*

(iv) $\sum_{i\in I} \psi_i(p) = 1$ *for all* $p \in M$.

Definition A.2.12. Integration of differential forms ([42], pp.402ff. and [40], pp.81ff.). First, consider an open set $U \subseteq \mathbb{R}^n$ and an on U compactly supported n-form $\omega = f\,\mathrm{d}x^1 \wedge \cdots \wedge \mathrm{d}x^n$ with $f : U \to \mathbb{R}$ being continuous. Then define

$$\int\limits_U \omega := \int\limits_U f\,\mathrm{d}x^1 \cdots \mathrm{d}x^n. \tag{A.64}$$

Now, lift this definition up to the case of an oriented n-dimensional manifold M. Let ω be a compactly supported n-form on M and (U_i, φ_i) positively oriented charts such that (U_i) is a finite open cover of $\mathrm{supp}(\omega)$. Using a smooth partition of unity (ψ_i) subordinate to (U_i) we define

$$\int\limits_M \omega := \sum_i \int\limits_M \psi_i\omega := \sum_i \int\limits_{\varphi_i(U_i)} (\varphi_i^{-1})^*(\psi_i\omega), \tag{A.65}$$

where this last integral is to be understood in the sense discussed above. One can show that this definition neither depends on the choice of charts nor on the choice of the partition of unity.

Appendix B

Review of Algebraic Concepts

Most proofs will be omitted in this appendix; those can be found in the provided references.

B.1 Tensor Products

The tensor product is most elegantly defined by the following universal property:

Theorem B.1.1. *Tensor Products ([42], pp.307ff. for a detailed proof and [47]. p.23). Let K be a number field and V_1, V_2 be finite dimensional K-vector spaces. The tensor product space is a tuple $(V_1 \otimes V_2, \tau)$ consisting of*

(i) a K-vector space $V_1 \otimes V_2$ and

(ii) a K-bilinear map $\tau : V_1 \times V_2 \to V_1 \otimes V_2,\ (v_1, v_2) \mapsto \tau(v_1, v_2) := v_1 \otimes v_2$

such that the following condition is met: For all K-vector spaces W and all K-bilinear maps $f : V_1 \times V_2 \to W$ there exists a unique linear *map $\hat{f} : V_1 \otimes V_2 \to W$ with $f = \hat{f} \circ \tau$, i.e. the following diagram commutes:*

$$\begin{tikzcd} V_1 \times V_2 \arrow[r, "f"] \arrow[d, "\tau"] & W \\ V_1 \otimes V_2 \arrow[ur, "\hat{f}"] & \end{tikzcd}$$

This condition specifies the tensor product space up to isomorphisms.

Proposition B.1.2. *Properties of tensor products ([47], pp.23f.) Let U, V, W be K-vector spaces.*

(i) The isomorphism

$$(U \otimes V) \otimes W \cong U \otimes (V \otimes W) \tag{B.1}$$

allows us to set $(U \otimes V) \otimes W =: U \otimes V \otimes W$ and generalize to tensor products of arbitrary but finitely many K-vector spaces. Furthermore we have

$$K \otimes V \cong V \cong V \otimes K. \tag{B.2}$$

(ii) The bilinearity of τ induces the following identities:

$$\forall u_1, u_2 \in U\ \forall v_1, v_2 \in V\ \forall \lambda \in K : \quad (u_1 + u_2) \otimes v_1 = u_1 \otimes v_1 + u_2 \otimes v_1, \tag{B.3}$$

$$u_1 \otimes (v_1 + v_2) = u_1 \otimes v_1 + u_1 \otimes v_2, \tag{B.4}$$

$$\lambda(u_1 \otimes v_1) = (\lambda u_1) \otimes v_1 = u_1 \otimes (\lambda v_1). \tag{B.5}$$

(iii) If $(u_i)_{i\in I}$ is a basis for U and $(v_j)_{j\in J}$ is a basis for V, then $(u_i \otimes v_j)_{(i,j)\in I\times J}$ is a basis for $U \otimes V$. As a result, $\dim(U \otimes V) = \dim(U) \cdot \dim(V)$.

Definition B.1.3. Tensor Products of Linear Maps ([47], p.26). Let V_1, V_2 and U_1, U_2 be K-vector spaces and $f : V_1 \to V_2$, $g : U_1 \to U_2$ linear maps. The tensor product map $f \otimes g : V_1 \otimes U_1 \to V_2 \otimes U_2$ is defined by

$$\forall v \in V_1\ \forall u \in U_1 : \quad (f \otimes g)(v \otimes u) := f(v) \otimes g(u) \tag{B.6}$$

and is itself a K-linear map on $V_1 \otimes U_1$.

B.2 Rings, Fields, Algebras and Modules

Some knowledge about groups is assumed. Reference [48] might be useful as a refresher.

Definition B.2.1. Rings ([48], p.184). Let R be a set and $+ : R \times R \to R$, $\cdot : R \times R \to R$ two maps called addition and multiplication. The triple $(R, +\cdot)$ is called a ring iff

(i) $(R, +)$ is an abelian group.

(ii) $(R, \cdot)$ is a semigroup.

(iii) Distributivity holds, i.e. for all $a, b, c \in R$ we have

$$a(b + c) = ab + ac \quad \text{and} \quad (a + b)c = ac + bc. \tag{B.7}$$

A ring is further called

- commutative, iff $(R, \cdot)$ is commutative.
- unital, iff $(R, \cdot)$ possesses a unit 1 which is different from the neutral element 0 of $(R, +)$.

In the future, we will oftentimes write just R instead of $(R, +, \cdot)$.

Definition B.2.2. Subrings ([48], pp.186f.). Let $(R, +, \cdot)$ be a ring and $S \subseteq R$ a subset. $(S, +, \cdot)$ is called a subring of $(R, +, \cdot)$ iff $(S, +)$ is a subgroup of $(R, +)$ and $(S, \cdot)$ is a sub-semigroup of $(R, \cdot)$, i.e.

$$\forall a, b \in S :\ a - b \in S \text{ and } ab \in S. \tag{B.8}$$

Proposition B.2.3. *Center of a ring ([48], p.187). The center of a ring R defined by*

$$C(R) := \{z \in R \mid \forall a \in R :\ az = za\} \tag{B.9}$$

is a commutative subring of R.

Definition B.2.4. Ring-Homomorphisms ([48], p.188). Let R, S be rings. A map $f : R \to S$ is called a ring-homomorphism iff

$$\forall a, b \in R : \quad f(a +_R b) = f(a) +_S f(b) \text{ and } f(a \cdot_R b) = f(a) \cdot_S f(b). \tag{B.10}$$

Example B.2.5. Polynomial Ring.

(i) Univariate case ([48], pp.201ff.). Let R be a commutative ring with unit 1. Then

$$R[X] = \left\{ \sum_{i\in\mathbb{N}_0} a_i X^i \mid a_i \in R \text{ and } a_i = 0 \text{ for almost all } i \in \mathbb{N}_0 \right\} \tag{B.11}$$

is a commutative ring with unit 1 called the polynomial ring. Addition and multiplication of polynomials are defined as usual:

$$\left(\sum_{i\in\mathbb{N}_0} a_i X^i\right) + \left(\sum_{i\in\mathbb{N}_0} b_i X^i\right) := \sum_{i\in\mathbb{N}_0} (a_i + b_i) X^i, \tag{B.12}$$

$$\left(\sum_{i\in\mathbb{N}_0} a_i X^i\right) \cdot \left(\sum_{i\in\mathbb{N}_0} b_i X^i\right) := \sum_{k\in\mathbb{N}_0} \left(\sum_{i+j=k} a_i b_j\right) X^k. \tag{B.13}$$

Formally, the objects X are modelled by maps

$$X : \mathbb{N}_0 \to R,\ i \mapsto \delta_{i,1} \tag{B.14}$$

and polynomials are understood as elements of the commutative ring with unit $(1, 0, 0, ...)$ of sequences in R.

(ii) Multivariate case ([48], pp.216f.). Let R be a commutative ring with unit 1. Then

$$R[X_1, ..., X_n] = \left\{ \sum a_{i_1 \ldots i_n} X_1^{i_1} \cdots X_n^{i_n} \mid a_{i_1 \ldots i_n} \in R\ \wedge\ a_{i_1 \ldots i_n} = 0 \text{ f.a.a.} (i_1, ..., i_n) \in \mathbb{N}_0^n \right\} \tag{B.15}$$

is a commutative ring with unit 1 (f.a.a. means for almost all). Formally, one can define this ring recursively by

$$R[X_1, ..., X_n] := (R[X_1, ..., X_{n-1}])[X_n]. \tag{B.16}$$

Definition B.2.6. Fields ([48], p.193). Let $(R, +, \cdot)$ be a commutative ring with unit 1. It is called a field iff every element $a \neq 0$ has a multiplicative inverse.

Example B.2.7. Quotient fields and rational functions.

(i) Quotient fields ([48], pp.194ff.). Let R be a commutative ring in which the product of two nonzero elements is also nonzero and set $S := R \setminus \{0\}$. Introduce on $R \times S$ the relation

$$(a, s) \sim (a', s') :\Longleftrightarrow\ as' = a's. \tag{B.17}$$

One can easily show that this is an equivalence relation. Set for an equivalence class $[(a, s)] := \frac{a}{s}$ and for the quotient set $Q(R) := \{\frac{a}{s} \mid a \in R,\ s \in S\}$. With the (indeed well-defined) operations

$$\frac{a}{s} + \frac{a'}{s'} := \frac{as' + a's}{ss'} \quad \text{and} \quad \frac{a}{s} \cdot \frac{a'}{s'} := \frac{aa'}{ss'} \tag{B.18}$$

we obtain a field $(Q(R), +\cdot)$ called the quotient field of R.

(ii) Rational functions ([48], p.209 and p.218). Specializing to $R = R[X_1, ..., X_n]$ (of which one can show that it has the zero-product property mentioned above) we can conclude that the set of rational functions forms a field.

Definition B.2.8. Algebras ([47], p.3). Let K be a field and A a ring. Two conditions have to be met in order for A to be a K-Algebra:

(i) There exists a ring-homomorphism $\eta_A : K \to A$ called unit such that $\eta_A(K) \subseteq C(A)$, i.e.
$$\forall \lambda \in K \ \forall a \in A : \quad \eta_A(\lambda)a = a\eta_A(\lambda), \tag{B.19}$$
One can informally think of η_A as the assignment $\lambda \mapsto \lambda \cdot 1_A$, hence the name unit. η_A allows to introduce vector space structure on A with vector space addition being the default addition in A and scalar multiplication being given by $K \times A \mapsto A$, $(\lambda, a) \mapsto \eta_A(\lambda)a$.

(ii) The multiplication $\mu_A : A \times A \to A$ has to be bilinear (A is thought to be equipped with the aforementioned vector space structure).

Remark. Using the universal property of the tensor product and recalling the definition of a ring, one can rephrase the definition of an algebra ([47], pp.39f. and [49], p.5) to a form that makes it more useful for the definition of Hopf algebras:

Let K be a field and A be a K-vector space. A K-algebra is a triple (A, μ, η) with K-linear maps
$$\mu : A \otimes A \to A \quad \text{and} \quad \eta : K \to A \tag{B.20}$$
such that

(i) Associativity:
$$\mu \circ (\mu \otimes \mathrm{id}_A) = \mu \circ (\mathrm{id}_A \otimes \mu). \tag{B.21}$$
In other words, the diagram

$$\begin{tikzcd} A \otimes A \otimes A \arrow[r, "\mu\otimes\mathrm{id}_A"] \arrow[d, "\mathrm{id}_A\otimes\mu"] & A \otimes A \arrow[d, "\mu"] \\ A \otimes A \arrow[r, "\mu"] & A \end{tikzcd}$$

commutes.

(ii) Unitality ($K \otimes A \cong A \otimes K \cong A$ is tacitly understood):
$$\mu \circ (\eta \otimes \mathrm{id}_A) = \mu \circ (\mathrm{id}_A \otimes \eta) = \mathrm{id}_A. \tag{B.22}$$
In other words, the following diagram commutes:

$$\begin{tikzcd} K \otimes A \arrow[r, "\eta\otimes\mathrm{id}_A"] \arrow[dr, "\cong"] & A \otimes A \arrow[d, "\mu"] & A \otimes K \arrow[l, "\mathrm{id}_A\otimes\eta"'] \arrow[dl, "\cong"] \\ & A & \end{tikzcd}$$

Definition B.2.9. Algebra-Homomorphisms ([47], p.3). Let A, B be K-algebras. A ring homomorphism $f : A \to B$ is called an algebra homomorphism iff $f \circ \eta_A = \eta_B$.

Remark. This definition, too, can be reformulated using the tensor product: Let (A, μ_A, η_A) and (B, μ_B, η_B) be K-Algebras in the sense of the preceding remark. A linear map $f : A \to B$ is called algebra homomorphism iff ([47], p.40)

$$\mu_B \circ (f \otimes f) = f \circ \mu_A \quad \text{and} \quad f \circ \eta_A = \eta_B \tag{B.23}$$

The first condition in conjunction with the linearity models the properties of a ring homomorphism whereas the the second condition is already known from the preceding definition. In the language of diagrams, the following two diagrams have to be commutative:

$$\begin{tikzcd} A \otimes A \arrow[r, "f\otimes f"] \arrow[d, "\mu_A"] & B \otimes B \arrow[d, "\mu_B"] \\ A \arrow[r, "f"] & B \end{tikzcd} \qquad \begin{tikzcd} K \arrow[r, "\eta_A"] \arrow[dr, "\eta_B"] & A \arrow[d, "f"] \\ & B \end{tikzcd}$$

Definition B.2.10. Modules ([47], p.4). Let A be a K-algebra. An A-module is a vector space V together with a bilinear map $A \times V \to V,\ (a, v) \mapsto av$ such that

$$\forall a, b \in A\ \forall v \in V : \quad a(bv) = (ab)v \quad \text{and} \quad 1v = v. \tag{B.24}$$

Definition B.2.11. Module-Homomorphisms a.k.a A-Linear Maps ([47], p.5). Let V, W be A-modules. An A-linear map $f : V \to W$ is linear (as a map between vector spaces) and additionally satisfies

$$\forall a \in A\ \forall v \in V : \quad f(av) = af(v). \tag{B.25}$$

Example B.2.12. Free Algebras and Tensor Algebras.

(i) Free Algebras ([47], pp.7ff. for free algebras and [42], pp.307f. for free vector spaces). Let K be a field and $X = (x_i)_{i\in I}$ be a set called the alphabet with the elements called letters. We construct a free vector space $K\langle X\rangle$ as follows:

- Define the set of words as the set of all ordered tuples

$$B = \{x_{i_1} x_{i_2} \cdots x_{i_p} \mid p \in \mathbb{N}_0 \text{ and } i_1, ..., i_p \in I\} =: (w_j)_{j\in J} \tag{B.26}$$

  where the empty word $\emptyset \in B$ is defined as the word with length $p = 0$.

- Define the set of maps

$$\Phi_B := \left\{ \delta_w : B \to \{0, 1\},\ v \mapsto \begin{cases} 1 & \text{if} \quad v = w \\ 0 & \text{if} \quad v \neq w \end{cases} \mid w \in B \right\} \tag{B.27}$$

  There is obviously a canonical bijection $w \mapsto \delta_w$ and we will identify w with its corresponding map δ_w.

- The free vector space is defined as (f.a.a. means for almost all)

$$K\langle X\rangle := \left\{ \sum_{j\in J} a_j \delta_{w_j} \mid a_j \in K \text{ and } a_j = 0 \text{ f.a.a. } j \in J \right\}. \tag{B.28}$$

  So $K\langle X\rangle$ consists of all formal linear combinations of words if one makes use of the identification of w with δ_w.

- One has the following characteristic property: Every map $f : B \to V$ into some vector space V can be uniquely extended to a linear map $\hat{f} : K\langle X\rangle \to V$ by setting

$$\hat{f}\left(\sum_{j\in J} a_j \delta_{w_j}\right) := \sum_{j\in J} a_j f(w_j). \tag{B.29}$$

Using the characteristic property mentioned above, the concatenation of words

$$\mu : B \times B \to B,\ (x_{i_1} \cdots x_{i_p}, x_{i_{p+1}} \cdots x_{i_n}) \mapsto x_{i_1} \cdots x_{i_p} x_{i_{p+1}} \cdots x_{i_n} \tag{B.30}$$

can be uniquely extended to a bilinear map $K\langle X\rangle \times K\langle X\rangle \to K\langle X\rangle$ and thus constitutes a multiplication on $K\langle X\rangle$. The unit is given by $\eta : K \to K\langle X\rangle,\ \lambda \mapsto \lambda\delta_\emptyset$. Hence, $K\langle X\rangle$ has K-algebra structure.

(ii) Tensor Algebras ([47], p.34). Let V be a K-vector space. Define

$$T^0(V) := K, \quad T^1(V) := V, \quad \forall k \geq 2 :\ T^k(V) := \underbrace{V \otimes \cdots \otimes V}_{k} =: V^{\otimes k}. \tag{B.31}$$

The tensor algebra is then given by the vectorspace

$$T(V) := \bigoplus_{k\geq 0} T^k(V) \tag{B.32}$$

together with the unit $1 \in K \subset T(V)$ and the (by linearity extended) multiplication

$$(x_1 \otimes \cdots \otimes x_p, x_{p+1} \otimes \cdots \otimes x_n) \mapsto x_1 \otimes \cdots \otimes x_p \otimes x_{p+1} \otimes \cdots \otimes x_n, \tag{B.33}$$

which makes use of the canonical isomorphism $T^n(V) \otimes T^m(V) \cong T^{n+m}(v)$ mentioned in Proposition B.1.2 (i).

Definition B.2.13. Graded Algebras ([47], p.12). Let A be an algebra. A is called graded if there are countably many subspaces $(A_i)_{i\in\mathbb{N}}$ such that

$$A = \bigoplus_{i\in\mathbb{N}} A_i \quad \text{and} \quad A_i \cdot A_j \subseteq A_{i+j}, \tag{B.34}$$

where $A_i \cdot A_j := \{a_i \cdot a_j \mid a_i \in A_i \text{ and } a_j \in A_j\}$.

Example B.2.14. The tensor algebra is graded by definition and the free algebra is graded by the length of words ([47], p.13 and p.34).

Proposition B.2.15. *Tensor Product of Algebras ([47], p.32). Let A and B be K-algebras. The tensor product space $A \otimes B$ (a vector space) can be equipped with algebra structure by defining a multiplication $\mu_\otimes : A \otimes B \times A \otimes B \to A \otimes B$ through*

$$\forall a_1, a_2 \in A \ \forall b_1, b_2 \in B : \quad \mu_\otimes(a_1 \otimes b_1, a_2 \otimes b_2) \mapsto (a_1 a_2) \otimes (b_1 b_2). \tag{B.35}$$

The unit is given by $\eta_\otimes = \eta_A \otimes \eta_B$.

B.3 Hopf-Algebras

Definition B.3.1. Coalgebras ([47], p.40 and [49], pp.21f.). Let K be a field and C be a K-vector space. A K-coalgebra is a triple (C, Δ, ϵ) with K-linear maps

$$\Delta : A \to A \otimes A \quad \text{and} \quad \epsilon : A \to K \tag{B.36}$$

called comultiplication and counit, respectively, such that

(i) Coassociativity:

$$(\mathrm{id}_C \otimes \Delta) \circ \Delta = (\Delta \otimes \mathrm{id}_C) \circ \Delta. \tag{B.37}$$

Or - equivalently - the following diagram commutes:

$$\begin{tikzcd} C \arrow[r, "\Delta"] \arrow[d, "\Delta"] & C \otimes C \arrow[d, "\mathrm{id}_C \otimes \Delta"] \\ C \otimes C \arrow[r, "\Delta \otimes \mathrm{id}_C"] & C \otimes C \otimes C \end{tikzcd}$$

(ii) Counitality:

$$(\epsilon \otimes \mathrm{id}_C) \circ \Delta = (\mathrm{id}_C \otimes \epsilon) \circ \Delta = \mathrm{id}_C, \tag{B.38}$$

where we have identified $K \otimes C$ and $C \otimes K$ with C. Equivalently, the diagram

$$\begin{tikzcd} K \otimes C & C \otimes C \arrow[l, "\epsilon \otimes \mathrm{id}_C"'] \arrow[r, "\mathrm{id}_C \otimes \epsilon"] & C \otimes K \\ & C \arrow[ul, "\cong"] \arrow[u, "\Delta"] \arrow[ur, "\cong"'] & \end{tikzcd}$$

commutes.

Remark. If one compares this definition with the alternative definition of an algebra given in the remark following Definition B.2.8, one notices that all arrows have been inverted. Hence the name *co*algebra.

It is helpful to discuss the conditions of coassociativity and counitality in more detail.

Example B.3.2. Meaning of coassociativity and counitality ([31], pp.12f. and [47], pp.43f.). Let (C, Δ, ϵ) be a coalgebra. For $x \in C$ the element $\Delta(x) \in C \otimes C$ can be written as

$$\Delta(x) = \sum_i x_i^{(1)} \otimes x_i^{(2)} \tag{B.39}$$

for some $x_i^{(1)}, x_i^{(2)} \in C$.

(i) Coassociativity means that

$$(\mathrm{id}_C \otimes \Delta) \circ \Delta(x) = (\mathrm{id}_C \otimes \Delta)\left(\sum_i x_i^{(1)} \otimes x_i^{(2)}\right) = \sum_i x_i^{(1)} \otimes (\Delta(x_i^{(2)})) =$$
$$= \sum_i x_i^{(1)} \otimes \left(\sum_j x_{i,j}^{(2,1)} \otimes x_{i,j}^{(2,2)}\right) \equiv \sum_{i,j} x_i^{(1)} \otimes x_{i,j}^{(2,1)} \otimes x_{i,j}^{(2,2)} \tag{B.40}$$

has to coincide with

$$(\Delta \otimes \mathrm{id}_C) \circ \Delta(x) = (\Delta \otimes \mathrm{id}_C)\left(\sum_i x_i^{(1)} \otimes x_i^{(2)}\right) = \sum_i (\Delta(x_i^{(1)})) \otimes x_i^{(2)} =$$
$$= \sum_i \left(\sum_j x_{i,j}^{(1,1)} \otimes x_{i,j}^{(1,2)}\right) \otimes x_i^{(2)} \equiv \sum_{i,j} x_{i,j}^{(1,1)} \otimes x_{i,j}^{(1,2)} \otimes x_i^{(2)}. \tag{B.41}$$

(ii) Similarly, counitality means that

$$(\epsilon \otimes \mathrm{id}_C) \circ \Delta(x) = \sum_i (\epsilon(x_i^{(1)})) \otimes x_i^{(2)} \equiv \sum_i \epsilon(x_i^{(1)}) x_i^{(2)} \tag{B.42}$$

has to coincide with

$$(\mathrm{id}_C \otimes \epsilon) \circ \Delta(x) = \sum_i x_i^{(1)} \otimes (\epsilon(x_i^{(2)})) \equiv \sum_i x_i^{(1)} \epsilon(x_i^{(2)}) \tag{B.43}$$

and with $\mathrm{id}_C(x) = x$.

Definition B.3.3. Coalgebra-Homomorphisms ([47], p.40). Let $(C_1, \Delta_1, \epsilon_1)$ and $(C_2, \Delta_2, \epsilon_2)$ be coalgebras and $f : C_1 \to C_2$ a linear map. f is a homomorphism of coalgebras iff

$$(f \otimes f) \circ \Delta_1 = \Delta_2 \circ f \quad \text{and} \quad \epsilon_2 \circ f = \epsilon_1. \tag{B.44}$$

In terms of diagrams we have that

$$\begin{tikzcd} C_1 \arrow[r, "\Delta_1"] \arrow[d, "f"] & C_1 \otimes C_1 \arrow[d, "f\otimes f"] \\ C_2 \arrow[r, "\Delta_2"] & C_2 \otimes C_2 \end{tikzcd} \qquad \begin{tikzcd} C_1 \arrow[r, "\epsilon_1"] \arrow[d, "f"] & K \\ C_2 \arrow[ur, "\epsilon_2"] & \end{tikzcd}$$

must be commutative.

Proposition B.3.4. *Tensor Product of Coalgebras ([47], p.42). Let $(C_1, \Delta_1, \epsilon_1)$ and $(C_2, \Delta_2, \epsilon_2)$ be two coalgebras. The tensor product $C_1 \otimes C_2$ can be endowed with coalgebra structure by setting*

$$\Delta_\otimes := (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2) \tag{B.45}$$

for the comultiplication ($\nu_{C_1,C_2} : C_1 \otimes C_2 \to C_2 \otimes C_1,\ x \otimes y \mapsto y \otimes x$ *is the flip) and*

$$\epsilon_{\otimes} := \epsilon_1 \otimes \epsilon_2 \tag{B.46}$$

for the counit.

Proof. It is a good exercise to do this proof. Clearly, $\Delta_{\otimes}$ and $\epsilon_{\otimes}$ are linear maps. Coassociativity and Counitality are to be verified.

(i) Coassociativity. Calculate for arbitrary $x \otimes y \in C_1 \otimes C_2$:

$$\begin{aligned} \Delta_{\otimes}(x \otimes y) &= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \left(\sum_{i,j} x_i^{(1)} \otimes x_i^{(2)} \otimes y_j^{(1)} \otimes y_j^{(2)} \right) = \\ &= \sum_{i,j} x_i^{(1)} \otimes y_j^{(1)} \otimes x_i^{(2)} \otimes y_j^{(2)}. \end{aligned} \tag{B.47}$$

Hence:

$$\begin{aligned} (\mathrm{id}_{C_1 \otimes C_2} \otimes \Delta_{\otimes}) \circ \Delta_{\otimes}(x \otimes y) &= (\mathrm{id}_{C_1 \otimes C_2} \otimes \Delta_{\otimes}) \left(\sum_{i,j} x_i^{(1)} \otimes y_j^{(1)} \otimes x_i^{(2)} \otimes y_j^{(2)} \right) = \\ &= \sum_{i,j} x_i^{(1)} \otimes y_j^{(1)} \otimes \left(\Delta_{\otimes}(x_i^{(2)} \otimes y_j^{(2)}) \right) = \\ &= \sum_{i,j} x_i^{(1)} \otimes y_j^{(1)} \otimes \left(\sum_{k,l} x_{i,k}^{(2,1)} \otimes y_{j,l}^{(2,1)} \otimes x_{i,k}^{(2,2)} \otimes y_{j,l}^{(2,2)} \right) = \\ &= (\mathrm{id}_{C_1 \otimes C_2} \otimes \mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\mathrm{id}_{C_1 \otimes C_2} \otimes \Delta_1 \otimes \Delta_2)(\Delta_{\otimes}(x \otimes y)). \end{aligned} \tag{B.48}$$

On the other hand

$$\begin{aligned} (\Delta_{\otimes} \otimes \mathrm{id}_{C_1 \otimes C_2}) \circ \Delta_{\otimes}(x \otimes y) &= \sum_{i,j} \left(\sum_{k,l} x_{i,k}^{(1,1)} \otimes y_{j,l}^{(1,1)} \otimes x_{i,k}^{(1,2)} \otimes y_{j,l}^{(1,2)} \right) \otimes x_i^{(2)} \otimes y_j^{(2)} = \\ &= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2} \otimes \mathrm{id}_{C_1 \otimes C_2}) \circ (\Delta_1 \otimes \Delta_2 \otimes \mathrm{id}_{C_1 \otimes C_2})(\Delta_{\otimes}(x \otimes y)). \end{aligned} \tag{B.49}$$

In summary, equations B.48 and B.49 prove

$$\begin{aligned} (\mathrm{id}_{C_1 \otimes C_2} \otimes \Delta_{\otimes}) \circ \Delta_{\otimes} = (\mathrm{id}_{C_1 \otimes C_2} \otimes \mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ \\ \circ (\mathrm{id}_{C_1 \otimes C_2} \otimes \Delta_1 \otimes \Delta_2) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2) \end{aligned} \tag{B.50}$$

and

$$\begin{aligned} (\Delta_{\otimes} \otimes \mathrm{id}_{C_1 \otimes C_2}) \circ \Delta_{\otimes} = (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2} \otimes \mathrm{id}_{C_1 \otimes C_2}) \circ \\ \circ (\Delta_1 \otimes \Delta_2 \otimes \mathrm{id}_{C_1 \otimes C_2}) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2), \end{aligned} \tag{B.51}$$

respectively. We want to use the coassociativity of Δ_1 and Δ_2 which implies

$$
\begin{aligned}
(\mathrm{id}_{C_1} \otimes \Delta_1 \otimes \mathrm{id}_{C_2} \otimes \Delta_2) \circ (\Delta_1 \otimes \Delta_2) &= [(\mathrm{id}_{C_1} \otimes \Delta_1) \circ \Delta_1] \otimes [(\mathrm{id}_{C_2} \otimes \Delta_2) \circ \Delta_2] = \\
&= [(\Delta_1 \otimes \mathrm{id}_{C_1}) \circ \Delta_1] \otimes [(\Delta_2 \otimes \mathrm{id}_{C_2}) \circ \Delta_2] = \\
&= (\Delta_1 \otimes \mathrm{id}_{C_1} \otimes \Delta_2 \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2).
\end{aligned}
\tag{B.52}
$$

In order to do this, we rewrite parts of equation B.50 to

$$
\begin{aligned}
(\mathrm{id}_{C_1\otimes C_2} \otimes \Delta_1 \otimes \Delta_2) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) &= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_1} \otimes \mathrm{id}_{C_2\otimes C_2}) \circ \\
\circ (\mathrm{id}_{C_1\otimes C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2\otimes C_2}) &\circ (\mathrm{id}_{C_1} \otimes \Delta_1 \otimes \mathrm{id}_{C_2} \otimes \Delta_2)
\end{aligned}
\tag{B.53}
$$

and parts of equation B.51 to

$$
\begin{aligned}
(\Delta_1 \otimes \Delta_2 \otimes \mathrm{id}_{C_1\otimes C_2}) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) &= (\mathrm{id}_{C_1\otimes C_1} \otimes \mathrm{id}_{C_2} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ \\
\circ (\mathrm{id}_{C_1\otimes C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2\otimes C_2}) &\circ (\Delta_1 \otimes \mathrm{id}_{C_1} \otimes \Delta_2 \otimes \mathrm{id}_{C_2}).
\end{aligned}
\tag{B.54}
$$

Both identities can be easily proven by evaluating the left and right hand side on a generic $x_1 \otimes x_2 \otimes y_1 \otimes y_2$ similarly to equations B.48 and B.49. Plugging the last three equations into B.50 and B.51 we find that all that is left to show is the identity

$$
\begin{aligned}
&(\mathrm{id}_{C_1\otimes C_2} \otimes \mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_1} \otimes \mathrm{id}_{C_2\otimes C_2}) \circ \\
&\quad \circ (\mathrm{id}_{C_1\otimes C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2\otimes C_2}) = \\
&= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2} \otimes \mathrm{id}_{C_1\otimes C_2}) \circ (\mathrm{id}_{C_1\otimes C_1} \otimes \mathrm{id}_{C_2} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ \\
&\quad \circ (\mathrm{id}_{C_1\otimes C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2\otimes C_2}).
\end{aligned}
\tag{B.55}
$$

But this is also readily verified by direct calculation which finishes the proof of coassociativity.

(ii) Counitality. Analogous to (i) the proof can be obtained by direct calculation.

$$
\begin{aligned}
(\epsilon_\otimes \otimes \mathrm{id}_{C_1\otimes C_2}) \circ \Delta_\otimes &= (\epsilon_1 \otimes \epsilon_2 \otimes \mathrm{id}_{C_1\otimes C_2}) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2) = \\
&= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\epsilon_1 \otimes \mathrm{id}_{C_1} \otimes \epsilon_2 \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2) = \\
&= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ [(\epsilon_1 \otimes \mathrm{id}_{C_1}) \circ \Delta_1] \otimes [(\epsilon_2 \otimes \mathrm{id}_2) \circ \Delta_2] = \\
&= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ [(\mathrm{id}_{C_1} \otimes \epsilon_1) \circ \Delta_1] \otimes [(\mathrm{id}_2 \otimes \epsilon_2) \circ \Delta_2] = \\
&= (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\mathrm{id}_{C_1} \otimes \epsilon_1 \otimes \mathrm{id}_{C_2} \otimes \epsilon_2) \circ (\Delta_1 \otimes \Delta_2) = \\
&= (\mathrm{id}_{C_1\otimes C_2} \otimes \epsilon_1 \otimes \epsilon_2) \circ (\mathrm{id}_{C_1} \otimes \nu_{C_1,C_2} \otimes \mathrm{id}_{C_2}) \circ (\Delta_1 \otimes \Delta_2) = \\
&= (\mathrm{id}_{C_1\otimes C_2} \otimes \epsilon_\otimes) \circ \Delta_\otimes.
\end{aligned}
\tag{B.56}
$$

□

Definition B.3.5. Bialgebras ([47], pp.45f.). If a K-vector space H is endowed with an algebra structure (H, μ, η) as well as a coalgebra structure (H, Δ, ϵ) and certain compatibility conditions are fulfilled, the quintuple $(H, \mu, \eta, \Delta, \epsilon)$ is called a bialgebra. Those compatibility conditions are:

(i) Equip $H \otimes H$ with the algebra structure $(H \otimes H, \mu_\otimes, \eta_\otimes)$ defined in B.2.15. Then $\Delta : H \to H \otimes H$ is required to be a homomorphism of algebras. I.e.

$$\begin{tikzcd} H \otimes H \arrow[r, "\Delta\otimes\Delta"] \arrow[d, "\mu"] & (H \otimes H) \otimes (H \otimes H) \arrow[d, "\mu_\otimes"] \\ H \arrow[r, "\Delta"] & H \otimes H \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} K \arrow[r, "\eta"] \arrow[d, "\mathrm{id}"] & H \arrow[d, "\Delta"] \\ K \otimes K \arrow[r, "\eta_\otimes"] & H \otimes H \end{tikzcd}$$

have to be commuting diagrams.

(ii) Also, $\epsilon : H \to K$ has to be a homomorphism of algebras. This means that

$$\begin{tikzcd} H \otimes H \arrow[r, "\epsilon\otimes\epsilon"] \arrow[d, "\mu"] & K \otimes K \arrow[d, "\mathrm{id}"] \\ H \arrow[r, "\epsilon"] & K \end{tikzcd} \quad \text{and} \quad \begin{tikzcd} K \arrow[r, "\eta"] \arrow[dr, "\mathrm{id}"] & H \arrow[d, "\epsilon"] \\ & K \end{tikzcd}$$

are required to commute.

Definition B.3.6. Hopf Algebras ([47], pp.49ff. and [5], p.34). Let $(H, \mu, \eta, \Delta, \epsilon)$ be a bialgebra. H is called a Hopf algebra if there exists an algebra homomorphism $S : H \to H$ called antipode such that

$$\mu \circ (S \otimes \mathrm{id}_H) \circ \Delta = \mu \circ (\mathrm{id}_H \otimes S) \circ \Delta = \eta \circ \epsilon. \tag{B.57}$$

Remark. If it exists, the antipode is uniquely determined by equation B.57 ([47], p.51).

Definition B.3.7. Graded Hopf Algebras ([13], p.188). Let $(H, \mu, \eta, \Delta, \epsilon)$ be a Hopf algebra. It is a graded Hopf Algebra if the following conditions hold:

(i) The ground K-vector space can be decomposed as

$$H = \bigoplus_{i \geq 0} H_i \tag{B.58}$$

(ii) Multiplication and comultiplication are compatible with this decomposition:

$$\forall i, j \in \mathbb{N}_0 : \quad \mu(H_i \otimes H_j) \subseteq H_{i+j} \quad \text{and} \quad \Delta(H_i) \subseteq \bigoplus_{n+m=i} H_n \otimes H_m. \tag{B.59}$$

Note that the first condition is a reformulation of the condition appearing in Definition B.2.13.

(iii) The antipode satisfies $S(H_i) \subseteq H_i$ for all $i \in \mathbb{N}_0$.

The following two examples give important Hopf algebras and show furthermore that there are in general many possible Hopf structures which can be imposed on one vector space.

Example B.3.8. Hopf Structure for Tensor Algebras ([47], p.47 and [49], pp.27,41). Take the tensor algebra $T(V)$ with the concatenation product (now called μ and thought of as a map $T(V) \otimes T(V) \to T(V)$) and the unit $\eta : K \to T(V)$ characterised by $1 \mapsto 1 \in V^{\otimes 0} = K \subset T(V)$. We've already noted in B.2.12 (ii) that $(T(V), \mu, \eta)$ forms an algebra. To proceed we first define the set of (l, r)-shuffles by

$$\Sigma(l,r) := \{\sigma \in S_{l+r} \mid \sigma^{-1}(1) < \cdots < \sigma^{-1}(l) \ \wedge \ \sigma^{-1}(l+1) < \cdots < \sigma^{-1}(l+r)\} \tag{B.60}$$

where S_n denotes the symmetric group. We can now define a unique coalgebra structure by imposing

$$\forall v \in V \ \forall \lambda \in K : \quad \Delta(v) = 1 \otimes v + v \otimes 1 \quad \text{and} \quad \epsilon(\lambda) = \lambda, \ \epsilon(v) = 0. \tag{B.61}$$

Using the fact that Δ has to be a homomorphism of algebras which implies $\Delta(v_1 \otimes \cdots \otimes v_n) = \Delta(v_1 \otimes \cdots \otimes v_{n-1}) \otimes \Delta(v_n)$ one can inductively show that $\Delta : T(V) \to T(V) \otimes T(V)$ and $\epsilon : T(V) \to K$ fulfill

$$\Delta(v_1 \otimes \cdots \otimes v_n) = \sum_{k=0}^{n} \sum_{\sigma \in \Sigma(l,r)} (v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(k)}) \otimes (v_{\sigma(k+1)} \otimes \cdots \otimes v_{\sigma(n)}), \tag{B.62}$$

$$\epsilon(v_1 \otimes \cdots \otimes v_n) = 0 \quad (n \geq 1) \tag{B.63}$$

for all $v_1, ..., v_n \in V$ (for convenience, empty tensor products are taken to be 1). By introducing the antipode $S : T(V) \to T(V)$ via

$$S(1) = 1 \quad \text{and} \quad S(v_1 \otimes \cdots \otimes v_n) = (-1)^n v_n \otimes \cdots \otimes v_1 \tag{B.64}$$

we finally arrive at a graded Hopf algebra.

Example B.3.9. Shuffle Hopf Algebra ([50], p.31 and [47], p.68). We return to the tensor algebra $T(V)$ over a vector space V defined in Example B.2.12 (ii). This time, however, we consider a slightly more complex multiplication given by the so called shuffle product:

$$ш : T(V) \times T(V) \to T(V), \quad (v_1 \otimes \cdots \otimes v_l) ш (v_{l+1} \otimes \cdots \otimes v_{l+1}) \mapsto \sum_{\sigma \in \Sigma(l,r)} v_{\sigma(1)} \otimes \cdots \otimes v_{\sigma(l+r)}. \tag{B.65}$$

Extending by linearity we end up with a bilinear map, which gives rise to a unique map $\mu_ш : T(V) \otimes T(V) \to T(V)$. The unit is again given by η as above. $(T(V), \mu_ш, \eta)$ constitutes the algebra structure. For the coalgebra part one defines first a comultiplication that takes the form of deconcatenation

$$\Delta_ш : T(V) \to T(V) \otimes T(V), \quad \Delta_ш(v_1 \otimes \cdots \otimes v_n) := \sum_{k=0}^{n} (v_1 \otimes \cdots \otimes v_k) \otimes (v_{k+1} \otimes \cdots \otimes v_n) \tag{B.66}$$

where empty products are defined to be 1 and we again extend by linearity. Note that we should distinguish between the (external) tensor product appearing in $T(V) \otimes T(V)$ and the (internal) tensor product appearing when writing down elements of $T(V)$. The counit $\epsilon_{\sqcup\!\sqcup}$ is as above defined to be the identity on $V^{\otimes 0}$ and the zero map for $V^{\otimes n}, n \geq 1$. Then $(T(V), \Delta_{\sqcup\!\sqcup}, \epsilon_{\sqcup\!\sqcup})$ is a coalgebra. One can show that $(T(V), \mu_{\sqcup\!\sqcup}, 1, \Delta_{\sqcup\!\sqcup}, \epsilon_{\sqcup\!\sqcup})$ together with the same antipode S as above forms a graded Hopf algebra.

A completely analogous construction can be done for the case of the free K-vector space over an alphabet X with set of words B, $K\langle X\rangle$. Here, one defines ([21], pp.66f.):

$$\sqcup\!\sqcup : K\langle X\rangle \times K\langle X\rangle \to K\langle X\rangle, \quad (x_1 \cdots x_l) \sqcup\!\sqcup (x_{l+1} \cdots x_{l+r}) \mapsto \sum_{\sigma \in \Sigma(l,r)} x_{\sigma(1)} \cdots x_{\sigma(l+r)} \tag{B.67}$$

and

$$\Delta_{\sqcup\!\sqcup} : K\langle X\rangle \to K\langle X\rangle \otimes K\langle X\rangle, \quad \Delta_{\sqcup\!\sqcup}(x_1 \cdots x_n) := \sum_{k=0}^{n} (x_1 \cdots x_k) \otimes (x_{k+1} \cdots x_n) \tag{B.68}$$

for multiplication and comultiplication. The unit is given by $\eta : 1 \mapsto \emptyset$ (with $\emptyset$ as the empty word) and the counit by $\epsilon : K\langle X\rangle \to K$, $\sum_{w \in B} \lambda_w w \mapsto \lambda_\emptyset$ (i.e. the counit yields the coefficient of the empty word). The antipode, finally, is defined by

$$S : K\langle X\rangle \to K\langle X\rangle, \quad x_1 \cdots x_n \mapsto (-1)^n x_n \cdots x_1. \tag{B.69}$$

B.4 De Rham Cohomology and Differential Graded Algebras

Definition B.4.1. Cochain Complex ([42], p.460). Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ be a field and $(A^p)_{p \in \mathbb{Z}}$ a sequence of $\mathbb{K}$-vector spaces. If there are $\mathbb{K}$-linear maps $d^p : A^p \to A^{p-1}$ called differentials connecting those $\mathbb{K}$-vector spaces

$$\cdots \xrightarrow{d^{-1}} A^0 \xrightarrow{d^0} A^1 \xrightarrow{d^1} A^1 \xrightarrow{d^2} \cdots \tag{B.70}$$

such that $d^p \circ d^{p-1} = 0$ for all $p \in \mathbb{Z}$, we say that $(A^\bullet, d^\bullet) := ((A^p, d^p)_{p \in \mathbb{Z}})$ forms a cochain complex. We often write just $A^\bullet$ for the complex.

Definition B.4.2. Cochain Maps ([42], p.461). Let $A^\bullet$ and $B^\bullet$ be cochain complexes. A cochain map $F : A^\bullet \to B^\bullet$ is understood to be a sequence of linear maps $(F^p : A^p \to B^p)_{p \in \mathbb{Z}}$ that is compatible with the differentials:

$$\forall p \in \mathbb{Z} : \quad F^{p+1} \circ d_A^p = d_B^p \circ F^p. \tag{B.71}$$

In other words, the following diagram commutes for all $p \in \mathbb{Z}$:

$$\begin{tikzcd}
\cdots \arrow[r, "d_A^{p-1}"] & A^p \arrow[r, "d_A^p"] \arrow[d, "F^p"] & A^{p+1} \arrow[r, "d_A^{p+1}"] \arrow[d, "F^{p+1}"] & \cdots \\
\cdots \arrow[r, "d_B^{p-1}"] & B^p \arrow[r, "d_B^p"] & B^{p+1} \arrow[r, "d_B^{p+1}"] & \cdots
\end{tikzcd}$$

Definition B.4.3. Cohomology Groups ([42], p.460). Let $A^\bullet$ be a cochain complex. Since

$$d^p \circ d^{p-1} = 0 \implies \mathrm{Im}(d^{p-1} : A^{p-1} \to A^p) \subseteq \mathrm{Ker}(d^p : A^p \to A^{p+1}) \tag{B.72}$$

we can define

$$H^p(A^\bullet) := \frac{\mathrm{Ker}(d^p)}{\mathrm{Im}(d^{p-1})}. \tag{B.73}$$

$H^p(A^\bullet)$ is called the p-th cohomology group of $A^\bullet$. The total cohomology of $A^\bullet$ is defined as

$$H^\bullet(A^\bullet) := \bigoplus_{p\in\mathbb{Z}} H^p(A^\bullet). \tag{B.74}$$

Proposition B.4.4. *Quasi-Isomorphism ([13], p.395 and [42], pp.442,461). Let $F : A^\bullet \to B^\bullet, G : B^\bullet \to C^\bullet$ be cochain maps. Then define for all $p \in \mathbb{Z}$:*

$$H(F^p) : H^p(A^\bullet) \to H^p(B^\bullet), \quad [x] \mapsto H(F^p)([x]) := [F^p(x)]. \tag{B.75}$$

This map has the properties

$$H(G^p \circ F^p) = H(F^p) \circ H(G^p) \quad \text{and} \quad H(\mathrm{id}) = \mathrm{id}. \tag{B.76}$$

The induced map $H(F) : H^\bullet(A^\bullet) \to H^\bullet(B^\bullet)$ is understood to be the collection of all $H(F^p)$. F is called a quasi-isomorphism if $H(F)$ is an isomorphism.

Example B.4.5. De Rham Complex and Cohomology ([42], pp.441,460). Let M be a differentiable real or complex n-dimensional manifold, $p \in \mathbb{N}_0$ and $\Omega^p(M)$ the vector space of p-forms on M. With the exterior derivative $\mathrm{d} : \Omega^p(M) \to \Omega^{p+1}(M)$ (we suppress indices) it is evident, that

$$0 \to \Omega^0(M) \stackrel{\mathrm{d}}{\to} \Omega^1(M) \stackrel{\mathrm{d}}{\to} \cdots \stackrel{\mathrm{d}}{\to} \Omega^p(M) \stackrel{\mathrm{d}}{\to} \cdots \stackrel{\mathrm{d}}{\to} \Omega^n(M) \to 0 \tag{B.77}$$

is a cochain complex called the de Rham complex of differential forms on M. The cohomology groups $H^p_{\mathrm{dR}}(M)$ are called de Rham cohomology groups and are actually vector spaces. If $H^p_{\mathrm{dR}}(M) = 0$ for $0 \leq p \leq n$ then every closed p-form on M is exact. It is furthermore clear that $H^p_{\mathrm{dR}} = 0$ always for $p < 0$ or $p > n$ since then $\Omega^p(M) = 0$.

Definition B.4.6. Differential Graded Algebra ([13], pp.237f.). Let $\mathbb{K} \in \{\mathbb{R}, \mathbb{C}\}$ be a field. A differential graded algebra is a triplet $(A^*, \wedge, d)$ such that the following properties are fulfilled:

(i) There exists a sequence of $\mathbb{K}$-vector spaces $(A^p)_{p\in\mathbb{Z}}$ such that

$$A^* = \bigoplus_{p\in\mathbb{Z}} A^p. \tag{B.78}$$

(ii) $\wedge : A^p \otimes A^q \to A^{p+q},\ p, q \in \mathbb{Z}$, is a multiplication and makes $(A^*, \wedge)$ into a graded algebra with unit $1 \in A^0$.

(iii) The differential $d : A^* \to A^{*+1}$ fulfills $d^2 = 0$ and $d(A^p) \subseteq A^{p+1}$. Furthermore, the graded Leibniz rule holds:

$$\forall a \in A^p, b \in A^q : \quad d(a \wedge b) = (da) \wedge b + (-1)^p a \wedge (db). \tag{B.79}$$

As usual, we will refer to A^* (and not the formal triple $(A^*, \wedge, d)$) as differential graded algebra. Finally, there might be additional structure:

- A^* is said to be graded anticommutative if

$$\forall a \in A^p, b \in A^q : \quad a \wedge b = (-1)^{pq} b \wedge a. \tag{B.80}$$

- A^* is called connected if $A^p = 0$ for all $p < 0$ and $A^0 \cong K$.

Example B.4.7. De Rham Differential Graded Algebra ([13], p.238). The obvious example for a differential graded algebra is given by the space of smooth differential forms $\Omega^*(M)$ together with the usual wedge product $\wedge$ and the exterior derivative d. It is also graded commutative but not connected (since $\Omega^0(M)$ is the space of smooth $\mathbb{K}$-valued functions on M and not $\mathbb{K}$.)

Remark. Note that every differential graded algebra can also be thought of as a cochain complex (with some additional structure). In particular, the notions of cohomology and quasi-isomorphisms carry over to differential graded algebras.

Example B.4.8. Real and complex projective spaces (compare [42], pp.6f.,21 and [40], p.29f.).

(i) Definition. Central is the following equivalence relation. Let $x, ybe \in \mathbb{R}^{n+1}$. Then

$$x \sim y :\iff \exists \lambda \in \mathbb{R} \setminus \{0\} : \ x = \lambda y. \tag{B.81}$$

One is easily convinced that this relation satisfies the three axioms of symmetry, reflexivity and transitivity for an equivalence relation. The real projective space is now defined by the quotient construction

$$\mathbb{RP}^n := \mathbb{R}^{n+1} \backslash \{0\} / \sim = \{[x]_\sim \mid x \in \mathbb{R}^{n+1} \backslash \{0\}\} \equiv \{\mathrm{span}(x) \mid x \in \mathbb{R}^{n+1} \backslash \{0\}\}; \tag{B.82}$$

moreover, $\mathbb{RP}^n$ is endowed with the quotient topology by means of the canonical projection

$$\pi : \mathbb{R}^{n+1} \setminus \{0\} \to \mathbb{RP}^n, \ x \mapsto [x] \tag{B.83}$$

and

$$U \subseteq \mathbb{RP}^n \text{ open} :\iff \pi^{-1}(U) \subseteq \mathbb{R}^{n+1} \setminus \{0\} \text{ open} \tag{B.84}$$

By definition, π satisfies the defining properties of a quotient mapping.

(ii) $\mathbb{RP}^n$ can be provided with structure of a toplogical manifold. We first construct the coordinate domains; the formal proof that $\mathbb{RP}^n$ has the Hausdorff property and satisfies the second axiom of countability will be omitted in this appendix (but cf. for example [43]). Define for each $j \in \{1, ..., n+1\}$ the sets

$$\tilde{U}_i := \{(x_1, ..., x_i, ..., x_{n+1}) \in \mathbb{R}^{n+1} \setminus \{0\} \mid x_i \neq 0\} \tag{B.85}$$

and from this the functions

$$\pi|_{\tilde{U}_i} : \tilde{U}_i \to \pi(\tilde{U}_i) =: U_i \subseteq \mathbb{RP}^n. \tag{B.86}$$

The sets $(U_i)_{i \in \{1,...,n\}}$ are open because $\pi^{-1}(U_i) = \tilde{U}_i$ is open. Moreover, $\bigcup_{i=1}^{n+1} U_i = \mathbb{RP}^n$ holds, as can be easily seen, so $(U_i)_i$ are indeed good candidates for coordinate domains. Now we still have to construct suitable coordinate mappings. It turns out that

$$\varphi_i : U_i \to \mathbb{R}^n, \ [x_1, ..., x_{n+1}] \mapsto \left(\frac{x_1}{x_i}, ..., \frac{x_{i-1}}{x_i}, \frac{x_{i+1}}{x_i}, ..., \frac{x_{n+1}}{x_i} \right) \tag{B.87}$$

is a correct choice. We first note that this definition is independent of the particular representative (possible factors truncate away in the quotient) and thus the mappings are well-defined. Moreover, $x \mapsto (\varphi_i \circ \pi)(x) = \varphi_i([x])$ is obviously continuous on $\tilde{U}_i$. Since $\pi|_{\tilde{U}_i}$ is a quotient mapping, as can be shown with a little topology, the continuity of φ_i follows with the universal property of quotient mappings (cf. [42], p.605). The bijectivity is also quickly shown by noting that through

$$\varphi_i^{-1}(u_1, ..., u_n) := [u_1, ..., u_{i-1}, 1, u_i, ..., u_n] \tag{B.88}$$

the inverse is defined. $(U_i, \varphi_i)_i$ are thus charts for $\mathbb{RP}^n$ and the real projective space becomes a topological manifold.

(iii) $\mathbb{RP}^n$ can be equipped with the structure of a differentiable manifold. It suffices to show that for $i, j \in \{1, ..., n+1\}$ with $i \neq j$ the transition maps $\varphi_j \circ \varphi_i^{-1}$ are diffeomorphisms. But this result can be easily obtained: for $i > j$ we get

$$\begin{aligned} \varphi_j \circ \varphi_i^{-1}(u_1, ..., u_n) &= \varphi_j([u_1, ..., u_{i-1}, 1, u_i, ..., u_n]) = \\ &= \left(\frac{u_1}{u_j}, ..., \frac{u_{j-1}}{u_j}, \frac{u_{j+1}}{u_j}, ..., \frac{u_{i-1}}{u_j}, \frac{1}{u_j}, \frac{u_i}{u_j}, ..., \frac{u_n}{u_j} \right) \end{aligned} \tag{B.89}$$

and for $i < j$ correspondingly

$$\varphi_j \circ \varphi_i^{-1}(u_1, ..., u_n) = \left(\frac{u_1}{u_j}, ..., \frac{u_{i-1}}{u_j}, \frac{1}{u_j}, \frac{u_{i+1}}{u_j}, ..., \frac{u_{j-1}}{u_j}, \frac{u_{j+1}}{u_j}, ..., \frac{u_n}{u_j} \right). \tag{B.90}$$

Both are smooth mappings from $\varphi_i(U_i \cap U_j)$ to $\varphi_j(U_i \cap U_j)$. The inverse map is given by $(\varphi_j \circ \varphi_i^{-1})^{-1} = \varphi_i \circ \varphi_j^{-1}$ and is also smooth as a transition map according to the calculation just done. So the $\varphi_j \circ \varphi_i^{-1}$ are indeed diffeomorphisms.

(iv) Complex case. Now define the equivalence relation in a very similar way as in (i)

$$\forall z, w \in \mathbb{C}^{n+1} : z \sim w :\Longleftrightarrow \exists \zeta \in \mathbb{C} \setminus \{0\} : \; z = \zeta w. \tag{B.91}$$

The complex projective space is then defined by

$$\mathbb{CP}^n := \mathbb{C}^{n+1} \setminus \{0\} / \sim . \tag{B.92}$$

Just as in steps (ii) and (iii) of this example, it can also be shown that $\mathbb{CP}^n$ is a complex differentiable manifold of dimension n. $\mathbb{CP}^1$ is also called a Riemann sphere.

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