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To my grandparents:
Ancina and Aron,
Iulia and Petru.

Abstract

In this thesis we present our contributions to symbolic summation, extending WZ-Fasenmyer methods to handle definite hypergeometric sums with nonstandard boundary conditions and to compute recurrences for multiple Mellin-Barnes integrals over hypergeometric terms. We also include concrete applications of these methods to Feynman integral calculus, as well as for proving identities involving definite integrals and special functions.

First we give a short introduction to WZ-summation methods, including K. Wegschaider's approach to this method and its implementation in the package `MultiSum`. Inspired by work of Sister Celine Fasenmyer, these techniques were introduced by H. Wilf and D. Zeilberger to algorithmically compute recurrences for multiple sums over hypergeometric terms. Their procedure is based on finding a certificate recurrence satisfied by the hypergeometric summand and summing over this difference equation to obtain a recurrence for the nested sum. Our proofs of two nontrivial special function identities involving Gegenbauer polynomials, provide classic applications of the method.

As part of the collaboration between RISC and DESY coordinated by C. Schneider, we developed an algorithmic approach to compute Feynman parameter integrals after rewriting them as multisums over hypergeometric terms to fit the input class of classic summation algorithms.

Since these definite sums have nonstandard boundary conditions, the WZ-method delivers inhomogeneous recurrence relations. We designed a recursive procedure to determine the inhomogeneous parts of these recurrences and implemented it in the Mathematica package `FSums` which builds on the already existing packages, `MultiSum` and C. Schneider's `Sigma`.

Another approach to evaluate Feynman integrals is by representating them in terms of nested Mellin-Barnes integrals. These complex contour integrals can also be viewed as sums of residues at certain poles of the integrands and they are connected to the inversion formula for the Mellin transform.

In the last part, we show how WZ-methods can be used to compute recurrences for multiple Mellin-Barnes integrals over hypergeometric terms, eliminating the need to search for sum representations. We applied this new algorithmic technique to prove typical entries from the Gradshteyn-Ryzhik table of integrals using the Mellin transform and to find recurrences for a class of Ising integrals.

Keywords: Symbolic summation, special functions, recurrences, difference equations, integral transforms, Mellin-Barnes integrals, Feynman integrals.

Zusammenfassung

In der vorliegenden Arbeit wird unser Beitrag, innerhald der symbolischer Summation, zur Erweiterung von WZ-Methoden, durch die Behandlung definiter Summen, die nicht Standardrandbedingungen erfüllen, sowie durch das Berechnen von Rekursionen für mehrfache Mellin-Barnes Integrale über hypergeometrische Terme, präsentiert. Außerdem werden konkrete Anwendungen dieser Methoden vorgestellt, sowohl für Feynman Integrale als auch zum Beweisen von Identitäten für definite Integrale und spezielle Funktionen.

Zunächst geben wir eine kurze Einführung in WZ-Summation inklusive einer Beschreibung von K. Wegschaiders Zugang und dessen Implementierung im Mathematica-Paket `MultiSum`. Diese Verfahren wurden von H.S. Wilf und D. Zeilberger entwickelt um algorithmisch Rekursionen für Mehrfachsummen über hypergeometrische Terme zu bestimmen. Sie basieren auf das Brechnen einer Zertifikatsrekursion, die vom hypergeometrischen Summanden erfüllt wird. Anschließend wird über diese Differenzengleichung summiert um so eine Rekursion für die verschachtelte Summe zu erhalten. Unsere Beweise zweier interessanter Identitäten für Gegenbauer Polynome demonstrieren klassische Anwendungen dieser Methode.

Im Rahmen einer Kollaboration zwischen RISC und DESY, haben wir einen algorithmischen Zugang zur Berechnung von Feynman Parameterintegralen entwickelt. Dazu verwenden wir eine Reformulierung der Integrale als Mehrfachsummen über hypergeometrische Terme, auf die dann die klassischen Summationsalgorithmen angewandt werden können.

Da wir es mit definiten Summen, die keine Standardrandbedingungen erfüllen, zu tun haben, sind die von der WZ-Methode gelieferten Rekursionen inhomogen. Wir haben ein rekursives Verfahren entwickelt, das die inhomogenen Terme dieser Rekursionen bestimmt und diese Prozedur im Mathematica-Paket `FSums` implementiert, welches auf die bereits existierende Pakte `MultiSum` und C. Schneiders `Sigma` aufbaut.

Ein anderer Zugang zur Evaluierung von Feynman Integralen nutzt eine Darstellung als verschachtelte Mellin-Barnes Integrale. Diese komplexen Kurvenintegrale können als Summen über Residuen an bestimmten Polen der Integranden betrachtet werden und hängen mit der Inversionsformel für die Mellin-Transformation zusammen.

Zum Abschluß zeigen wir wie WZ-Methoden eingesetzt werden können, um Rekursionen für mehrfache Mellin-Barnes Integrale über hypergeometrische Terme zu berechnen. Dieser Zugang vermeidet es erst Summendarstellungen der Integrale bestimmen zu müssen. Diese neue algorithmische Technik haben wir angewandt um typische Einträge der Gradshteyn-Ryzhik Integraltafel zu beweisen, indem wir die Mellin-Transformation verwenden, und um Rekursionen für eine Klasse von Ising-Integralen zu ermitteln.

Stichwörter: Symbolische Summation, spezielle Funktionen, Rekurrenzen, Differenzengleichungen, Integraltransformationen, Mellin-Barnes Integrale, Feynman Integrale.

Contents

1 Introduction

The domain of symbolic summation concentrates on the development of algorithmic methods for finding and proving identities involving special functions. One of the first generic approaches to this problem was presented by Sister Celine Fasenmyer in her thesis [25, 54] from 1945. Later, Gosper's algorithm for indefinite summation [31] which he implemented in Macsyma [42] became a cornerstone of the field and made it popular as part of an emerging interest in computer mathematics systems.

Zeilberger's generalization [75] of Gosper's algorithm to handle definite sums and the Wilf-Zeilberger (WZ) summation methods [76] extending Sister Celine's technique to multiple sums over proper hypergeometric summands in an algorithmic fashion gave the decisive impulse for further developments of the field. These classic techniques are the focus of this thesis and in this context, we present practical extensions of WZ-methods.

After these starting points there were many developments, both by extending the input class, through Karr's summation analog [35] for the Risch integration algorithm [55] or Zeilberger's holonomic approach [79], and from the point of view of efficiency [27,28,51,71,72]. Further extensions and improvements of these methods can be found in [2, 4, 21, 22, 29, 48, 49, 52, 62].

As a result of the latest theoretical advances and their implementations in mainstream computer algebra systems [3,36,41,51,72], summation methods became strong enough for real-world applications. For instance in combinatorics [50, 61], finite element methods [39, 53] or our proofs of two special function identities presented in Section 2.2.

Even in the light of these developments, numerical [30] or table look-up methods [26] are still preferred over their symbolic counter parts for summation problems. A similar situation holds for differential equation solving or integration methods. The reason for this phenomenon, apart from efficiency considerations, may be the subtle missing links in the usage of symbolic algorithms, mostly related to analytical issues.

In this thesis we will concentrate on some of these analytic issues such as considering definite nested sums with nonstandard boundary conditions where the summation range needs to be adjusted according to the set of well-defined values of the summands. Another aspect of our work concerns algorithmically finding recurrence relations for Mellin-Barnes integrals without the need to look for sum representations first.

In the next chapter we give a short description of WZ-summation methods, including Wegschaider's approach to this method and its implementation in the package

MultiSum. The rest of Chapter 2 contains proofs for some special functions identities obtained via these methods [66].

Chapter 3 is dedicated to our work on the evaluation of a class of Feynman parameter integrals as part of the collaboration between RISC and DESY under the direction of C. Schneider. Our contribution to the project was to introduce WZ-summation to improve the computation of these intricate integrals after suitable representations in terms of multisums over proper hypergeometric terms were found. In this context we develop an algorithmic approach to sums with nonstandard bounds for which we set up inhomogeneous recurrence relations. Our techniques are implemented in the package FSums which relies on other summation packages like MultiSum and C. Schneider's Sigma.

In chapter 4 we present a new method to apply WZ-summation techniques for multiple Mellin-Barnes integrals over hypergeometric integrands. These complex contour integrals, related to the inversion formula for the Mellin transform, provide an alternative way to compute Feynman integrals. Our procedure to determine homogeneous and inhomogeneous recurrences for contour integrals of this type eliminates the need to find sum representations which was a crucial non-algorithmic step in the computational approach presented in Chapter 3. We also apply this new algorithmic technique to prove typical entries from the Gradshteyn-Ryzhik table of integrals [32] using the Mellin transform [38] and to find recurrences for a class of Ising integrals [65].

The work presented in this thesis has lead to four papers [15, 38, 65, 66], three of which are accepted for publication.

1.1 An illustrative example

One can summarize the theme of this thesis as finding new symbolic summation methods for computing Feynman parameter integrals. Namely, we look for strategies to apply WZ-Fasenmyer summation techniques to large real-world problems of this type. To illustrate our main procedures let us consider the following simple Feynman parameter integral of the type described in [15],

$$I = \int_0^1 \int_0^1 \frac{(1-w)^{-1-\epsilon/2} z^{\epsilon/2} (1-z)^{-\epsilon/2}}{(1-wz)^{1-\epsilon}} (1-w)^{N+1}\, dw\, dz,$$

where the Mellin moment $N \in \mathbb{N}$ is a discrete variable which becomes important in the application of our symbolic methods. In this context, our collaborators from DESY are interested in determining the first few coefficients of the Laurent series expansion for the analytic object defined by the integral in $\epsilon > 0$, the dimension regularization parameter.

For this purpose, one looks for equivalent representations in terms of nested sums over hypergeometric terms. In this case, we observe a resemblance between I and the integral representation for a ${}_3F_2$ hypergeometric series which leads to rewriting the integral as

$$I = \frac{\Gamma\left(1-\frac{\epsilon}{2}\right)\Gamma\left(1+\frac{\epsilon}{2}\right)}{2\left(N+1-\frac{\epsilon}{2}\right)} \sum_{\sigma\geq 0} \frac{(1-\epsilon)_\sigma \left(1+\frac{\epsilon}{2}\right)_\sigma}{(2)_\sigma \left(N+2-\frac{\epsilon}{2}\right)_\sigma}. \tag{1.1}$$

This summation problem fits the input class of WZ-summation techniques. By calling Wegschaider's package `MultiSum` we compute a certificate recurrence satisfied by its summand, denoted here by `F[N, σ]`,

Out[0]= $(N+1)(2N-\epsilon+2)F[N,\sigma]-(N-\epsilon+1)(2N+\epsilon+2)F[N+1,\sigma] = \Delta_\sigma[(-\sigma-1)(2N-\epsilon+2)F[N,\sigma]]$

where Δ_σ is the forward shift operator in the variable σ. Note that the left hand side coefficients of this recurrence are free of summation variables. When we sum the recurrence over the given range, the delta part on the right will telescope and we obtain a recurrence satisfied by the sum representing I.

However, in the case of definite nested sums related to Feynman integral calculus, we often encounter summands that do not satisfy a finite support condition. These sums are said to have *nonstandard summation bounds*. We can only assume that these proper hypergeometric terms are well defined inside the original range. Therefore, the size and analytic structure of the sums we are computing make it unfeasible to reformulate them as even larger summation problems with standard boundary conditions, and force us to manipulate and solve inhomogeneous recurrence relations.

Coming back to our simple example, we obtain the following recurrence for the integral I, now denoted by `SUM[N]`,

Out[0]= $\text{rec} = (N+1)(2N-\epsilon+2)\text{SUM}[N]-(N-\epsilon+1)(2N+\epsilon+2)\text{SUM}[N+1] == \Gamma\left(1-\frac{\epsilon}{2}\right)\Gamma\left(\frac{\epsilon}{2}+1\right).$

In chapter 3, we present an algorithmic approach to determine the inhomogeneous side of recurrences for multiple sums with nonstandard bounds, implemented in our package `FSums`. Using these inhomogeneous recurrences and procedures from the packages `Sigma`, `EvaluateMultiSums` and `HarmonicSums`, we have developed a strategy to answer the question of finding the coefficients in the Laurent series expansion in ϵ mentioned above in terms of multiple harmonic sums.

Another approach to Feynman integral calculus is via *Mellin-Barnes integrals.* For the integral I we find a reformulation as a contour integral by using the following special case of a result going back to Barnes [63, Chapter 4]

$$\frac{1}{(1-wz)^{1-\epsilon}} = \frac{1}{2\pi i}\int_{\mathcal{C}_s} \frac{\Gamma(-s)\,\Gamma(1-\epsilon+s)}{\Gamma(1-\epsilon)}(-wz)^s ds,$$

where the contour is drawn such that the ascending chain of poles of the function $\Gamma(-s)$ is separated from the descending chain coming from $\Gamma(1-\epsilon+s)$ as we sketched in

Figure 1.1: The integration contours $\mathcal{C}_s$ and Λ_m

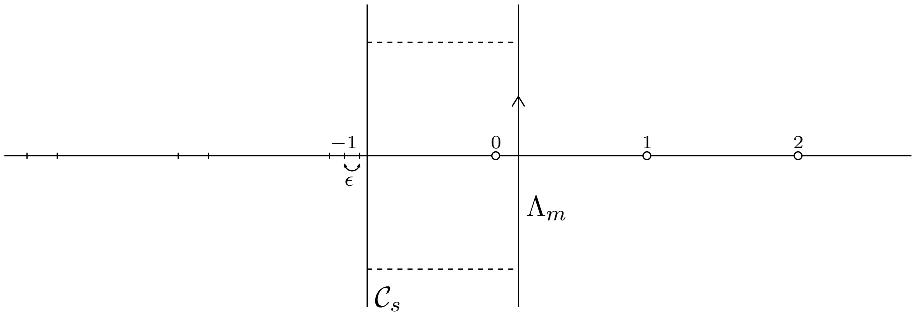


figure 1.1. Moreover, we are allowed to reverse the order of integration and using the property (1.4) of the beta function, we obtain the following contour integral of Barnes' type

$$I = \frac{\Gamma\left(1-\frac{\epsilon}{2}\right)\Gamma\left(N-\frac{\epsilon}{2}+1\right)}{4\pi i\Gamma(1-\epsilon)}\int_{\mathcal{C}_s}\frac{\Gamma(-s)\Gamma(s+1-\epsilon)\Gamma\left(s+1+\frac{\epsilon}{2}\right)}{(s+1)\Gamma\left(N+s-\frac{\epsilon}{2}+2\right)}(-1)^s\,ds \qquad (1.2)$$

which has a hypergeometric integrand satisfying the same certificate recurrence as the summand of the sum representation (1.1) with respect to the discrete parameter N and the integration variable s. Next we integrate this certificate recurrence over the contour $\mathcal{C}_s$ and compute the integral over the Δ_s-part.

We end up with an improper integral defined as

$$\int_{\mathcal{C}_s}\Delta_s[(-s-1)(2N-\epsilon+2)F[N,s]] := -(2N-\epsilon+2)\lim_{m\to\infty}\int_{\Lambda_m}(s+1)F[N,s]\,ds$$

where, `F[N,s]` denotes the integrand from (1.2). We evaluate the integrals over the closed contours Λ_m by using Cauchy's residue theorem and get the recurrence relation `rec`, this time satisfied by the Mellin-Barnes integral representation of I.

In chapter 4, we give more details about this method of finding recurrences for nested Mellin-Barnes integrals over proper hypergeometric terms. Moreover we apply it to compute recurrences for a class of Ising integrals and to prove typical entries involving definite integrals over various special functions from the Gradshteyn-Ryzhik table of integrals using the Mellin transform.

1.2 Notation and preliminary notions

We will denote the set of natural numbers $\{0, 1, \dots\}$ with $\mathbb{N}$, positive natural numbers $\{1, 2, \dots\}$ with $\mathbb{N}^*$, ring of integers with $\mathbb{Z}$, field of rational numbers with $\mathbb{Q}$, real numbers with $\mathbb{R}$, and complex numbers with $\mathbb{C}$.

The notation $[a \dots b]$ for integers $a, b \in \mathbb{Z}$ will be used for the closed integer interval $\{\, i \in \mathbb{Z} \,|\, a \le i \le b \,\}$. We will also write $[a \dots \infty)$ to denote $\{\, i \in \mathbb{Z} \,|\, a \le i \,\}$.

1.2.1 Multi indices

We will often use tuples as indices to sums or arguments to functions. This allows us to work with multisums while keeping the notation similar to the single sum case. For instance, we write $\mu \in S^k$ to indicate μ is a k-tuple with elements from a set S. In this case, the same letter with sub-indices will be used to denote the components of the tuple, as in $\mu = (\mu_1, \dots, \mu_k)$.

Let $i, j \in S^n$ be two n-tuples with elements in S. The sum and exponents of these tuples will be taken componentwise. More precisely, we have

$$i + j = (i_1 + j_1, \dots, i_n + j_n) \quad \text{and} \quad i^j = (i_1^{j_1}, \dots, i_n^{j_n}).$$

For $c \in S$, addition and multiplication of a tuple with c will be used to denote the application of this operation to each component of the n-tuple. Then we have

$$i + c = (i_1 + c, \dots, i_n + c) \quad \text{and} \quad ci = (ci_1, \dots, ci_n).$$

Another operation we will use is the dot product, i.e., $i \cdot j = i_1 j_1 + \cdots i_n j_n$.

In Chapter 3, when discussing summation problems with nonstandard boundary conditions, we take the norm of a tuple $i \in \mathbb{N}^n$ as the sum of its components

$$|i| = \sum_{l=1}^{n} i_l.$$

Tuples will also be used to denote multi-dimensional intervals. The range represented by the tuple interval $[i \dots j]$ is the Cartesian product of the intervals defined by the components. More precisely,

$$[i \dots j] = [i_1 \dots j_1] \times [i_2 \dots j_2] \times \cdots \times [i_n \dots j_n].$$

Often when working with multisums, summation ranges for inner sums will depend on the value of a variable for an outer sum. Intervals whose endpoints are defined by tuples are not enough to represent the summation ranges for these sums, since they are not simple cartesian products of coordinate sets. For example, in the sum

$$\sum_{j_0=1}^{N-2} \sum_{j_1=0}^{N-j_0-2} \sum_{j_2=0}^{j_0} \sum_{j_3=0}^{j_1+2} \mathcal{F}(N, j_0, j_1, j_2, j_3)$$

the ranges of the inner sums all depend on a summation variable from a previous sum. We will use a variant of the cartesian product notation above to denote such a summation range. In order to be able to refer to a variable associated to a range, we will specify it as a subscript to the corresponding interval. To indicate that we are using this shorthand notation, we will use $\ltimes$ signs instead of the $\times$ symbols. For example, the range for the sum above can be written as

$$[1 \dots N-2]_{j_0} \ltimes [0 \dots N-j_0-2]_{j_1} \ltimes [0 \dots j_0] \ltimes [0 \dots j_1+2].$$

1.2.2 Hypergeometric series

A series $\sum_{k \geq 0} c_n$ is called a *hypergeometric series* if the ratio of two consecutive terms is a rational function, i.e., if there exist two polynomials in $p(k), q(k)$ such that

$$\frac{c_{n+1}}{c_n} = \frac{p(k)}{q(k)}.$$

In this case the terms c_n will be called *hypergeometric terms.*

By factorizing the polynomials p and q completely, we can write the ratio of two terms in the form

$$\frac{p(k)}{q(k)} = \frac{(k+a_1)(k+a_2)\cdots(k+a_p)x}{(k+b_1)(k+b_2)\cdots(k+b_q)(k+1)},$$

where the constant x is the leading coefficient of $p(k)$ in case it is not monic. Even if the factor $(k+1)$ doesn't occur in $q(k)$, it can be added to the numerator to obtain this traditional form.

Now we can write an explicit formula for the series. More precisely,

$$\sum_{k=0}^{\infty} c_n = c_0 \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_2)_k}{(b_1)_k \cdots (b_q)_k} \frac{x^k}{k!}$$

where $(a)_k$ is the rising factorial.

This last generic form is encapsulated in the notation

$${}_pF_q\left(\begin{matrix} a_1, \dots, a_p \\ b_1, \dots, b_q \end{matrix}; x\right) = \sum_{k=0}^{\infty} \frac{(a_1)_k \cdots (a_2)_k}{(b_1)_k \cdots (b_q)_k} \frac{x^k}{k!}$$

where the b_i's are not negative integers or zero.

Hypergeometric series play a central role in the study of special functions. Extensive information about them can be found in classical texts like [7, 54]. More information on hypergeometric terms and their applications in symbolic summation can be found in [76, 78].

1.2.3 Operators

Since we will be studying recurrences, operators will be an indispensable tool. Given a function $F(k) : \mathbb{C}^r \to \mathbb{C}$, with variables $k = (k_1, \ldots, k_r)$, we say that F satisfies a homogeneous polynomial recurrence relation if there exist a finite nonempty set $\mathbb{S} \subset \mathbb{Z}^r$ and a polynomial $a_i(k) \in \mathbb{C}[k] \setminus \{0\}$ for each $i \in \mathbb{S}$ such that

$$\sum_{i \in \mathbb{S}} a_i(k) F(k + i) = 0 \tag{1.3}$$

for all $k \in \mathbb{C}^r$ where $F(k + i)$ is well defined for all $i \in \mathbb{S}$. More precise definitions of the domain of validity of the recurrence will be provided in Section 2.1.2 in the context of hypergeometric summation.

Another way to write this recurrence relation is to consider operators which act on the variables k_i by shifting them forward by 1, i.e., $K_i k_i = (k_i + 1)K_i$ for all $i \in \{0, \ldots, r\}$. Extending the multi-index notation to operators, we can write $K^i k = k + i$ where $K = (K_0, \ldots, K_r)$, $k = (k_0, \ldots, k_r)$ and $i \in \mathbb{Z}^r$ as above. Now the recurrence relation (1.3) becomes

$$\sum_{i \in \mathbb{S}} a_i(k) K^i F(k) = 0.$$

To provide a formal setting for the manipulation of recurrences, we consider the operator ring $\mathbb{C}[k]\langle K \rangle$ with elements of the form

$$\sum_{i \in \mathbb{S}} a_i(k) K^i.$$

for a finite nonempty set $\mathbb{S} \subset \mathbb{N}^r$ and nonzero polynomials $a_i(k) \in \mathbb{C}[k]$. In this ring, addition is performed by adding the coefficients of monomials with the same degree, i.e., $a_i(k)N^i + a_i'(k)N^i = (a_i(k) + a_i'(k))N^i$. Multiplication on monomials is defined by $a_i(k)N^i * a_j(k)N^j = (a_i(k) * a_j(k + i))N^{i+j}$ and extended linearly to polynomials. We can also perform right or left Euclidean division [20]. Note that we restricted the exponents to $\mathbb{N}^r$ which gives only forward shift operators.

We say that a function $F(k)$ is annihilated by an operator $\mathcal{P} \in \mathbb{C}[k]\langle K \rangle$, if $\mathcal{P}F = 0$. Functions that are annihilated by operators with polynomial coefficients as we defined here are called *P-recursive* [67] or *holonomic* [79]. This class covers a wide range of special functions and it is computationally interesting due to its closure properties. Packages such as `GeneratingFunctions` [41] and `gfun` [56] provide tools to manipulate recurrences obtained for these objects.

Note that a hypergeometric sequence $f(n)$ satisfies a first order linear recurrence with polynomial coefficients. More precisely, there exist polynomials $p_0(n), p_1(n)$ such that $p_1(n)f(n + 1) + p_0(n)f(n) = 0$ for all $n \in \mathbb{N}$.

1.2.4 Rising factorials

We define the rising factorial $(a)_n$ for $a \in \mathbb{C}$, and $n \in \mathbb{Z}$ as

$$(a)_n := \begin{cases} a(a+1)\cdots(a+n-1) & \text{if } n > 0 \\ 1 & \text{if } n = 0 \\ \frac{1}{(a-1)(a-2)\cdots(a+n)} & \text{if } n < 0 \text{ and } a \notin \{1, 2, \ldots, -n\}. \end{cases}$$

Rising factorials are also known as the *Pochhammer symbol.* We also use the following identity

$$(a)_n = \frac{\Gamma(a+n)}{\Gamma(a)} \text{ if } a \in \mathbb{C} \text{ and } a+n \notin \{0, -1, -2, \ldots\}$$

1.2.5 Beta function

We define the Beta function [5, 6.2] by

$$B(p,q) := \int_0^1 t^{p-1}(1-t)^{q-1}dt$$

for $Re(p) > 0$ and $Re(q) > 0$. Another useful representation of this function can be obtained using its relation to the Gamma function

$$B(p,q) = \frac{\Gamma(p)\Gamma(q)}{\Gamma(p+q)}. \tag{1.4}$$

1.2.6 Multiple harmonic sums

Harmonic numbers of order k, denoted by $H_n^{(k)}$, are defined as the sum

$$H_n^{(k)} = \sum_{i=1}^{n} \frac{1}{i^k}.$$

In the order one case, we will omit k and just write H_n. The nested harmonic sums occur frequently in physics applications [1,16,70,73]. We use the shorthand $S_{a_1,\ldots,a_k}(n)$ for $a_i \in \mathbb{Z} \setminus \{0\}$ to denote multiple harmonic sums of the form

$$\sum_{i_1=1}^{n} \sum_{i_2=1}^{i_1} \cdots \sum_{i_k=1}^{i_{k-1}} \frac{\text{sign}(a_1)^{i_1}}{i_1^{|a_1|}} \frac{\text{sign}(a_2)^{i_2}}{i_2^{|a_2|}} \cdots \frac{\text{sign}(a_k)^{i_k}}{i_k^{|a_k|}}.$$

For example, $S_{-1,2}(n)$ is

$$\sum_{i=1}^{n} \sum_{j=1}^{i} \frac{(-1)^i}{i} \frac{1}{j^2} = \sum_{i=1}^{n} \frac{(-1)^i \sum_{j=1}^{i} \frac{1}{j^2}}{i}.$$

Note that $S_1(n) = H_n$. In Mathematica output, $S_{a_1,\ldots,a_k}(n)$ will be represented by $\texttt{S}[a_1, \ldots, a_n, n]$.

2 Proving special functions identities with WZ summation methods

This chapter contains a general introduction to WZ-Fasenmyer summation [76] and describes Wegschaider's algorithm [72] which we use throughout the thesis. The following chapters rely on some notions defined in the introductory Section 2.1.

The second section presents direct proofs for two interesting special function identities involving Gegenbauer polynomials. These proofs provide an example of the application of WZ-methods in this domain. These identities were proved by E. Symeonidis in [69] in an indirect fashion by showing that both sides of the equality define the same analytic object.

2.1 A short introduction to WZ summation

Wegschaider's algorithm [72] is an extension of multivariate WZ summation [76]. In this chapter it is used to compute recurrences for sums of the form

$$Sum\,(\mu,\alpha) = \sum_{\kappa_1\in\mathcal{R}_1}\cdots\sum_{\kappa_r\in\mathcal{R}_r}\mathcal{F}\,(\mu,\kappa_1,\ldots,\kappa_r,\alpha)\,. \tag{2.1}$$

Under some mild side conditions described in [72], it can be applied if the summands $\mathcal{F}\,(\mu,\kappa,\alpha)$ are hypergeometric in all integer variables μ_i from $\mu=(\mu_1,\ldots,\mu_p)$ and in all summation variables κ_j from $\kappa=(\kappa_1,\ldots,\kappa_r)\in\mathcal{R}$ where $\mathcal{R}:=\mathcal{R}_1\times\cdots\times\mathcal{R}_r\subseteq\mathbb{Z}^r$ is the summation range. The sums we consider can also depend on some additional parameters α_i from $\alpha\in\mathbb{C}^l$.

Remark 2.1. Recall from Section 1.2.2 that an expression $\mathcal{F}\,(\mu,\kappa,\alpha)$ is called hypergeometric, if there exists a rational function $r_{m,k}(\mu,\kappa,\alpha)$ such that $\frac{\mathcal{F}(\mu,\kappa,\alpha)}{\mathcal{F}(\mu+m,\kappa+k,\alpha)} = r_{m,k}(\mu,\kappa,\alpha)$ at the points $m\in\mathbb{Z}^p$ and $k\in\mathbb{Z}^r$ where this ratio is defined.

As described in [76], WZ-summation is based on Sister Celine's method [54] of finding a κ-free recurrence for the hypergeometric summand $\mathcal{F}\,(\mu,\kappa,\alpha)$

$$\sum_{(u,v)\in\mathbb{S}} c_{u,v}\,(\mu,\alpha)\,\mathcal{F}(\mu+u,\kappa+v,\alpha)=0 \tag{2.2}$$

where the finite set of shifts $\mathbb{S}\subset\mathbb{Z}^{p+r}$ is called the structure set of the recurrence.

Denoting the forward-shift operators with respect to the variables from μ by $M = (M_1, \ldots, M_p)$ and those from κ by $K = (K_1, \ldots, K_r)$ and using the multi-index notation from Section 1.2.1, the left hand side of (2.2) can be viewed as applying to $\mathcal{F}$ the operator

$$\mathcal{P}(\mu, \alpha, M, K) := \sum_{(u,v)\in\mathbb{S}} c_{u,v}(\mu, \alpha)\, M^u K^v. \tag{2.3}$$

The next step consists of successively dividing the polynomial recurrence operator $\mathcal{P}$ by all forward-shift difference operators

$$\Delta_{\kappa_j}\mathcal{F}(\mu,\kappa,\alpha) := (K_i - 1)\,\mathcal{F}(\mu,\kappa,\alpha) = \mathcal{F}(\mu, \kappa_1, \ldots, \kappa_j + 1, \ldots, \kappa_r, \alpha) - \mathcal{F}(\mu, \kappa, \alpha)$$

to obtain an operator free of shifts in the summation variables κ_j from $\kappa = (\kappa_1, \ldots, \kappa_r)$, called the principal part of the recurrence (2.2).

Given a structure set $\mathbb{S}$ together with the hypergeometric summand $\mathcal{F}(\mu, \kappa, \alpha)$, Wegschaider's algorithm [72] computes a certificate recurrence of the form

$$\sum_{m\in\mathbb{S}'} a_m(\mu,\alpha)\,\mathcal{F}(\mu+m,\kappa,\alpha) = \sum_{j=1}^{r} \Delta_{\kappa_j}\left(\sum_{(m,k)\in\mathbb{S}_j} b_{m,k}(\mu,\kappa,\alpha)\,\mathcal{F}(\mu+m,\kappa+k,\alpha)\right), \tag{2.4}$$

where the polynomials $a_m(\mu, \alpha)$, not all zero, and $b_{m,k}(\mu, \kappa, \alpha)$, as well as the sets of shifts $\mathbb{S}_j \subset \mathbb{Z}^{p+r}$ and $\mathbb{S}' \subset \mathbb{Z}^p$ are determined algorithmically.

Here some more details on Wegschaider's approach to WZ-summation, which will be used throughout this thesis, are in order.

Wegschaider first observes in [72, Section 3.2] that during the chain of divisions of the k-free operator (2.3) by the Δ_{κ_j}'s, we can obtain a zero remainder at any point. To fix this shortcoming and prove that from a k-free recurrence one always obtains a nontrivial certificate recurrence [72, Theorem 3.2], we need to consider more general certificate recurrences of the form (2.4), with non-k-free polynomial coefficients in the delta parts.

Remark 2.2. Wegschaider went even further along this path, by starting with an Ansatz for a non-k-free recurrence of the form

$$\sum_{(u,v)\in\mathbb{S}} c'_{u,v}(\mu,\kappa,\alpha)\,\mathcal{F}(\mu+u,\kappa+v,\alpha) = 0 \tag{2.5}$$

instead of the k-free one (2.2), which lead to smaller recurrences and much better computation times [72, Section 3.5]. Therefore, by expanding the certificate recurrence (2.4) we obtain precisely an operator of the form

$$\mathcal{P}'(\mu,\kappa,\alpha,M,K) := \sum_{(u,v)\in\mathbb{S}} c'_{u,v}(\mu,\kappa,\alpha)\,M^u K^v \tag{2.6}$$

with coefficients $c'_{u,v}(\mu, \kappa, \alpha) \in \mathbb{C}[\mu, \kappa, \alpha]$.

Note also that in [76], a certification procedure is introduced, based on rewriting the right hand side as

$$\sum_{j=1}^{r}\Delta_{\kappa_j}\left(\sum_{(m,k)\in\mathbb{S}_j} b_{m,k}\left(\mu,\kappa,\alpha\right)\mathcal{F}(\mu+m,\kappa+k,\alpha)\right)= \sum_{j=1}^{r}\Delta_{\kappa_j}\left(r_j\left(\mu,\kappa,\alpha\right)\mathcal{F}(\mu,\kappa,\alpha)\right), \quad (2.7)$$

where the certificates, r_j for all $1\le j\le r$, are rational functions with respect to all variables.

Remark 2.3. As we mentioned above, the left side of (2.4) constitutes the principal part of the k-free recurrence (2.2) and its coefficients $a_m\left(\mu,\alpha\right)$ are polynomials free of the summation variables κ_j from κ, while the coefficients $b_{m,k}\left(\mu,\kappa,\alpha\right)$ of the delta-parts are polynomials involving all variables.

Remark 2.4. Since the right side of (2.4) contains the quotients of the successive divisions by the delta operators, in each expression inside a delta-part Δ_{κ_j}, the summand $F(\mu,\kappa,\alpha)$ will appear free of shifts in the summation variables κ_i with $1\le i<j$. This implies that the sets $\mathbb{S}_j$ are of the form

$$\mathbb{S}_j=\left\{(m,k_1,\dots,k_r)\in\mathbb{Z}^{p+r}: k_i=0 \text{ for } 1\le i<j\right\}$$

for all $1\le j\le r$.

2.1.1 Proper hypergeometric functions

Another important remark is that we find a certificate recurrence for the hypergeometric term $\mathcal{F}\left(\mu,\kappa,\alpha\right)$, if such a recurrence exists. To be more precise, the algorithm [72] terminates successfully, for a large enough structure set, if we restrict our input class to *proper* hypergeometric summands.

Definition 2.5. *[72, Definition 2.1] A proper hypergeometric term takes the form*

$$\mathcal{F}\left(\mu,\kappa,\alpha\right)=\psi(\mu,\kappa,\alpha)\frac{\prod_{i=1}^{ii}\Gamma\left(a_i\mu+b_i\kappa+c_i(\alpha)\right)}{\prod_{j=1}^{jj}\Gamma\left(u_j\mu+v_j\kappa+w_j(\alpha)\right)}x_1(\alpha)^{\mu_1}\dots x_p(\alpha)^{\mu_p}y_1(\alpha)^{\kappa_1}\dots y_r(\alpha)^{\kappa_r} \quad (2.8)$$

with $ii,jj\in\mathbb{N}^*$ and $a_i,u_j\in\mathbb{Z}^p$, $b_i,v_j\in\mathbb{Z}^r$, $c_i,w_j\in\mathbb{C}[\alpha]$ for all $1\le i\le ii$ and $1\le j\le jj$. Additionally, $x_1\dots x_p,y_1,\dots y_r\in\mathbb{C}[\alpha]$ are polynomials in the additional parameters α and $\psi(\mu,\kappa,\alpha)\in\mathbb{C}[\mu,\kappa,\alpha]$.

In contrast to the notion of "simple" hypergeometric, if a proper hypergeometric term should contain, instead of a polynomial, a rational function $\psi(\mu,\kappa,\alpha) \in \mathbb{C}(\mu,\kappa,\alpha)$, its denominator would factor completely into integer-linear factors of the form $u\mu+v\kappa+w$ with $u \in \mathbb{Z}^p, v \in \mathbb{Z}^r$ and $w \in \mathbb{C}[\alpha]$. Factors of this type can be always rewritten as quotients of gamma functions $\frac{1}{u\mu+v\kappa+w} = \frac{\Gamma(u\mu+v\kappa+w)}{\Gamma(u\mu+v\kappa+w+1)}$.

Many important special functions can be represented as sums of proper hypergeometric terms, such as, the Bessel function

$$J_n(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!\Gamma(n+k+1)} \left(\frac{x}{2}\right)^{n+2k} \tag{2.9}$$

or the Jacobi polynomials

$$P_n^{(a,b)}(x) = \binom{n+a}{n} \sum_{k=0}^{n} \frac{(-n)_k (n+a+b+1)_k}{k!(a+1)_k} \left(\frac{1-x}{2}\right)^k, \tag{2.10}$$

with $a, b > -1$, where $(a)_l$ denotes the Pochhammer symbol defined in Section 1.2.4.

As a side-remark, the Gegenbauer polynomials appearing in the next section, are a special case of Jacobi polynomials defined for $\lambda > -\frac{1}{2}$ by

$$C_n^{\lambda}(x) = \frac{(2\lambda)_n}{\left(\lambda+\frac{1}{2}\right)_n} P_n^{(\lambda-\frac{1}{2},\lambda-\frac{1}{2})}(x).$$

Especially in chapter 3, we will regard proper hypergeometric terms as complex valued functions in all parameters. For this we need to exclude from the definition domain the poles of the numerator gamma functions and use the complex logarithm function to define the function x^k for complex values of x and k. Like in [72], we choose $\log : \mathbb{C}^* \to \mathbb{C}$

$$\log z = \ln|z| + i \arg z \quad \text{with} \quad -\pi < \arg z < \pi. \tag{2.11}$$

Definition 2.6. *[72, Definition 2.3] Let $\mathcal{F}(\mu,\kappa,\alpha)$ be a proper hypergeometric term as in Definition 2.5 and denote by*

$$\begin{aligned} D_{\mathcal{F}} := \{(m,k,a) \in \mathbb{C}^{p+r+l} : \quad & a_i\mu + b_i\kappa + c_i(a) \notin \mathbb{Z}\setminus\mathbb{N}^* \text{ for all } 1 \le i \le ii, \\ & x_j(a) \neq 0, j \in [1\ldots p] \text{ and } y_n(a) \neq 0, \text{ for } n \in [1\ldots r]\} \end{aligned}$$

the set of its well-defined values. The proper hypergeometric function in μ and κ of $\mathcal{F}$ is $\tilde{\mathcal{F}} : D_{\mathcal{F}} \to \mathbb{C}$ defined as

$$\begin{aligned} \tilde{\mathcal{F}}(\mu,\kappa,\alpha) =& \psi(\mu,\kappa,\alpha) \frac{\prod_{i=1}^{ii} \Gamma\left(a_i\mu + b_i\kappa + c_i(\alpha)\right)}{\prod_{j=1}^{jj} \Gamma\left(u_j\mu + v_j\kappa + w_j(\alpha)\right)} \\ & \times e^{\mu_1 \log x_1(\alpha)} \cdots e^{\mu_p \log x_p(\alpha)} e^{\kappa_1 \log y_1(\alpha)} \cdots e^{\kappa_r \log y_r(\alpha)} \end{aligned}$$

where the complex logarithm is given by (2.11).

In [76], Wilf and Zeilberger show the existence of k-free recurrences for every proper hypergeometric function and used this fact to prove the fundamental theorem of hypergeometric summation.

Theorem 2.7. *[76, Section 2] Every proper hypergeometric function $\tilde{\mathcal{F}}(\mu, \kappa, \alpha)$ satisfies a nontrivial certificate recurrence (2.4) in μ with delta parts in κ.*

Remark 2.8. This certificate recurrence will hold for well-defined values from $D_{\mathcal{F}}$. There are several strategies, presented in [72, Section 2.7], to extend a k-free recurrence for singular values of $\tilde{\mathcal{F}}$. The most general approach is to introduce a new variable $\epsilon > 0$ and compute a recurrence for a new function $\tilde{\mathcal{F}_1}$ having the property $\lim_{\epsilon \to 0} \tilde{\mathcal{F}}_1(\mu, \kappa, \alpha, \epsilon) = \tilde{\mathcal{F}}(\mu, \kappa, \alpha)$ at the singular point (μ, κ, α). For example, the binomial coefficient for $n, k \in \mathbb{C}$ is defined as

$$\binom{n}{k} = \lim_{\varepsilon \to 0} \frac{\Gamma(n+1+\varepsilon)}{\Gamma(k+1)\Gamma(n-k+1+\varepsilon)},$$

which also exists, for $k \in \mathbb{Z}$, when $n \in \{-1, -2, \dots\}$. See also [33, Section 5.5, (5.90)].

2.1.2 Summing over certificate recurrences

Coming back to the algorithmic point of view, a k-free recurrence (2.2) was found by Sister Celine's technique, after making an Ansatz about its structure set $\mathbb{S}$. Comparing coefficients for all appearing power products of the form $\kappa_1^{s_1} \dots \kappa_r^{s_r}$ in this equation with zero, we ended up with a homogeneous system of linear equations for the coefficients $c_{u,v}(\mu, \alpha)$ over the field of rational functions $\mathbb{C}(\mu, \alpha)$. If the set of solutions for this equation system was empty, we have to extend the structure set $\mathbb{S}$ in our Ansatz.

The existence theory from [76] assures the termination of this procedure, but the proven bounds for structure sets are far bigger than the ones arising in practice. Although, Wegschaider improved this approach by using Verbaeten's P-maximal structure sets [72, Section 2.5], instead of rectangular ones, in non-elementary applications it was a still time and space consuming.

Nowadays, we use a very efficient method based on modular computation to guess a candidate structure set, which was introduced and implemented in the Mathematica package `MultiSum` by A. Riese and B. Zimmermann. This package which includes an implementation of Wegschaider's algorithm [72] can be loaded within a Mathematica session by

In[1]:= **<< MultiSum.m**

MultiSum Package by Kurt Wegschaider (enhanced by Axel Riese and Burkhard Zimmermann) – © RISC Linz – V2.02β (02/21/05)

Finally, the recurrence for the multisum (2.1) is obtained by summing the certificate recurrence (2.4) over all variables from κ in the given summation range $\mathcal{R} \subseteq \mathbb{Z}^r$. Since it can be easily checked whether the summand $\mathcal{F}(\mu, \kappa, \alpha)$ indeed satisfies the recurrence (2.4), the certificate recurrence also provides an algorithmic proof of the recurrence for the multisum $Sum(\mu, \alpha)$.

However, in most situations human inspection is needed to pass from the recurrence (2.4) to a homogeneous or inhomogeneous recurrence for the sum. To investigate the type of sums satisfying homogeneous recurrence relations, the notion of admissible functions was introduced in [76, Section 3.3]. We present it here in Wegschaider's slightly more general context [72, Section 3.3].

For this purpose, let us consider a function $\mathcal{F}(\mu, \kappa, \alpha)$ defined on $D \subseteq \mathbb{Z}^{p+r} \times \mathbb{C}^l$ satisfying a non-k-free recurrence given by an operator $\mathcal{P}'(\mu, \kappa, \alpha, M, K)$ of the form (2.6) with maximal shifts $\tau = (\tau_1, \ldots, \tau_p)$ and $\delta = (\delta_1, \ldots, \delta_r)$ in μ and κ, respectively. With respect to this recurrence operator, using only parameters from the set

$$\mathcal{D}^{\alpha}_{\mathcal{F},\mu,\tau} = \{(\mu, \alpha) \in \mathbb{Z}^p \times \mathbb{C}^l : \text{for all } m \in [0 \ldots \tau] \\ \exists \kappa \in \mathbb{Z}^r \text{ such that } (\mu + m, \kappa, \alpha) \in D\}, \quad (2.12)$$

we define the support

$$Supp_{\mathcal{F}}(\mu, \alpha) = \{\kappa \in \mathbb{Z}^r : (\mu, \kappa, \alpha) \in D \text{ and } \mathcal{F}(\mu, \kappa, \alpha) \neq 0\} \quad (2.13)$$

and the summation range of $\mathcal{F}$

$$Summ_{\mathcal{F},\tau,\delta}(\mu, \alpha) = \{\kappa \in \mathbb{Z}^r : \quad (\mu + m, \kappa + k, \alpha) \in D \\ \text{for all } m \in [0 \ldots \tau] \text{ and } k \in [0 \ldots \delta]\}. \quad (2.14)$$

After introducing the summation range such that we can formally consider all the sums

$$\sum_{\kappa \in Summ_{\mathcal{F},\tau,\delta}(\mu,\alpha)} \mathcal{P}'(\mu, \kappa, \alpha, M, K)\mathcal{F}(\mu, \kappa, \alpha), \quad (2.15)$$

the notion of summability is necessary for the case when the support of $\mathcal{F}$ is infinite.

Definition 2.9. *The summand $\mathcal{F} : D \subseteq \mathbb{Z}^{p+r} \times \mathbb{C}^l \to \mathbb{C}$ is called summable with respect to the recurrence operator (2.6) of shifting orders $\tau \in \mathbb{N}^p$ and $\delta \in \mathbb{N}^r$ if and only if for all $(\mu, \alpha) \in \mathcal{D}^{\alpha}_{\mathcal{F},\mu,\tau}$ we have $(\mu+1, \alpha) \in \mathcal{D}^{\alpha}_{\mathcal{F},\mu,\tau}$ and all the sums (2.15) exist.*

While summability assures only that for all $(\mu, \alpha) \in \mathcal{D}^{\alpha}_{\mathcal{F},\mu,\tau}$ the sum

$$\sum_{\kappa \in Supp_{\mathcal{F}}(\mu,\alpha)} \mathcal{F}(\mu, \kappa, \alpha)$$

exists, an admissible function will have a large enough zone of zero values around its support.

Definition 2.10. *Using the same setting as in the definition above, the function $\mathcal{F}$ is called admissible with respect to the recurrence given by the operator (2.6) if and only if for all parameters $(\mu, \alpha) \in \mathcal{D}^{\alpha}_{\mathcal{F},\mu,\tau}$ and for all shifts $(m, k) \in [0 \ldots \tau] \times [0 \ldots \delta]$ we have*

$$Supp_{\mathcal{F}}(\mu + m, \alpha) - k \subseteq Summ_{\mathcal{F},\tau,\delta}(\mu, \alpha).$$

Summation problems with standard boundary conditions, introduced in [76, Section 3.3], have summable and admissible summands with respect to every k-free recurrence (2.2). These conditions are for instance satisfied by all everywhere defined functions with compact support, like our examples (2.9) and (2.10). In these lucky situations, after summing the relation (2.2) over a domain that is larger then the support of the summand we get a homogeneous recurrence for $Sum(\mu, \alpha)$

$$\sum_{m\in[0\ldots\tau]} \left(\sum_{k\in[0\ldots\delta]} c_{m,k}(\mu, \alpha) \right) Sum(\mu + m, \alpha) = 0 \tag{2.16}$$

However, we need to ensure that not all the coefficients in (2.16) are zero. Wegschaider showed in [72, Theorem 3.5], that if a function $\mathcal{F}$, annihilated by the certificate recurrence (2.4), is summable and admissible with respect to the expanded form (2.5) of this recurrence, by summing over (2.4), the Δ-parts on the right hand side telescope and the remaining boundary values lie outside its support. Hence from the summand recurrence one obtains a non-trivial homogeneous recurrence for the sum

$$\sum_{m\in\mathbb{S}} a_m(\mu, \alpha)\, Sum(\mu + m, \alpha) = 0. \tag{2.17}$$

For example, using the package `MultiSum`, we proceed as follows to find a recurrence satisfied by the Bessel function

In[2]:= $\mathbf{JSmnd}[n\_, k\_, x\_] := \dfrac{(-1)^k}{k!\Gamma(n + k + 1)} \left(\dfrac{x}{2}\right)^{n+2k}$

In[3]:= **FindRecurrence[JSmnd[n, k, x], n, k]**

Out[3]= $\{xF[n-1,k-1] - 2nF[n,k-1] + xF[n+1,k-1] = \Delta_k[2nF[n,k-1] - xF[n-1,k-1]]\}$

In[4]:= **CRec = ShiftRecurrence[%[[1]], {n, 1}, {k, 1}]**

Out[4]= $xF[n,k] - 2(n+1)F[n+1,k] + xF[n+2,k] = \Delta_k[2(n+1)F[n+1,k] - xF[n,k]]$

while the Sister Celine type of relation is returned by the command

In[5]:= **CertificateToRecurrence[CRec]**

Out[5]= $xF[n,k+1] - 2(n+1)F[n+1,k+1] + xF[n+2,k] = 0.$

Note that, in this particular situation, the recurrence for the sum (2.9) can be obtained by summing over either of these two recurrence relations. Since this will not be the case in general, we read off the final result from the principal part of the certificate recurrence using another procedure from the package `MultiSum`

In[6]:= **SumCertificate[CRec]**

Out[6]= $x\mathrm{SUM}[n] - 2(n+1)\mathrm{SUM}[n+1] + x\mathrm{SUM}[n+2] = 0$

where SUM[n] denotes $J_n(x)$. Note also that before we sum over this certificate recurrence, we need to check the limit behaviour as the summation variable k tends to $+\infty$ which is here implicitly assumed to be zero.

Remark 2.11. Especially in the case of large single summation problems from this input class, such as the ones presented in Chapter 3, we find recurrences in one parameter by calling Zeilberger's algorithm [78] and its efficient implementation [51]

In[7]:= **<< zb.m;**

Fast Zeilberger Package by Peter Paule, Markus Schorn and Axel Riese – © RISC Linz – V 3.52 (01/12/05)

Using Zeilberger's algorithm for the sum (2.9), we obtain again the recurrence

In[8]:= **Zb[JSmnd[*n*, *k*], {*k*, 0, **Infinity**}, *n*]**

Out[8]= $\{x\mathrm{SUM}[n] - 2(n+1)\mathrm{SUM}[n+1] + x\mathrm{SUM}[n+2] = 0\}.$

During the next chapters, we mostly study applications involving sums with nonstandard boundary conditions, for which WZ-methods deliver inhomogeneous recurrences. For example, when proving Theorem 2.12 below, we encounter identity (2.30) which is of this type and for which we need a homogeneous recurrence relation.

As we discuss in Remark 2.16, relatively small applications with nonstandard boundary conditions can be transformed into larger problems with standard boundary conditions [72, Section 3.4]. This is done, for instance, by a variation of the ϵ-trick, described in Remark 2.8 for extending the recurrence to singular values of the summand.

Let us apply the classic WZ-proving strategy to the following identity[1]

$$1 + (-1)^{n+k} \sum_{m=0}^{k-1} (-1)^m \binom{k-1-n}{m} \binom{n}{k-1-m} = 2^k \sum_{m=k}^{n} \binom{-k}{n-m}, \tag{2.18}$$

where $n \geq k \geq 1$. Given its structure, it suffices to search for recurrences in the integer parameter $n \geq 1$ for the single sums

$$T(n) := \sum_{m=k}^{n} \binom{-k}{n-m} \quad \text{and} \quad S(n) := \sum_{m=0}^{k-1} (-1)^{n+m} \binom{k-1-n}{m} \binom{n}{k-1-m}.$$

[1]This question was emailed to Prof. Paule by Dr. Peter van der Kamp in July 2007.

Using again Zeilberger's algorithm [78] one finds for all $n \geq k \geq 1$ the following recurrences:

In[9]:= $\mathbf{Zb}[(-1)^{n+m}\binom{k-1-n}{m}\binom{n}{k-1-m}, \{m, 0, k-1\}, n]$

Out[9]= $\{(-n-1)\text{SUM}[n] + (k-1)\text{SUM}[n+1] + (-k+n+2)\text{SUM}[n+2] = 0\}$

In[10]:= $\mathbf{Zb}[\binom{-k}{n-m}, \{m, k, n\}, n]$

Out[10]= $\{-\text{SUM}[n] + \text{SUM}[n+1] = \frac{n}{k-1}\binom{1-k}{1-k+n}\}.$

However, we started out to find a recurrence satisfied by both sides of the identity (2.18). Using the continuity of its summand on the set of well-defined values, we extend the sum $T(n)$ to a summation problem with standard boundary conditions, i.e.,

$$T(n) := \sum_{m=k}^{n} \binom{-k}{n-m} = \lim_{\epsilon \to 0} \sum_{m=-\infty}^{\infty} t(n, \epsilon)$$

where $t(n, \epsilon) = \binom{-k}{n-m}\frac{(m-k+\epsilon)!}{(m-k)!}$ and $\epsilon \in \mathbb{C} \setminus \mathbb{Z}$. Now Zeilberger's algorithm delivers a new recurrence

In[11]:= $\mathbf{Zb}[t[n, \epsilon], \{m, -\text{Infinity}, n\}, n]$

Out[11]= $\{(\epsilon + n + 1)\text{SUM}[n] + (\epsilon - k + 1)\text{SUM}[n+1] + (k-n-2)\text{SUM}[n+2] = 0\}$

which holds for all $n \geq 1$ and sufficiently small $\epsilon > 0$. Moreover, by letting ϵ tend to zero, it follows that $T(n)$ also satisfies the order two recurrence computed above for $S(n)$. At last, initial values are easy to check.

This general ϵ-strategy to avoid inhomogeneous recurrences increases the complexity of the input and is undesirable in the case of large multiple sums. In chapter 3, we present a systematic treatment of inhomogeneous recurrences coming from nested definite sums with nonstandard boundary conditions, related to the evaluation of Feynman parameter integrals.

2.2 Two special function identities related to Poisson integrals

The following two special function identities were obtained in [69] while computing expressions of the Poisson kernel for geodesic balls in the cases of spheres and real hyperbolic spaces of arbitrary dimension. By showing that the two sides of each identity express one and the same Poisson kernel, E. Symeonidis [69] has proven the following two theorems.

Theorem 2.12. *For real x and t such that $|x| < 1$, $|t| < 1$ and $n \in \mathbb{N}$ with $n \geq 3$,*

$$\sum_{k\geq 0} \frac{\binom{k+n-2}{k}}{\binom{k+\frac{n}{2}-2}{k}} t^k \, {}_2F_1\left(\begin{matrix} k, 1-\frac{n}{2} \\ k+\frac{n}{2} \end{matrix}; t^2\right) C_k^{\frac{n-2}{2}}(x) = \left(\frac{1-t^2}{1-2tx+t^2}\right)^{n-1}. \tag{2.19}$$

Theorem 2.13. *For real x and t such that $|x| < 1$, $|t| < 1$ and $n \in \mathbb{N}$ with $n \geq 3$,*

$$\sum_{k\geq 0} \frac{\Gamma\left(\frac{k+n}{2}\right)\Gamma\left(\frac{k+1}{2}\right)}{\Gamma\left(\frac{n}{2}+k-1\right)} t^k \, {}_2F_1\left(\begin{matrix} k, k+n-1 \\ k+\frac{n}{2} \end{matrix}; \frac{1-\sqrt{1-t^2}}{2}\right) C_k^{\frac{n-2}{2}}(x) =$$
$$= \frac{(n-2)\Gamma\left(\frac{n+1}{2}\right)}{2\Gamma\left(\frac{n}{2}+1\right)} \sqrt{1-t^2} \, {}_2F_1\left(\begin{matrix} n, 1 \\ \frac{n}{2}+1 \end{matrix}; \frac{xt+1}{2}\right). \tag{2.20}$$

More details on the classical hypergeometric series

$${}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix}; z\right) := \sum_{l\geq 0} \frac{(a)_l (b)_l}{(c)_l} \frac{z^l}{l!}$$

can be found, for instance, in [7, Chapter 2].

Moreover, in the above theorems, the following notation has been used to denote the ultraspherical or Gegenbauer polynomials [7, 6.4.12],

$$C_k^{\lambda}(x) = \frac{(\lambda)_k}{\Gamma(k+1)} (2x)^k \, {}_2F_1\left(\begin{matrix} -\frac{k}{2}, \frac{1-k}{2} \\ 1-k-\lambda \end{matrix}; \frac{1}{x^2}\right). \tag{2.21}$$

Independent of Symeonidis' original derivation and the background of these identities we present a direct approach based on computer algebra methods which is easy to follow and could be applied when proving other similar identities.

The basic idea for our proofs is to transform the problem into that of proving equality of sequences of coefficients defined by multiple sums. Then, such a multisum identity is proven by finding a recurrence satisfied by both sides of the identity and checking the equality of finitely many initial values. The structure of the identities in question will allow us the use of WZ-summation methods to compute the necessary recurrences.

By Taylor expansion around the origin, any side of the identities (2.19) and (2.20) can be rewritten as

$$\sum_{i,j\geq 0} c_{i,j}(\mu) t^i x^j \tag{2.22}$$

where the coefficients $c_{i,j}(\mu)$ are multiple sums of the form

$$c_{i,j}(\mu) = \sum_{\kappa_1} \cdots \sum_{\kappa_r} \mathcal{F}_{i,j}(\mu, \kappa_1, \ldots, \kappa_r), \tag{2.23}$$

and the summands $\mathcal{F}_{i,j}(\mu, \kappa_1, \ldots, \kappa_r)$ are hypergeometric terms in all integer variables μ_n from $\mu = (\mu_1, \ldots, \mu_p)$ and in all summation variables κ_l from $\kappa = (\kappa_1, \ldots, \kappa_r)$.

Since we are dealing with sums over proper hypergeometric summands of the form (2.1) or of the more general form (2.22), recurrences in even more than one variable μ_n can be found, as we described in Section 2.1, using the Mathematica implementation of Wegschaider's algorithm [72] which is an extension of multivariate WZ-summation [76].

Given a term $\mathcal{F}(\mu, \kappa)$, proper hypergeometric in all parameters, Wegschaider's algorithm computes a recurrence of the type (2.4)

$$\sum_{m \in \mathbb{S}'} a_m(\mu)\, \mathcal{F}(\mu - m, \kappa) = \sum_{l=1}^{r} \Delta_{\kappa_l} \left(R_l(\mu, \kappa)\, \mathcal{F}(\mu, \kappa) \right), \tag{2.24}$$

where $a_m(\mu)$ are polynomials, not all zero, $R_l(\mu, \kappa)$ are rational functions and the forward shift operators Δ_{κ_l} are defined as in Section 2.1.

Further remarks are in place. First, by summing over the certificate recurrence (2.24), we obtain a recurrence for the sum (2.1) because the coefficients $a_m(\mu)$ are free of the summation variables from κ and the Δ-parts on the right hand side telescope.

However, when we want to pass from these certificate recurrences to recurrences for infinite sums over some parameters κ_l from κ, we have to study the behavior of expressions of the form $R_l(\mu, \kappa)\, \mathcal{F}(\mu, \kappa)$ when the parameter κ_l tends to $\pm\infty$. Only after these limit considerations we can decide if the recurrence for the sum $\sum_{\kappa} \mathcal{F}(\mu, \kappa)$ is homogeneous. Throughout the proofs of the above theorems, we will always check the homogeneity of the recurrences we have computed algorithmically.

As it was mentioned in Section 2.1, in order to provide the input for the algorithm [72], we determine a small structure set using the procedure `FindStructureSet` included in the package `MultiSum` and already used in [40]. After making an Ansatz about their structure, certificate recurrences are computed by solving a large system of linear equations over a field of rational functions. If the input of the algorithm is involved, computations will be time consuming; in addition, we might find only high order recurrences which require many initial values to be checked. Consequently, *directly* applying this algorithm for large and intricately nested multiple sums of the more general type (2.22), for example, such as the ones appearing in the identities (2.19) and (2.20), is not advisable in practice.

Moreover, the initial values for such output recurrences might again be complicated sums. In this case, the algorithm can be applied again, provided that for these new identities an independent variable μ_n from μ is left. Iterating this procedure, we will end up with single sum representations of initial values that still need to be proven. If at this last step, recurrences in a single parameter μ_n are sufficient, one can use Zeilberger's algorithm [78].

To avoid involved computations, before searching algorithmically for recurrences, we apply coefficient comparison with respect to the additional real variables x and

t and we end up with identities whose sides are of type (2.1). This is a well-known strategy to eliminate summation quantifiers and to reduce the number of variables. Coefficient comparisons might lead to case distinctions, but in either case, the input for the algorithm [72] becomes significantly smaller. In this way, we reduce the identity (2.20) to a single summation problem and use the implementation [51] of Zeilberger's algorithm which is more efficient than the one described by Wegschaider in [72].

Another advantage of coefficient comparison is that it introduces "useful" discrete variables. For instance, in view of (2.22), if we compare coefficients with respect to $t^i x^j$, these arbitrarily chosen powers $i, j \in \mathbb{Z}$ will be further independent variables in addition to those of μ. Furthermore, the recurrences in these new variables often are of low order, so the initial values are easier to check.

Remark 2.14. In order to keep proofs readable, we sometimes use the notation

$$\mathcal{F}(\mu, \kappa)|_{\kappa_l = p} := \mathcal{F}(\mu, \kappa_1, \ldots, \kappa_{l-1}, p, \kappa_{l+1}, \ldots, \kappa_r)$$

where $p \in \mathbb{Z}$ and, as above, $\kappa = (\kappa_1, \ldots, \kappa_r)$ and $\mathcal{F}(\mu, \kappa)$ is the summand of an arbitrary coefficient $c_{i,j}(\mu)$ from (2.22).

2.2.1 Proof of the first theorem

First, we observe that a change of variable $y := 1 - x$ is useful when expanding the denominator of the right hand side of the identity (2.19),

$$\left(1 - 2tx + t^2\right)^{n-1} = \sum_{l=0}^{n-1} \binom{n-1}{l} (2ty)^{n-1-l} (1-t)^{2l}. \tag{2.25}$$

In view of this substitution, it is convenient to use the following representation for the Gegenbauer polynomials [7, 6.4.9 and 6.3.5],

$$C_k^{\frac{n-2}{2}}(x) = \binom{k+n-3}{k} {}_2F_1\left(\begin{matrix} -k, k+n-2 \\ \frac{n-1}{2} \end{matrix}; \frac{1-x}{2}\right).$$

Using this form for the orthogonal polynomials $C_k^{\frac{n-2}{2}}(x)$ and multiplying both sides of the identity (2.19) with the expression (2.25), it remains to prove that

$$\sum_{k \geq 0} \frac{\binom{k+n-2}{k}\binom{k+n-3}{k}}{\binom{k+\frac{n}{2}-2}{k}} t^k \sum_{j \geq 0} \frac{(k)_j \left(1 - \frac{n}{2}\right)_j}{\left(k + \frac{n}{2}\right)_j \Gamma(j+1)} t^{2j} \sum_{i \geq 0} \frac{(-k)_i (k+n-2)_i}{\left(\frac{n-1}{2}\right)_i \Gamma(i+1) 2^i} y^i$$
$$\times \sum_{l=0}^{n-1} \binom{n-1}{l} (2ty)^{n-1-l} (1-t)^{2l} = \left(1 - t^2\right)^{n-1} \tag{2.26}$$

holds for all $n \in \mathbb{N}$ with $n \geq 3$ and for all real variables t, y with $|t| < 1$ and $0 < y < 2$.

Remark 2.15. In [69] it was proven that for every fixed t with $|t| < 1$ the left hand side of (2.19) is a uniformly convergent series in the interval $-1 \leq x \leq 1$. Hence, we can proceed with the coefficient comparison with respect to the new variable y; see also [74, 3.32].

One needs to deal with the constant coefficient with respect to y separately, so we continue with the following case distinction, cases (a) and (b).

(a) In the multisum expression on the left hand side of (2.26), the constant coefficient with respect to y is obtained when $l = n-1$ and $i = 0$. Consequently, this case reduces to proving that

$$\sum_{k\geq 0} \frac{\binom{k+n-2}{k}\binom{k+n-3}{k}}{\binom{k+\frac{n}{2}-2}{k}} t^k \sum_{j\geq 0} \frac{(k)_j\left(1-\frac{n}{2}\right)_j}{\left(k+\frac{n}{2}\right)_j \Gamma(j+1)} t^{2j} = \left(\frac{1+t}{1-t}\right)^{n-1} \tag{2.27}$$

holds for all $|t| < 1$ and $n \geq 3$.

Furthermore, using the binomial theorem, the right hand side of (2.27) can be written as

$$\left(\tfrac{1+t}{1-t}\right)^{n-1} = \sum_{m\geq 0} (-t)^m \sum_{s=0}^{m} \binom{n-1}{s}\binom{-n+1}{m-s}(-1)^s.$$

Via coefficient comparison with respect to t^m for an arbitrary $m \geq 0$, we obtain the equality of two single sum expressions

$$\sum_{j\geq 0} \frac{\binom{k+n-2}{k}\binom{k+n-3}{k}}{\binom{k+\frac{n}{2}-2}{k}} \frac{(k)_j\left(1-\frac{n}{2}\right)_j}{\left(k+\frac{n}{2}\right)_j \Gamma(j+1)}\Bigg|_{k=m-2j} = (-1)^m \sum_{s=0}^{m} \binom{n-1}{s}\binom{-n+1}{m-s}(-1)^s. \tag{2.28}$$

Note here that both sides of this last identity are terminating sums and that in classical hypergeometric notation, we relate a ${}_7F_6$ to a ${}_2F_1$ series. However, proceeding algorithmically, we prefer to use Zeilberger's algorithm to prove this identity. The Mathematica implementation [51] delivers the same recurrence,

$$m\text{SUM}[m] + 2(n-1)\text{SUM}[1+m] - (2+m)\text{SUM}[2+m] = 0$$

for both sides of (2.28). At last, it is trivial to check that the identity (2.28) holds for $m = 0$ and $m = 1$.

(b) We also need to show that the coefficients of all the powers $r \geq 1$ of the real variable y are zero. To determine the coefficient of y^r with $r \geq 1$, we choose in the multisum on the left hand side of (2.26) the term where $l = n-1+i-r$. Consequently, the identity

$$\sum_{k\geq 0} \frac{\binom{k+n-2}{k}\binom{k+n-3}{k}}{\binom{k+\frac{n}{2}-2}{k}} t^k \sum_{j\geq 0} \frac{(k)_j\left(1-\frac{n}{2}\right)_j}{\left(k+\frac{n}{2}\right)_j \Gamma(j+1)} t^{2j} \times \sum_{i=0}^{r} \frac{(-k)_i (k+n-2)_i}{\left(\frac{n-1}{2}\right)_i \Gamma(i+1) 4^i} \binom{n-1}{r-i} t^{r-i}(1-t)^{2i} = 0 \tag{2.29}$$

must hold for $|t| < 1$ and integers $r \geq 1$, $n \geq 3$.

Moreover, in (2.29) the coefficient of an arbitrary power $p \geq 0$ of the variable t must be zero. Therefore, we will prove that

$$\sum_{k\geq 0} \frac{\binom{k+n-2}{k}\binom{k+n-3}{k}}{\binom{k+\frac{n}{2}-2}{k}} \sum_{j\geq 0} \frac{(k)_j\left(1-\frac{n}{2}\right)_j}{\left(k+\frac{n}{2}\right)_j \Gamma(j+1)} \times \sum_{i=0}^{r} \frac{(-k)_i\,(k+n-2)_i}{\left(\frac{n-1}{2}\right)_i \Gamma(i+1)4^i} \binom{n-1}{r-i} \binom{2i}{p-r+i-k-2j} (-1)^{i-k} = 0 \tag{2.30}$$

holds for all integer variables $r \geq 1$, $p \geq 0$ and $n \geq 3$.

Since there is no obvious further simplification of this expression, we now algorithmically compute a recurrence satisfied by the left hand side of (2.30). The triple sum in (2.30) comes in three parameters; to indicate this explicitly we denote it as a function of r, p and n,

$$S[r,p,n] := \sum_{k\geq 0}\sum_{j\geq 0}\sum_{i\geq 0} \mathcal{F}[r,p,n,k,j,i]. \tag{2.31}$$

We will only search for a recurrence in the parameters r and p, so we view the triple sum (2.31) as a function SUM$[\cdot,\cdot]$ defined on lattice points $(r,p) \in [1\ldots\infty)\times[0\ldots\infty)$. Note that the value of SUM$[r,p]$ at an arbitrary integer lattice point is a finite sum and is dependent on the integer variable $n \geq 3$.

Because the new integer variables r and p have been introduced when comparing coefficients, finding a recurrence and showing that sufficiently many initial values are zero corresponds to proving that in (2.26) the coefficients of $y^r t^p$ for all $r \geq 1$ and $p \geq 0$ are zero. This proof strategy, motivated by the induction principle, has also a significant computational advantage since the sums arising from the coefficient comparison are finite.

As it was mentioned in the introduction, before applying Wegschaider's algorithm [72] we determine a suitable set of shifts, called structure set, for the desired recurrence. An algorithm for computing small structure sets is implemented in the Mathematica package `MultiSum`; see also [40]. The following command determines 8 candidate structure sets for a recurrence in r and p satisfied by the summand $\mathcal{F}[r,p,n,k,j,i]$ of the triple sum from (2.30):

```
In[12]:= FindStructureSet[F[r, p, n, k, j, i], {r, p}, {0, 0}, {k, j, i}, {0, 1, 1}, 1]
```

Settling, for instance, on the first candidate structure set, Wegschaider's algorithm [72] computes a recurrence for the summand $\mathcal{F}[r,p,n,k,j,i]$, called certificate recurrence. In less than 300 seconds on an average personal computer one obtains a recurrence for the summand as output of the command

```
In[13]:= FindRecurrence[F[r, p, n, k, j, i], {r, p}, {k, j, i}, %[[1]], 1, WZ → True].
```

The certificate recurrence has as coefficients polynomials free of the summation variables k, j and i. Therefore, by summing over the certificate recurrence in the given summation range we obtain the desired recurrence for the sum SUM$[r,p]$ from (2.30).

More precisely, with respect to the variables k and j, we sum over domains that are larger than the finite support of the summand $\mathcal{F}[r,p,n,k,j,i]$ for fixed integers r,p,n and $0 \leq i \leq r$. This assures that, after summing over the Δ_k and Δ_j parts on the right hand side of any certificate recurrence, these will vanish. When it comes to the variable i we have a nonstandard lower boundary condition which, in general, leads from the certificate recurrence to an inhomogeneous recurrence for the triple sum (2.31).

Remark 2.16. The classic technique to avoid inhomogeneous recurrence relations is to introduce a new variable $\epsilon > 0$ and transforming (2.31) into a problem with standard boundary conditions with respect to all summation variables. After computing a homogeneous recurrence for the new triple sum

$$S'[r,p,n,\epsilon] = \sum_{k\geq 0}\sum_{j\geq 0}\sum_{i=-\infty}^{r} \mathcal{F}[r,p,n,k,j,i]\frac{\Gamma(i+1+\epsilon)}{\Gamma(i+1)},$$

we get a recurrence for $S[r,p,n]$ using the fact that $\lim\limits_{\epsilon\to 0} S'[r,p,n,\epsilon] = S[r,p,n]$. This method is described for instance in [72, Section 3.4]. The disadvantage of this elegant strategy is that it increases the computation time. Since our original problem (2.30) is already large, we can not afford to introduce an additional parameter.

Coming back to our concrete problem, inspection shows that we do not need to apply this general ϵ-strategy. Namely, we can utilize the fact that the function to which the Δ_i operator is applied, vanishes for the lower bound $i = 0$. This becomes clear by rewriting the Δ_i part of our certificate recurrence as

$\Delta_i\,[\,2(n-r-1)(n+2r-1)(r+1)^2\,\{F[r+1,p+3,n,k,i,j]-F[r+1,p+2,n,k,i,j]\}+2(r+1)$
$(n-r-1)(n^2+2in+rn-2n-2r^2-r+1)\,\{F[r,p+1,n,k,i,j]-F[r,p+2,n,k,i,j]\}\,]$
$=\Delta_i\left[\frac{2in(2i+n-3)(r+1)(-n+r+1)(4j+2k-2p+2r-3)}{(i-r-1)(i-2j-k+p-r+2)}F[r,1+p,n,k,i,j]\right].$

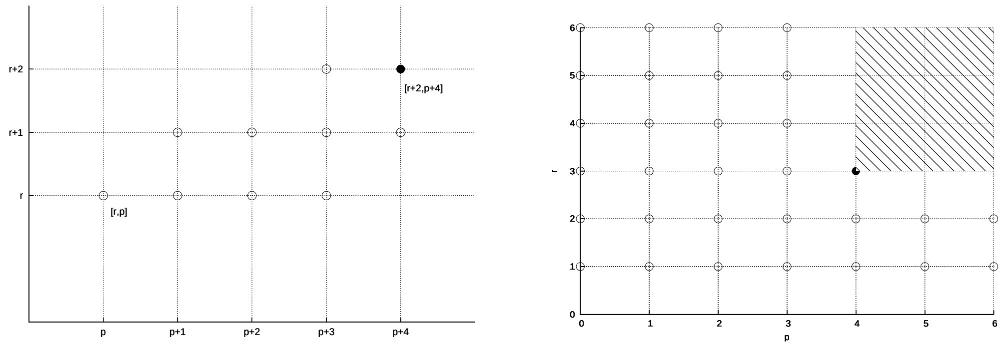
Note that the poles of the rational function do not cause any trouble, since

$$\tfrac{n}{i-r-1}\tfrac{2i+1}{i-2j-k+p-r+2}\tbinom{n-1}{r-i}\tbinom{2i}{p+1-r+i-k-2j} = -\tbinom{n}{r-i+1}\tbinom{2i+1}{p+2-r+i-k-2j}.$$

Therefore, by summing over $(k,j,i)\in\mathbb{N}^3$ this certificate recurrence leads to a homogeneous recurrence for the sum SUM$[r,p]$ and now we can use the command

In[14]:= **SumCertificate** [%]

Out[14]= $\{-(n+p-3r)(p-r)\text{SUM}[r,p]+\left(2n^2+3pn-9rn-n-p^2+5r^2-6p+10r-3\right)$
$\text{SUM}[r,p+1]+\left(-2n^2+3pn+3rn+10n+p^2-r^2-4pr-10r-6\right)\text{SUM}[r,p+2]$
$-(n-p-r-3)(p-r+3)\text{SUM}[r,p+3]+(p-r)(n-p+3r)\text{SUM}[r+1,p+1]$
$+\left(-2n^2+pn-5rn+n-p^2+9r^2-6p+20r+1\right)\text{SUM}[r+1,p+2]$



(a) The multivariate recurrence (b) The initial values

$$+\left(2n^2+pn+3rn+2n+p^2-5r^2-4pr-20r-10\right)\mathrm{SUM}[r+1,p+3]$$
$$+(p-r+3)(n+p+r+3)\mathrm{SUM}[r+1,p+4]+2(r+2)(n+2r+1)$$
$$\mathrm{SUM}[r+2,p+3]-2(r+2)(n+2r+1)\mathrm{SUM}[r+2,p+4]=0\ \}\,.$$

One can see that the value of $\mathrm{SUM}[r+2,p+4]$ can be computed from the recurrence if the values of the function $\mathrm{SUM}[\cdot,\cdot]$ in all the integer lattice points marked with $\circ$ in Figure 2.1(a) are known.

We observe that the leading term coefficient of the recurrence is non-zero for all positive values of r and n. Having a visualization of the recurrence at hand, it is also clear which initial values need to be checked; see Figure 2.1(b).

For an arbitrary $r \geq 1$ we need to show that (2.30) holds in cases $p \in \{0,1,2,3\}$. Note that in all these cases the triple sum (2.30) becomes a finite sum with summation bounds being fixed integers. At last we look at the situations when $p \geq 0$ is fixed and $r=1$ or $r=2$. Since $i \leq r$ and $p-r-i \leq k+2j \leq p-r+i$, we can rewrite $S[1,p,n]$ and $S[2,p,n]$ as the sum of 4, respectively 9, terminating ${}_7F_6$ series. After distinguishing between even and odd values of the parameter p, all these hypergeometric series have closed forms given by Dougall's terminating ${}_7F_6$ formula [7, Theorem 3.5.1].

In order to avoid such cumbersome calculations, we prefer to compute recurrences in the parameter $p \geq 0$ for $r=1$ and $r=2$. Checking the initial values for those recurrences is trivial. For instance, if $r=1$, we can separate the left hand side of (2.30) into the following finite sums:

$$S[1,p,n]=\sum_{j\geq 0}\mathcal{F}[1,p,n,p-2j-1,j,0]+\sum_{k\geq 0}\sum_{j\geq 0}\mathcal{F}[1,p,n,k,j,1].$$

Zeilberger's algorithm [78] and Wegschaider's MultiSum package [72] deliver recurrences in p for the single and double sum, respectively. It only remains to compute a recurrence for $S[1,p,n]$ from the recurrences of its two components. To this end, we use another Mathematica package

In[15]:= **<< GeneratingFunctions.m**

GeneratingFunctions Package by Christian Mallinger – © RISC Linz – V 0.68 (07/17/03)

Given two sequences which satisfy linear recurrences with polynomial coefficients, the command `REPlus` delivers a recurrence for their sum; see [41, 56] for more details. Taking as input the recurrences in p determined by the above summation algorithms, we obtain the desired recurrence for $S[1,p,n](=\mathrm{SUM}[p])$.

In[16]:= **REPus [recZb, recMsum, SUM[p]]**

Out[16]= $(n-2p)(p-1)\mathrm{SUM}[p]-2\left(n^2-2pn-n+2p^2+4p\right)\mathrm{SUM}[p+1]+6(n-2)(p+1)\mathrm{SUM}[p+2]$
$+2\left(n^2+2pn+3n+2p^2+4p\right)\mathrm{SUM}[p+3]+(p+3)(n+2p+4)\mathrm{SUM}[p+4]=0.$

Since our recurrence has order 4, we have reduced the problem to checking initial values for $r=1$ and $p\in\{0,1,2,3\}$. case $r=2$ can be handled in a similar manner.

2.2.2 Proof of the second theorem

Since $|t|<1$, the following quadratic transformation that goes back to Gauss [7, 3.1.3]

$$ {}_2F_1\left(\begin{matrix} k, k+n-1 \\ k+\frac{n}{2} \end{matrix}; \tfrac{1-\sqrt{1-t^2}}{2}\right) = {}_2F_1\left(\begin{matrix} \frac{k}{2}, \frac{k+n-1}{2} \\ k+\frac{n}{2} \end{matrix}; t^2\right) $$

can be applied to the identity (2.20).

Furthermore, we use the representation (2.21) for the Gegenbauer polynomials and the identity (2.20) is brought to a more convenient form for the purpose of coefficient comparison:

$$ \sum_{k\geq 0} \frac{\Gamma\left(\frac{k+n}{2}\right)\Gamma\left(\frac{k+1}{2}\right)}{\Gamma(k+1)} (2xt)^k\, {}_2F_1\left(\begin{matrix} \frac{k}{2}, \frac{k+n-1}{2} \\ k+\frac{n}{2} \end{matrix}; t^2\right) {}_2F_1\left(\begin{matrix} -\frac{k}{2}, \frac{1-k}{2} \\ 2-k-\frac{n}{2} \end{matrix}; \frac{1}{x^2}\right) $$
$$ = \frac{2}{n}\Gamma\left(\frac{n+1}{2}\right)\sqrt{1-t^2}\, {}_2F_1\left(\begin{matrix} n, 1 \\ \frac{n}{2}+1 \end{matrix}; \tfrac{xt+1}{2}\right). $$

Thus, we will prove that

$$ \sum_{k\geq 0} \frac{\Gamma\left(\frac{k+n}{2}\right)\Gamma\left(\frac{k+1}{2}\right)}{\Gamma(k+1)} (2xt)^k \sum_{j\geq 0} \frac{\left(\frac{k}{2}\right)_j \left(\frac{k+n-1}{2}\right)_j}{\left(\frac{n}{2}+k\right)_j \Gamma(j+1)} t^{2j} \sum_{i\geq 0} \frac{\left(-\frac{k}{2}\right)_i \left(\frac{1-k}{2}\right)_i}{\left(2-\frac{n}{2}-k\right)_i \Gamma(i+1)} x^{-2i} $$
$$ = \frac{2}{n}\Gamma\left(\frac{n+1}{2}\right)\sqrt{1-t^2} \sum_{s\geq 0} \frac{(n)_s}{\left(\frac{n}{2}+1\right)_s 2^s} (1+xt)^s \tag{2.32} $$

holds for all $|x|<1$, $|t|<1$ and $n\in\mathbb{N}$ with $n\geq 3$.

After exchanging the order of summation, on the left hand side of (2.32) the coefficient of x^m for any $m \geq 0$ can be determined by setting $k = m + 2i$. Comparing coefficients with respect to x^m on both sides of (2.32), reduces the problem to showing that

$$\sum_{i\geq 0} \frac{\Gamma\left(\frac{k+n}{2}\right)\Gamma\left(\frac{k+1}{2}\right)}{\Gamma(k+1)} (2t)^k \frac{\left(-\frac{k}{2}\right)_i \left(\frac{1-k}{2}\right)_i}{\left(2-\frac{n}{2}-k\right)_i \Gamma(i+1)} \sum_{j\geq 0} \frac{\left(\frac{k}{2}\right)_j \left(\frac{k+n-1}{2}\right)_j}{\left(\frac{n}{2}+k\right)_j \Gamma(j+1)} t^{2j} \Bigg|_{k=m+2i}$$
$$= \frac{2}{n}\Gamma\left(\frac{n+1}{2}\right) t^m \sqrt{1-t^2} \sum_{s\geq m} \binom{s}{m} \frac{(n)_s}{\left(\frac{n}{2}+1\right)_s 2^s} \qquad (2.33)$$

holds for all integers $m \geq 0$, $n \geq 3$ and real $|t| < 1$.

To determine a closed form for the sum on the right hand side of (2.33) we use a classic summation formula proven, for instance, in [7, Theorem 3.5.4(i)]. More precisely, we have

$$\sum_{s\geq m} \binom{s}{m} \frac{(n)_s}{\left(\frac{n}{2}+1\right)_s 2^s} = \frac{2^{-m}(n)_m}{\left(\frac{n}{2}+1\right)_m} {}_2F_1\left(\begin{matrix} m+1, m+n \\ m+\frac{n}{2}+1 \end{matrix}; \frac{1}{2}\right) = \frac{\Gamma\left(\frac{n}{2}+1\right)\Gamma\left(\frac{m}{2}+\frac{n}{2}\right)}{2^{1-n}\Gamma\left(\frac{m}{2}+1\right)\Gamma(n)}.$$

Note that to simplify this non-terminating series one could also use Zeilberger's algorithm [78].

Plugging in this closed form, (2.33) is equivalent to

$$\sum_{i\geq 0} \frac{\Gamma\left(\frac{k+n}{2}\right)\Gamma\left(\frac{k+1}{2}\right)}{\Gamma(k+1)} 2^k t^{2i} \frac{\left(-\frac{k}{2}\right)_i \left(\frac{1-k}{2}\right)_i}{\left(2-\frac{n}{2}-k\right)_i \Gamma(i+1)} \sum_{j\geq 0} \frac{\left(\frac{k}{2}\right)_j \left(\frac{k+n-1}{2}\right)_j}{\left(\frac{n}{2}+k\right)_j \Gamma(j+1)} t^{2j} \Bigg|_{k=m+2i}$$
$$= \sqrt{\pi} \frac{\Gamma\left(\frac{m+n}{2}\right)}{\Gamma\left(1+\frac{m}{2}\right)} \sum_{q\geq 0} \binom{1/2}{q} \left(-t^2\right)^q. \qquad (2.34)$$

On the left hand side of (2.34) the coefficient of an arbitrary power $q \geq 0$ of t^2 is obtained by setting $j = q - i$. Comparing the coefficients of t^{2q} in (2.34) leads to the following identity

$$\sum_{i\geq 0} \frac{\Gamma\left(\frac{k+n}{2}\right)\Gamma\left(\frac{k+1}{2}\right)}{\Gamma(k+1)} 2^k \frac{\left(-\frac{k}{2}\right)_i \left(\frac{1-k}{2}\right)_i}{\left(2-\frac{n}{2}-k\right)_i \Gamma(i+1)} \frac{\left(\frac{k}{2}\right)_j \left(\frac{k+n-1}{2}\right)_j}{\left(\frac{n}{2}+k\right)_j \Gamma(j+1)} \Bigg|_{\substack{k=m+2i \\ j=q-i}}$$
$$= \sqrt{\pi} \frac{\Gamma\left(\frac{m+n}{2}\right)}{\Gamma\left(1+\frac{m}{2}\right)} (-1)^q \binom{1/2}{q}. \qquad (2.35)$$

To prove that (2.35) holds for all integers $q \geq 0$ and $n \geq 3$, we use again Zeilberger's algorithm [78]. The Mathematica implementation described in [51] delivers a first order recurrence for the single terminating sum on the left hand side of (2.35):

$$(2q-1)\mathrm{SUM}[q] - 2(q+1)\mathrm{SUM}[q+1] = 0.$$

We can easily check that the expression on the right hand side of (2.35) also satisfies this output recurrence. At last, we verify the identity (2.35) at the initial value $q = 0$ and we obtain

$$2^m \Gamma\left(\frac{m+1}{2}\right)\Gamma\left(\frac{m}{2}+1\right) = \sqrt{\pi}\Gamma\left(m+1\right). \tag{2.36}$$

The identity (2.36) is known as Legendre's duplication formula [7, 1.5] and it holds for all $m \geq 0$. Herewith, the proof of Theorem 2.13 is complete.

Summary

We use WZ-summation methods to prove two theorems that go back to the work of Symeonidis [69]. These are, to our knowledge, the first direct proofs of the identities (2.19) and (2.20).

Our method of proof uses coefficient comparisons with respect to certain parameters to reduce the complexity of the identities. Coefficient comparisons lead to case distinctions and in most cases we have single sum expressions to which Zeilberger's algorithm [78] can be applied because of the structure of the identities. In the situations where nested multisums remain, we can use Wegschaider's algorithm [72] to compute recurrences for both sides of the reduced identity. To complete the proofs we only need to check finitely many initial values.

Note that both algorithms delivered recurrences for the summand of the given sums $\sum_{\kappa} \mathcal{F}(\mu, \kappa)$. Summing the certificate recurrence over all the variables from κ, we obtained the desired recurrences for the sum. In each case one can easily check that the algorithmically computed certificate recurrence holds, so the algorithms also deliver a proof for the recurrence satisfied by the sum.

On the other hand there are several non algorithmic aspects involved in the proofs. In the case of Theorem 2.12, a change of variables is necessary. The proof of Theorem 2.13 becomes straight-forward after applying a quadratic transformation to one of the hypergeometric terms involved. Also convergence issues, such as absolute convergence for exchanging the order of summation needed to be considered at various steps of the proofs. We have omitted these details that can be supplied by routine analysis.

3 Symbolic summation for Feynman parameter integrals

In this chapter we present our work in the FWF project "Symbolic Summation in Perturbative Quantum Field Theory," a collaboration between RISC and DESY, coordinated by Priv.-Doz. Dr. Carsten Schneider (RISC), with research partners Prof. Dr. Peter Paule (RISC) and Priv.-Doz. Dr. Johannes Blümlein (DESY).

One important goal of the project was to develop algorithmic strategies for the computation of multi-sums arising in Feynman integral calculus. Our symbolic methods have been efficiently implemented in a summation toolbox combining several Mathematica packages like Carsten Schneider's `Sigma`, Jakob Ablinger's `HarmonicSums`, the Paule-Schorn implementation of Zeilberger's algorithm, Kurt Wegschaider's `MultiSum`, described in Section 2.1 of this thesis, and my recent package `FSums` on which we will focus in this chapter. At the moment our toolbox bundles together the following components:

In[17]:= << **Sigma.m;**

Sigma - A summation package by Carsten Schneider – © RISC Linz – V0.8 (02/05/10)

In[18]:= << **EvaluateMultiSums.m;**

A package by Carsten Schneider – © RISC Linz – (02/05/10)

In[19]:= << **HarmonicSums.m;**

A package by Jakob Ablinger – © RISC Linz – (02/05/10)

In[20]:= << **zb.m;**

Fast Zeilberger Package by Peter Paule, Markus Schorn and Axel Riese – © RISC Linz – V 3.52 (01/12/05)

In[21]:= << **MultiSum.m;**

MultiSum Package by Kurt Wegschaider (enhanced by Axel Riese and Burkhard Zimmermann) – © RISC Linz – V2.02β (02/21/05)

In[22]:= << **FSums.m;**

A package for nested sums with nonstandard boundary conditions by Flavia Stan – © RISC Linz – V2.09 (02/02/09)

I would like to remark here that this work is ongoing, since we plan to optimize and extend our procedures such that even larger problems of this type can be handled. At the moment, we have analysed and computed all the sums coming from the two-loop integrals described in [11]. These results will appear in the joint publication [15].

As we see in the next section, the first step in our procedure is rewriting Feynman parameter integrals as multisums over hypergeometric terms to fit the input class of classic summation algorithms. In chapter 4, we describe a new approach which can be used for Mellin-Barnes integral representations of Feynman integrals.

In this context, my package `FSums` takes as input a multi-sum over proper hypergeometric terms and uses the WZ-summation strategy to obtain a recurrence for its summand. An overview of WZ-summation and Wegschaider's `MultiSum` package [72] can be found in the introductory section 2.1.

However, the summation problems we considered are highly nested sums with non-standard boundary conditions. Hence, after summing over the algorithmically computed certificate recurrence (2.4), one obtains an inhomogeneous recurrence for the sum (2.1). The right hand side of this recurrence will contain special instances of the original multi-sum of lower nested depth. Applying the same method on these new sums recursively, we get new recurrences. This procedure sets up a tree of recurrences with leaves made of relations with only hypergeometric terms on their right hand sides.

For the next step of the method we are relying on the package `Sigma`. Namely, these last inhomogeneous difference equations can be viewed in special difference fields introduced by M. Karr [35] and extended significantly by C. Schneider [57–62]. In this setting, it is possible to find solutions of such recurrences [4, 60] and plugging in these answers into the recurrences from the previous level, we can recursively compute a solution to the initial recurrence satisfied by the multisum (2.1).

This chapter will first discuss the input delivered by our collaborators from DESY. We present the types of multi-sums to be computed and how sum representations for Feynman parameter integrals are found. Section 3.3 describes the package `FSums` and our new approach to multi-sums with nonstandard summation bounds. We also talk about the procedures we use from the powerful `Sigma` package. Illustrative examples and several strategies to optimize our methods are also presented in these sections.

3.1 Multisums coming from Feynman integral calculus

Let us start by introducing the class of multisums delivered by our DESY collaborators and give some examples of sum representations for Feynman parameter integrals. A pragmatic approach to Feynman integral calculus and an account of the algorithmic strategies used by physicists for these computations can be found in [64].

We consider a class of integrals related to the heavy flavor Wilson coefficients in unpolarized deeply inelastic scattering, as it was described in [11], where representative problems of this type were already computed using sum representations. A detailed account on how to find suitable sum representations for parameter integrals of this form is given in [14, 37]. We limit ourselves here to an intuitive example which we simply computed by hand.

From our point of view, Feynman parameter integrals are functions depending on two important parameters. On the one hand, we have the Mellin moment, $N \in \mathbb{N}$, needed as a free discrete variable for our summation methods. On the other hand, we want to determine the first few coefficients of the Laurent series expansion with respect to the dimension regularization parameter $\epsilon > 0$ for the analytic object represented by the Feynman integral.

The following Feynman parameter integral arises as part of a 3-loop ladder graph computation described in [37, Chapter 10].

Example 3.1.

$$I_2 = \int_0^1 \dots \int_0^1 \frac{(xy)^{1-\epsilon}(1-x)^{\epsilon/2}(1-y)^{\epsilon/2}}{(xy - z_1 - z_2 + z_1 x + z_2 y)^{2-3/2\epsilon}} (1 - z_1 - z_2)^{N+3} dz_1 dz_2 dx dy$$

where the integration variables $z_1, z_2 \in [0,1]$ must satisfy the condition $z_1 + z_2 < 1$.

We already mentioned that the first step of our strategy consists in finding a reformulation of the problem in terms of multiple sums over hypergeometric terms. In this particular instance we find

$$I_2 = \int_0^1 \dots \int_0^1 \frac{x^{\epsilon/2-1}(1-x)^{\epsilon/2} y^{\epsilon/2-1}(1-y)^{\epsilon/2}}{z_1^{\epsilon/2} z_2^{\epsilon/2}\left(1 - z_1 \frac{1-x}{x} - z_2 \frac{1-y}{y}\right)^{2-3/2\epsilon}} (1 - z_1 - z_2)^{N+3} dz_1 dz_2 dx dy.$$

Using the Appell function of the first kind with its integral representation [63, Chapter 8 and 9]

$$F_1\left[a; b, b'; c; \alpha, \beta\right] := \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} \frac{(a)_{m+n}(b)_m(b')_n}{(c)_{m+n} m! n!} \alpha^m \beta^n$$
$$= \frac{\Gamma(b)\Gamma(b')\Gamma(c-b-b')}{\Gamma(c)} \int_0^1 \int_0^1 \frac{z_1^{b-1} z_2^{b'-1}(1 - z_1 - z_2)^{c-b-b'-1}}{(1 - \alpha z_1 - \beta z_2)^a} dz_1 dz_2 \qquad (3.1)$$

and, for the remaining integrals, the beta function introduced in Section 1.2.5, we obtain a reformulation of the integral in terms of a double sum

$$I_2 = \frac{\Gamma(N+6-\epsilon)}{\Gamma(N+4)\Gamma(1-\frac{ep}{2})^2} \sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \frac{\left(2 - \frac{3}{2}\epsilon\right)_{m+n}\left(1 - \frac{\epsilon}{2}\right)_m \left(1 - \frac{\epsilon}{2}\right)_n}{(N+6-\epsilon)_{m+n}\, m! n!} \times$$
$$\frac{\Gamma\left(\frac{\epsilon}{2} - m\right)\Gamma\left(\frac{\epsilon}{2} + m + 1\right)}{\Gamma(\epsilon+1)} \frac{\Gamma\left(\frac{\epsilon}{2} - n\right)\Gamma\left(\frac{\epsilon}{2} + n + 1\right)}{\Gamma(\epsilon+1)}.$$

Note that the Appell function F_1 is convergent for arguments $|z_1| < 1$ and $|z_2| < 1$. The convergence of the double series explains the additional condition imposed on the integration variables in I_2.

However, in most examples the binomial theorem is used to split the integrands to a convenient form. Therefore we end up with some sums with finite summation bounds besides the ones generated by the pattern matching procedure for generalized hypergeometric functions. For example, in the case of the same 3-loop topology, we also need to consider integrals of the form

$$I_3 = \int_0^1 \dots \int_0^1 \frac{(xy)^{1-\epsilon}(1-x)^{\epsilon/2}(1-y)^{\epsilon/2}}{(xy - z_1 - z_2 + z_1 x + z_2 y)^{2-3/2\epsilon}} (z_1+z_2)^{N+3} dz_1 dz_2 dx dy$$

with $z_1, z_2 \in [0,1]$ such that $z_1 + z_2 < 1$. In this case we use the binomial theorem to obtain the integral representation (3.1). Namely,

$$(z_1+z_2)^{N+3} = \sum_{j=0}^{N+3} \binom{N+3}{j} (-(1-z_1-z_2))^j$$

which leads to a triple sum representation

$$\begin{aligned} I_3 = & \sum_{j=0}^{N+3} \binom{N+3}{j} (-1)^j \frac{\Gamma(j-\epsilon+3)}{\Gamma(1-\epsilon/2)^2 \Gamma(j+1)} \\ & \times \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{\left(2-\frac{3}{2}\epsilon\right)_{m+n} (1-\epsilon/2)_m (1-\epsilon/2)_n}{(j-\epsilon+3)_{m+n} m! n!} \\ & \times \frac{\Gamma(\epsilon/2-m)\Gamma(\epsilon/2+m+1)\Gamma(\epsilon/2-n)\Gamma(\epsilon/2+n+1)}{\Gamma(\epsilon+1)^2}. \end{aligned}$$

3.1.1 A class of summation problems

As we have seen from the above examples, the general approach, when calculating integrals coming from specific Feynman diagrams, is to identify integral representations for known generalized hypergeometric functions and reformulate the integration problem in terms of nested sums over hypergeometric terms.

Using this procedure, for the Feynman parameter integrals described in [11] one finds sum representations of the form

$$\sum_{\sigma_1=p_1}^{\infty} \cdots \sum_{\sigma_s=p_s}^{\infty} \sum_{j_0=q_0}^{N+c} \sum_{j_1=q_1}^{B_1} \cdots \sum_{j_r=q_r}^{B_r} \mathcal{F}(N, \sigma, j, \epsilon) \tag{3.2}$$

where

(i) $N \geq b$ is a non-negative discrete variable, $\epsilon > 0$ is a real parameter and c, b are given integers;

(ii) the upper summation bounds $B_i := \gamma_i N + (j_0, j_1, \ldots, j_{i-1}) \cdot \eta_i + \nu_i$ depend on the given constants $\gamma_i, \nu_i \in \mathbb{Z}$ and $\eta_i \in \mathbb{Z}^i$ for all $1 \leq i \leq r$;

(iii) the lower summation bounds are given constants $p_i, q_l \in \mathbb{N}$ for all $1 \leq i \leq s$ and $0 \leq l \leq r$, respectively;

(iv) $\mathcal{F}$ is a proper hypergeometric term with respect to the integer variable N and all summation variables from $(\sigma, j) \in \mathbb{Z}^{s+r+1}$;

(v) for all $1 \leq i \leq s$ we have

$$\lim_{\sigma_i \to \infty} \mathcal{F}(N, \sigma, j, \epsilon) = 0. \tag{3.3}$$

Remark 3.2. All applications we have encountered so far in our work with DESY, are a special case of the summation problems (3.2). Since the sums with finite bounds result by applying the binomial theorem several times, we have for the upper summation bounds N_i the condition $\gamma_i \in \{0, 1\}$ for all $1 \leq i \leq r$ and for the η_i's

$$\eta_i = (\eta_{i,1}, \eta_{i,2}, \ldots, \eta_{i,i}) \text{ with components } \eta_{i,l} \in \{-1, 0, 1\} \text{ for all } 1 \leq l \leq i.$$

Moreover, we impose the additional structural restriction on our sums (3.2)

$$(\eta_i, \gamma_i) \in \{(\eta_i, \gamma_i) \in \{-1, 0, 1\}^i \times \{0, 1\} : \exists! \quad l \in [1 \ldots i] \text{ such that } \eta_{i,l} \neq 0 \\ \text{and } \gamma_i = 0 \Rightarrow \eta_{i,l} > 0 \text{ and } \gamma_i = 1 \Rightarrow \eta_{i,l} < 0\} \tag{3.4}$$

for all $1 \leq i \leq r$.

Note that the restriction (3.4) together with the conditions (i-v) assure the following property for the finite summation range

$$[q_0 \ldots N + c] \ltimes [q_1 \ldots B_1] \cdots \ltimes [q_r \ldots B_r] \subseteq [q_0 \ldots N + d]^{r+1}.$$

with $d \in \mathbb{N}$ a given constant. The notation $\ltimes$ is introduced in Section 1.2.1 for a nested range with summation bounds depending on other summation variables.

The implementation of our methods in the package `FSums` treats the particular case of summation problems (3.2) which fulfill condition (3.4). In the next sections we will describe a strategy to handle this special case. A generalization of our methods is straight-forward but technically more involved.

Example 3.3. *The following 4-fold sum is a typical entry from the list of sums representations for a class of Feynman parameter integrals we computed as part of the work* *described in [15].*

$$\mathcal{U}(N,\epsilon) := (-1)^N \sum_{\sigma_0=0}^{\infty} \sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-j_0-3} \sum_{j_2=0}^{j_0+1} \binom{j_0+1}{j_2} \binom{N-j_0-3}{j_1} \times \frac{\left(\frac{\epsilon}{2}+1\right)_{\sigma_0} (-\epsilon)_{\sigma_0} (j_1+j_2+3)_{\sigma_0} \left(3-\frac{\epsilon}{2}\right)_{j_1}}{(j_1+4)_{\sigma_0} \left(-\frac{\epsilon}{2}+j_1+j_2+4\right)_{\sigma_0} \left(4-\frac{\epsilon}{2}\right)_{j_1+j_2}} \times \frac{\Gamma(j_1+j_2+2)\Gamma(j_1+j_2+3)\Gamma(N-j_0-1)\Gamma(N-j_1-j_2-1)}{\Gamma(\sigma_0+1)\Gamma(j_1+4)\Gamma(N-j_0-2)}$$

where $N \geq 3$ is the Mellin moment and $\epsilon > 0$ the dimension regularization parameter.

3.2 Summation with nonstandard boundary conditions

The summation problem (3.2) fits the input class of WZ-methods [76], which we shortly introduced in Section 2.1. For the proper hypergeometric summand $\mathcal{F}$, Wegschaider's algorithm [72] delivers a certificate recurrence of the form (2.4) in N with delta parts in the summation variables from (σ, j), i.e.,

$$\sum_{m\in\mathbb{S}'} a_m(N,\epsilon)\mathcal{F}(N+m,\sigma,j,\epsilon) = \sum_{i=1}^{s} \Delta_{\sigma_i} \left(\sum_{(m,k,n)\in\mathbb{S}_i} b_{m,k,n}(N,\sigma,j,\epsilon)\mathcal{F}(N+m,\sigma+k,j+n,\epsilon) \right) + \sum_{l=0}^{r} \Delta_{j_l} \left(\sum_{(m,0,n)\in\mathbb{S}_{s+l+1}} c_{m,n}(N,\sigma,j,\epsilon)\mathcal{F}(N+m,\sigma,j+n,\epsilon) \right) \tag{3.5}$$

where the coefficients a_m, not all zero, $b_{m,k,n}$ and $c_{m,n}$ are polynomials.

This recurrence can be expanded in the form (2.5) as

$$\sum_{(u,v,w)\in\mathbb{S}} c'_{u,v,w}(N,\sigma,j,\epsilon)\,\mathcal{F}(N+u,\sigma+v,j+w,\epsilon) = 0 \tag{3.6}$$

with polynomial coefficients and $\mathbb{S} \subset \mathbb{N}^{s+r+2}$ a structure set containing only positive shifts. Let $\tau \in \mathbb{N}$ and $\delta \in \mathbb{N}^{n+m+1}$ denote the maximal shifts in $\mathbb{S}$ for the discrete parameter N and the summation variables, respectively.

Moreover, denoting the forward-shift operators with respect to the summation variables from σ by $S = (S_1, \ldots, S_s)$ and from j by $J = (J_0, \ldots, J_r)$, as well as the one in N by $\mathcal{N}$, we obtain the operator

$$\mathcal{P}'(N,\sigma,j,\epsilon,\mathcal{N},S,J) := \sum_{(u,v,w)\in\mathbb{S}} c'_{u,v,w}(N,\sigma,j,\epsilon)\mathcal{N}^u S^v J^w, \tag{3.7}$$

of orders τ and δ, representing the expanded form (3.6) of the certificate recurrence.

In the case of Example 3.3, we use the package `MultiSum` to determine a certificate recurrence and shift it accordingly

In[23]:= **FindStructureSet[summandU, N, {σ_0, j_0, j_1, j_2}, 1];**

In[24]:= **strSet = %[[1]]**

Out[24]= $\{\{0,0,0,0,0\},\{0,1,0,0,0\},\{0,1,1,0,0\},\{1,0,0,0,0\},\{1,1,0,0,0\},\{1,1,1,0,0\}\}$

In[25]:= **FindRecurrence[summandU, N, {σ_0, j_0, j_1, j_2}, strSet, 1, WZ → True];**

In[26]:= **certRecU = ShiftRecurrence[%[[1]], {N, 1}, {j_0, 1}, {σ_0, 1}]**

Out[26]= $(N-2)(N+1)F[N,\sigma_0,j_0,j_1,j_2] + (N-2)F[N+1,\sigma_0,j_0,j_1,j_2] = \Delta_{j_0}[(j_0-N+1)(N-2)F[N,\sigma_0,j_0,j_1,j_2] + (2-N)F[N+1,\sigma_0,j_0,j_1,j_2]] + \Delta_{j_1}[0] + \Delta_{j_2}[0] + \Delta_{\sigma_0}[(j_0+j_1-N+3)F[N+1,\sigma_0,j_0+1,j_1,j_2] - (j_0-N+2)(j_1+j_2-N+1)F[N,\sigma_0,j_0+1,j_1,j_2]]$

The expanded form (3.6) is returned by the following command and in this situation we have $\tau = 1$ and $\delta = (1,1,0,0)$.

In[27]:= **expandRecU = CertificateToRecurrence[certRecU]**

Out[27]= $(j_0+2)(N-2)F[N,\sigma_0,j_0,j_1,j_2] - (j_1+j_2-1)(j_0-N+2)F[N,\sigma_0,j_0+1,j_1,j_2] - (j_0-N+2)(-j_1-j_2+N-1)F[N,\sigma_0+1,j_0+1,j_1,j_2] + (j_0+j_1+1)F[N+1,\sigma_0,j_0+1,j_1,j_2] + (-j_0-j_1+N-3)F[N+1,\sigma_0+1,j_0+1,j_1,j_2] = 0.$

Note that the structure set `strSet` which we use to make an Ansatz for the computation does not need to coincide with the resulting structure set $\mathbb{S}$ of the non-k-free recurrence (3.6) because some coefficients become zero.

In the next sections we are designing an algorithmic approach for the general class of summation problems (3.2), satisfying the range restriction (3.4). Our computational approach will be applied to several hundreds of sums of this form. Since it is not possible to analyze each sum individually, we will work under more restrictive assumptions which hold for our entire input class.

The most important assumption is that the support and summation range of our problem (3.2) do not satisfy the admissibility condition stated in Definition 2.10. Since we deal with large problems it is not feasible to transform these into sums with standard boundary conditions by introducing several new variables. Therefore, after summing over the certificate recurrences (3.5), we need to compute the inhomogeneous parts for the recurrence relations satisfied by the sums (3.2). Section 3.3 explains how these inhomogeneous recurrences are constructed.

Before summing over the certificate recurrence, we need to analyze the summability conditions given in Definition 2.9 and pre-determine the summation range (2.14) for which all the sums (2.15) exist. For this purpose, the first condition imposed on our input sum (3.2) sets the range of the free parameters N and ϵ as a set of the form (2.12), i.e.,

$$\mathcal{D}^{\epsilon}_{\mathcal{F},N,\tau} = [b \ldots \infty) \times (0, \infty)$$

with $b \in \mathbb{N}$ a given constant.

Our next task is to determine a range of the form (2.14) such that $\mathcal{F}$ is summable with respect to the recurrence (3.6). Here we intervene with a second assumption for the class of sums (3.2). Namely, their summands are well-defined only inside the initial input range

$$\mathcal{R} := \mathcal{R}_\sigma \times \mathcal{R}_j \subseteq D_{\mathcal{F}} \tag{3.8}$$

where $D_{\mathcal{F}}$ is the set of well-defined values, given by Definition 2.6. We also introduce notations for the infinite and the finite range of the sum (3.2) as $\mathcal{R}_\sigma := [p \ldots \infty)$ and $\mathcal{R}_j = [q_0 \ldots N + c] \ltimes [q_1 \ldots B_1] \ltimes \cdots \ltimes [q_r \ldots B_r]$, respectively.

Under these two assumptions, we can only sum the non-k-free recurrence (3.6) with respect to a possibly smaller summation range

$$Summ'_{\mathcal{F},\tau,\delta}(N,\epsilon) := \{(\sigma, j) \in \mathbb{Z}^{s+r+1} : \quad (N + u, \sigma + v, j + w, \epsilon) \in \mathcal{R} \text{ for all } 0 \leq u \leq \tau \text{ and } (\sigma, j) \in [0 \ldots \delta]\}. \tag{3.9}$$

When trying to determine this more restrictive range, we observe that only sums over the summation variables from $j = (j_0, j_1, \ldots, j_r)$ which have finite upper summation bounds will play a role. In this context we introduce a grading function $\varphi_{N,j}$ with respect to the free variable N defined on the structure set of the recurrence. This function assigns an integer value to each term of the recurrence (3.6) assessing by how much we go beyond the summation bounds when summing over the input range $\mathcal{R}$.

Definition 3.4. *Given a ring of operators $R[N, \sigma, j, \epsilon]\langle \mathcal{N}, S, J\rangle$, let the grading function on the monomials of this ring*

$$\varphi_{N,j} : \mathbb{M}\left(R[N, \sigma, j, \epsilon]\langle \mathcal{N}, S, J\rangle\right) \to \mathbb{Z}$$

be defined as

$$\mathcal{N}^u S^v J^w \mapsto |w| - u$$

where $u \in \mathbb{N}$, $v \in \mathbb{N}^s$, $w \in \mathbb{N}^{r+1}$. Moreover, we introduce the grade of an operator $\mathcal{P} \in R[N, \sigma, j, \epsilon]\langle \mathcal{N}, S, J\rangle$ through the function

$$\Phi_{N,j} : R[N, \sigma, j, \epsilon]\langle \mathcal{N}, S, J\rangle \to \mathbb{Z}$$

defined by

$$\Phi_{N,j}(\mathcal{P}) = \max_{(u,v,w) \in \mathbb{S}_{\mathcal{P}}} \varphi_{N,j}(\mathcal{N}^u S^v J^w),$$

where $\mathbb{S}_{\mathcal{P}}$ is the structure set associated to the recurrence operator $\mathcal{P}$.

Note that all operators from the ring $R[N,\sigma,j,\epsilon]\langle\mathcal{N},S,J\rangle$ have structure sets containing only positive shifts, as we described in Section 1.2.3.

Moreover, the grading function $\varphi_{N,j}$ returns the difference between the sum of shifts in the summation variables from j and the shift in N for a term of the non-k-free recurrence (3.6). The integer returned by $\Phi_{N,j}$ as the grade of the recurrence operator $\mathcal{P}'$ is the maximum value the grading function takes over the entire structure set of the recurrence.

Using these concepts we can determine the range (3.9), $Summ'_{\mathcal{F},\tau,\delta}(N,\epsilon)$, for which the summability condition holds with respect to the recurrence $\mathcal{P}'$. For this we need to prove the following theorems

Theorem 3.5. *Let $\mathcal{F}(N,\sigma,j,\epsilon)$ be a proper hypergeometric summand of the form (3.2), well-defined on the input range $\mathcal{R}$ and let $\mathcal{P}' \in R[N,\sigma,j,\epsilon]\langle\mathcal{N},S,J\rangle$ be the expanded form of a nontrivial certificate recurrence (3.5) which annihilates $\mathcal{F}$ for all $(N,\epsilon)\in\mathcal{D}^{\epsilon}_{\mathcal{F},N,\tau}$. Denoting with $g\in\mathbb{Z}$ the grade $\Phi_{N,j}(\mathcal{P}')$ of this recurrence operator, for all $(N,\epsilon)\in\mathcal{D}^{\epsilon}_{\mathcal{F},N,\tau}$ we have*

(i) if $g\le 0$ then the summable range, $Summ'_{\mathcal{F},\tau,\delta}(N,\epsilon)$, is the whole range $\mathcal{R}$;

(ii) if $g>0$ then

$$Summ'_{\mathcal{F},\tau,\delta}(N,\epsilon)=\mathcal{R}_\sigma\times\mathcal{R}'_j$$

with restricted range for the sums with finite summation bounds given by

$$\mathcal{R}'_j=[q_0\ldots N+c-g]\ltimes[q_1\ldots B_1-g]\ltimes\cdots\ltimes[q_r\ldots B_r-g].$$

Proof. Let (u,v,w) be a point from the structure set $\mathbb{S}$ of the operator $\mathcal{P}'$. Since we consider upper summation bounds under the restrictions of Remark 3.2 we know that for all $1\le i\le r$ we find an integer $0\le l<i$ such that $B_i\in\{N-j_l,j_l\}$.

In the case (i), using several changes of variables we have

$$\begin{aligned}&\sum_{\sigma\in\mathcal{R}_\sigma}\sum_{j_0=q_0}^{N+c}\sum_{j_1=q_1}^{B_1}\cdots\sum_{j_r=q_r}^{B_r}\mathcal{F}(N+u,\sigma+v,j+w,\epsilon)\\&\quad=\sum_{\sigma\in\mathcal{R}_\sigma}\sum_{j_0=q_0+w_0}^{N+c+w_0}\sum_{j_1=q_1+w_1}^{B_1+w_1}\cdots\sum_{j_r=q_r+w_r}^{B_r+w_r}\mathcal{F}(N+u,\sigma+v,j,\epsilon).\end{aligned}$$

Let us denote the new summation bounds with $B'_i:=B_i+w_i$ for all $0\le i\le r$ and analyse this new summation range.

If it contains no bound of the form $B'_i=j_l+w_i$ with $l<i$ and $i\in[1\ldots r]$, then we can make a change of variables from N to $N-|w|$. The grade condition will assure a left-over positive shift in N, i.e., $u-|w|\ge 0$, while the resulting range is included in or equal to the original range $\mathcal{R}$.

In the case of summation bounds of the form $B'_i = j_l + w_i$ with $l < i$ and $i \in [1 \dots r]$, we use a change of variables from j_l to $j_l + w_i$ which leads to a new l-th summation range $[q_l + w_l + w_i \dots B'_l + w_i]$. Using changes of variables of this form we walk through all problematic summation bounds till we have eliminated all of them and find a B'_i depending on N. We will make at most r such changes of variables and stop at latest with a change of variables for j_0. In any of these cases, a last change of variables from N to $N - |w|$ and the condition $g \leq 0$ assures a final range smaller or equal to $\mathcal{R}$.

Note that, in this process we never make the same transformation j_l to $j_l + w_i$ twice, since i is decreasing. Therefore, each of the positive shifts w_i will contribute at most once to the final shift in j_l.

To prove (ii), we take the point $(u, v, w) \in \mathbb{S}$ for which the grade $g > 0$ is attained. By making a change of variables for N to $N + d$ we have

$$\sum_{\sigma \in \mathcal{R}_\sigma} \sum_{j_0=q_0}^{N+c-g} \sum_{j_1=q_1}^{B_1-g} \cdots \sum_{j_r=q_r}^{B_r-g} \mathcal{F}(N + u, \sigma + v, j + w, \epsilon)$$
$$= \sum_{\sigma \in \mathcal{R}_\sigma} \sum_{j_0=q_0}^{N+c} \sum_{j_1=q_1}^{B'_1} \cdots \sum_{j_r=q_r}^{B'_r} \mathcal{F}(N + u + g, \sigma + v, j + w, \epsilon).$$

In this way, we obtained a new operator of grade zero and a summation range included in $\mathcal{R}$. Hence, the conditions from (i) are fullfiled. □

Note that in the case (ii) of the theorem, we end up with a recurrence for a smaller sum

$$\sum_{\sigma \in \mathcal{R}_\sigma} \sum_{j \in \mathcal{R}'_j} \mathcal{F}(N, \sigma, j, \epsilon)$$

to which we need to add several sums of lower nested depth, so-called sore spots, in order to obtain our initial sum (3.2). In the next section we present algorithms to generate these additional sums. On the other hand, if the grade of the operator $\mathcal{P}'$ is negative or zero, the function $\mathcal{F}$ is summable over the initial summation range and there are no sore spots with respect to the given recurrence (3.6).

Returning to Example 3.3, the parameter range is given by

$$\mathcal{D}^{\epsilon}_{\mathcal{F},N,1} = [3 \dots \infty) \times (0, \infty)$$

and the input range can be split into

$$\mathcal{R}_\sigma = [0 \dots \infty) \text{ and } \mathcal{R}_j = [0 \dots N-3]_{j_0} \ltimes [0 \dots N - j_0 - 3] \ltimes [0 \dots j_0 + 1].$$

For the non-k-free recurrence **`expandRecU`** of orders $\tau = 1$ and $\delta = (1, 1, 0, 0)$, the grading function returns $\varphi_{N,j}(\mathbb{S}) = \{-1, 0, 1\}$ and condition (ii) is satisfied. Therefore we are only allowed to sum the certificate recurrence over a smaller summation range

$$Summ'_{\mathcal{F},1,(1,1,0,0)}(N, \epsilon) = [0 \dots \infty) \times [0 \dots N-4]_{j_0} \ltimes [0 \dots N - j_0 - 4] \ltimes [0 \dots j_0]. \quad (3.10)$$

However we obtain two additional sums, the so called sore sports, namely

$$\begin{aligned}\mathcal{U}(N,\epsilon) = &\sum_{\sigma_0=0}^{\infty}\sum_{j_0=0}^{N-4}\sum_{j_1=0}^{N-j_0-4}\sum_{j_2=0}^{j_0}\mathcal{F}(N,\sigma_0,j_0,j_1,j_2,\epsilon)\\ &+\sum_{\sigma_0=0}^{\infty}\sum_{j_0=0}^{N-3}\sum_{j_1=0}^{N-j_0-3}\mathcal{F}(N,\sigma_0,j_0,j_1,j_0+1,\epsilon)\\ &+\sum_{\sigma_0=0}^{\infty}\sum_{j_0=0}^{N-3}\sum_{j_2=0}^{j_0}\mathcal{F}(N,\sigma_0,j_0,N-j_0-3,j_2,\epsilon).\end{aligned}\tag{3.11}$$

Remark 3.6. Since we are dealing with definite summation problems, we can also view Definition 2.9 as a question of finding a large enough recurrence such that the function $\mathcal{F}$ is summable over the initial summation range $\mathcal{R}$. Since the range (2.14) depends on the orders of the recurrence, we can shift the recurrence in the free variable N, whenever condition (ii) holds.

In this case, the summation range with respect to the shifted recurrence will be equal the original range, i.e.,

$$\begin{aligned}Summ_{\mathcal{F},\tau',\delta}(N,\epsilon) := \{(\sigma,j)\in\mathbb{Z}^{s+r+1}:\quad &(N+u,\sigma+v,j+w,\epsilon)\in D_{\mathcal{F}}\\ &\text{for all } 0\le u\le\tau' \text{ and } (\sigma,j)\in[0\ldots\delta]\}=\mathcal{R}\end{aligned}$$

where $\tau'=\tau+\Phi_{N,j}(\mathcal{P}')$ and $\Phi_{N,j}(\mathcal{P}')>0$.

By avoiding the computation of sore spots, this leads to an elegant strategy. However, the inhomogeneous side of the shifted recurrence becomes larger and since we are aiming at solving this recurrence, the approach is computationally more challenging.

Although we have not yet encountered this situation in applications, it is interesting to consider what happens when we need recurrences (3.6) in more than one parameter for sums of the form (3.2). For example, if $N=(N_1,\ldots,N_l)\in\mathbb{N}^l$, we will apply the grading function with respect to each of the free variables and generalize the condition (ii) to

$$\max\{\Phi_{N_1,j}(\mathcal{P}'),\ldots,\Phi_{N_l,j}(\mathcal{P}')\}>0.$$

To use the approach described in Remark 3.6, we shift the recurrence in all parameters N_i, with $1\le i\le l$, for which condition (ii) holds by the positive integers $\Phi_{N_i,j}(\mathcal{P}')$, respectively.

3.3 Inhomogeneous recurrences

In this section we present our algorithmic strategy, implemented in the package `FSums`, to determine the inhomogeneous part for the recurrences satisfied by definite sums of the form (3.2). We start by considering a simple example and go through all the steps of our procedure.

Note that all the examples in this chapter are typical entries chosen from the list of 1420 sums delivered to us by our collaborators from DESY, which we needed to compute for our work at [15]. Let us start with the sum number 75 from this list

Example 3.7. *For $N \geq 3$ a discrete parameter and $\epsilon > 0$ we introduce the sum*

$$\mathcal{S}(N,\epsilon) := \sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-3-j_0} (-1)^{j_1}(j_1+1)\binom{N-2-j_0}{j_1+1} \frac{\Gamma(j_0+j_1+1)\left(1-\frac{\epsilon}{2}\right)_{j_0}\left(3-\frac{\epsilon}{2}\right)_{j_1}}{(4-\epsilon)_{j_0+j_1}\left(\frac{\epsilon}{2}+4\right)_{j_0+j_1}}.$$

As it was mentioned above, the first step is to apply WZ-summation techniques included in the Wegschaider's Mathematica package `MultiSum` [72]

In[28]:= **<< MultiSum.m**

MultiSum Package by Kurt Wegschaider (enhanced by Axel Riese and Burkhard Zimmermann) – © RISC Linz – V2.02β (02/21/05)

to compute a certificate recurrence for its summand

In[29]:= $\mathbf{termS} = (-1)^{j_1}(j_1+1)\binom{N-2-j}{j_1+1}\frac{\Gamma(j_0+j_1+1)\left(1-\frac{\epsilon}{2}\right)_{j_0}\left(3-\frac{\epsilon}{2}\right)_{j_1}}{(4-\epsilon)_{j_0+j_1}\left(\frac{\epsilon}{2}+4\right)_{j_0+j_1}}.$

For this, we find a suitable structure set using the command

In[30]:= **FindStructureSet[termS,** N**,** $\{j_0, j_1\}$**, 1];**

In[31]:= **strSetS = %[[1]]**

Out[31]= $\{\{0,0,1\},\{0,1,0\},\{0,1,1\},\{1,1,0\},\{1,1,1\}\}$

and calling further procedures from the package `MultiSum`

In[32]:= **FindRecurrence[termS,** N**,** $\{j_1, j_0\}$**, strSetS, 1, WZ → True];**

In[33]:= **certRecS = ShiftRecurrence[%[[1]],** $\{N, 1\}$**,** $\{j_0, 1\}$**,** $\{j_1, 1\}$**]**

Out[33]= $(\epsilon-2N)NF[N,j_0,j_1]-(\epsilon-N-3)(\epsilon+2N+2)F[N+1,j_0,j_1]=\Delta_{j_0}[(\epsilon^2+j_0\epsilon+\epsilon-2j_1-2j_0N-4j_1N-12N-6)F[N+1,j_0,j_1]]+\Delta_{j_1}[(\epsilon-2N)(j_0+j_1-N+1)F[N,j_0,j_1]+(-2N^2+\epsilon N+2j_0N+4j_1N+4N-2\epsilon-\epsilon j_0+2j_1)F[N+1,j_0,j_1]]$

we obtained a certificate recurrence which we afterwards shift to get only positive shifts in the recursion parameter N and in the summation variables.

Note that the precomputed structure set was used as input for the `FindRecurrence` function, since it translates into an Ansatz for the non-k-free recurrence (3.6). As it was described in Section 2.1, finding a small Ansatz for our computation proves to be vital from the efficiency point of view when dealing with more involved sums of the form (3.2).

Note also that the shifts of the resulting non-k-free recurrence do not necessarily coincide with the structure set `strSetS`, since some coefficients of the Ansatz might be zero. In this case we obtain the following expanded form of the certificate recurrence

In[34]:= **expandRecS = CertificateToRecurrence[certRecS]**

Out[34]= $(j_0 + j_1 + 1)(\epsilon - 2N)F[N, j_0, j_1] + (\epsilon - 2N)(-j_0 - j_1 + N - 2)F[N, j_0, j_1 + 1] + (2N^2 - \epsilon N - 2j_0N - 4j_1N - 8N + 2\epsilon + \epsilon j_0 - 2j_1 - 2)F[N + 1, j_0, j_1 + 1] + (-\epsilon^2 - j_0\epsilon - 2\epsilon + 2j_1 + 2j_0N + 4j_1N + 14N + 6)F[N + 1, j_0 + 1, j_1] = 0.$

The recurrence `certRecS` is of the form (2.4) and has the properties described in Remark 2.3. Therefore, summing over this certificate leads to a recurrence for the sum $\mathcal{S}(N, \epsilon)$ with its inhomogeneous part containing special instances of the double sum with lower nested depth, i.e., single sums and simple hypergeometric terms.

Moreover, we impose on our summation problem the assumptions described in Section 3.2, regarding nonstandard summation bounds. Therefore, we need to find the range (3.9) over which we can sum the certificate and determine the inhomogeneous part of the recurrence satisfied by the sum. If the range is smaller then the input range of the initial sum $\mathcal{S}(N, \epsilon)$, we additionally need to compute some extra sums, called sore spots. In the next subsections we present the main steps of this strategy for setting up inhomogeneous recurrence relations for sums of the form (3.2).

3.3.1 Delta boundary sums and sore spots

Let us start by summing over the initial summation range

$$\mathcal{R} = [0 \ldots N - 3]_{j_0} \ltimes [0 \ldots N - 3 - j_0]$$

over the delta parts on the right hand side of the recurrence. For this we denote the polynomial coefficients inside the delta parts Δ_{j_0} and Δ_{j_1} with $e[N, j_0, j_1, \epsilon]$ and $d_1[N, j_0, j_1, \epsilon]$, $d_2[N, j_0, j_1, \epsilon]$, respectively.

When summing over the Δ_{j_0}-part we generate two type of sums on the right side of the recurrence, the Δ-boundary sums and so-called telescoping compensating sums.

$$\sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-3-j_0} \Delta_{j_0}[e[N, j_0, j_1, \epsilon]F[N + 1, j_0, j_1]] =$$

$$
\begin{aligned}
&= \sum_{j_0=1}^{N-2} \sum_{j_1=0}^{N-2-j_0} e[N, j_0, j_1, \epsilon] F[N+1, j_0, j_1] - \sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-3-j_0} e[N, j_0, j_1, \epsilon] F[N+1, j_0, j_1] \\
&= \sum_{j_1=0}^{N-3-j_0} \left(e[N, j_0, j_1, \epsilon] F[N+1, j_0, j_1]\right) \Bigg|_{j_0=0}^{j_0=N-2} \\
&\quad + \sum_{j_0=1}^{N-2} e[N, j_0, N-2-j_0, \epsilon] F[N+1, j_0, N-2-j_0].
\end{aligned} \tag{3.12}
$$

Let us also consider the first term inside the Δ_{j_1}-part where no telescoping compensation is necessary

$$
\begin{aligned}
&\sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-3-j_0} \Delta_{j_1}[d_1[N, j_0, j_1, \epsilon] F[N, j_0, j_1]] = \sum_{j_0=0}^{N-3} \left(d_1[N, j_0, j_1, \epsilon] F[N, j_0, j_1]\right) \Bigg|_{j_1=0}^{j_1=N-2-j_0} \\
&\quad = \sum_{j_0=0}^{N-3} d_1[N, j_0, N-2-j_0, \epsilon] F[N, j_0, N-2-j_0] - \sum_{j_0=0}^{N-3} d_1[N, j_0, 0, \epsilon] F[N, j_0, 0].
\end{aligned}
$$

We observe that, after telescoping, the upper bound $N-2-j_0$ for j_1 translates into a term outside the original summation range, under the assumption that our summand `termS` is well-defined only inside this range $\mathcal{R}$. As we showed in Section 3.2, we need to adjust the range over which we sum the certificate recurrence or shift this relation with respect to the free parameter N.

We can compute the grade of the non-k-free recurrence operator $\mathcal{P}'$ for `expandRecS`, by looking at its structure set

$$
\mathbb{S} = \{\{0,0,0\}, \{0,0,1\}, \{1,0,1\}, \{1,1,0\}\}.
$$

In this case the grade is

$$
\Phi_{N,j}(\mathcal{P}') = \max_{(u,w)\in\mathbb{S}} |w| - u = \max\{1, 0\} = 1.
$$

Therefore, we generate the new range

$$
Summ'_{\mathcal{F},1,(1,1)}(N, \epsilon) = [0 \ldots N-4]_{j_0} \ltimes [0 \ldots N-j_0-4]
$$

and we will consider separately the sore spot

$$
\mathcal{S}(N, \epsilon) = \sum_{j_0=0}^{N-4} \sum_{j_1=0}^{N-4-j_0} F[N, j_0, j_1] + \sum_{j_0=0}^{N-3} F[N, j_0, N-j_0-3]. \tag{3.13}
$$

The package `FSums` contains a general strategy to obtain the necessary sore spots for sums of the form (3.2) over a summand $\mathcal{F}(N,\sigma,j,\epsilon)$ with input range

$$\mathcal{R} = \mathcal{R}_\sigma \times [q_0 \dots B_0] \ltimes \dots \ltimes [q_r \dots B_r]$$

where $\mathcal{R}_\sigma$ denotes the range corresponding to the infinite sums. Let g be the grade returned by $\Phi_{N,j}(\mathcal{P}')$ for a given certificate recurrence operator $\mathcal{P}'$ of the form (3.7) which annihilates $\mathcal{F}$.

Algorithm 1 SoreSpots [$F[N,\sigma,j,\epsilon], [q_0 \dots B_0] \ltimes \dots \ltimes [q_r \dots B_r], g, N, \mathcal{R}_\sigma$]

soreSpots =0;
for $i \in [r \dots 0]$ **do**
  soreSpots += $\sum_{\sigma\in\mathcal{R}_\sigma} \sum_{j_0=q_0}^{B_0} \cdots \sum_{j_{i-1}=q_{i-1}}^{B_{i-1}} \sum_{j_i=B_i-g+1}^{B_i} \sum_{j_{i+1}=q_{i+1}}^{B_{i+1}-g} \cdots \sum_{j_r=q_r}^{B_r-g} F[N,\sigma,j,\epsilon]$
end for
return soreSpots

The procedure `SoreSpots` will also deliver the new sum we consider, i.e., for our running example it returns precisely the equivalent formulation (3.13) or, in the case of the 4-fold sum $\mathcal{U}(N,\epsilon)$, the right hand side of identity (3.11).

3.3.2 Shift and telescoping compensation

As we described above, we continue from now on with the new sum

$$\mathcal{S}'(N,\epsilon) = \sum_{j_0=0}^{N-4} \sum_{j_1=0}^{N-4-j_0} F[N,j_0,j_1].$$

Shift compensating sums are another side-effect of nonstandard summation bounds. They appear when we sum over the left hand side of the recurrence over a given definite range, because our upper summation bounds depend on the other summation parameters.

Hence, in the case of the certificate recurrence `certRecS` summing over the restricted range $Summ'_{\mathcal{F},1,(1,1)}(N,\epsilon)$, we obtain

$$\sum_{j_0=0}^{N-4} \sum_{j_1=0}^{N-4-j_0} F[N+1,j_0,j_1] = \mathcal{S}'(N+1,\epsilon) - \sum_{j=0}^{N-3} F[N+1,j,N-3-j]. \qquad (3.14)$$

Compensating sums of this form are more cumbersome to generate since they appear only in the case of upper summation bounds depending on the free variable N. They are also very similar to the telescoping compensating sums which appeared for instance in (3.12).

Denoting by $sh \in \mathbb{N}$ the shift in a generic parameter p and mixing the two sets of summation parameters (σ, j) into κ with the summable range $\mathcal{R}$, let us first introduce the strategy for determining the shift compensating sums which is implemented in a procedure of the package `FSums`.

Algorithm 2 CompensatingSums [$F[p, \kappa, \epsilon], \mathcal{R}, sh, p$]

```
if R is empty then
  return F[p + sh, j, ε]
end if
{comment: separate the first sum from all the other ones in R}
currentRange = R[1]
lowerRange = R[2 . . . ]
rest = CompensatingSums [ F[p, j, ε], lowerRange, sh, p]
{comment: let's process the current range}
read from currentRange variable v, lower bound q and upper bound B
if B free of N then
  return Σ_{currentRange} rest
end if
{comment: see Remark 3.2 regarding structure of
          upper bounds → coefficient of p in B is either 1 or -1 }
if Coefficient[B, N] = 1 then
  CSums = Σ_{currentRange} rest - Σ_{v=B+1}^{B+sh} rest
else
  CSums = Σ_{currentRange} rest + Σ_{v=B-sh+1}^{B} rest
end if
return Σ_{v=q}^{B+sh} rest[1] + CSums
```

We have again included the new shifted sum as the first term of the output. For example,

In[35]:= **CompensatingSums**$[F[N, j_0, j_1], \{\{j_0, 0, N-4\}, \{j_1, 0, N-4-j_0\}\}, N, 1]$

Out[35]= $\{\{F[1+N, j_0, j_1], \{\{j_0, 0, -3+N\}, \{j_1, 0, -3-j_0+N\}\}\}, \{-F[1+N, j_0, -3-j_0+N], \{\{j_0, 0, -3+N\}\}\}, \{-F[1+N, -3+N, j_1], \{\{j_1, 0, -1\}\}\}\}$

delivers the right hand side of (3.14) since the last term represents a trivial sum.

Note that we represent a sum in the form of a list with two elements, where the elements are the summand and the range. We also store the range as a list of lists each containing the summation variable, the lower bound and the upper bound. In some situations we introduce a data structure `FSum` to encapsulate this list representation.

Moreover, after summing over the left hand side of the recurrence, we will move the resulting compensating sums, with a change of sign, to the inhomogeneous part of the recurrence. We have also implemented a short function which renames the first term of the output.

Algorithm 3 ShiftCompensatingSums [$F[N,\kappa,\epsilon],\mathcal{R},N,sh$]

```
CSums = CompensatingSums[ F[N, κ, ε], R, N, sh ]
if Length[CSums] > 1 then
   CSums = FSum ( CSums[2...] )
   eliminate trivial sums from CSums
   return SUM[N + sh] + CSums
else
   return SUM[N + sh]
end if
```

Therefore, we will have

In[36]:= **ShiftCompensatingSums[$F[N, j_0, j_1]$, {{j_0, 0, $N-4$}, {j_1, 0, $N-4-j_0$}}, N, 1]**

Out[36]= $\mathrm{SUM}[N+1]+\mathrm{FSum}[-F[1+N,j_0,-3-j_0+N],\{\{j_0,0,-3+N\}\}]$.

As we mentioned above, we also use the `CompensatingSums` procedure to generate the telescoping compensating sums which appear when summing over the Δ-parts on the right hand side of the certificate recurrence, again because of the structure of the summation bounds for the nested sums (3.2).

To illustrate this connection more clearly, let us go back to the example (3.3) and sum over the first term from the Δ_{j_0}-part of the certificate recurrence `certRecU` using its restricted range (3.10)

$$
\begin{aligned}
&\sum_{\sigma_0=0}^{\infty}\sum_{j_0=0}^{N-4}\sum_{j_1=0}^{N-j_0-4}\sum_{j_2=0}^{j_0}\Delta_{j_0}\left[(N-j_0+1)(N-2)F[N,\sigma_0,j_0,j_1,j_2]\right]\\
&\quad=\sum_{\sigma_0=0}^{\infty}\sum_{j_1=0}^{N-j_0-4}\sum_{j_2=0}^{j_0}(N-j_0+1)(N-2)F[N,\sigma_0,j_0,j_1,j_2]\Bigg|_{j_0=0}^{j_0=N-3}\\
&\quad+\sum_{\sigma_0=0}^{\infty}\sum_{j_0=1}^{N-3}\sum_{j_2=0}^{j_0-1}(N-j_0+1)(N-2)F[N,\sigma_0,j_0,N-j_0-3,j_2]\\
&\quad-\sum_{\sigma_0=0}^{\infty}\sum_{j_0=1}^{N-3}\sum_{j_1=0}^{N-j_0-4}(N-j_0+1)(N-2)F[N,\sigma_0,j_0,j_1,j_0].
\end{aligned}
\tag{3.15}
$$

Note that the first element on the right side of this identity denotes the Δ-boundary sums while the last two are due to telescoping compensation. These last sums are delivered by

In[37]:= $\mathbf{CompensatingSums}[F[N,\sigma_0,j_0-1,j_1,j_2],\{\{\sigma_0,0,\infty\},\{j_1,0,N-j_0-4\},\{j_2,0,j_0\}\}/.j_0\to(j_0-1),j_0,1]$

Out[37]= $\{\{F[N,\sigma_0,j_0,j_1,j_2],\{\{\sigma_0,0,\infty\},\{j_1,0,-4-j_0+N\},\{j_2,0,j_0\}\}\},\{F[N,\sigma_0,j_0,-3-j_0+N,j2],\{\{\sigma_0,0,\infty\},\{j_2,0,-1+j_0\}\}\},\{-F[N,\sigma_0,j_0,j_1,j_0],\{\{\sigma_0,0,\infty\},\{j_1,0,-4-j_0+N\}\}\}\}.$

Note that we obtain the delta boundary sums by evaluating this first entry for $j_0=0$ and $j_0=N-3$ and the compensating sums by adding the shifted sum $[1\dots N-3]_{j_0}$ to the range of the other terms of the output. This strategy is implemented in a simple function which can handle the entire right hand side of a certificate recurrence.

Algorithm 4 ProcessDeltas [RHS, $\mathcal{R}$]

```
boundarySums = 0
compSums = 0
{comment: for each of the deltas we generate the boundary sums
                                   and the telescoping compensating sums}
for i ∈ [1... Length[RHS]] do
   var = RHS [i][1]
   insideDelta = RHS [i][2]
   read from R the range of var in the form [q ... B]
   restOfRange = R\ [q ... B]
   if B = ∞ then
      newRange = [q+1 ... ∞]
   else
      newRange = [q+1 ... B+1]
      boundarySums = boundarySums + Σ_{restOfRange} insideDelta /. var → (B + 1)
   end if
   boundarySums = boundarySums - Σ_{restOfRange} insideDelta /. var → q
   newCompSums = CompensatingSums [ insideDelta /. var → (var - 1),
                              restOfRange /. var → (var - 1), var, 1] [2 ...]
   compSums = compSums + Σ_{newRange} newCompSums
end for
return FSum (boundarySums + compSums)
```

Using this function we can generate, for instance, the sums appearing on the right hand side of (3.15). Note that the delta boundary sum resulting in the case $j_0=N-3$ is again a trivial sum.

In[38]:= $\mathbf{ProcessDeltas[Delta[}j_0, (N - j_0 + 1)(N - 2)F[N, \sigma_0, j_0, j_1, j_2]], N, \{\{\sigma_0, 0, \mathrm{Infinity}\}, \{j_0, 0, N - 4\}, \{j_1, 0, N - 4 - j_0\}, \{j_2, 0, j_0\}\}]$

Out[38]= $\mathrm{FSum}[-(-2 + N)(1 + N)F[N, \sigma_0, 0, j_1, 0], \{\{\sigma_0, 0, \mathrm{Infinity}\}, \{j_1, 0, -4 + N\}\}] + \mathrm{FSum}[-(-2 + N)(1 - j_0 + N)F[N, \sigma_0, j_0, j_1, j_0], \{\{\sigma_0, 0, \mathrm{Infinity}\}, \{j_0, 1, -3 + N\}, \{j_1, 0, -4 - j_0 + N\}\}] + \mathrm{FSum}[(-2+N)(1-j_0+N)F[N, \sigma_0, j_0, -3-j_0+N, j_2], \{\{\sigma_0, 0, \mathrm{Infinity}\}, \{j_0, 1, -3+N\}, \{j_2, 0, -1 + j_0\}\}].$

3.3.3 An outline of the method

The above sections introduced the types of sums, i.e., shift and telescoping compensating sums as well as delta boundary sums, which will appear on the right hand side of the inhomogeneous recurrences satisfied by summation problems of the form (3.2) after summing over corresponding certificate recurrences (3.5).

A procedure to generate these inhomogeneous recurrences is implemented in the package `FSums`. For example, the recurrence satisfied by the sum $\mathcal{S}'(N, \epsilon)$, which we denote by simply SUM$[N]$, is returned by

In[39]:= $\mathbf{finalRecS = InhomogenRec[certRecS, \{\{}j_0, 0, -4 + N\}, \{j_1, 0, -4 - j_0 + N\}\}, N]$

Out[39]= $(\epsilon - 2N)N\mathrm{SUM}[N] + (3 - \epsilon + N)(2 + \epsilon + 2N)\mathrm{SUM}[1 + N] == \mathrm{FSum}[(1 + j_0 - N)(-\epsilon + 2N)F[N, j_0, 0], \{\{j_0, 0, -4+N\}\}] + \mathrm{FSum}[-2(\epsilon-2N)F[N, j_0, -3-j_0+N], \{\{j_0, 0, -4+N\}\}] + \mathrm{FSum}[(6 - \epsilon - \epsilon^2 + 2j_1 + 12N + 4j_1N)F[1 + N, 0, j_1], \{\{j_1, 0, -4 + N\}\}] + \mathrm{FSum}[(\epsilon - 2N)(2 + j_0 - N)F[1 + N, j_0, 0], \{\{j_0, 0, -4 + N\}\}] + \mathrm{FSum}[(3 - \epsilon + N)(2 + \epsilon + 2N)F[1 + N, j_0, -3 - j_0 + N], \{\{j_0, 0, -3 + N\}\}] + \mathrm{FSum}[(\epsilon + \epsilon^2 + 2j_0 + \epsilon j_0 - 2N + 2j_0N - 4N^2)F[1 + N, j_0, -3 - j_0 + N], \{\{j_0, 1, -3 + N\}\}] + \mathrm{FSum}[-((6 + 2\epsilon + 2j_0 + \epsilon j_0 + 6N - \epsilon N + 2j_0N - 2N^2)F[1 + N, j_0, -3 - j_0 + N]), \{\{j_0, 0, -4 + N\}\}]$

Note that we use the structure `FSum` to store sums with nonstandard boundary conditions of the form (3.2). This data type contains two components, the summand and a list structure for the summation range. The nested range is stored in the order given in (3.2), starting with the infinite sums and ending with the sums with finite summation bounds in the order of their dependence.

We have implemented this procedure using the short functions introduced in the sections above. The procedure `InhomogenRec` takes as input a certificate recurrence, the range of our summation problem and the free parameter N. The output will be the corresponding inhomogeneous recurrence containing special instances of our initial sum on its right hand side.

In the package `FSums` we use this procedure further, to compute recurrences for all the single sums appearing on the right hand side of the inhomogeneous relation `finalRecS`. These last inhomogeneous recurrences, delivered by Zeilberger's algorithm

Algorithm 5 InhomogenRec [rec, $\mathcal{R}$, N]

```
LHS = rec[1]/.F[N + sh_, a_] → ShiftCompensatingSums[F[N, a], R, N, sh]
lhsSums = LHS /. SUM[_] → 0
LHS = LHS - lhsSums;
RHS = rec[2]/. Delta[_,0] → 0
deltaSums = ProcessDeltas[RHS,R ]
RHS = deltaSums - lhsSums;
return LHS == RHS
```

[78], can be viewed in special difference fields introduced by M. Karr [35] and it is possible to find solutions of such recurrences [60] using the `Sigma` package. Moreover, for these solutions we find alternative representations in terms of generalized harmonic sums [70] using the package `HarmonicSums`.

By plugging in these answers into the recurrences from the previous level, `Sigma` computes a solution to the initial recurrence satisfied by the double sum $\mathcal{S}'(N,\epsilon)$. The solution is returned in the form of the first few coefficients of the Laurent series expansion around the parameter $\epsilon > 0$. However to obtain the initial sum we need to compute one sore spot given by (3.13). Using procedures from the packages `Sigma` and `EvaluateMultiSums` we have implemented this approach in the following function

In[40]:= **ComputeFSum[termS, $\{N\}, \{\{j_0, 0, -4+N\}, \{j_1, 0, -4-j_0+N\}\}, \{4\}, \{\epsilon, 0, 1\}$, Printing → Minimal, Splitting → 0, SigmaLevel → 0, Reorder → *False*]//Timing**

Out[40]= $\{67.5562\text{Second}, \{\frac{9(-2+N)(-1+N))}{2N^2}, \frac{3(24-32N-28N^2-13N^3+N^4)}{8N^3(2+N)} + \frac{9(3+N)S[1,N]}{N(1+N)(2+N)}\}\}$

Note that we use the notation from Section 1.2.6 for generalized harmonic sums, in this basic case we have

$$S[1,N] = \sum_{i=1}^{N} \frac{(-1)^i}{i}.$$

Hence, we obtained the following result for the sum from the Example 3.7

$$\mathcal{S}(N,\epsilon) = \frac{9(-2+N)(-1+N))}{2N^2} + \frac{3(24-32N-28N^2-13N^3+N^4)}{8N^3(2+N)}\epsilon + \frac{9(3+N)\epsilon}{N(1+N)(2+N)}\sum_{i=1}^{N}\frac{(-1)^i}{i} + \mathcal{O}(\epsilon^2).$$

Note also that in order to use the procedure `ComputeFSum` from our package, we need to first load all the components of the symbolic summation toolbox mentioned in the introduction to this chapter. In the next sections we present the `Sigma` approach to

Algorithm 6 ComputeFSum [term, vars, $\mathcal{R}$, $\{\epsilon$, start, end$\}$, opt]

```
N = vars[1] and read from R the list of summation variables sumVars
split R in R_σ × R_j as in (3.8)
{in case we have no sum}
if sumVars = {} then
  return the ε^start till the ε^end coefficients of the Laurent series expansion for term
  simplified by Sigma
end if
{in case we have only infinite sums}
if R = R_σ then
  return the ε^start till the ε^end coefficients of the Laurent series expansion for
  ∑_{R_σ} term determined by EvaluateMultiSums
end if
{in case we have sums with finite bounds}
if Length[sumVars] = 1 then
  rec = Zb[term, R, N]
else if Length[sumVars] > 1 then
  if Reorder then
    rec = UseMultiSum[ term, N, Reorder[ sumVars, R ] ]
    rec = Rearrange[ rec, R ]
  else
    rec = UseMultiSum[ term, N, sumVars ]
  end if
  {let's compute the sore spots}
  determine the grade d of the recurrence rec given by Definition 3.4
  if d > 0 then
    soreSpots = SoreSpots[ term, R_j, d, N, R_σ ]
    newRange = R_σ × R'_j
    apply ComputeFSum [ spot, vars, R_spot, {ε, start, end}, opt ] to each sore spot
  else
    soreSpots =0
    newRange = R
  end if
  rec= InhomogenRec[ rec, newRange, N, SplitRHSOpt]
  rec= SubstituteSummand[ rec, term, N, sumVars ]
  {compute the sums on the right hand side of rec}
  rec = rec/.FSum[f_, r_] → ComputeFSum[ f, vars, r, {ε, start, end}, opt]
end if
use Sigma and EvaluateMultiSums to solve rec ⇒ the ε^start till the ε^end coefficients
of the Laurent series expansion for the input sum
result = result + soreSpots
use HarmonicSums to find representations in terms of S-sums for result
return result
```

solving recurrences of this type and give more details about the procedure implemented in `ComputeFSum`.

Using the simple Example 3.7, we also notice that the procedure of shifting the recurrence instead of separating sore spots, described in Remark 3.6, will indeed lead to a larger inhomogeneous part for the recurrence that we later need to solve.

In[41]:= **InhomogenRec[ShiftRecurrence[certRecS, {N, 1}], {{j_0, 0, $N-3$}, {j_1, 0, $N-3-j_0$}}, N];**

In[42]:= **ShiftRecurrence[%, {N, −1}]**

Out[42]= $(\epsilon-2N)N\mathrm{SUM}[N]+(3-\epsilon+N)(2+\epsilon+2N)\mathrm{SUM}[1+N] == \mathrm{FSum}[(1+j_0-N)(-\epsilon+2N)F[N,j_0,0],\{\{j_0,0,-4+N\}\}]+\mathrm{FSum}[-2(\epsilon-2N)F[N,j_0,-3-j_0+N],\{\{j_0,0,-4+N\}\}]+\mathrm{FSum}[(\epsilon-2N)NF[N,j_0,-3-j_0+N],\{\{j_0,0,-3+N\}\}]+\mathrm{FSum}[(6-\epsilon-\epsilon^2+2j_1+12N+4j_1N)F[1+N,0,j_1],\{\{j_1,0,-4+N\}\}]+\mathrm{FSum}[(\epsilon-2N)(2+j_0-N)F[1+N,j_0,0],\{\{j_0,0,-4+N\}\}]+\mathrm{FSum}[(3-\epsilon+N)(2+\epsilon+2N)F[1+N,j_0,-3-j_0+N],\{\{j_0,0,-2+N\}\}]+\mathrm{FSum}[(\epsilon+\epsilon^2+2j_0+\epsilon j_0-2N+2j_0N-4N^2)F[1+N,j_0,-3-j_0+N],\{\{j_0,1,-3+N\}\}]+\mathrm{FSum}[(-6-2\epsilon-2j_0-\epsilon j_0-6N+\epsilon N-2j_0N+2N^2)F[1+N,j_0,-3-j_0+N],\{\{j_0,0,-4+N\}\}]+\mathrm{FSum}[(3-\epsilon+N)(2+\epsilon+2N)F[1+N,j_0,-2-j_0+N],\{\{j_0,0,-2+N\}\}]$

In[43]:= **Length[%[[2]]] − Length[finalRecS[[2]]]**

Out[43]= 2.

where the last command returns the difference between the number of sums in the inhomogeneous parts of the recurrences.

3.4 The `Sigma` package - solving recurrences and more

As presented above, the package `FSums` uses several procedures from C. Schneider's packages `Sigma` and `EvaluateMultiSums` to solve the inhomogeneous recurrences for the sums (3.2). We will focus here on the `Sigma` package [61] which combines several different symbolic summation approaches to automatically simplify nested sums and products.

Based on Karr's algorithm [35], the summation analogue of the Risch integration algorithm [55], the `Sigma` package contains further application-oriented extensions [59–62]. In this section we limit ourselves to the very basic concepts involved in this method, as described by Karr in [35], in order to specify the class of expressions that can be handled by our package `FSums` which relies on `Sigma`.

The main idea behind Karr's method is trying to find an antidifference for a given summand which is similar to how integrals can be solved by finding a primitive function. This strategy of algorithmically simplifying expressions refers to the elimination of summation and product quantifiers, if feasible, or else reduction of the nested depth, as remarked by C. Schneider in [62].

Suppose we're looking for a simpler representation, a *closed form* solution, $g(n)$ of the given a sum

$$g(n) = \sum_{i=a}^{n} f(i).$$

We can rewrite this to get an expression of $g(n)$ in terms of the summand $f(n)$,

$$\Delta g(n) = g(n+1) - g(n) = f(n). \tag{3.16}$$

Once we know such a function g satisfying the equality above, using the telescoping property, we obtain the value of the sum by evaluating g at the end points of the sum, in a similar fashion to evaluating a definite integral after finding a primitive function

$$\sum_{i=a}^{n} f(i) = g(n+1) - g(a).$$

Karr's strategy for finding the antidifference g works by first constructing an algebraic domain, a *difference field* to model the summand f and the shift behavior associated to the given sum structure. Hence, the starting point of this construction is finding a shift function which models the given structure and determining a field of constants, denoted here by K, containing elements that remain unchanged under this shift.

Definition 3.8. *[23] A difference field is a field F together with an automorphism σ of F. The constant field $K \subset F$ is the fixed field of σ.*

The map σ encapsulates the action of the shift. For example, given the sum $\sum_{i=1}^{n} i$, we take $F = \mathbb{Q}(n)$ with constant field $\mathbb{Q}$ and $\sigma(n) = n+1$. In order to simplify a given sum, we need to find a g satisfying equation (3.16). In the difference field setting, this equation can be written as a first order linear difference equation,

$$\sigma(g) - g = f. \tag{3.17}$$

Going back to our simple example, we have $f = i(n) = n$, where i is considered as a polynomial function on F. One can easily see that $g = \frac{n(n-1)}{2}$ satisfies the equation above. Then our sum $\sum_{i=1}^{n} i$ is equal to $g(n+1) - g(1) = \frac{(n+1)n}{2}$.

In general the summand f contains nested indefinite sums and products. In this case, we construct the difference field recursively, extending the domain by a new indeterminate to represent the current sum or product at each step. In [35], we find algorithms to solve equation (3.17) over certain towers of difference fields. These towers can be constructed by extending the given difference fields in one of two ways at each step.

Given a difference field F, σ, both extensions add a new transcendental indeterminate, say t, such that $\sigma(t) = \alpha t + \beta$ for some $\alpha, \beta \in F$. They also require that the constant field is not extended by this addition. Extensions with these properties are called *first order linear* by Karr [35, Definition 5]. We further divide first order linear extensions into two categories. If there is an element $w \in F(t)$ such that $\sigma(w) = aw$ for some $a \in F$, then the extension is called *homogeneous*. If there is no such element, we call the extension *inhomogeneous*. Homogeneous first order linear extensions are called Π extensions. Whereas Σ extensions are a special case of inhomogeneous first order linear extensions.

When constructing a tower, at each step the properties of a first order linear extension have to be verified. To accomplish this we first check if the extension is inhomogeneous. If this is the case, it will also be a first order linear extension which was proven in [35, Theorem 3]. In order to check if a homogeneous extension is first order linear, or if an inhomogeneous extension is a Σ extension, we verify a more technical condition described in Theorem 2 and Section 2.6 of [35].

In case they cannot already be represented by an element of the field at that stage, nested sums over the summand f are introduced as new Σ extensions in the tower of difference fields. For example, in order to extend the difference field $F = \mathbb{Q}(n)$ where $\sigma(n) = n + 1$ with the harmonic sums $H_n = \sum_{i=1}^{n} \frac{1}{n}$, we construct $F(h) = \mathbb{Q}(n, h)$ such that $\sigma(h) = h + \frac{1}{n+1}$. The image of h under σ is determined by shifting the harmonic sums,

$$\sigma(\sum_{i=1}^{n} \frac{1}{i}) = \sum_{i=1}^{n+1} \frac{1}{i} = (\sum_{i=1}^{n} \frac{1}{i}) + \frac{1}{n+1}.$$

Products in the function f are represented by Π extensions. For example, to add the expression 2^n, which can be written in product form $\prod_{i=1}^{n} 2$, to a difference field $F = \mathbb{Q}(n)$ where $\sigma(n) = n+1$, we construct $F(t) = \mathbb{Q}(n, t)$ with $\sigma(t) = 2t$. The image of $\sigma(t)$ is determined by the shift behavior of 2^n. Namely, $\sigma(2^n) = 2^{n+1} = 2 \cdot 2^n$.

For a small but nontrivial example of this construction, we try to find a simple formula for the double sum

$$\sum_{i=1}^{n} H_n^2 = \sum_{i=1}^{n} \left(\sum_{j=1}^{i} \frac{1}{j} \right)^2 .$$

The summand f is H_n^2 in this case. To represent f, we construct the difference field $F = \mathbb{Q}(n, h)$ with constant field $\mathbb{Q}$, $\sigma(n) = n + 1$ and $\sigma(h) = 1 + \frac{1}{n+1}$ as above. Now we need to solve

$$\sigma(g) - g = h^2$$

for $g \in F$. This can be accomplished by Karr's algorithm from [35], or a simplified version provided in [60]. We get the solution

$$g = h^2 n - 2hn - h + 2n,$$

which represents $H_n^2 n - 2H_n n - H_n + 2n$. Now we only need to evaluate g at the end points of the given sum,

$$\sum_{i=1}^{n} H_i^2 = g(n+1) - g(1) = H_n^2(n+1) - 2H_n n - H_n + 2n.$$

Note that Karr's approach to symbolic summation was extended by C. Schneider in many new directions [57, 58, 62] and the powerful package `Sigma` [61] is already used to solve large summation problems related to Feynman parameter integrals [11,13,44]. The computations described in this chapter rely on `Sigma` for solving the class of inhomogeneous recurrence relations set up during the procedure `ComputeFSum`.

Using generalizations of algorithms for solving difference equations [4, 52, 60], `Sigma` finds solutions for the recurrences satisfied by our class of summation problems (3.2). Combining these solutions with initial values computed by the `EvaluateMultiSums` package, we find an alternative representation for the input sum. These results can be rewritten in terms of harmonic sums [16, 70], using the package `HarmonicSums` [1].

3.5 Examples and variations on this theme

In this section we present the options `Reorder, Splitting`, and `SigmaLevel` which we have implemented to optimize the function `ComputeFSum`. We will also discuss the following 3-fold sum.

Example 3.9.

$$\mathcal{T}(\epsilon, N) := \sum_{j_0=1}^{N-2} \sum_{j_1=0}^{j_0} \sum_{j_2=0}^{j_1+1} (-1)^{j_0-j_1+j_2+N} \binom{j_0}{j_1} \binom{j_1+1}{j_2} \times \frac{\Gamma(-j_0+j_1+N+1)\Gamma(-j_0+j_2+N) \left(-\frac{\epsilon}{2}\right)_{j_2} \left(N-\frac{\epsilon}{2}\right)_{-j_0}}{\Gamma(-j_0+j_1+N+2)(N-\epsilon)_{j_2-j_0} \left(\frac{\epsilon}{2}+N+1\right)_{j_2-j_0}}$$

where $N \geq 3$ is the Mellin moment and $\epsilon > 0$ the dimension regularization parameter.

Recall from Section 2.1 that the certificate recurrence was obtained by sucessively dividing a k-free or a non-k-free recurrence by the Δ-operators of all the summation variables. The last remainder in this chain of division being the principal part which will become the left hand side of the corresponding certificate recurrence (2.4). Note also that, the principal part of the certificate recurrence will be independent of the order in which we choose to perform the divisions. Only the quotients, the contents of the Δ-parts, will differ under such a formal permutation of the summation variables.

Since the finite summation bounds in the ranges of the problems (3.2) originate from successive applications of the binomial theorem, the inner summation variables will be less spread in factors of the summand. Therefore we arrive faster at the principal part if we divide by the Δ-operators of the inner variables first and move to the outer sums. Experiments showed that for faster results the σ variables should be placed at the end of this chain. The option `Reorder` for the function `ComputeFSum` will reorder the variables for this purpose. Afterwards, by using the procedure `Rearrange` we reverse the variable permutation back such that `F[N, σ, j]` denotes the summand in any computed certificate recurrence.

Another shortcut we use is the `SigmaLevel` option. As we explained above, by summing over the computed certificate recurrence (3.5) satisfied by a sum of the form (3.2), one obtains an inhomogeneous recurrence. The right hand side of this recurrence will contain special instances of the original multi-sum of lower nested depth. Applying the same method on these new sums recursively, we get new recurrences. This procedure sets up a tree of recurrences with leaves made of relations with only hypergeometric terms on their right hand sides which we can solve using `Sigma`.

Even when we start with only a relatively small sum, the tree of recurrences will contain many branches that need to be pursued. In the case of Example 3.9, Wegschaider's algorithm solves an equation system of size 302×83 to determine a certificate recurrence of grade 2 and order 3 with respect to N. This leads to a number of 6 sore spots which needs to be considered separately. Moreover, after summing over the certificate recurrence, its inhomogeneous side will contain 87 double and single sums which need to be computed.

In this context, we have introduced the `SigmaLevel` option which cuts some branches of the recurrences tree and passes them over to `Sigma`. We have successfully used this idea for double sums on the right hand side of recurrence for many triple sums. For our running example we have

In[44]:= $\mathbf{ComputeFSum[termT, \{\mathit{N}\}, \{\{\mathit{j}_0, 1, -2{+}\mathit{N}\}, \{\mathit{j}_1, 0, \mathit{j}_0\}, \{\mathit{j}_2, 0, 1{+}\mathit{j}_1\}\}, \{4\}, \{\epsilon, 0, 1\},}$
$\mathbf{Printing \rightarrow Minimal, Splitting \rightarrow 0, SigmaLevel \rightarrow 2, Reorder \rightarrow \mathit{True}]//Timing}$

Out[44]= $$\{9574.13\text{Second}, \{N!\frac{1-(-1)^N}{N(1+N)^2}, N!\left(\frac{2+2N-5N^2-2N^3}{2N^2(1+N)^3}+\frac{3(-1)^N}{2(1+N)^3}+\frac{2}{1+N}\sum_{i=1}^{N}\frac{(-1)^i}{i^2}-\frac{S[2,N]}{1+N}\right)\}\}.$$

For the case of more then 4 summation quantifiers we have introduced the `Splitting` option which allows to split off some sums from the input problem (3.2). We regard the last split summation variable as the free parameter, in which we compute recurrences, for the remaining inner kernel. After finding a close form representation for these inner sums by setting up the tree of recurrences and solving them, as described above, we will add the split sum on the top of the result by using the `Sigma` package. Note also that all the optimization techniques we describe in this section lay more weight on the usage of the efficient package `Sigma`.

Summary

The collaboration between RISC and DESY, lead by C. Schneider, represents a breakthrough in applications of symbolic summation tools to Feynman integral calculus [11,13,44]. We contribute in this endeavor by applying WZ-Fasenmyer methods [25,76] to sum representations for a class of Feynman parameter integrals described in [15].

The summation problems we consider are highly nested definite sums with non-standard boundary conditions which satisfy inhomogeneous recurrences determined by summing over the certificate recurrences returned by Wegschaider's algorithm [72].

After constructing the range for which we can sum over a certificate recurrence without stepping out of the domain where the summand is well defined, we set up the inhomogeneous side of the recurrence relation satisfied by the multisum. The procedures described in sections 3.3 and 3.2 are also implemented in the Mathematica package `FSums`.

Our implementation in `FSums` became part of a symbolic summation toolbox for the computation of Feynman parameter integrals which also contains the packages `Sigma, EvaluateMultiSums, HarmonicNumbers, MultiSum` and the Paule-Schorn implementation of Zeilberger's algorithm.

Moreover, the question of setting up inhomogeneous recurrences for sums with non-standard boundary conditions is interesting in itself. For instance using the package `FSums` we can easily find the inhomogeneous recurrence for a double sum with finite bounds which is needed in [6, Section 4].

4 Recurrences for Mellin-Barnes integrals

This chapter presents how WZ-Fasenmyer summation methods [25, 76] can be used to determine recurrences for multiple contour integrals of Barnes' type, where in analogy to the summation case, the integrands need to be hypergeometric in all integration variables and contain free hypergeometric parameters.

As explained in section 4.2, we determine these recurrences by successively integrating the certificate recurrence (2.4) over the Barnes paths of integration $\mathcal{C}_{\kappa_j}$ for $1 \leq j \leq r$ and analyzing the behavior of the contour integrals over Δ-parts on the left hand side. By a different choice of the integration contours, this method will lead to homogeneous or inhomogeneous recurrences satisfied by the integrals.

These ideas go back to a question stated in [9, Section7] which presents an approach by W. Zudilin for the recurrences satisfied by a class of Ising integrals. We answer this question in section 4.4 of this chapter.

We start by introducing the Mellin transform and its inverse as well as generalized Mellin transforms which can be constructed for polynomial functions. In section 4.3 we prove entries involving definite integrals from the Gradshteyn-Ryzhik table of integrals [32]. By using the Mellin transform method, we find Mellin-Barnes integral representations for these problems and afterwards Wegschaider's algorithm [72] delivers recurrences satisfied by both sides of the identities.

4.1 The Mellin transform and its inverse

In this introductory section we give the definition of the Mellin transform and some of its elementary properties. We also discuss the inversion theorem, the Parseval formula and the Mellin transform method which we will later combine with algorithmic tools like WZ-summation techniques [76]. Chapters dedicated to this classic integral transform and its applications can be found in [12, 24, 34, 47, 63, 77].

Let us first recall that a function is said to be locally integrable on $(0, \infty)$ if and only if it is integrable on all closed subintervals of $(0, \infty)$. The *Mellin transform* of a locally integrable function $f : (0, \infty) \to \mathbb{C}$ is defined by

$$\tilde{f}(z) = \int_0^\infty t^{z-1} f(t) dt =: M[f; z] \tag{4.1}$$

wherever the integral converges. We first note that it can be expressed as a bilateral Laplace transform [34, Section 10.11] through the substitution $t = e^{-u}$, i.e.,

$$M[f; z] = \int_{-\infty}^{\infty} e^{-zu} f(e^{-u}) du \tag{4.2}$$

from which we know that it converges absolutely and it is analytic on the infinite strip $\alpha < Re(z) < \beta$ where

$$\alpha = \inf \left\{ a \,\middle|\, f(t) = \mathcal{O}(t^{-a}) \text{ as } t \to 0_+ \right\}$$
$$\beta = \sup \left\{ b \,\middle|\, f(t) = \mathcal{O}(t^{-b}) \text{ as } t \to +\infty \right\}. \tag{4.3}$$

Our main tool will be the inversion formula, which also follows directly from that for the two-sided Laplace transform,

$$f(t) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} t^{-z} \tilde{f}(z) dz \tag{4.4}$$

and uniquely determines $f(t)$ from $\tilde{f}(z)$ at all points $t \geq 0$ where $f(t)$ is continuous. The contour of integration is a vertical line in the z-plane and must be placed in the *strip of analyticity* $\alpha < c < \beta$, whose boundaries are determined by the asymptotic behaviour of f at the limits of its domain of definition.

Remark 4.1. Using (4.2) and the Riemann-Lebesgue lemma [8, Section 15-6], one can show that for all $\alpha \leq x \leq \beta$ we have

$$\lim_{y \to \pm\infty} M[f, x + iy] = 0.$$

In other words, $M[f, z]$ tends to zero as z goes to infinity along any vertical line within the strip of absolute convergence.

To introduce our approach to identities involving definite integrals, we prove the main property of the *Mellin convolution*, i.e.,

$$\int_0^{\infty} g(xt)h(t)dt = \frac{1}{2\pi i} \int_{\delta-i\infty}^{\delta+i\infty} x^{-z} \tilde{g}(z)\tilde{h}(1-z)dz, \tag{4.5}$$

where $g, h : (0, \infty) \to \mathbb{C}$ are defined such that the left hand side integral exists and the Mellin transforms $\tilde{g}(z)$ and $\tilde{h}(1-z)$ have a common domain of analyticity with δ lying in this common domain. Note that the special case $x = 1$ of (4.5) is called the *Parseval formula* for the Mellin transform [47, Section 3.1].

To prove (4.5), we start with the Mellin convolution on the left-hand side and use the inversion formula to insert $\tilde{g}(z)$. Next we reverse the order of integration, using the absolute convergence of the double integral and applying Fubini's theorem. Hence, we have

$$\int_0^\infty g(xt)h(t)dt = \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} x^{-z}\tilde{g}(z)\left(\int_0^\infty t^{-z}h(t)dt\right)dz$$

and since the inner definite integral is precisely $\tilde{h}(1-z)$ the proof is complete.

This simple proof strategy is based on the *Mellin transform method* for integration problems, mostly used to obtain equivalent Mellin-Barnes integral representations which can be rewritten as sums of residues at certain poles of the integrands. These sums lead to asymptotic expansions for the original integrals.

In this case, if the Mellin transforms $\tilde{g}(z)$ and $\tilde{h}(1-z)$ can be analytically continued to meromorphic functions in a left half plane and the contour of integration can be shifted to $Re\,z = d < \delta$, we have

$$\int_0^\infty g(xt)h(t)dt = \sum_{d<Re\,z<\delta} Res[x^{-z}\tilde{g}(z)\tilde{h}(1-z)] + E(x)$$

where $E(x)$ denotes the integral over the shifted contour

$$E(x) = \frac{1}{2\pi i}\int_{d-i\infty}^{d+i\infty} x^{-z}\tilde{g}(z)\tilde{h}(1-z)dz.$$

The resulting sum of residues yields the asymptotic expansion of the integral for small values of x. In a similar way, by shifting the contour to the right, we can construct the asymptotic expansion for $x \to +\infty$.

We use the Mellin transform technique to prove identities from the table of integrals [32]. For this purpose we only need the definition of the reciprocal pair (4.1) and (4.4). The proof of property (4.5) serves merely an introductory purpose here.

In Section 4.3, we rewrite the definite integrals appearing in entries from the table [32] by inserting a Mellin-Barnes integral representation of type (4.4) for a factor of the integrand using the method introduced above. This is done in the hope that after interchanging the order of integration, the inner integral becomes an easily computable definite integral and we end up with a contour integral of Barnes' type over a hypergeometric integrand.

For example, when proving the identity [32, **3.383.1**]

$$\int_0^u x^{\nu-1}(u-x)^{\mu-1}e^{\beta x}dx = B(\mu,\nu)u^{\mu+\nu-1}\,{}_1F_1\left(\nu;\nu+\mu;\beta u\right), \quad [Re\,\mu > 0, Re\,\nu > 0] \tag{4.6}$$

we rewrite the left-hand side by plugging in the Mellin-Barnes integral representation

$$e^{\beta x} = \frac{1}{2\pi i}\int_{\delta-i\infty}^{\delta+i\infty} \frac{1}{(-\beta)^z}\Gamma(z)x^{-z}dz, \quad \delta > 0.$$

This representation of the exponential function is to be found in [46] or can be obtained by observing that its Mellin transform is given by ([7], 1.1.18)

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx, \quad Re\, z > 0 \tag{4.7}$$

and using the inversion formula (4.4) afterwards.

Hence, the left-hand side of (4.6) becomes

$$\int_0^u x^{\nu-1}(u-x)^{\mu-1} e^{\beta x} dx = \frac{1}{2\pi i} \int_{\delta - i\infty}^{\delta + i\infty} \frac{1}{(-\beta)^z} \Gamma(z) \left(\int_0^u x^{\nu - z - 1}(u-x)^{\mu-1} dx \right) dz.$$

After several changes of variables, the inner definite integral is given by

$$\int_0^u x^{\nu-z-1}(u-x)^{\mu-1} dx = u^{\nu+\mu-1-z} B(\nu - z, \mu),$$

where B denotes the beta function. The identity (4.6) is equivalent to

$$\frac{\Gamma(\nu+\mu)}{2\pi i \Gamma(\nu)} \int_{\delta-i\infty}^{\delta+i\infty} \frac{\Gamma(\nu - z)}{\Gamma(\nu+\mu-z)} \Gamma(z)(-u\beta)^{-z} dz = {}_1F_1\left(\nu; \nu+\mu; \beta u\right),$$

which is the Barnes' integral representation for the confluent hypergeometric function ${}_1F_1$; see for instance section 4.2 in [7]. Note that identity (4.6) constitutes the base case for a proof by induction in n of the table entry [32, **3.478.3**].

Proving more involved identities from [32] via the Mellin transform method requires inserting the Mellin-Barnes type integral representations for two or more factors of the integrand. In this case, we will end up with nested contour integrals over hypergeometric terms and a sum representation for such integrals is not always easily determined. Examples of such situations are included in section 4.3.

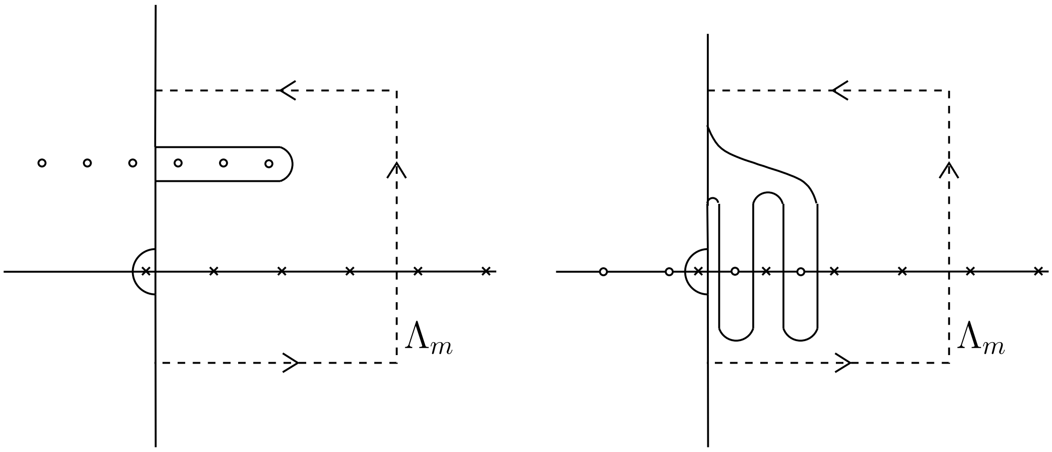
In this context, *Mellin-Barnes integrals* [34, 47] are complex contour integrals with integrands involving products of gamma functions and paths of integration, usually, running along the imaginary axis and curving, if necessary, to put the poles of $\Gamma(a+s)$ functions to the left and those of $\Gamma(b-s)$ functions to the right of the path, where z denotes the integration variable.

A simple example, for a Mellin-Barnes integral is

$$I_a := \int_{-i\infty}^{i\infty} \Gamma(a+s)\Gamma(-s) y^s ds$$

where a is neither zero nor a negative integer and possible contours of integration along the imaginary axis, separating ascending from descending chains of poles, are

Figure 4.1: Integration contours for I_a



(a) (b)

presented in Figure 4.1. Moreover, by integrating over the rectangular curves Λ_m, with corners $\pm im$, $m + \frac{1}{2} \pm im$, for large integers m, we can prove that

$$\frac{1}{2\pi i} I_a = \Gamma(a)(1+y)^{-a},$$

for $|y| < 1$ and $|\arg(y)| < \pi$. To show this result, we use Cauchy's residue theorem to express the integrals over the closed curves Λ_m as the sums of residues at the first poles of the ascending chain

$$\frac{1}{2\pi i} \int\limits_{\Lambda_m} \Gamma(a+s)\Gamma(-s) y^s ds = -\Gamma(a) \sum_{n=0}^{m} \frac{(a)_n}{n!} (-y)^n.$$

Next we investigate the asymptotic properties of the integrand using Stirling's formula [74, Section 13.6],

$$\log \Gamma(z+a) = (z + a - \frac{1}{2})\, Log\, z - z + \mathcal{O}(1) \tag{4.8}$$

which holds for large $|z|$ in the region where $|\arg(z)| < \pi$ and $|\arg(z+a)| < \pi$. Denoting the integrand of I_a by $\psi_{a,y}(s)$, we have for $|s| \to \infty$

$$\psi_{a,y}(s) = \mathcal{O}\left(|y|^{Re(s)} e^{-|\, Im\, s|(\pi - \arg(y))} |s|^{Re(a)-1} \right).$$

This asympotic behaviour implies that the integrals to the right of the contour Λ_m, as well as along the top and the bottom parts to tend to zero as $m \to \infty$. Hence we have the existence of I_a as an improper integral given by

$$\lim_{m\to+\infty}\int_{\Lambda_m}\psi_{a,y}(s)ds = I_a.$$

Thus, we have proved the Mellin-Barnes integral representation for a ${}_1F_0$ hypergeometric series. In the following sections we will use Barnes integrals of this form for other generalized hypergeometric series which can be proved using a similar argument [54, Theorem 35] or found in tables of Mellin transforms like [46].

Section 4.2 describes how WZ-Fasenmayer summation methods [76] can be used to compute homogeneous and inhomogeneous recurrences not only for nested sums but also for multiple Mellin-Barnes integrals over hypergeometric terms. This algorithmic aspect adds more power to the Mellin transform method and we are able to prove more involved entries from the table.

4.1.1 Analytic continuation of Mellin transforms

For the functions considered so far, the Mellin transform existed as defined in (4.1) and the contour of integration for its Mellin-Barnes integral representation passing through $c\in\mathbb{R}$ lay in the strip $\alpha < c < \beta$ defined by (4.3). In the case of a polynomial function $f(x) = (1-x)^n$ we have $\alpha = 0$ and $\beta = -n$ which implies that a strip of analyticity and the defining integral for the Mellin transform (4.1) do not exist.

An extension of the Mellin transform to deal with this problem is presented in [12, Section 4.3]. The procedure is based on the decomposition of the input function $f(x)$ into two functions defined on disjoint intervals such that $f(x) = f_1(x) + f_2(x)$. We can choose an arbitrary point and truncate f in the following way

$$f_1(x) = \begin{cases} f(x), & x\in[0,1) \\ 0, & x\in[1,\infty)\end{cases}, \quad f_2(x) = \begin{cases} 0, & x\in[0,1) \\ f(x), & x\in[1,\infty)\end{cases}.$$

Moreover, the Mellin transforms of these new functions are analytic in $Re(z) > \alpha$ and in $Re(z) < \beta$, respectively, where α, β are defined by (4.3). In the simple case when $\alpha < \beta$, we have

$$M[f;z] = M[f_1;z] + M[f_2;z].$$

Using the work of Handelsman and Lew, as presented in [77, Section 3.4], we extend this definition to the case $\alpha > \beta$ by imposing additional asymptotic conditions such that either $M[f_1;z]$ or $M[f_2;z]$ can be continued analytically to meromorphic functions on the entire z-plane. Indeed for the function $f(x) = (1-x)^n$ with $Re(n) > 0$, we have

$$\tilde{f}(z) = \Gamma(n+1)\left[\frac{\Gamma(z)}{\Gamma(n+z+1)} + (-1)^n\frac{\Gamma(-n-z)}{\Gamma(1-z)}\right], \tag{4.9}$$

for all $z\in\mathbb{C}$ except at its simple poles. The Parseval formula and other considerations for generalized Mellin transforms of this type is presented in [12, Section 4.5].

Remark 4.2. From our algorithmic point of view, the Mellin transform (4.9) is particularly interesting as it is the sum of two proper hypergeometric terms which are shadows of each other [75, Section 4]. Therefore, we find the same certificate recurrence for both terms which is also satisfied by their sum.

From (4.9) and Euler's integral representation [7, Theorem 2.2.1] we determine the Barnes' type integral form of the terminating ${}_2F_1$

$$ {}_2F_1\left(\begin{matrix} -n, b \\ c \end{matrix}; x\right) = \frac{\Gamma(c)\Gamma(n+1)}{2\pi i \Gamma(b)} \left[\int_{\delta - i\infty}^{\delta + i\infty} \frac{\Gamma(z)}{\Gamma(n+z+1)} \frac{\Gamma(b-z)}{\Gamma(c-z)} x^{-z} dz \right. \\ \left. + (-1)^n \int_{\eta - i\infty}^{\eta + i\infty} \frac{\Gamma(-n-z)}{\Gamma(1-z)} \frac{\Gamma(b-z)}{\Gamma(c-z)} x^{-z} dz \right] \quad (4.10)$$

where $Re(c) > Re(b) > 0$, $Re(b) > \delta > 0$ and $\eta < -Re(n)$.

4.2 From summation to integration

In this section we will show how Wegschaider's algorithm [72] can be used to determine recurrences for multiple contour integrals of Barnes' type

$$ Int(\mu) = \int_{\mathcal{C}_{\kappa_1}} \dots \int_{\mathcal{C}_{\kappa_r}} \mathcal{F}(\mu, \kappa_1, \dots, \kappa_r, \alpha)\, d\kappa_1 \dots d\kappa_r, \quad (4.11)$$

where the integrands $\mathcal{F}(\mu, \kappa, \alpha)$ are proper hypergeometric in all integer variables μ_i from $\mu = (\mu_1, \dots, \mu_p)$ and in all integration variables κ_j from $\kappa = (\kappa_1, \dots, \kappa_r) \in \mathbb{C}^r$, while $\alpha = (\alpha_1, \dots, \alpha_l) \in \mathbb{C}^l$ are additional parameters.

As in the case of the summation problem (2.1), the fundamental theorem of hypergeometric summation, Theorem 2.7, stated by Wilf and Zeilberger in [76] proves the existence of non-trivial certificate recurrences of the form (2.4) for the function $\mathcal{F}(\mu, \kappa, \alpha)$. Using WZ summation methods, Wegschaider's algorithm [72] delivers recurrences of the form (2.4) for the hypergeometric integrand from (4.11). As remarked in Section 2.1, the coefficients on the left hand side of this recurrence are free of all integration variables $\kappa = (\kappa_1, \dots, \kappa_r)$.

Although discrete functions are our main interest, one can also evaluate the function $\mathcal{F}(\mu, \kappa, \alpha)$ for complex values of the variables μ_i and κ_j for all $1 \le i \le p$ and $1 \le j \le r$ except at certain points. In our case, the singularities of the numerator gamma functions need to be excluded from the evaluation domain. The function $\mathcal{F}(\mu, \kappa, \alpha)$ is then continuous on its evaluation domain and by taking limits it can be shown that the computed recurrences (2.4) hold in $\mathbb{C}^{p+r+l}$.

Therefore, after successively integrating over the Barnes paths of integration $\mathcal{C}_{\kappa_j}$ for $1 \le j \le r$, (2.4) leads, in some cases, to a homogeneous recurrence for the integration problem (4.11), i.e.,

$$\sum_{m\in\mathbb{S}} a_m(\mu)\, Int(\mu+m) = 0. \tag{4.12}$$

However, again in analogy to the summation case, after integrating over the contours of integration $\mathcal{C}_{\kappa_j}$ for $1 \le j \le r$, it is not clear in general that we obtain a homogeneous equation of the type (4.12). Consequently, one needs to analyze the behavior of the contour integrals over the left hand side of (2.4).

For this purpose, we study the following integration problems:

$$I_j := \int_{\mathcal{C}_{\kappa_j}} \Delta_{\kappa_j}\mathcal{F}(\mu,\kappa)\, d\kappa_j = \int_{\mathcal{C}'_{\kappa_j}} \mathcal{F}(\mu,\kappa,\alpha)\, d\kappa_j - \int_{\mathcal{C}_{\kappa_j}} \mathcal{F}(\mu,\kappa,\alpha)\, d\kappa_j, \tag{4.13}$$

where the Barnes path $\mathcal{C}_{\kappa_j}$ runs vertically over $(c_j - i\infty, c_j + i\infty)$ while $\mathcal{C}'_{\kappa_j}$ denotes the shifted path $(1 + c_j - i\infty, 1 + c_j + i\infty)$ for all $1 \le j \le r$.

For any $1 \le j \le r$, consider now the contour integral I_j^N over a rectangle with vertices at the points $c_j - iN$, $c_j + iN$, $1 + c_j + iN$ and $1 + c_j - iN$ with $N \in \mathbb{N}$; i.e.,

$$\begin{aligned} I_j^N = &\int_{1+c_j-iN}^{1+c_j+iN} \mathcal{F}(\mu,\kappa,\alpha)\, d\kappa_j + \int_{1+c_j+iN}^{c_j+iN} \mathcal{F}(\mu,\kappa,\alpha)\, d\kappa_j \\ &+ \int_{c_j+iN}^{c_j-iN} \mathcal{F}(\mu,\kappa,\alpha)\, d\kappa_j + \int_{c_j-iN}^{1+c_j-iN} \mathcal{F}(\mu,\kappa,\alpha)\, d\kappa_j. \end{aligned} \tag{4.14}$$

If in any such rectangular region of integration, we have the asymptotic behavior

$$\mathcal{F}(\mu,\kappa) = \mathcal{O}\left(|\kappa_j|^{-d} e^{-c|\kappa_j|}\right) \quad \text{as} \quad |\kappa_j| \to \infty \quad \text{with} \quad c \ge 0, \quad d > 0, \tag{4.15}$$

then $I_j^N \to I_j$ as $N \to \infty$. Since the function $\mathcal{F}(\mu,\kappa,\alpha)$ is dominated by an exponential with negative exponent, it suffices to analyze the integrals (4.13) instead of the integrals over the right hand side of (2.7).

On the other hand, we can calculate the integrals (4.14) by considering the residues of the function $\mathcal{F}(\mu,\kappa,\alpha)$ at the poles lying inside the closed rectangular contours. Therefore, if for all $1 \le j \le r$, the Barnes paths of integration $\mathcal{C}_{\kappa_j}$ can be chosen such that the function $\mathcal{F}(\mu,\kappa,\alpha)$ has no poles inside these rectangular regions, then the integrals (4.13) will be zero. This is why conditions (4.37) are imposed on the integral representation of $C_{n,k}$ for $n, k \ge 1$.

Under these restrictions, we obtain from the certificate recurrence (2.4) a homogeneous recurrence (4.12) for the multiple Barnes' type integral (4.11). Note that by a different choice of the integration contours this method will lead to inhomogeneous recurrences for multiple Barnes integrals which satisfy the asymptotic condition (4.15).

Let us consider the entry [32, **6.512.3**] as a simple example

$$\int_0^\infty J_\nu(\alpha x)J_{\nu-1}(\beta x)dx = \frac{\beta^{\nu-1}}{\alpha^\nu}, \quad [\beta < \alpha] \tag{4.16}$$

where J_ν denotes the Bessel function of the first kind of order ν; see for instance [7, 4.5.2]. The Mellin-Barnes integral representation of J_ν is given by [46, 10.1]

$$J_\nu(\alpha x) = \frac{1}{4\pi i}\int_{\delta-i\infty}^{\delta+i\infty} \frac{\Gamma\left(\frac{\nu+z}{2}\right)}{\Gamma\left(1+\frac{\nu-z}{2}\right)}\left(\frac{\alpha x}{2}\right)^{-z}. \tag{4.17}$$

Using the Mellin transform method presented in Section 4.1, we obtain a simple Mellin-Barnes integral representation for the left hand side of (4.16)

$$\int_0^\infty J_\nu(\alpha x)J_{\nu-1}(\beta x)dx = \frac{1}{2\pi i\beta}\int_{\delta-i\infty}^{\delta+i\infty}\left(\frac{\beta}{\alpha}\right)^z \frac{dz}{\nu-z}, \tag{4.18}$$

where $-\nu < \delta < \frac{3}{2}$. We denote the integral on the right hand side of (4.18) by

$$Int[\nu] = \int F[\nu, z]dz \tag{4.19}$$

and observe that $F[\nu, z] = \mathcal{O}\left(|z|^{-1}\, e^{|z|\, log\, \frac{\beta}{\alpha}}\right)$.

Once we input the integrand

In[45]:= $\boldsymbol{F[\nu\_, z\_] := \frac{1}{2\pi i\beta(\nu-z)}\left(\frac{\beta}{\alpha}\right)^z}$

we compute a certificate recurrence in the integer parameter ν using either the Mathematica implementation of Zeilberger's algorithm [51] or the command

In[46]:= **FindRecurrence** $[\boldsymbol{F[\nu, z], \nu, z, 1}]$;

from the package `MultiSum` and shift this recurrence accordingly:

In[47]:= **ShiftRecurrence** $[\%[[1]], \{\nu, 1\}, \{z, 1\}]$

Out[47]= $\beta F[\nu, z] - \alpha F[\nu+1, z] = \Delta_z\left[\alpha F[\nu+1, z]\right].$

Here we need to think about the contour of integration. Since δ can be chosen such that the rectangular regions described above do not contain the pole of the function $F[\nu+1, z]$, we find the homogeneous recurrence satisfied by the left hand side of (4.16) as the output of the following command:

In[48]:= $\boldsymbol{rec1}$ = **SumCertificate** [%] /.**SUM** → **INT**

Out[48]= $\beta\mathrm{INT}[\nu] - \alpha\mathrm{INT}[\nu+1] = 0.$

In this simple case we can either read off the solution of the recurrence relation or, since the right side of the identity (4.16) is given, we also can check whether it satisfies the recurrence above:

In[49]:= $\mathbf{RHS}[\nu\_] := \frac{\beta^{\nu-1}}{\alpha^{\nu}}$

In[50]:= $\mathbf{CheckRecurrence}\,[rec\mathbf{1}, \mathbf{RHS}[\nu]]$

Out[50]= True.

The initial value that needs to be checked is a known property of the Bessel function. A similar approach works for the other two cases given in the table for this identity.

4.3 Back to proving special functions identities

Considerable work on proving and verifying the entries in the Table of Integrals, Series and Products [32] is being done by Victor Moll, et.al., in a series of articles, the latest being [19, 43, 45]. Moreover, an introduction to the art of evaluating definite integrals using a variety of techniques can be found in [17].

In joint work with K. Kohl [38], we contributed with an approach based on the Mellin transform method for rewriting definite integration problems in terms of nested Mellin-Barnes integrals. Viewing the identities in [32] from the perspective of the Mellin transform method seems natural, especially since most entries from the table of Mellin transforms [46] are also found there. In this section we present some short examples illustrating our approach.

4.3.1 A simple example

To prove the identity [32, **7.245.1**]

$$\int_0^{2\pi} P_{2m+1}(\cos\theta)\cos\theta d\theta = \frac{\pi}{2^{4m+1}}\binom{2m}{m}\binom{2m+2}{m+1} \tag{4.20}$$

we use the change of variable $\sin\theta =: x$ and the following representation for the Legendre function of the first kind

$$P_\nu(z) = {}_2F_1\left(\begin{matrix} -\frac{\nu}{2}, \frac{\nu+1}{2} \\ 1 \end{matrix}; 1-z^2\right).$$

Since, in our case, $\nu = 2m+1$ with $m \in \mathbb{N}$ by converting the ${}_2F_1$ to a Barnes integral, reversing the order of integration and evaluating the innermost integral, we rewrite (4.20) as

$$\frac{1}{2\pi i\Gamma(-m-\frac{1}{2})\Gamma(m+1)}\int_{\delta-i\infty}^{\delta+i\infty}\frac{\Gamma(-m-\frac{1}{2}+s)\Gamma(m+1+s)\Gamma(-s)}{\Gamma(1+s)}\frac{(-1)^s}{(2s+1)}ds$$
$$= \frac{\pi}{2^{4m+3}}\binom{2m}{m}\binom{2m+2}{m+1}. \tag{4.21}$$

This path of integration is curved to put the poles of the gamma functions $\Gamma(-m-\frac{1}{2}+s)$ and $\Gamma(m+1+s)$ to the left of the path and the poles of $\Gamma(-s)$ to the right.

Using Wegschaider's algorithm [72], we find a recurrence for the integrand:

In[51]:= $\mathrm{F}\,[m\_, s\_] := \dfrac{\boldsymbol{\Gamma(-m-1/2+s)\Gamma(m+1+s)\Gamma(-s)(-1)^s}}{\boldsymbol{2\pi i\Gamma(-m-1/2)\Gamma(m+1)\Gamma(1+s)(2s+1)}}$

In[52]:= **FindRecurrence** $[F[m,s], m, \{s\}, 1]$

In[53]:= $rec1$ = **ShiftRecurrence** $[\%[[1]], \{m, 1\}, \{s, 1\}]$

Out[53]= $2(1+m)(1+2m)(3+2m)(9+4m)F[m,s]+3(7+4m)(11+14m+4m^2)F[1+m,s]$
$-4(2+m)(3+m)(5+2m)(5+4m)F[2+m,s]=\Delta_s[2(1+2m)(3+2m)(9+4m)sF[m,s]$
$-2(300+610m+446m^2+140m^3+16m^4+297s+510ms+276m^2s+48m^3s)F[1+m,s]$
$+4(2+m)(3+m)(5+2m)(5+4m)F[2+m,s]]$

To check the asymptotic condition we use Stirling's formula (4.8). Since $|e^{i\pi y}| = 1$ for any real y, we denote with PI the pure imaginary terms and we obtain

$$\log F[m,s] = -\frac{5}{2}\log|s| + (arg(-s) - arg(s) - \pi)\, Im\, s + PI + \mathcal{O}(1).$$

Here we distinguish two cases, either $Im(s) > 0$ or $Im(s) < 0$, and in either of these cases the function $F[m,s]$ is of the form (4.15).

Integrating over the certificate recurrence with a suitable contour leads to a zero integral over the Δ_s part and we obtain a homogeneous recurrence for the left hand side of (4.21):

In[54]:= $rec2$ = **SumCertificate**[$rec1$]/.**SUM** → **INT**

Out[54]= $2(1+m)(1+2m)(3+2m)(9+4m)\mathrm{INT}[m]+3(7+4m)(11+14m+4m^2)\mathrm{INT}[1+m]-4(2+m)(3+m)(5+2m)(5+4m)\mathrm{INT}[2+m]=0$

Now we check that the right hand side of (4.21) also satisfies the recurrence:

In[55]:= **RHS**[$m\_$] := $\dfrac{\pi}{2^{4m+3}}\binom{2m}{m}\binom{2m+2}{m+1}$

In[56]:= **CheckRecurrence**[$rec2$, $RHS[m]$]

Out[56]= True.

At last, we only need to show that identity (4.20) holds for two initial values $m = 0$ and $m = 1$, and this is done by looking up the appropriate Legendre functions.

4.3.2 Examples involving orthogonal polynomials

Next we consider two more examples from the table [32] involving Gegenbauer polynomials. We start with identity **7.318**

$$\int_0^1 x^{2\nu}(1-x^2)^{\sigma-1} C_n^{\nu}\left(1-x^2 y\right) dx = \frac{\Gamma(2\nu+n)\Gamma\left(\nu+\frac{1}{2}\right)\Gamma(\sigma)}{2\Gamma(2\nu)\Gamma\left(n+\nu+\sigma+\frac{1}{2}\right)} P_n^{\left(\nu+\sigma-\frac{1}{2},\nu-\sigma-\frac{1}{2}\right)}(1-y) \tag{4.22}$$

for $Re(\nu) > -\frac{1}{2}$ and $Re(\sigma) > 0$.

Using the definition of the Jacobi polynomials [7], we have

$$P_n^{\left(\nu+\sigma-\frac{1}{2},\nu-\sigma-\frac{1}{2}\right)}(1-y) = \frac{\left(\nu+\sigma+\frac{1}{2}\right)_n}{n!} {}_2F_1\left(\begin{matrix}-n, n+2\nu \\ \nu+\sigma+\frac{1}{2}\end{matrix}; \frac{y}{2}\right). \tag{4.23}$$

On the left hand side of (4.22), it is convenient to make the change of variable $x^2 = z$ and use the representation (2.2.1) for the Gegenbauer polynomials. After this preprocessing step, identity (4.22) can be rewritten as

$$\int_0^1 z^{\nu-\frac{1}{2}}(1-z)^{\sigma-1} {}_2F_1\left(\begin{matrix}-n, n+2\nu \\ \nu+\frac{1}{2}\end{matrix}; \frac{zy}{2}\right) dz = \frac{\Gamma\left(\nu+\frac{1}{2}\right)\Gamma(\sigma)}{\Gamma\left(\nu+\sigma+\frac{1}{2}\right)} {}_2F_1\left(\begin{matrix}-n, n+2\nu \\ \nu+\sigma+\frac{1}{2}\end{matrix}; \frac{y}{2}\right). \tag{4.24}$$

Next, we represent the ${}_2F_1$ on the left hand side as a sum of Barnes' type integrals (4.10) and identity (4.24) becomes

$$\frac{\Gamma(n+1)}{2\pi i\Gamma(n+2\nu)}\left[\int_{\delta-i\infty}^{\delta+i\infty} \frac{\Gamma(s)}{\Gamma(n+s+1)} \frac{\Gamma(n+2\nu-s)}{\Gamma\left(\sigma+\nu-s+\frac{1}{2}\right)}\left(\frac{y}{2}\right)^{-s} ds + (-1)^n \times \int_{\eta-i\infty}^{\eta+i\infty} \frac{\Gamma(-n-s)}{\Gamma(1-s)} \frac{\Gamma(n+2\nu-s)}{\Gamma\left(\sigma+\nu-s+\frac{1}{2}\right)}\left(\frac{y}{2}\right)^{-s} ds\right] = \frac{1}{\Gamma\left(\nu+\sigma+\frac{1}{2}\right)} {}_2F_1\left(\begin{matrix}-n, n+2\nu \\ \nu+\sigma+\frac{1}{2}\end{matrix}; \frac{y}{2}\right), \tag{4.25}$$

where we also used the closed form of the Beta integral

$$\int_0^1 z^{\nu-s-\frac{1}{2}}(1-z)^{\sigma-1} dz =: B(\nu-s+\frac{1}{2},\sigma) = \frac{\Gamma(\nu-s+\frac{1}{2})\Gamma(\sigma)}{\Gamma(\nu-s+\sigma+\frac{1}{2})}.$$

At last, identity (4.25) is equivalent to the Barnes type integral representation of the ${}_2F_1$ appearing on the right hand side.

As a last example, we prove the more involved identity [32, **7.314.1**]

$$\int_{-1}^{1} (1-x)^{\nu-\frac{3}{2}}(1+x)^{\nu-\frac{1}{2}} \left[C_n^\nu(x)\right]^2 dx = \frac{\pi^{1/2}\Gamma\left(\nu-\frac{1}{2}\right)\Gamma(2\nu+n)}{n!\Gamma(\nu)\Gamma(2\nu)}. \tag{4.26}$$

We first make a change of variable $\frac{1-x}{2} =: y$ and then use the duplication formula [7, 1.5.1] to write (4.26) as

$$\int_{0}^{1} y^{\nu-\frac{3}{2}}(1-y)^{\nu-\frac{1}{2}} \left[C_n^\nu(1-2y)\right]^2 dy = \frac{\Gamma\left(\nu-\frac{1}{2}\right)\Gamma\left(\nu+\frac{1}{2}\right)\Gamma(2\nu+n)}{n!\Gamma(2\nu)^2}. \tag{4.27}$$

For the Gegenbauer polynomials we have the representation (2.2.1) with $z=2$ and the Barnes' type integral representation for the terminating ${}_2F_1$ given by (4.10). Therefore (4.27) can be rewritten as

$$\frac{\Gamma\left(\nu+\frac{1}{2}\right)^2}{(2\pi i)^2} \sum_{i,j\in\{1,2\}} \int_{C_i}\int_{C_j} \tilde{f}_i(s)\tilde{f}_j(t)\frac{\Gamma\left(\nu-s-t-\frac{1}{2}\right)}{\Gamma(2\nu-s-t)} ds\ dt = \frac{\Gamma\left(\nu-\frac{1}{2}\right)\Gamma(2\nu+n)}{n!}, \tag{4.28}$$

where for simplicity of presentation, we introduced the notations

$$\tilde{f}_1(s) = \frac{\Gamma(s)}{\Gamma(n+s+1)}\frac{\Gamma(n+2\nu-s)}{\Gamma\left(\nu+\frac{1}{2}-s\right)},$$
$$\tilde{f}_2(s) = (-1)^n\frac{\Gamma(-n-s)}{\Gamma(1-s)}\frac{\Gamma(n+2\nu-s)}{\Gamma\left(\nu+\frac{1}{2}-s\right)}$$

and the contours of integrations are of the form $C_1 = (\delta - i\infty, \delta + i\infty)$ and $C_2 = (\eta - i\infty, \eta + i\infty)$.

Since all the integrands on the left hand side of (4.28) are shadows of each other and will satisfy the same certificate recurrence, we denote a generic integral of the four by

$$INT[n] = \int\int F[n,s,t] \quad ds\ dt. \tag{4.29}$$

Wegschaider's algorithm [72] delivers the following certificate recurrence

In[57]:= **FindRecurrence** $[F[n,s,t], n, \{s,t\}, 1]$;

In[58]:= **ShiftRecurrence** $[\%[[1]], \{n,2\}, \{s,1\}, \{t,1\}]$

Out[58]= $(n+1)(2n+2\nu+3)(n+2)^2F[n+2,s,t]+(n+1)(n+2\nu)^2(2n+2\nu+1)F[n,s,t]-2(n+1)(n+\nu+1)(2n^2+4\nu n+4n+6\nu+3)F[n+1,s,t] = \Delta_s[2(n+\nu+1)(4\nu n^2-4sn^2-6tn^2-4n^2+4\nu^2n-4\nu n-$

$4\nu sn-4sn-8\nu tn-2stn-8tn-7n-4\nu^2-8\nu-4\nu t-4st-2t-3)F[n+1,s,t]-2(n+1)(n+\nu+1)(4n+6\nu+3)(2\nu-2s-2t-3)F[n+1,s,t+1]+4(n+2)(n+\nu+1)(n+s+2)(t+1)F[n+2,s,t]]+\Delta_t[4(n+\nu+1)(2n^3+6\nu n^2-sn^2+8n^2+4\nu^2 n+18\nu n-2\nu sn-3sn+stn-tn+10n+8\nu^2+12\nu-4\nu s-2s-2\nu t+2st-t+4)F[n+1,s,t]-4(n+2)(n+\nu+1)(2n+s+3)(n+t+2)F[n+2,s,t]].$

By integrating over this certificate recurrence, we obtain a recurrence for the sum of integrals from (4.28). This homogeneous recurrence is the output of the following command

In[59]:= $\boldsymbol{rec2} = $ **SumCertificate** [%] /.**SUM** → **INT**

Out[59]= $(2n+2\nu+3)(n+2)^2\mathrm{INT}[n+2]+(n+2\nu)^2(2n+2\nu+1)\mathrm{INT}[n]-2(n+\nu+1)\left(2n^2+4\nu n+4n+6\nu+3\right)\mathrm{INT}[n+1]=0.$

and it is also satisfied by the right hand side of (4.28)

In[60]:= **RHS** $[\nu\_, n\_] := \dfrac{\Gamma\left(\nu-\frac{1}{2}\right)\Gamma(2\nu+n)}{n!}$

In[61]:= **CheckRecurrence** $[\boldsymbol{rec2}, \boldsymbol{RHS}[n,\nu]]$

Out[61]= True.

At last, we only need consider two initial values. In the case $n=0$, we have $C_0^\nu(x)=1$ and (4.26) is equivalent to the duplication formula. For $n=1$, we have $C_1^\nu(x)=2\nu x$ and the calculations are again trivial.

4.4 Recurrences for a class of Ising integrals

In [9], it was asked whether an already conjectured recurrence for the member $C_{5,k}$ of the Ising-class integrals

$$C_{n,k} := \frac{1}{n!}\int_0^\infty \cdots \int_0^\infty \frac{dx_1 dx_2 \dots dx_n}{(\cosh x_1 + \cdots + \cosh x_n)^{k+1}} \tag{4.30}$$

could be proven with WZ summation methods, after transforming it to a two-fold nested Barnes integral. As described in [9, Section 7], this idea goes back to W. Zudilin. We have obtained the conjectured recurrences in $k \geq 1$ for the integrals $C_{5,k}$ and $C_{6,k}$ using WZ-summation [76] and the approach to compute recurrences for multiple nested Barnes' type integrals presented in Section 4.2. Moreover, we will show that using this method one can in principle obtain recurrences with respect to $k \geq 1$ for any integral of the form (4.30) with $n \in \mathbb{N}$.

Note that, in [18], J. M. Borwein and B. Salvy show the existence of linear recurrences with polynomial coefficients for the integrals (4.30) using the theory of D-finite series and a Bessel-kernel representation given in [10]. They also describe a very efficient algorithm to compute recurrences in $k \geq 1$ for the integrals $C_{n,k}$ for given $n \in \mathbb{N}$.

4.4.1 Mellin-Barnes integral representations

For the statement of the problem we invoke the renormalization

$$c_{n,k} := \frac{n!}{2^n} \Gamma(k+1) C_{n,k}$$

used in [9]. The idea of W. Zudilin presented in [9, Section 7] relies on the following analytic convolution theorem.

Theorem 4.3. *([9], Theorem 7) For $k \in \mathbb{C}$ with $Re(k) > 0$ and $n, q \in \mathbb{N}$ such that $n \geq 1$ and $1 \leq q \leq n-1$, we have*

$$c_{n,k} = \frac{1}{2\pi i} \int_{\mathbf{C}} c_{n-q,k+s} c_{q,-1-s} ds$$

where the contour $\mathbf{C}$ runs over the vertical line $(-\lambda - i\infty, -\lambda + i\infty)$ with $\lambda \in \mathbb{R}$ such that $-1 - Re(k) < -\lambda < -1$.

Also in [9] the closed forms

$$C_{1,k} = \frac{2^k \Gamma\left(\frac{k+1}{2}\right)^2}{\Gamma(k+1)} \tag{4.31}$$

and

$$C_{2,k} = \frac{\sqrt{\pi}\Gamma\left(\frac{k+1}{2}\right)^3}{2\Gamma\left(\frac{k}{2}+1\right)\Gamma(k+1)} \tag{4.32}$$

were computed. In the following sections, we will compute the homogeneous recurrences satisfied by $C_{3,k}$ and $C_{6,k}$ for $k \geq 1$. By applying Theorem 4.3, using the closed forms (4.31) and (4.32), and making substitutions $(s,t) \to (2s, 2t)$, we are able to rewrite these as the Barnes' type integrals

$$C_{3,k} = \frac{1}{12i\sqrt{\pi}\Gamma(k+1)} \int_{\mathcal{C}_s} \frac{\Gamma\left(\frac{k+1}{2}+s\right)^3 \Gamma(-s)^2}{\Gamma\left(\frac{k}{2}+s+1\right) 4^s} ds \tag{4.33}$$

and, respectively,

$$C_{6,k} = \frac{-1}{720\sqrt{\pi}\Gamma(k+1)} \int_{\mathcal{C}_s} \int_{\mathcal{C}_t} \frac{\Gamma\left(\frac{k+1}{2}+s\right)^3 \Gamma(t-s)^3 \Gamma(-t)^3}{\Gamma\left(\frac{k}{2}+s+1\right)\Gamma\left(t-s+\frac{1}{2}\right)\Gamma\left(-t+\frac{1}{2}\right)} dsdt. \tag{4.34}$$

The vertical contours $\mathcal{C}_s := (-\lambda - i\infty, -\lambda + i\infty)$ separate the poles of $\Gamma\left(\frac{k+1}{2} + s\right)$ from the poles of $\Gamma(-s)$ and, respectively, from those of $\Gamma(t-s)$. Similarly, $\mathcal{C}_t := (-\rho - i\infty, -\rho + i\infty)$ splits the descending set of poles coming from $\Gamma(t-s)$ from the ascending poles of $\Gamma(-t)$. For reasons that become clear in Section 4.4.2, we choose $\lambda, \rho \in \mathbb{R}$ such that the following conditions are satisfied:

$$-\frac{1 + Re(k)}{2} < -\lambda < -\rho < -1. \tag{4.35}$$

Successively applying Theorem 4.3, we prove the following integral representation:

Theorem 4.4. *For arbitrary integers $n, k \geq 1$, we have*

$$C_{n,k} = \frac{2^n}{n!\,(2\pi i)^q} \frac{1}{\Gamma(k+1)} \int_{\mathbf{C}_{t_1}} \cdots \int_{\mathbf{C}_{t_q}} c_{2,k+t_1} \left(\prod_{j=1}^{q-1} c_{2,-1-t_j+t_{j+1}} \right) c_{\epsilon,-1-t_q} dt_1 \ldots dt_q, \tag{4.36}$$

where $q := \left\lceil \frac{n}{2} \right\rceil - 1$ and $\epsilon := n - 2q$.

We use the closed forms (4.31) and (4.32), and the substitutions $t_j \to 2t_j$ for all $1 \leq j \leq q$, to obtain from (4.36) the final representation of $C_{n,k}$ for arbitrary $k, n \geq 1$. At last, we choose new integration contours $\mathcal{C}_{t_j} := (-\lambda_j - i\infty, -\lambda_j + i\infty)$ for all $1 \leq j \leq q$ which run over vertical lines separating the poles of gamma functions of the form $\Gamma(a + t_j)$ from the poles of gamma functions of the form $\Gamma(b - t_j)$. For reasons presented later, we choose these Barnes paths of integration such that the following conditions are satisfied:

$$-\frac{1 + Re(k)}{2} < -\lambda_1 < -\lambda_2 < \cdots < -\lambda_q < -1. \tag{4.37}$$

4.4.2 Recurrences for the integrals $C_{n,k}$

After distinguishing between odd and even values of the parameter k, for an arbitrary Ising-class integral $C_{n,k}$, $n, k \geq 1$, one obtains two representations of the form

$$C_{n,\mu} = \frac{2^{n+2q}}{n!\,(2\pi i)^q} \frac{1}{\Gamma(\mu+1)} \int_{\mathcal{C}_{t_1}} \cdots \int_{\mathcal{C}_{t_q}} \Psi(\mu, t_1, \ldots, t_q)\, dt_1 \ldots dt_q, \tag{4.38}$$

where $\mu = \frac{k}{2}$, respectively, $\mu = \frac{k-1}{2}$ such that $\mu \in \mathbb{N}$. In both cases the integrand $\Psi(\mu, \mathbf{t})$ is proper hypergeometric in $\mu \geq 0$ and in all integration variables t_j from $\mathbf{t} = (t_1, \ldots, t_q)$.

Therefore, Wegschaider's algorithm [72] can be applied to deliver a certificate recurrence of the form (2.4), that can always be rewritten as

$$\sum_{m \in \mathbb{S}} a_m(\mu)\, \Psi(\mu + m, \mathbf{t}) = \sum_{j=1}^{r} \Delta_{t_j} \left(\sum_{(m,\tau) \in \mathbb{S}_j} b_{m,\tau}(\mu, \mathbf{t})\, \Psi(\mu + m, \mathbf{t} + \tau) \right), \tag{4.39}$$

where $\mathbb{S}$ is a pre-computed structure set, where $b_{m,\tau}(\mu, \mathbf{t})$ and the coefficients $a_m(\mu)$ are polynomials, the latter free of the integration variables and not all zero. Next we discuss when the recurrence relation, obtained after integrating over the certificate (4.39), is homogeneous.

Proposition 1. *If the integration contours $\mathcal{C}_{t_j} := (-\lambda_j - i\infty, -\lambda_j + i\infty)$ satisfy the conditions (4.37) and the sets of shifts $\mathbb{S}_j$ are of the form*

$$\mathbb{S}_j = \left\{(m, \tau) \in \mathbb{Z}^{q+1} : m \geq 0, \tau_j < \tau_{j+1} \text{ and } \tau_i = 0 \text{ for } 1 \leq i < j\right\},$$

for $1 \leq j < q$ and

$$\mathbb{S}_q = \left\{(m, \tau) \in \mathbb{Z}^{q+1} : m \geq 0 \text{ and } \tau_i = 0 \text{ for } 1 \leq i \leq q\right\},$$

then we have

$$\int_{\mathcal{C}_{t_j}} \Delta_{t_j} \left(\sum_{(m,\tau)\in\mathbb{S}_j} b_{m,\tau}(\mu, \mathbf{t}) \Psi(\mu + m, \mathbf{t} + \tau) \right) dt_j = 0, \tag{4.40}$$

for all $1 \leq j \leq q$ and $\mu \geq 1$.

Proof: Given the iterative construction of the integral representation (4.36), computed in Section 4.4.1, it suffices to study the behavior of the following two integrals

$$I_1 := \int_{\mathcal{C}_1} \Delta_t \left(\frac{\Gamma(t-r)^3}{\Gamma\left(t-r+\frac{1}{2}\right)} \frac{\Gamma(-t)^2}{4^t} \right) dt, \tag{4.41}$$

$$I_2 := \int_{\mathcal{C}_2} \Delta_t \left(\frac{\Gamma(t-r)^3}{\Gamma\left(t-r+\frac{1}{2}\right)} \frac{\Gamma(s+1-t)^3}{\Gamma\left(s-t+\frac{3}{2}\right)} \right) dt, \tag{4.42}$$

where $r, s \in \mathbb{C}$ are given constants.

We will prove here that both integrals

$$I_l = \int_{\mathcal{C}_l} \Delta_t \left(F_l(t)\right) dt, \quad l \in \{1, 2\}$$

are zero if the contours of integration $\mathcal{C}_l$ are the vertical lines $(-\rho_l - i\infty, -\rho_l + i\infty)$ separating the increasing from the decreasing sequences of poles of the gamma functions appearing in the numerators of the integrands $F_l(t)$. The Barnes paths of integration $\mathcal{C}_l$ also fulfill the conditions (4.37); i.e., $Re(r) < -\rho_l < Re(s) < -1$ for $l \in \{1, 2\}$.

Using the transformation $t + 1 \to t$ we can write the integrals (4.41) and (4.42) as

$$I_l = \int_{\mathcal{C}_l'} F_l(t)\, dt - \int_{\mathcal{C}_l} F_l(t)\, dt, \quad l \in \{1, 2\}$$

where the shifted contours $\mathcal{C}'_l$ run vertically on the line $(1-\rho_l-i\infty, 1-\rho_l+i\infty)$.

Next we define integrals of the form (4.14),

$$I_l^N := \int_{1-\rho_l-iN}^{1-\rho_l+iN} F_l(t)\,dt + \int_{1-\rho_l+iN}^{-\rho_l+iN} F_l(t)\,dt + \int_{-\rho_l+iN}^{-\rho_l-iN} F_l(t)\,dt + \int_{-\rho_l-iN}^{1-\rho_l-iN} F_l(t)\,dt,$$

for $N>0$ an arbitrary integer and $l \in \{1,2\}$.

Since conditions (4.37) are fulfilled, there are no poles of the functions $F_l(t)$ within these closed rectangular contours of integration. Therefore I_l^N are zero for any integer $N \in \mathbb{N}$. It only remains to show that $I_l^N \to I_l$ as $N \to \infty$ for $l \in \{1,2\}$. For this we need to prove that the integrals

$$J_l^N := \int_{1-\rho_l+iN}^{-\rho_l+iN} F_l(t)\,dt \quad \text{and} \quad L_l^N := \int_{-\rho_l-iN}^{1-\rho_l-iN} F_l(t)\,dt$$

tend to zero as $N \to \infty$. Using (4.8) one obtains when $|t| \to \infty$ and $|\arg(t)| < \pi$,

$$F_l(t) = \mathcal{O}\left(e^{\mathrm{Im}(t)[\arg(-t)-\arg(t)]}\right), \quad l \in \{1,2\}.$$

Here we distinguish two cases, either $\mathrm{Im}(t) > 0$ or $\mathrm{Im}(t) < 0$, and in any of these cases the functions $F_l(t)$ fulfill the condition (4.15) which assures that the integrals J_l^N and L_l^N tend to zero as $N \to \infty$ for $l \in \{1,2\}$.

Remark: The conditions of our proposition are very restrictive; especially the condition imposed on the set of shifts appearing inside the last delta part Δ_{t_q} rarely occurs in practice. For example, for the integral $C_{3,k}$ in the case $k=2K$ we use the integral form (4.33) and the following commands, from the package `MultiSum`, to compute a certificate recurrence and shift it accordingly

In[62]:= $\mathrm{F}[\boldsymbol{k\_}, \boldsymbol{s\_}] := \dfrac{\boldsymbol{\Gamma\left[\frac{k+1}{2}+s\right]^3 \Gamma[-s]^2}}{\boldsymbol{12 i\sqrt{\pi}\Gamma[k+1]\Gamma\left[\frac{k}{2}+s+1\right]4^s}};$

In[63]:= **FindRecurrence** $[\boldsymbol{F[2K, s], K, s, 1}]$;

In[64]:= **ShiftRecurrence** $[\%[[1]], \{\boldsymbol{K, 2}\}, \{\boldsymbol{s, 2}\}]$

Out[64]= $-(2K+1)^3F[K,s]+4(K+1)(20K^2+40K+21)F[K+1,s]-36(K+1)(K+2)(2K+3)F[K+2,s] = \Delta_s[(2K+1)^3F[K,s]+(2K+1)^3F[K,s+1]-4(K+1)(20K^2+40K+21)F[K+1,s]-16(K+1)(2K^2-4sK-K-5s-4)F[K+1,s+1]+48(K+1)(K+2)(2K+3)F[K+2,s]]$.

Note that in this case one can also compute a certificate recurrence using the more efficient algorithm [78]. After integrating both sides of this certificate recurrence with respect to the variable s, we can apply Proposition 1 only to some of the terms appearing inside the delta part. At last, on the remaning terms, Cauchy's residue theorem and the asymptotic property (4.15) will be used to evaluate the left-over contour integrals occuring on the right hand side of the recurrence. In this way, after computing the following two Mellin-Barnes integrals

$$\int_{\mathcal{C}_s} \Delta_s[(2K+1)^3 F[K,s+1] - 16(K+1)(2K^2-4sK-K-5s-4)$$
$$F[K+1,s+1]]ds = (2K+1)^3 2\pi i \underset{s=-1}{Res}\, F[K,s+1] -$$
$$16(K+1)(2K^2+3K+1)2\pi i \underset{s=-1}{Res}\, F[K+1,s+1],$$

the final recurrence satisfied by $C_{3,2K}$ turns out to be homogeneous. In more general situations, the necessary residue computations tend to be involved but packages such as `Sigma` [61] and `HarmonicSums` [1] can algorithmically simplify the resulting expressions.

4.4.3 The Recurrence for the integral $C_{6,k}$

In [9], the following recurrence for the integral $C_{6,k}$ was conjectured

$$\begin{aligned} &-(k+1)^6 C_{6,k} + 8(k+2)^2(7k^4+56k^3+182k^2+280k+171)\\ &C_{6,k+2} - 16(k+2)(k+3)^2(k+4)(49k^2+294k+500)C_{6,k+4}\\ &+2304(k+2)(k+3)(k+4)^2(k+5)(k+6)C_{6,k+6} = 0. \end{aligned} \tag{4.43}$$

To prove that the integral (4.30) for $n=6$ satisfies the above recurrence, we use the representation (4.34). First, we input in Mathematica its integrand as a function of $k \geq 0$ and complex variables s and t

In[65]:= $$\boldsymbol{F[k\_,s\_,t\_] := \frac{-\left(\Gamma\left[\frac{k+1}{2}+s\right]\Gamma[t-s]\Gamma[-t]\right)^3}{720\sqrt{\pi}\Gamma[k+1]\Gamma\left[\frac{k}{2}+s+1\right]\Gamma\left[t-s+\frac{1}{2}\right]\Gamma\left[-t+\frac{1}{2}\right]}}.$$

In the first part of the proof we want to apply Wegschaider's algorithm [72] which was already introduced in Section , to obtain a certificate recurrence for $F[k,s,t]$. For this we need the function to be *proper* hypergeometric not only with respect to the integration variables s,t but also with respect to the additional parameter k. This leads to a case distinction between even and odd values of k. In each of the two cases, $C_{6,k}$ can be expressed as a double Barnes type integral over a proper hypergeometric term

$$C_{6,2K+\epsilon} = \frac{-1}{720\pi}\int_{\mathcal{C}_s}\int_{\mathcal{C}_t} \mathcal{F}(K,s,t)dsdt,$$

with $K \geq 0$, $\epsilon \in \{0,1\}$ and integration contours satisfying the condition (4.35).

As already pointed out, one can reduce the running time of the summation algorithm [72] by first making an Ansatz for a small structure set of the recurrence. For example, before computing a recurrence relation for $F[2K,s,t]$, we find a structure set with the command

In[66]:= **FindStructureSet** [F[2K, s, t], K, {s, t} , {2, 2} , 1]

which gives us two candidates. Using the first candidate we already succeed in finding a certificate recurrence which can be shifted accordingly to obtain a relation of the form (4.39), i.e.,

In[67]:= **FindRecurrence** [F[2K, s, t], K, {s, t} , %[[1]], 1, WZ → True] ;

In[68]:= rec = **ShiftRecurrence** [%[[1]], {K, 3} , {s, 2} , {t, 1}] .

The sets of shifts appearing inside the delta parts, Δ_s and Δ_t can be inspected by using the simple Mathematica commands

In[69]:= **Cases** [rec[[2, 1]], F[__], Infinity]

Out[69]= $\{F[K,s,1+t], F[K,1+s,1+t], F[K,2+s,1+t], F[1+K,s,t], F[1+K,s,1+t], F[1+K,1+s,t], F[1+K,1+s,1+t], F[1+K,2+s,1+t], F[2+K,s,t], F[2+K,s,1+t], F[2+K,1+s,t], F[2+K,1+s,1+t], F[2+K,2+s,1+t], F[3+K,s,t], F[3+K,s,1+t], F[3+K,1+s,t], F[3+K,1+s,1+t]\}$

In[70]:= **Cases** [rec[[2, 2]], F[__], Infinity]

Out[70]= $\{F[K,s,t], F[1+K,s,t], F[2+K,s,t], F[3+K,s,t]\}$.

When integrating with respect to the variables s and t over this certificate recurrence, the conditions of Proposition 1 are fullfilled by the set of shifts appearing in the Δ_t-part and by a subset of the set shifts contained in Δ_s. At last, we evaluate the remaining contour integrals and again we obtain a homogeneous recurrence satisfied by $\mathrm{INT}[K] := C_{6,2K}$. This is returned by the command

In[71]:= **SumCertificate** [rec] /.SUM → INT

Out[71]= $(1+2K)^6\mathrm{INT}[K] - 32(1+K)^2(171+560K+728K^2+448K^3+112K^4)\mathrm{INT}[1+K] + 256(1+K)(2+K)(3+2K)^2(125+147K+49K^2)\mathrm{INT}[2+K] - 36864(1+K)(2+K)^2(3+K)(3+2K)(5+2K)\mathrm{INT}[3+K] = 0.$

Similarly, in the case $k = 2K + 1$ and $K \geq 0$ the computed recurrence is

Out[71]= $(1+K)^6\mathrm{INT}[K] - (3+2K)^2(87+210K+196K^2+84K^3+14K^4)\mathrm{INT}[1+K] + (2+K)^2(3+2K)(5+2K)(843+784K+196K^2)\mathrm{INT}[2+K] - 144(2+K)(3+K)(3+2K)(5+2K)^2(7+2K)\mathrm{INT}[3+K] = 0,$

where $\mathrm{INT}[K]$ now denotes $C_{6,2K+1}$.

The last step of the proof consists of obtaining the recurrence for the sequence of integrals $C_{6,k}$ with $k \geq 0$. To this end, we utilize the fact that the sequences $C_{6,2K}$ and $C_{6,2K+1}$ defined for all $K \geq 0$ are P-recursive (also called holonomic [68, 79]); i.e., they satisfy linear recurrences with polynomial coefficients. To compute the desired recurrence, we load, for instance, the Mathematica package

In[72]:= **<< GeneratingFunctions.m**

GeneratingFunctions Package by Christian Mallinger – © RISC Linz – V 0.68 (07/17/03)

From this package, the command `REInterlace` computes a recurrence that is satisfied by the sequence obtained by interlacing the input recurrences (see [41] for more details). This means, we input the recurrence relations satisfied by $(C_{6,2K})_{K\geq 0}$ and $(C_{6,2K+1})_{K\geq 0}$, respectively, and obtain a polynomial recurrence for the sequence $C_{6,k}$ with $k \geq 0$. The computed recurrence is exactly (4.43) and herewith the proof is complete.

Summary

In this chapter we introduced an algorithmic approach to prove and compute recurrences for Mellin-Barnes integrals by using WZ-Fasenmyer summation techniques, as we show in [65], and used this technique in combination with the Mellin transform method.

In analogy with the summation case, we prove entries from [32] by first using the Mellin transform method to bring the integrals to a suitable input form and then algorithmically finding a recurrence satisfied by both sides of the identity. We demonstrate that the idea can be successfully used to enlarge the domain of applicability for this classic integral transform.

This algorithmic method was also used to determine recurrences for members of the Ising-class integrals. Wegschaider's algorithm [72] delivers the recurrence conjectured in [9] for $C_{5,k}$ in completely analogous manner. Neglecting practical issues like computation time, this method applies to all $n \geq 1$.

Though, we need to remark that the algorithm [72] determines recurrences, after making an Ansatz about their structure set (i.e., fixing the set of shifts that they contain), by solving a large system of equations over a field of rational functions. Therefore, if the input of the algorithm is too involved, computations might become time consuming.

Basic ingredients of the approach are the representation of the Ising integrals $C_{n,k}$ for $k, n \geq 1$ as nested Barnes' type integrals and the convolution theorem stated in Section 7 of [9], ideas going back W. Zudilin. In addition, the method presented in Section 4.2 has a wider range of applications that deserve to be explored further.

My Mathematica package FSums

We present the main functions from the Mathematica package `FSums`, described and used in Chapter 3 which relies on several procedures from the packages `MultiSum` [72], `Sigma` [61], `HarmonicNumbers` [1], `zb` [51] and the new `EvaluateMultiSums` package by C. Schneider.

```
ComputeFSum[fIn_, N_, rangeIn_List, lb_, {ep_, start_Integer,
end_Integer}, opt___Rule]
```

To call this procedure one needs to load all the packages mentioned above. We take as input a summation problem of the form (3.2) which depends on the Mellin moment $N \geq lb$ and on the dimension regularization parameter $\epsilon > 0$. As output we obtain the ϵ^{start} till the ϵ^{end} coefficients of the Laurent series expansion for $\sum_{\text{rangeIn}}$ fIn. The options for this function, as described in Section 3.5 are `Printing`, `Splitting`, `SigmaLevel`, `Reorder`. In the case when the `Splitting` option is set to be nonzero, the summation variables of the split sums will be added to a list in the second parameter, the Mellin moment becoming the first element of this list. See also Algorithm 6.

```
UseZb[fIn_, range_List, N_]
```

is used in `ComputeFSum` to call Zeilberger's algorithm as implemented in the Mathematica package `zb.m`. After computing a recurrence for the single sum $\sum_{range}$ fIn with the `Zb` procedure, we set it up in the form needed for further computations.

```
UseMultiSum[fIn_, N_, listSumVars_List]
```

calls the functions `FindStructureSet` and `FindRecurrence` from the package `MultiSum` to determine a certificate recurrence. Afterwards we shift this recurrence to contain only positive shifts in all summation variables from listSumVars and in the free parameter N.

```
Reorder[range_List]
```

As described in Section 3.5, this function is used when the `Reorder` option is set to True in the `ComputeFSum` procedure. It determines a new order of the summation variables which will be used in the `UseMultiSum` procedure.

```
Arrange[rec_, range_]
```

used when the `Reorder` option is set to True in the `ComputeFSum` procedure. After calling the `UseMultiSum` procedure with a rearranged order of variables, the `Arrange` function restores the order in the computed recurrence.

```
ShiftToPositive[rec_, N_, varList_List]
```

is called inside the `UseMultiSum` function. It determines by how much we need to shift the computed certificate recurrence such that it contains only positive shifts and afterwards calls the `ShiftRecurrence` procedure from the package `MultiSum` to achieve this goal.

```
SoreSpots[fIn_, finRange_List, d_Integer, N_, infinRange_List]
```

implements Algorithm 1 to compute the sore spots of a sum with summand `fIn` and range `infinRange` $\times$ `finRange` after adjusting with grade $d > 0$.

```
CompensatingSums[fIn_, range_List, shift_Integer, N_]
```

using Algorithm 2 computes the compensating sums after shifting with `shift` in the parameter N.

```
InhomogenRec[rec_, N_, range_List, CoeffSplitBound_]
```

As described in Section 3.3, given a certificate recurrence returned by the `UseMultiSum` function we determine the sums appearing on the right hand side after summing over `range` assuming nonstandard summation bounds. The option `CoeffSplitBound` can be used to split the sums appearing in the inhomogeneous part for large polynomial coefficients in the Δ-parts.

```
SubstituteSummandInRec[rec_,fIn_,N_,listSumVars_List]
```

substitutes the summand fIn as `F [N, listSumVars]` in the inhomogeneous part of the recurrence returned by the `InhomogenRec` function.

```
TrivialSums[fIn_, rangeIn_List]
```

sets to zero sums which contain ranges of the form $[q \dots B]$ with $q > B$.

```
TestingFction[fIn_, range_List, N_List, lb_List, {ep_, start_,
end_}, splitPoints_List, opt___Rule]
```

This procedure is used for testing, by calling the `ComputeFSum` procedure with different `Splitting` options given in the list `splitPoints`.

Notation and symbols

$\mathbb{N} = \{0, 1, 2, \ldots\}$	-	The set of natural numbers
$\mathbb{Z}, \mathbb{Q}, \mathbb{R}$	-	Sets of integers, rational, real numbers
$R[k]\langle K\rangle$	-	Ring of difference operators with $Kk = (k+1)K$
$(a)_n$	-	Pochhammer symbol or rising factorial, $(a)_n = a(a+1) \cdot \ldots \cdot (a+n-1)$
${}_pF_q\left(\begin{matrix} a_1 & \ldots & a_p \\ b_1 & \ldots & b_q \end{matrix}; z\right)$	-	The generalized hypergeometric function, ${}_pF_q\left(\begin{matrix} a_1 & \ldots & a_p \\ b_1 & \ldots & b_q \end{matrix}; z\right) = \sum_{n\geq 0} \frac{(a_1)_n \cdot \ldots \cdot (a_p)_n}{(b_1)_n \cdot \ldots \cdot (b_q)_n} \frac{z^n}{n!}$
H_n	-	Harmonic number, $H_n = \sum_{j=1}^n \frac{1}{j}$
$S_{a_1,\ldots,a_k}(n)$	-	Multiple harmonic sum $\sum_{i_1=1}^n \sum_{i_2=1}^{i_1} \cdots \sum_{i_k=1}^{i_{k-1}} \frac{\mathrm{sign}(a_1)^{i_1}}{i_1^{\lvert a_1\rvert}} \cdots \frac{\mathrm{sign}(a_k)^{i_k}}{i_k^{\lvert a_k\rvert}}$
$P_n^{(\alpha,\beta)}(x), P_n(x), C_n^\lambda(x)$	-	The families of Jacobi, Legendre and Gegenbauer polynomials, respectively
Δ_n	-	The forward difference operator in n
$\lvert i\rvert$	-	Norm of a multi-index tuple $\sum_{l=1}^n i_l$ for $i = (i_1, \ldots, i_n)$
$[a \ldots b]$	-	integer range $\{\, i \in \mathbb{Z} \,\vert\, a \leq i \leq b \,\}$ for $a, b \in \mathbb{Z}$ $[a_1 \ldots b_1] \times [a_2 \ldots b_2] \times \cdots \times [a_n \ldots b_n]$ for $a, b \in \mathbb{Z}^n$
$[0 \ldots a]_i \ltimes [0 \ldots i]$	-	range for the sum $\sum_{i=0}^a \sum_{j=0}^i$
$\Phi_{N,j}(\mathcal{P}')$	-	$\max\limits_{(u,v,w)\in\mathbb{S}_{\mathcal{P}}} \varphi_{N,j}(\mathcal{N}^u S^v J^w)$ for $\mathcal{P}'$ in $R[N, \sigma, j, \epsilon]\langle \mathcal{N}, S, J\rangle$
$\varphi_{N,j}$	-	grading function on monomials of the operator ring $R[N, \sigma, j, \epsilon]\langle \mathcal{N}, S, J\rangle$, $\varphi_{N,j} : \mathcal{N}^u S^v J^w \mapsto \lvert w\rvert - u$
$\mathcal{D}_{\mathcal{F}}$	-	Set of well-defined values of $\mathcal{F}$
$Supp_{\mathcal{F}}(\mu, \alpha)$	-	Support of $\mathcal{F}$
$Summ_{\mathcal{F}}(\tau, \delta)$	-	Summation range of $\mathcal{F}$
$C_{n,k}$	-	Ising integral $\frac{1}{n!} \int_0^\infty \cdots \int_0^\infty \frac{dx_1 dx_2 \ldots dx_n}{(\cosh x_1 + \cdots + \cosh x_n)^{k+1}}$

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Eidesstattliche Erklärung

Ich erkläre an Eides statt, daß ich die vorliegende Dissertation selbstständig und ohne fremde Hilfe verfaßt, andere als die angegebenen Quellen und Hilfsmittel nicht benutzt bzw. die wörtlich oder sinngemäß entnommenen Stellen als solche kenntlich gemacht habe.

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