DESY 10–185
TTK–10–49
SFB-CPP/10–107
November 2010

A Symbolic Summation Approach to Feynman Integral Calculus

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arXiv:1011.2656v1 [cs.SC] 11 Nov 2010

Abstract

Given a Feynman parameter integral, depending on a single discrete variable N and a real parameter ε, we discuss a new algorithmic framework to compute the first coefficients of its Laurent series expansion in ε. In a first step, the integrals are expressed by hypergeometric multi-sums by means of symbolic transformations. Given this sum format, we develop new summation tools to extract the first coefficients of its series expansion whenever they are expressible in terms of indefinite nested product-sum expressions. In particular, we enhance the known multi-sum algorithms to derive recurrences for sums with complicated boundary conditions, and we present new algorithms to find formal Laurent series solutions of a given recurrence relation.

Key words: Feynman integrals, multi-summation, recurrence solving, formal Laurent series

⋆ Supported in part by the Austrian Science Fund (FWF) grants P20162-N18, P20347-N18, DK W1214, the German Research Fund SFB-TR-9, and EU TMR Network Heptools.

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1. Introduction

Starting with single summation over hypergeometric terms developed, e.g., in Gosper (1978); Zeilberger (1990a); Petkovšek (1992); Abramov and Petkovšek (1994); Paule (1995) symbolic summation has been intensively enhanced to multi-summation like, e.g., the holonomic approach of Zeilberger (1990b); Chyzak (2000); Schneider (2005a); Koutschan (2009). In this article we use –among various different approaches– the techniques of Fasenmyer (1945); Wilf and Zeilberger (1992) which lead to efficient algorithms developed, e.g., in Wegschaider (1997) to compute recurrence relations for hypergeometric multi-sums. Besides this, we rely on multi-summation algorithms presented in Schneider (2007) that generalize the summation techniques worked out in Petkovšek et al. (1996); the underlying algorithms are based on a refined difference field theory elaborated in Schneider (2008, 2011) that is adapted from Karr's $\Pi\Sigma$-fields originally introduced in Karr (1981).

In this article we aim at combining these summation approaches which leads to a new framework assisting in the task to evaluate Feynman integrals in an automatic fashion. We show in a first step that Feynman parameter integrals, which contain local operator insertions, in D-dimensional Minkowski space with one time- and $(D-1)$ Euclidean space dimensions, $\varepsilon = D-4$ and $\varepsilon \in \mathbb{R}$ with $|\varepsilon| \ll 1$, can be transformed by means of symbolic computation to hypergeometric multi-sums.

Given these integrals in form of hypergeometric multisums $\mathcal{S}(\varepsilon, N)$, with N an integer parameter, one can check by analytic arguments wether the integrals can be expanded in a Laurent series w.r.t. the parameter ε, and we seek for summation algorithms to compute the first coefficients of its Laurent series expansion whenever they are representable in terms of indefinite nested sums and products. If we obtain such solutions, they usually can be transformed –due the special input class of Feynman integrals– to harmonic sums or S-sums; see Blümlein and Kurth (1999); Vermaseren (1999); Moch et al. (2002); Ablinger (2009).

In general, we present an algorithm (see Theorem 3) that decides constructively, if these first coefficients of the ε–expansion can be written in such indefinite nested product-sum expressions. Here one first computes a homogeneous recurrence by WZ-theory and Wegschaider's approach, and afterwards derives the coefficients (see Corollary 1) by ansatz and solving incrementally linear recurrences by the algorithms given in Petkovšek (1992); Abramov and Petkovšek (1994); Schneider (2001, 2005b). The found solutions are highly nested by construction, and finding sum representations with minimal depth using the algorithms from Schneider (2011) is an essential subproblem in our recurrence solver.

From the practical point of view there is one crucial drawback of the proposed solution: looking for such recurrences is extremely expensive, even worse, for our examples arising form particle physics the proposed algorithm is not applicable considering the available computer and time resources. On that score we relax this very restrictive requirement and search for possibly inhomogeneous recurrence relations. By a careful analysis of the involved input sums and dealing with the problem that the summand has poles almost everywhere outside of the summation range, we can compute with Wegschaider's package `MultiSum.m` and the new package `FSums.m` presented in Stan (2010) a recurrence where the inhomogeneous side consists of multi-sums with less sum quantifiers. Applying our

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method to these simpler sums by recursion will eventually lead to an expansion of the right hand side of the starting recurrence. Finally, we compute the coefficients of the original input sum by our new recurrence solver mentioned above.

The outline of the article is as follows. In Section 2 we explain all computation steps that lead from Feynman integrals to hypergeometric multi-sums of the form (13) which can be expanded in a Laurent expansion (17) where the coefficients $F_i(N)$ can be represented in the form (18). In the beginning of Section 3 we face the problem that the multi-sums (13) have to be split further in the form (19) to fit the input class of our summation algorithms. We first discuss convergent sums only. The treatment of those sums which diverge in this special format or sums with several infinite summations that have difficult convergence properties will be dealt with later, cf. Remark 5. In the remaining parts of Section 3 we present the general mechanisms to compute the first coefficients $F_i(N)$ for a given hypergeometric multi-sum. In Section 4 we enhance the ideas of Wegschaider (1997) in order to deal with infinite sums and sums with non-trivial boundary conditions in an automatic fashion. Finally, in Section 5 we combine the ideas of the previous sections to obtain a method that is capable to compute the coefficients $F_i(N)$ in reasonable time. Conclusions are given in Section 6.

2. Multiple sum representations of Feynman integrals

We consider two–point Feynman integrals in D-dimensional Minkowski space with one time- and $(D-1)$ Euclidean space dimensions, $\varepsilon = D-4$ and $\varepsilon \in \mathbb{R}$ with $|\varepsilon| \ll 1$ of the following structure [1] :

$$\mathcal{I}(\varepsilon, N, p) = \int \frac{d^D p_1}{(2\pi)^D} \dots \int \frac{d^D p_k}{(2\pi)^D} \frac{\mathcal{N}(p_1, \dots p_k; p; m_1 \dots m_k; \Delta, N)}{(-p_1^2 + m_1^2)^{l_1} \dots (-p_k^2 + m_k^2)^{l_k}} \prod_V \delta_V \ . \tag{1}$$

Here the external momentum p and the loop momenta p_i denote D-dimensional vectors, $m_i > 0, m_i \in \mathbb{R}$ are scalars (masses), $m_i \in \{0, M\}$, $k, l_i \in \mathbb{N}$, $k \geq 2, l_i \geq 1$, and Δ is a light-like D-vector, $\Delta.\Delta = 0$. The numerator function $\mathcal{N}$ is a polynomial in the scalar products $p.p_i$, $p_i.p_k$ and of monomials $(\Delta.p_{(i)})^{n_i}$, $n_i \in \mathbb{N}, n_i \geq 0$. $N \in \mathbb{N}$ denotes the spin of a local operator stemming from the light cone expansion, see, e.g., Frishman (1971) and references therein, which contributes to the numerator function $\mathcal{N}$ with a polynomial in $\Delta.p_i$ of maximal degree N, cf. Bierenbaum et al. (2009b). Furthermore we assume for simplicity that only one of the loops is formed of massive lines. These integrals are mathematically well defined, while they would not in natural space-time dimensions, where they usually exhibit singularities. The change of the space dimension from $3 \to 3 + \varepsilon$ is a minimal modification, in accordance with the conservation laws, cf. Noether (1918). The integrals are evaluated setting $p^2 = 0$, the on-shell condition for external massless lines. The distributions δ_V assure D-momentum conservation at any of the $(P - L + 1)$ vertices of the Feynman graph, where P is the number of propagator lines (edges) and L the number of closed loops. Denoting the momenta which belong to the vertex V and are all incoming as $r_1, ..., r_a$, δ_V is given by

[1] We only display the essential parameters as arguments in the integrals $\mathcal{I}$.

$$\delta_V = \delta^{(D)}(r_1 + ... + r_a) \ , \tag{2}$$

with $\delta^{(D)}$ Dirac's δ-distribution in D dimensions.

In the following we device an algorithm to transform $\mathcal{I}$ into nested sum representations. All the following steps can be executed efficiently in a standard computer algebra system, like, e.g., Maple, Mathematica or Form.

Step 1: Performing all momentum integrals

The distributions δ_V imply momentum correlations and can be integrated out trivially changing the momentum structure of the denominator functions $D_i = (-p_i^2 + m_i^2)$. To be able to perform the remaining D–momentum integrals analytically one has to form quadratic forms in the momenta p_i, which are successively integrable. A necessary step consists in performing the Wick-rotation of the one dimensional energy components $p_k^0 \to ip_k^0$ to obtain D-dimensional Euclidean integrals. Next, the n denominator factors $D_c^{l_c}$, which contain the momentum p_i, are combined introducing Feynman parameters via

$$\frac{1}{\prod_{c=1}^n D_c^{l_c}} = \frac{\Gamma(\sum_{k=1}^n l_k)}{\prod_{k=1}^n \Gamma(l_k)} \int_0^1 dx_1 \ldots \int_0^1 dx_n \delta\left(\sum_{k=1}^n x_k - 1\right) \frac{\prod_{k=1}^n x_k^{l_k-1}}{(x_1 D_1 + \ldots x_n D_n)^{\sum_{k=1}^n l_k}} \ . \tag{3}$$

Here $\Gamma(z)$ denotes the Euler Gamma-function. The momentum integral for p_i can now be carried out and the procedure is repeated until all momentum integrals are performed. As a result one is left with the Feynman parameter integrals over $x_i \in [0,1]$.

Step 2: From Feynman parameter integrals to Mellin–Barnes integrals and multinomial series.

Parts of these scalar integrals again can be performed trivially related to the δ-distributions $\delta\left(\sum_{k=1}^n x_k - 1\right)$,

$$\int_0^1 dx_l \delta\left(\sum_{k=1}^n x_k - 1\right) = \theta\left(1 - \sum_{k=1, k\neq l}^n x_k\right) \prod_{m=1, m\neq l}^n \theta(x_m), \tag{4}$$

$$\theta(z) = \begin{cases} 1, z \geq 0 \\ 0, z < 0. \end{cases} \tag{5}$$

There may be more integrals, which can be computed, usually as indefinite integrals, without special effort.

Mapping all Feynman-parameter integrals onto the m-dimensional unit cube one obtains the following structure :

$$\mathcal{I}(\varepsilon, N) = C(\varepsilon, N, M) \int_0^1 dy_1 \ldots \int_0^1 dy_m \frac{\sum_{i=1}^k \prod_{l=1}^{r_i} [P_{i,l}(y)]^{\alpha_{i,l}(\varepsilon,N)}}{[Q(y)]^{\beta(\varepsilon)}} \ , \tag{6}$$

with $k \in \mathbb{N}$, $r_1, \ldots, r_k \in \mathbb{N}$ and where $\beta(\varepsilon)$ is given by a rational function in ε, i.e., $\beta(\varepsilon) \in \mathbb{R}(\varepsilon)$, and similarly $\alpha_{i,l}(\varepsilon, N) = n_{i,l} N + \overline{\alpha}_{i,l}$ for some $n_{i,l} \in \{0, 1\}$ and $\overline{\alpha}_{i,l} \in \mathbb{R}(\varepsilon)$, see also Bogner and Weinzierl (2010) in the case no local operator insertions are present. $C(\varepsilon, N, M)$ is a factor, which depends on the dimensional parameter ε, the integer

parameter N and the mass M. $P_i(y), Q(y)$ are polynomials in the remaining Feynman parameters $y = (y_1, \ldots, y_m)$ written in multi-index notation. In (6) all terms which stem from local operator insertions were geometrically resummed; see Bierenbaum et al. (2009b).

Remark. **(1)** After splitting the integral (6) (in particular, the k summands), the resulting integrals fit into the input class of the multivariate Almkvist-Zeilberger algorithm, see Apagodu and Zeilberger (2006). Hence, if the splitted integrals are properly defined, the integrals obey homogeneous recurrence relations[2] in N due to the existence theorems in Apagodu and Zeilberger (2006). However, so far we failed to compute these recurrences due to time and space resources.

Remark. **(2)** Usually the calculation of $\mathcal{I}(\varepsilon, N)$ for fixed integer values of N is a simpler task. If a large enough number of these values is known, one may guess these recurrences and with this input derive closed forms for $\mathcal{I}(\varepsilon, N)$ using the techniques applied in Blümlein et al. (2009). This has been illustrated for a large class of 3-loop quantities. However, at present no method is known to calculate the amount of moments needed.

To compute the integrals (6) over the variables $y_1, \ldots, y_m$ we proceed as follows :

- decompose the denominator function using Mellin–Barnes integrals, see Paris and Kaminski (2001) and references therein,
- decompose the numerator functions, if needed, into multinomial series.

The y_i-integrals finally turn into Euler integrals. Here we line out a general framework, despite in practice, different algorithms are used in specific cases, cf. e.g. Ablinger et al. (2010a,b).

The denominator function is of the structure

$$[Q(y)]^{\beta(\varepsilon)} = \left[\sum_{k=1}^{n} q_k(y)\right]^{\beta(\varepsilon)} , \tag{7}$$

with $q_k(y) = a_1 \ldots a_m$ where $a_i \in \{1, y_i, 1 - y_i\}$ for $1 \leq i \leq m$. This function can be decomposed applying its Mellin-Barnes integral representation $(n-1)$ times,

$$\frac{1}{(A+B)^q} = \frac{1}{2\pi i} \int_{\gamma - i\infty}^{\gamma + i\infty} d\sigma \; A^\sigma \; B^{-q-\sigma} \frac{\Gamma(-\sigma)\Gamma(q+\sigma)}{\Gamma(q)} \; . \tag{8}$$

Here γ denotes the real part of the contour. Often Eq. (8) has to be considered in the sense of its analytic continuation, see Whittaker and Watson (1996).

The numerator factors $[P_{i,l}(y)]^{\alpha_{i,l}(\varepsilon,N)}$ obey

$$[P_{i,l}(y)]^{\alpha_{i,l}(\varepsilon,N)} = \left[\sum_{k=1}^{w} p_k(y)\right]^{\alpha_{i,l}(\varepsilon,N)} , \tag{9}$$

[2] Recursions of this type may be established and solved by various methods in specific cases, cf. Bierenbaum et al. (2007b).

where the monomials $p_k(y)$ have the same properties as $q_k(y)$. One expands

$$[P_{i,l}(y)]^{\alpha_{i,l}(\varepsilon,N)} = \sum_{k_1,\ldots,k_{w-1}\geq 0} \binom{\alpha_{i,l}(\varepsilon,N)}{k_1,\ldots,k_{w-1}} \prod_{l=1}^{w-1} p_l(y)^{k_l} p_w(y)^{\alpha_{i,l}(\varepsilon,N)-\sum_{r=1}^{w-1} k_r} . \quad (10)$$

Now all integrals over the variables y_j can be performed. They are of the type

$$\int_0^1 dy y^{\alpha-1}(1-y)^{\beta-1} = B(\alpha,\beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)} . \quad (11)$$

One obtains

$$\begin{aligned}\mathcal{I}(\varepsilon,N) = \frac{1}{(2\pi i)^n} \int_{\gamma_1-i\infty}^{\gamma_1+i\infty} d\sigma_1 \ldots \int_{\gamma_n-i\infty}^{\gamma_n+i\infty} d\sigma_n \\ \sum_{k_1=1}^{L(N)} \ldots \sum_{k_v=1}^{L(N,k_1,\ldots,k_{v-1})} \sum_{k=1}^{l} C_k(\varepsilon,N,M) \frac{\Gamma(z_{1,k})\ldots\Gamma(z_{u,k})}{\Gamma(z_{u+1,k})\ldots\Gamma(z_{v,k})}.\end{aligned} \quad (12)$$

Here $l \in \mathbb{N}$ and the summation over k_i comes from the multinomial sums, i.e., the upper bounds $L(N),\ldots,L(N,k_1,\ldots,k_{v-1})$ are integer linear in the depending parameters or ∞. Moreover, the $z_{u,k}$ are linear functions with rational coefficients in terms of the Mellin-Barnes integration variables $\sigma_1,\ldots,\sigma_n$, the summation variables $k_1,\ldots,k_v$, and ε.

Step 3: Representation in multi–sums:

The Mellin-Barnes integrals are carried out applying the residue theorem in Eq. (12). The following representation is obtained :

$$\mathcal{I}(\varepsilon,N) = \sum_{n_1=1}^{\infty} \ldots \sum_{n_r=1}^{\infty} \sum_{k_1=1}^{L(N)} \ldots \sum_{k_v=1}^{L(N,k_1,\ldots,k_{v-1})} \sum_{k=1}^{l} C_k(\varepsilon,N,M) \frac{\Gamma(t_{1,k})\ldots\Gamma(t_{v',k})}{\Gamma(t_{v'+1,k})\ldots\Gamma(z_{w',k})}. \quad (13)$$

Here the $t_{l,k}$ are linear functions with rational coefficients in terms of the $n_1,\ldots,n_r$, of the $k_1,\ldots,k_v$, and of ε. Note that the residue theorem may imply more than one infinite sum per Mellin-Barnes integral, i.e., $r \geq n$. In general, this approach leads to a highly nested multi-sum. Fixing the loop order of the Feynman integrals and restricting to certain special situations usually enables one to find sum representations with less summation quantifiers. E.g., as worked out in Bierenbaum et al. (2008), one can identify the underlying sums in terms of generalized hypergeometric functions, i.e., can reduce the number of infinite sums to one or in some cases to zero.

Step 4: Laurent series in ε:

Eq. (13) can now be expanded in the dimensional parameter ε using

$$\Gamma(n+1+\varepsilon) = \frac{\Gamma(n)\Gamma(1+\varepsilon)}{B(n,1+\varepsilon)} \quad (14)$$

and

$$B(n,1+\varepsilon) = \frac{1}{n} \exp\left(\sum_{k=1}^{\infty} \frac{(-\varepsilon)^k}{k} S_k(n)\right) = \frac{1}{n} \sum_{k=0}^{\infty} (-\varepsilon)^k \underbrace{S_{1,\ldots,1}}_{k}(n) \quad (15)$$

and other well-known transformations for the Γ-functions. The harmonic sums $S_{\vec{a}}(n)$ Blümlein and Kurth (1999); Vermaseren (1999) are recursively defined by

$$S_{b,\vec{a}}(N) = \sum_{k=1}^{N} \frac{(\mathrm{sign}(b))^k}{k^{|b|}} S_{\vec{a}}(k), \quad S_\emptyset = 1 \ . \tag{16}$$

In (14) n stands for a linear combination of summation quantifiers with coefficients in $\mathbb{Q}$. In case of non-integer weight factors r_i for n analytic continuations of harmonic sums have to be considered Blümlein (2000, 2009, 2011); Blümlein and Moch (2005).

Remark 1. In order to guarantee correctness of this construction, i.e., performing the expansion first on the summand level of (13) and afterwards applying the summation on the coefficients of the summand expansion (i.e., exchanging the differential operator D_ε and the summation quantifiers) analytic arguments have to be considered. For all our computations this construction was possible.

Usually $\mathcal{I}(\varepsilon, N)$ has the form

$$\mathcal{I}(\varepsilon, N) = \sum_{l=-L}^{\infty} \varepsilon^l I_l(N) \ , \tag{17}$$

with $L \geq 0$ the loop order in case of infra-red finite integrals. Otherwise, L may be larger. For physical reasons the contributions to different powers in ε have to be treated separately.

The general expression of the functions $I_l(N)$ in terms of nested sums are

$$I_l(N) = \sum_{n_1=1}^{\infty} ... \sum_{n_r=1}^{\infty} \sum_{k_1=1}^{L(N)} ... \sum_{k_v=1}^{L(N,k_1,...,k_{v-1})} \sum_{j=1}^{s} \times H_j(N; n_1, ..., n_r; , k_1, ..., k_v) \prod_i S_{\vec{a}_{i,j}}(L_{i,j}(N; n_1, ..., n_r; , k_1, ..., k_v)) \ , \tag{18}$$

where $H_j(N; n_1, ..., k_v)$ denote proper hypergeometric terms [3] and $S_{\vec{a}_{i,j}}(L_{i,j}(N; n_1, ..., k_v))$ are harmonic sums to the index set $\vec{a}_{i,j}$ and $L_{i,j}$ (usually linear) functions of the arguments $(N; n_1, ..., k_v)$. The sum-structure in (18) is usually obtained performing the synchronization of arguments, see Vermaseren (1999), and applying the associated quasi–shuffle algebra, see Blümlein (2004). Due to the infinite sums, frequently the limit of summation parameters k to infinity has to be performed for intermediary sums which results into Euler-Zagier or multiple zeta values, respectively, see Blümlein et al. (2010) and references therein. In more involved cases, e.g. for various different masses, also other special constants appear, see Broadhurst (1999) and references therein.

[3] For a precise definition of proper hypergeometric terms we refer, e.g., to Wegschaider (1997). For all our applications it suffices to know that H_j might be a product of Gamma-functions (occurring in the numerator and denominator) with linear dependence on the variables N, n_i, k_i times a rational function in these variables where the denominator factors linearly.

3. A first approach for the problem

In the following we limit the investigation to a sub-class of integrals of the type (1) and consider two- and simpler three-loop diagrams, which occurred in the calculation of the massive Wilson coefficients for deep-inelastic scattering in Ref. Ablinger et al. (2010b); Blümlein et al. (2006); Bierenbaum et al. (2007a, 2009a, 2008).

Looking at the reduction steps of the previous section we obtain the following result. If we succeed in finding the representation (17) with (18) it follows constructively that for each $N \in \mathbb{N}$ with $N \geq \lambda$ for some $\lambda \in \mathbb{N}$ the integral $\mathcal{I}(\varepsilon, N)$ has a Laurent expansion in ε and thus it is an analytic function in ε throughout an annular region centered by 0 where the pole at $\varepsilon = 0$ has order L. In Bierenbaum et al. (2008); Ablinger et al. (2010b) we started with the sum representation of the coefficients (18) and the main task was to simplify the expressions in terms of harmonic sums.

In this article, we follow a new approach that directly attacks the sum representation (13) and searches for the first coefficients of its ε-expansion (17). By splitting the sum (13) accordingly (and pulling out constants such as $C_k(\varepsilon, N, m)$) our integral can be written as a linear combination of hypergeometric multi-sums of the following form.

Assumption 1.

$$\mathcal{S}(\varepsilon, N) = \sum_{\sigma_1=p_1}^{\infty} \cdots \sum_{\sigma_s=p_s}^{\infty} \sum_{j_0=q_0}^{N+c} \sum_{j_1=q_1}^{B_1} \cdots \sum_{j_r=q_r}^{B_r} \mathcal{F}(N, \sigma, j, \varepsilon) \tag{19}$$

where

(1) $N \geq \lambda$ is a discrete variable, $\varepsilon > 0$ is a real parameter and $\lambda \in \mathbb{N}, c \in \mathbb{Z}$;
(2) 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 $1 \leq i \leq r$;
(3) 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;
(4) $\mathcal{F}$ is a proper hypergeometric term (see Footnote 3) with respect to the integer variable N and all summation variables from $(\sigma, j) \in \mathbb{Z}^{s+r+1}$.

Remark 2. While splitting the sum (13) into sums of the form (19) it might happen that the infinite sums over individual monomials diverge for fixed values of ε, despite the complete expression converges, i.e., one obtains a representation of the form (17) in an asymptotic expansion for large upper bounds of the summation variables $\sigma_1, \ldots, \sigma_s$. We will deal with these cases in Section 5 and consider only those sums which are convergent at the moment.

In other words, we assume that (19) itself is analytic in ε throughout an annular region centered by 0 and we try to find the first coefficients $F_t(N), F_{t+1}(N), \ldots, F_u(N)$ in terms of indefinite nested product-sum expressions of its expansion

$$\mathcal{S}(\varepsilon, N) = F_t(N) + F_{t+1}(N)\varepsilon + F_{t+2}(N)\varepsilon^2 + \ldots. \tag{20}$$

with $t \in \mathbb{Z}$. In all our computations it turns out that the summand $\mathcal{F}(N, \sigma, j, \varepsilon)$ satisfies besides properties (1)–(4) the following asymptotic behavior:

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

$$\mathcal{F}(N, \sigma, j, \varepsilon) = \mathcal{O}\left(\sigma_i^{-d_i} e^{-c_i \sigma_i}\right) \quad \text{as} \quad \sigma_i \to \infty \quad \text{with} \quad c_i \geq 0, \quad d_i > 0. \tag{21}$$

For later considerations in Section 4 we suppose that such constants c_i and d_i are given explicitly. E.g., using the behaviour (Whittaker and Watson, 1996, Section 13.6) of $\log\Gamma(z)$ for large $|z|$ in the region where $|\arg(z)| < \pi$ and $|\arg(z+a)| < \pi$:

$$\log\Gamma(z+a) = (z+a-\frac{1}{2})\log z - z + \mathcal{O}(1), \tag{22}$$

such constants can be easily computed. If not all $c_i > 0$ for $1 \leq i \leq s$, things get more complicated and –for simplicity– we restrict ourself to the case that $s = 1$ and $c_1 = 0$; we refer again to Section 5 for further details how one can treat the more general case.

(6) If $s = 1$ and $c_1 = 0$, we suppose that we are given a constant $e \in \mathbb{N}$ such that

$$\mathcal{S}(\varepsilon, N) = \sum_{\sigma_1=p_1}^{\infty} \sigma_1^e \mathcal{F}(N, \sigma, j, \varepsilon) \tag{23}$$

converges absolutely for any small nonzero ε around 0, $N \geq B$ and any j that runs over the summation range.

Using, e.g., hypergeometric function results from (Andrews et al., 1999, Thm. 2.1.1) such a maximal constant e can be determined.

The following sum is a typical entry from the list of sum representations for a class of Feynman parameter integrals we computed:

$$\begin{aligned}\mathcal{U}(\varepsilon, N) := (-1)^N \sum_{\sigma_1=0}^{\infty} \sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-j_0-3} \sum_{j_2=0}^{j_0+1} \binom{j_0+1}{j_2} \binom{N-j_0-3}{j_1} \\ \times \frac{\left(\frac{\varepsilon}{2}+1\right)_{\sigma_1} (-\varepsilon)_{\sigma_1} (j_1+j_2+3)_{\sigma_1} \left(3-\frac{\varepsilon}{2}\right)_{j_1}}{(j_1+4)_{\sigma_1} \left(-\frac{\varepsilon}{2}+j_1+j_2+4\right)_{\sigma_1} \left(4-\frac{\varepsilon}{2}\right)_{j_1+j_2}} \\ \times \frac{\Gamma(j_1+j_2+2)\Gamma(j_1+j_2+3)\Gamma(N-j_0-1)\Gamma(N-j_1-j_2-1)}{\Gamma(\sigma_1+1)\Gamma(j_1+4)\Gamma(N-j_0-2)};\end{aligned} \tag{24}$$

here $(x)_k = x(x+1)\ldots(x+k-1)$ denotes the Pochhammer symbol defined for non-negative integers k. Then using formulas such as $(x)_k = \Gamma(x+k)/\Gamma(x)$ and $\binom{x}{k} = \Gamma(x+1)/\Gamma(x-k+1)/\Gamma(k+1)$ and applying (22) we get the asymptotic behavior $\mathcal{O}(\sigma_1^{-5})$ of the summand. Moreover, we choose the maximal $e = 3$ such that condition (23) is satisfied.

Restricting the $\mathcal{O}$-notation to formal Laurent series $f = \sum_{i=r}^{\infty} f_i \varepsilon^i$ and $g = \sum_{i=s}^{\infty} g_i \varepsilon^i$ the notation

$$f = g + O(\varepsilon^t)$$

for some $t \in \mathbb{Z}$ means that the order of $f - g$ is larger or equal to t, i.e., $f - g = \sum_{i=t}^{\infty} h_i \varepsilon^i$. Subsequently, $\mathbb{K}$ denotes a field with $\mathbb{Q} \subseteq \mathbb{K}$ in which the usual operations can be computed.

3.1. Single nested sums

First, we look for single nested sums over proper hypergeometric terms, such as

$$\begin{aligned}\mathcal{S}(\varepsilon, N) &= \sum_{k=0}^{N-1} \frac{(-2)^k (k+2)\Gamma(4-\varepsilon)\Gamma\left(\frac{\varepsilon}{2}+3\right)\Gamma(N)\Gamma\left(-\frac{\varepsilon}{2}+k+2\right)}{\Gamma\left(2-\frac{\varepsilon}{2}\right)\Gamma(-\varepsilon+k+4)\Gamma\left(\frac{\varepsilon}{2}+k+3\right)\Gamma(N-k)} \\ &\stackrel{?}{=} F_0(N) + F_1(N)\varepsilon + F_2(N)\varepsilon^2 + O(\varepsilon^3);\end{aligned} \tag{25}$$

note that the existence of the coefficients follows by arguments given in Remark 1. In order to obtain the coefficients F_i, we compute in a first step a recurrence relation. This task can be accomplished for instance by the packages Paule and Schorn (1995), Wegschaider (1997) or Schneider (2007) which are based on the creative telescoping paradigm presented in Zeilberger (1990a) or the paradigm presented in Fasenmyer (1945). In our example it turns out that $\mathcal{S}(\varepsilon, N)$ satisfies for all $N \geq 1$ the recurrence

$$a_0(\varepsilon,N)\mathcal{S}(\varepsilon,N) + a_1(\varepsilon,N)\mathcal{S}(\varepsilon,N+1) + a_2(\varepsilon,N)\mathcal{S}(\varepsilon,N+2) \\ = -24N - 48 + (2N-20)\varepsilon + (2N+6)\varepsilon^2 + 2\varepsilon^3 \quad (26)$$

with

$$\begin{aligned} a_0(\varepsilon,N) &= 2N(N+1)(\varepsilon+2N+5), \\ a_1(\varepsilon,N) &= (N+1)\big(\varepsilon^2+2\varepsilon N+5\varepsilon+4N+12\big), \\ a_2(\varepsilon,N) &= (\varepsilon-N-4)(\varepsilon+2N+3)(\varepsilon+2N+6). \end{aligned} \quad (27)$$

Then together with the first two initial values $N = 1, 2$,

$$\mathcal{S}(\varepsilon,1) = 2 \qquad \text{and} \qquad \mathcal{S}(\varepsilon,2) = 2 + \frac{6}{\varepsilon+6} = 1 + \frac{1}{6}\varepsilon - \frac{1}{36}\varepsilon^2 + O(\varepsilon^3), \quad (28)$$

we use the following algorithm to compute, e.g., the first three coefficients of the series expansion (25).
Namely, by setting $\varepsilon = 0$ in (26), it follows that the constant term $F_0(N)$ satisfies the recurrence

$$a_0(0,N)F_0(N) + a_1(0,N)F_0(N+1) + a_2(0,N)F_0(N+2) = -24N - 48. \quad (29)$$

At this point we exploit algorithms from Petkovšek (1992); Abramov and Petkovšek (1994); Schneider (2001, 2005b) which can constructively decide if a solution with certain initial values is expressible in terms of indefinite nested products and sums [4] . To be more precise, with the algorithms implemented in the summation package `Sigma` one can solve the following problem.

Problem RS: **R**ecurrence **S**olver for indefinite nested product-sum expressions.
Given $a_0(N), \dots, a_d(N) \in \mathbb{K}[N]$; given $\mu \in \mathbb{N}$ such that $a_d(k) \neq 0$ for all $k \in \mathbb{N}$ with $N \geq \mu$; given an expression $h(N)$ in terms of indefinite nested product-sum expressions which can be evaluated for all $N \in \mathbb{N}$ with $N \geq \mu$; given the initial values $(c_\mu, \dots, c_{\mu+d-1})$ which produces the sequence $(c_i)_{i\geq\mu} \in \mathbb{K}^{\mathbb{N}}$ by the defining recurrence relation

$$a_0(N)c_N + a_1(N)c_{N+1} + \cdots + a_d(N)c_{N+d} = h(N) \quad \forall N \geq \mu.$$

Find, if possible, $\lambda \in \mathbb{N}$ with $\lambda \geq \mu$ and an indefinite nested product-sum expression $g(N)$ such that $g(k) = c_k$ for all $k \geq \lambda$.

Remark. Later, we will give further details only for a special case that occurred in almost all instances of our computations related to Feynman integrals; see Theorem 2.

[4] This means in particular indefinite nested sums over hypergeometric terms (like binomials, factorials, Pochhammer symbols) that may occur as polynomial expressions with the additional constraint that the summation index i_j of a sum $\sum_{i_j=1}^{i_{j+1}} f(i_j)$ may occur only as the upper index of its inner sums and products, but not inside of the inner sums itself; for a formal but lengthy definition see Schneider (2011). Typical examples are sums of the form (16), (39), or (40).

In our concrete example, Sigma finds that for all $N \geq 1$ we have

$$F_0(N) = \frac{3\big(2N^2+4N+1\big)}{2N(N+1)(N+2)} - \frac{3(-1)^N}{2N(N+1)(N+2)}. \tag{30}$$

Remark. The correctness follows from the following fact: The expression given in (30) is a solution of (29) for all $N \geq 1$ and has the same initial values as $F_0(N)$ for $N = 1, 2$.

Now, plugging in the partial solution

$$\mathcal{S}(\varepsilon, N) = \frac{3\big(2N^2+4N+1\big)}{2N(N+1)(N+2)} - \frac{3(-1)^N}{2N(N+1)(N+2)} + F_1(N)\varepsilon + \dots$$

into (26) gives

$$a_0(\varepsilon,N)(F_1(N)\varepsilon+\dots) + a_1(\varepsilon,N)(F_1(N+1)\varepsilon+\dots) + a_2(\varepsilon,N)(F_1(N+2)\varepsilon+\dots) = h(N)\varepsilon + O(\varepsilon^2)$$

with $h(N) = \frac{-10N^4-98N^3-344N^2-511N-267}{(N+2)(N+3)(N+4)} - \frac{3(-1)^N(3N+7)}{(N+2)(N+3)(N+4)}$. As a consequence, by coefficient comparison $F_1(N)$ is uniquely determined by

$$a_0(0,N)F_1(N) + a_1(0,N)F_1(N+1) + a_2(0,N)F_1(N+2) = h(N)$$

and the initial values given in (28). Solving the recurrence with these initial values, i.e., solving the corresponding problem RS, leads for all $N \geq 1$ to the sum representation

$$F_1(N) = \frac{10N^3+52N^2+63N+10}{8N(N+1)(N+2)^2} - \frac{3S_1(N)}{2N\ (N+2)} + \frac{3S_{-1}(N)}{2N(N+2)} + \frac{(-1)^N(N-10)}{8N(N+1)(N+2)^2}; \tag{31}$$

recall the definition (16). Repeating this procedure, one gets the quadratic term

$$\begin{aligned} F_2(N) = {} & \big(\tfrac{3}{4N(N+2)} - \tfrac{3(-1)^N}{4N(N+1)(N+2)}\big)S_{1,-1}(N) + \big(\tfrac{N^3-14N^2-43N-34}{8N(N+1)^2(N+2)^2} \\ & + \tfrac{3(-1)^N S_{-1}(N)}{4N(N+1)(N+2)}\big)S_1(N) + \tfrac{\big(-N^3+14N^2+43N+34\big)S_{-1}(N)}{8N(N+1)^2(N+2)^2} + \tfrac{3(-1)^N S_{-2}(N)}{4N(N+1)(N+2)} \\ & + \tfrac{3N^6+41N^5+206N^4+478N^3+541N^2+267N+30}{8N(N+1)^3(N+2)^3} - \tfrac{3S_1(N)^2}{8N(N+2)} - \tfrac{3(-1)^N S_{-1}(N)^2}{8N(N+1)(N+2)} \\ & + \big(\tfrac{-3}{8N(N+2)} - \tfrac{3(-1)^N}{8N(N+1)(N+2)}\big)S_2(N) + \tfrac{(-1)^N\big(7N^4+37N^3+47N^2-7N-30\big)}{8N(N+1)^3(N+2)^3} \end{aligned} \tag{32}$$

of the series expansion (25).

3.2. A recurrence solver for ε-expansions

Looking at the construction above (not necessarily assuming that the sequences can be represented in terms of indefinite nested product-sum expressions), we can extract the following consequences.

Lemma 1. Let $\mu \in \mathbb{N}$, and let $a_0(\varepsilon,N), \dots, a_d(\varepsilon,N) \in \mathbb{K}[\varepsilon,N]$ such that $a_d(0,k) \neq 0$ for all $k \in \mathbb{N}$ with $k \geq \mu$. Let $h_t, \dots, h_u : \mathbb{N} \to \mathbb{K}$ ($t, u \in \mathbb{Z}$ with $t \leq u$) be functions, and let $c_{i,k} \in \mathbb{K}$ with $t \leq i \leq u$ and $\mu \leq k < \mu + d$. Then there are unique functions $F_t, \dots, F_u : \mathbb{N} \to \mathbb{K}$ (up to the first μ evaluation points) such that $F_i(k) = c_{i,k}$ for all $t \leq i \leq u$ and $\mu \leq k < d + \mu$ and such that for $T(\varepsilon,N) = \sum_{i=t}^{u} F_i(N)\varepsilon^i$ we have

$$a_0(\varepsilon,N)T(\varepsilon,N) + \dots + a_d(\varepsilon,N)T(\varepsilon,N+d) = h_0(N) + \dots, +h_u(N)\varepsilon^u + O(\varepsilon^{u+1}) \tag{33}$$

for all $N \geq \mu$. If the $h_i(N)$ are computable, the values of the $F_i(N)$ with $N \geq \mu$ can be computed by recurrence relations.

Proof. Plugging in the ansatz $T(\varepsilon, N) = \sum_{i=t}^{u} F_i(N)\varepsilon^i$ into (33) and doing coefficient comparison w.r.t. ε^t yields the constraint

$$a_0(0,N)F_t(N) + \cdots + a_d(0,N)F_t(N+d) = h_t(N). \tag{34}$$

Since $a_d(0,N)$ is non-zero for any integer evaluation $N \geq \mu$, the function $F_0 : \mathbb{N} \to \mathbb{K}$ is uniquely determined with the initial values $F_t(\mu) = c_{t,\mu}, \ldots, F_t(\mu+d-1) = c_{t,\mu+d-1}$ – up to the first μ evaluation points; in particular the values $F_t(k)$ for $k \geq \mu$ can be computed by the recurrence relation (34). Moving the $F_t(N)\varepsilon^t$ in (33) to the right hand side gives $a_0(\varepsilon,N)\sum_{i=t+1}^{u} F_i(N)\varepsilon^i + \cdots + a_d(\varepsilon,N)\sum_{i=t+1}^{u} F_i(N+d)\varepsilon^i = -\Big[a_0(\varepsilon,N)h_t(N)\varepsilon^t + \cdots + a_d(\varepsilon,N)h_t(N+d)\varepsilon^t\Big] + \sum_{i=t}^{u} h_i(N)\varepsilon^i$; denote the coefficient of ε^i on the right side by $\tilde{h}_i$. Since the coefficient of ε^t on the left side is 0, it is also 0 on the right side and we can write

$$a_0(\varepsilon,N)\sum_{i=t+1}^{u} F_i(N)\varepsilon^i + \cdots + a_d(\varepsilon,N)\sum_{i=t+1}^{u} F_{i+1}(N+d)\varepsilon^i = \sum_{i=t+1}^{u} \tilde{h}_i(N)\varepsilon^i + O(\varepsilon^{u+1})$$

for all $N \in \mathbb{N}$ with $N \geq \mu$. Repeating this process proves the lemma. □

Moreover, using in addition the algorithms for problem RS we obtain the following constructive version.

Algorithm FLSR (**F**ormal **L**aurent **S**eries solutions of linear **R**ecurrences)
Input: $\mu \in \mathbb{N}$; $a_0(\varepsilon,N), \ldots, a_d(\varepsilon,N) \in \mathbb{K}[\varepsilon,N]$ such that $a_d(0,k) \neq 0$ for all $k \in \mathbb{N}$ with $k \geq \mu$; indefinite nested product-sum expressions $h_t(N), \ldots, h_u(N)$ ($t, u \in \mathbb{Z}$ with $t \leq u$) which can be evaluated for all $N \in \mathbb{N}$ with $N \geq \mu$; $c_{i,j} \in \mathbb{K}$ with $t \leq i \leq u$ and $\mu \leq j < \mu + d$
Output $(r, \lambda, \tilde{T}(N))$: The maximal number $r \in \{t-1, 0, \ldots, u\}$ such that for the unique solution $T(N) = \sum_{i=t}^{u} F_i(N)\varepsilon^i$ with $F_i(k) = c_{i,k}$ for all $\mu \leq k < \mu + d$ and with the relation (33) the following holds: there are indefinite nested product-sum expressions that compute the $F_t(N), \ldots, F_r(N)$ for all $N \geq \lambda$ for some $\lambda \geq \mu$; if $r \geq 0$, return such an expression $\tilde{T}(N)$ for $T(N)$ together with λ.

(1) (Preprocessing) By Lemma 1 we can compute as many initial values $c_{i,k} := F_i(k)$ for $k \geq \mu$ as needed for the steps given below (at most $\lambda - \mu$ extra values are needed).
(2) Set $r := t$, $\lambda := \mu$, and $\tilde{T}(N) := 0$.
(3) Note that the sequence $(F_r(N))_{N \geq \mu}$ is defined by the initial values $F_i(N)$ for $\lambda \leq N < d+\lambda$ and its defining relation

$$a_0(0,N)F_r(N) + \cdots + a_d(0,N)F_r(N+d) = h_r(N) \tag{35}$$

for all $N \in \mathbb{N}$ with $N \geq \lambda$; see the proofs of Lemma 1 or Theorem 1. By solving problem RS decide constructively if there is a $\lambda' \geq \lambda$ such that $F_r(N)$ can be computed in terms of an indefinite nested product-sum expression $\tilde{F}_r(N)$ for all $N \in \mathbb{N}$ with $N \geq \lambda'$.
(4) If this fails, RETURN $(r-1, \lambda, \tilde{T}(N))$. Otherwise, set $\tilde{T}(N) := \tilde{T}(N) + \tilde{F}_r(N)\varepsilon^r$.
(5) If $r = u$, RETURN $(r, \lambda, \tilde{T}(N))$.
(6) Collect the coefficients (product-sum expressions) w.r.t. ε^i for all i ($r+1 \leq i \leq u$):

$$h_i'(N) := \mathrm{coeff}(-\Big[a_0(\varepsilon,N)F_r(N) + \cdots + a_d(\varepsilon,N)F_r(N+d)\Big] + \sum_{i=r+1}^{u} h_i(N)\varepsilon^i, \varepsilon^i).$$

(7) Set $h_i := h_i'$ for all $r+1 \leq i \leq u$, set $r := r+1$ and GOTO Step 2.

Theorem 1. The algorithm terminates and fulfills the input–output specification.

Proof. We show that entering the rth loop ($r \geq t$) we have for all $N \geq \lambda$ that

$$a_0(\varepsilon, N) \sum_{i=r}^{u} F_i(N)\varepsilon^i + \cdots + a_d(\varepsilon, N) \sum_{i=r}^{u} F_i(N+d)\varepsilon^i = \sum_{i=r}^{u} h_i(N)\varepsilon^i + O(\varepsilon^{u+1}) \quad (36)$$

where the $h_r(N), \ldots, h_u(N)$ are given explicitly in terms of indefinite nested product-sum expressions. Moreover, we show that the found expression $\tilde{T}(N) = \sum_{i=t}^{r-1} \tilde{F}_i(N)\varepsilon^i$ computes the values $\sum_{i=t}^{r-1} F_i(N)\varepsilon^i$ for each $N \geq \lambda$. For $r = t$ this holds by assumption. Now suppose that these properties hold when entering the rth loop ($r \geq t$). Then coefficient comparison in (36) w.r.t. ε^r yields the constraint (35) for all $N \geq \lambda$ as claimed in Step 3 of the algorithm. Solving problem RS decides constructively if there is a $\lambda' \geq 0$ such that $F_r(N)$ can be computed by an expression in terms of indefinite nested product-sum expressions, say $\tilde{F}_r(N)$, for all N with $N \geq \lambda'$. If this fails, $F_r(N)$ cannot be represented with such an expression and the output $(r-1, \lambda, \tilde{T}(N))$ with $\tilde{T}(N) = \sum_{i=t}^{r-1} \tilde{F}_i(N)$ is correct. Otherwise, the indefinite nested product-sum expressions $\tilde{F}_i(N)$ for $t \leq i \leq r$ compute the values $F_i(N)$ for all $N \in \mathbb{N}$ with $N \geq \lambda'$. Now move the term $F_r(N)\varepsilon^r$ in (36) to the right hand side and replace it with $\tilde{F}_r(N)\varepsilon^r$. This gives

$$\begin{aligned} a_0(\varepsilon, N) \sum_{i=r+1}^{u} F_i(N)\varepsilon^i + \cdots + a_d(\varepsilon, N) \sum_{i=r+1}^{u} F_i(N+d)\varepsilon^i &= -\sum_{i=0}^{d} a_i(\varepsilon, N)\tilde{F}_r(N+i) \\ + \sum_{i=r}^{u} h_i(N)\varepsilon^i + O(\varepsilon^{u+1}) &=: \tilde{h}_{r+1}(N)\varepsilon^{r+1} + \cdots + \tilde{h}_u(N)\varepsilon^u + O(\varepsilon^{u+1}) \end{aligned}$$

for all $N \geq \lambda'$ where $\tilde{h}_{r+1}(N), \ldots, \tilde{h}_u(N)$ are given in terms of indefinite nested product-sum expressions that can be evaluated for all $N \in \mathbb{N}$ with $N \geq \lambda'$. By redefining the $h_i(N)$ as in Step 7 of the algorithm we obtain the relation (36) for the case $r+1$. □

Note that Algorithm FLSR has been implemented within the summation package `Sigma`. E.g., the expansion for the sum (25) with $s = 0$, $t = 2$ and `start` $= 1$ is computed by

```
GenerateExpansion[a0(ε,N)S[N] + a1(ε,N)S[N+1] + a2(ε,N)S[N+2],
                  {-24N - 48, 2N - 20, 2N + 6, 2}, S[N], {ε, s, t},
                    {start, {{2, 1, 4/5}, {0, 1/6, 19/150}, {0, -1/36, -119/18000}}}];
```

here the $a_i(\varepsilon, N)$ stand for the polynomials (27), $\{-24N-48, 2N-20, 2N+6, 2\}$ is the list of the first coefficients on the right hand side of (26), and `start` tells the procedure that the list of initial values $\{\{2, 1, 4/5\}, \{0, 1/6, 19/150\}, \{0, -1/36, -119/18000\}\}$ from (28) starts with $N = 1, 2, 3$.

The following application is immediate.

Corollary 1. For each nonnegative N, let $\mathcal{S}(\varepsilon, N)$ be a an analytic function in ε throughout an annular region centered by 0 with the Laurent expansion $\mathcal{S}(\varepsilon, N) = \sum_{i=t}^{\infty} f_i(N)\varepsilon^i$ for some $t \in \mathbb{Z}$, and suppose that $\mathcal{S}(\varepsilon, N)$ satisfies the recurrence (33) with coefficients and inhomogeneous part as stated in Algorithm FLSR for some $\mu \in \mathbb{N}$; define $c_{i,k} := F_i(k)$ for $t \leq i \leq u$ and $\mu \leq k < \mu + d$. Let $(r, \lambda, \sum_{i=t}^{r} F_i(N)\varepsilon^i)$ be the output of Algorithm FLSR. Then $f_i(k) = F_i(k)$ for all $t \leq i \leq r$ and all $k \in \mathbb{N}$ with $k \geq \lambda$.

For further considerations we restrict to the following important special case. Namely, we observed –to our surprise– in almost all examples arising from Feynman integrals that the operator

$$a_0(0,N) + a_1(0,N)S_N + \cdots + a_d(0,N)S_{N+d} \\ = c(N)(S_N - b_d(N))(S_N - b_{d-1}(N)) \dots (S_N - b_1(N)) \quad (37)$$

with the shift operator S_N factorizes completely for some $b_1, \dots, b_d, c \in \mathbb{K}(N)$; the rational functions can be computed by Petkovšek's algorithm Petkovšek (1992). In this particular instance we can construct immediately the complete solution space of

$$a_0(0,N)F(N) + \cdots + a_d(0,N)F(N+d) = X(N) \quad (38)$$

for a generic sequence $X(N)$. Namely, choose $\mu_i \in \mathbb{N}$ such that the numerator and denominator polynomial of $b_i(j)$ have no zeros for all evaluations $j \in \mathbb{N}$ with $j \geq \mu_i$, and take $\lambda := \max_{1 \leq i \leq d} \mu_i + 1$. Now define for $1 \leq i \leq d$ the hypergeometric terms $h_i(N) = \prod_{j=\lambda}^{N} b_i(j-1)$. Then by Abramov and Petkovšek (1994) one gets the d linearly independent solutions

$$H_1(N) := h_1(N), \quad H_2(N) := h_1(N) \sum_{i_1=\lambda}^{N-1} \frac{h_2(i_1)}{h_1(i_1+1)}, \dots, \\ H_d(N) := h_1(N) \sum_{i_1=\lambda}^{N-1} \frac{h_2(i_1)}{h_1(i_1+1)} \cdots \sum_{i_{d-1}=\lambda}^{i_{d-2}-1} \frac{h_d(i_{d-1})}{h_d(i_{d-1}+1)} \quad (39)$$

of the homogeneous version of (38), and the particular solution

$$P(N) := \frac{h_1(N)}{c(N)} \sum_{i_1=\lambda}^{N-1} \frac{h_2(i_1)}{h_1(i_1+1)} \cdots \sum_{i_{d-1}=\lambda}^{i_{d-2}-1} \frac{h_d(i_{d-1})}{h_{d-1}(i_{d-1}+1)} \sum_{i_d=\lambda}^{i_{d-1}-1} \frac{X(i_d)}{h_d(i_d+1)} \quad (40)$$

of (38) itself. In other words, the solution space of (38) is explicitly given by

$$\{c_1 H_1(N) + \cdots + c_d H_d(N) + P(N) | c_1 \dots, c_d \in \mathbb{K}\}; \quad (41)$$

here the nesting depth (counting the nested sums) of H_i is $i-1$ and of P is d.

Given this explicit solution space (41) we end up with the following result.

Theorem 2. Let $h_t(N), h_1(N), \dots$ with $t \in \mathbb{Z}$ be functions that are computable in terms of indefinite nested product-sum expressions where the nesting depth of the summation quantifiers of $h_i(N)$ is d_i; let $a_0(\varepsilon, N), \dots, a_d(\varepsilon, N) \in \mathbb{K}[\varepsilon, N]$ such that the operator factors as in (37) for some $b_1, \dots, b_d, c \in \mathbb{K}(N)$. If $\mathcal{S}(\varepsilon, N) = \sum_{i=t}^{\infty} F_i(N)\varepsilon^i$ is a solution of

$$a_0(\varepsilon, N)\mathcal{S}(\varepsilon, N) + \cdots + a_d(\varepsilon, N)\mathcal{S}(\varepsilon, N+d) = h_0(N) + h_1(N)\varepsilon^1 + \dots, \quad (42)$$

for some functions $F_i(N)$, then the values of $F_i(N)$ can be computed by indefinite nested product-sum expressions $\tilde{F}_i(N)$. The depth of the $\tilde{F}_i(N)$ is $\leq \max_{t \leq j \leq i}(d_j + (i-j+1)d))$.

Proof. Choose $\mu \in \mathbb{N}$ with $\mu \geq d$ such that $a_d(k) \neq 0$ for all integers $k \geq \mu$ and such that the sequences $h_i(k)$ can be computed for indefinite nested product-sum expressions for each $k \geq \mu$. Consider the rth loop of Algorithm FLSR. Since $F_r(N)$ is a solution of (38) with $X(N) = h_r(N)$ for all $N \geq \gamma$, $F_r(N)$ is a linear combination of (41). Taking the

first d initial values $F_r(\mu), \dots, F_r(\mu+d-1)$ the c_i are uniquely determined. Applying this construction inductively for each $r \in \mathbb{N}$ proves the theorem. The bound of the depth is immediate. $\square$

In particular, if the operator (35) factorizes as stated in (37), the following considerations of Algorithm FLSR are relevant.

Simplification 1. The factorization (37) needs to be computed only once and the solutions $F_i(N)$ can be obtained in terms of indefinite nested product-sum expressions by simply plugging in the results of the previous steps. E.g., for our running example, we get the generic solution

$$\frac{c_1}{N(N+2)} + c_2 \frac{\sum_{i_1=1}^{N} \frac{-(-1)^{i_1}(2i_1+1)}{i_1\left(i_1+1\right)}}{2N(N+2)} - \frac{\sum_{i_1=1}^{N} \frac{(-1)^{i_1}(2i_1+1)}{i_1\left(i_1+1\right)} \sum_{i_2=1}^{i_1} \frac{(-1)^{i_2} i_2^2 X\left(i_2-2\right)}{\left(2i_2-1\right)\left(2i_2+1\right)}}{2N(N+2)} \tag{43}$$

of the recurrence

$$a_0(0,N)F(N) + a_1(0,N)F(N+1) + a_2(0,N)F(N+2) = X(N)$$

where the coefficients are defined as in (27). In this way, one gets the solution $F_0(N)$ in terms of a double sum by setting $c_1 = c_2 = 0$ and $X(i_2) = -24i_2 + 48$ in (43), i.e.,

$$F_0(N) = \frac{-1}{2N(N+2)} \sum_{i_1=1}^{N} \frac{(-1)^{i_1}(1+2\ i_1)}{i_1(1+i_1)} \sum_{i_2=1}^{i_1} \frac{-(-1)^{i_2} 24 i_2^3}{\left(-1+2i_2\right)\left(1+2i_2\right)}. \tag{44}$$

One step further, one gets the solution $F_1(N)$ in terms of a quadruple sum by setting $c_1 = c_2 = 0$ and plugging in the double sum expression

$$X(i_2) = 2i_2 - 20 - \operatorname{coeff}(a_0(\varepsilon, i_2)F_0(i_2) + a_1(\varepsilon, i_2)F_0(i_2+1) + a_2(\varepsilon, i_2)F_0(i_2+2), \varepsilon)$$

into (43). Similarly, one obtains a sum expressions of $F_2(N)$ with nesting depth 6.

Minimizing the nesting depth. Given such highly nested sum expressions, the summation package `Sigma` finds alternative sum representations with minimal nesting depth. The underlying algorithms are based on a refined difference field theory worked out in Schneider (2008, 2011) that is adapted from Karr's $\Pi\Sigma$-fields originally introduced in Karr (1981). E.g., with this machinery, we simplify the double sum (44) to (30), and we reduce the quadruple sum expression for $F_1(N)$ and the 6–fold sum expression for $F_2(N)$ to expressions in terms of single sums (31) and double sums (32).

Simplification 2: The solutions (39) of the homogeneous version of the recurrence (38) can be pre-simplified to expressions with minimal nesting depth by the algorithms mentioned above. Moreover, using the algorithmic theory described in Kauers and Schneider (2006) the algorithms in Schneider (2008) can be carried over to the sum expressions like (40) involving an unspecified sequence $X(i_d)$. With this machinery, the generic solution (43) can be simplified to

$$\frac{c_1}{N(N+2)} + \frac{c_2(-1)^{N+1}}{2N(N+1)(N+2)} - \frac{\sum_{i_1=1}^{N} \frac{i_1 X\left(i_1-2\right)}{\left(2i_1-1\right)\ \left(2i_1+1\right)}}{2N(N+2)} - \frac{(-1)^N \sum_{i_1=1}^{N} \frac{(-1)^{i_1}\ i_1^2 X\left(i_1-2\right)}{\left(2i_1-1\right)\left(2i_1+1\right)}}{2N(N+1)\ (N+2)}.$$

Performing this extra simplification, the blow up of the nesting depth for the solutions $F_0(N), F_1(N), F_2(N), \ldots$ reduces considerably: instead of nesting depth $2, 4, 6, \ldots$ we get the nesting depths $1, 2, 3, \ldots$. In particular, given these representations the simplification to expressions with optimal nesting depth in Step 2 also speeds up.

For simplicity we restricted ourself to the situation that the $a_i(\varepsilon, N)$ are polynomials in ε. However, all arguments can be carried over immediately to the situation that the $a_i(\varepsilon, N)$ are formal power series where the first coefficients are given explicitly.
Moreover, our algorithm is applicable for more general sequences $a_i(N)$ and $h_i(N)$ whenever there are algorithms available that solve problem RS. E.g. if the coefficients $a_i(N)$ itself are expressible in terms of indefinite nested product-sum expression, problem RS can be solved by Abramov et al. (2011), and hence Algorithm FLSR is executable.

3.3. An effective method for multi-sums

For a multisum $\mathcal{S}(\varepsilon, N)$ with the properties (1)–(6) from Assumption 1 and with the assumption that it has a series expansion (20) for all $N \geq \lambda$ for some $\lambda \in \mathbb{N}$, the ideas of the previous section can be carried over as follows.

Step 1: Finding a recurrence. By WZ-theory (Wilf and Zeilberger, 1992, Cor. 3.3) and ideas given in (Wegschaider, 1997, Theorem 3.6) it is guaranteed that there is a recurrence

$$a_0(\varepsilon, N)\mathcal{S}(\varepsilon, N) + \cdots + a_d(\varepsilon, N)\mathcal{S}(\varepsilon, N + d) = 0 \tag{45}$$

for the multi-sum $\mathcal{S}(\varepsilon, N)$ in N that can be computed, e.g., by Wegschaider's algorithm; for infinite sums similar arguments have to be applied as in Step 2.2 of Section 4. Given such a recurrence, let $\mu \in \mathbb{N}$ with $\mu \geq \lambda$ s.t. $a_d(0, N) \neq 0$ for all $N \in \mathbb{N}$ with $N \geq \mu$.

Step 2: Determining initial values. If the sum (19) contains no infinite sums, i.e., $s = 0$, the initial values $F_i(k)$ in $\mathcal{S}(\varepsilon, k) = \sum_{i=t}^{\infty} F_i(k)\varepsilon^i$ for $k = \mu, \mu + 1, \ldots$ can be computed immediately and simplify usually to rational numbers. However, if infinite sums occur it is not so obvious to which values these infinite sums evaluate for our general input class– by assumption we only know that the $F_i(k)$ for a specific integer $k \geq \mu$ are real numbers. At this point we emphasize that our approach works independently to the fact whether we express these sums in terms of well known constants or if we just keep the symbolic form in terms of infinite sums. In a nutshell, if we do not know how to represent these values in a better way, we keep the sum representation. However, whenever possible it is desirable to write these values in terms of special numbers or functions. Examples are harmonic sums which are known as limits for the external index $N \to \infty$ for harmonic sums, see Blümlein and Kurth (1999); Vermaseren (1999), to yield Euler-Zagier and multiple zeta values, cf. Blümlein et al. (2010), and generalized harmonic sums, see Moch et al. (2002) which give special values of S-sums. In massive 2-loop computations and for the simpler 3-loop topologies these are the only known classes, whereas extensions are known in case of more massive lines, cf. e.g. Broadhurst (1999).

Step 3: Recurrence solving. Given such a recurrence (45) together with the initial values of $\mathcal{S}(\varepsilon, N)$ (hopefully in a nice closed form) we can activate Algorithm FLSR. Then by Corollary 1, we have a procedure that decides if the first coefficients of the expansion are expressible in terms of indefinite nested product-sum expressions.

Summarizing, we obtain the following theorem.

Theorem 3. Let $\mathcal{S}(\varepsilon, N)$ be a sum with Assumption 1 which forms an analytic function in ε throughout an annular region centered by 0 with the Laurent expansion $\mathcal{S}(\varepsilon, N) = \sum_{i=t}^{\infty} f_i(N)\varepsilon^i$ for some $t \in \mathbb{Z}$ for each nonnegative N; let $u \in \mathbb{N}$. Then there is an algorithm which finds the maximal $r \in \{t-1, 0, \ldots, u\}$ such that the $f_t(N), \ldots, f_r(N)$ are expressible in terms of indefinite nested product-sums; it outputs such expressions $F_t(N), \ldots, F_r(N)$ and $\lambda \in \mathbb{N}$ s.t. $f_i(k) = F_i(k)$ for all $0 \leq i \leq r$ and all $k \in \mathbb{N}$ with $k \geq \lambda$.

As mentioned already in the introduction, the proposed algorithm is not applicable for our examples arising form particle physics: forcing Wegschaider's implementation to find a homogeneous recurrence is extremely expensive and usually fails by the given computer and time resources. Subsequently, we relax this restriction and search for recurrence relations which are not necessarily homogeneous.

4. Find recurrence relations for multi-sums

Given a multi-sum $\mathcal{S}(N)$ of the form (19) we present a general method to compute a linear recurrence of $\mathcal{S}(N)$. Here the challenges are to deal with the infinite sums and struggling with the fact that the summand in almost all instances is not well defined outside the summation range. We proceed as follows using WZ–summation.

Step 1: Finding a summand recurrence. The summation problem (19) fits the input class of the algorithm Wegschaider (1997), an extension of multivariate WZ-summation due to Wilf and Zeilberger (1992). This allows us to compute a certificate recurrence for the hypergeometric summand $\mathcal{F}$.

Let us first recall that an expression $\mathcal{F}(N, \sigma, j, \varepsilon)$ is called hypergeometric in N, σ, j, if there are rational functions $r_{\nu,\mu,\eta}(N, \sigma, j, \varepsilon) \in \mathbb{K}(N, \sigma, j, \varepsilon)$ such that $\frac{\mathcal{F}(N,\sigma,j,\varepsilon)}{\mathcal{F}(N+\nu,\sigma+\mu,j+\eta,\varepsilon)} = r_{\nu,\mu,\eta}(N, \sigma, j, \varepsilon)$ at the points $(\nu, \mu, \eta) \in \mathbb{Z}^{r+s+2}$ where this ratio is defined. Then the Mathematica package `MultiSum` described in Wegschaider (1997) solves the following problem by coefficient comparison and solving the underlying system of linear equations.

Given a hypergeometric term $\mathcal{F}(N, \sigma, j, \varepsilon)$, a finite structure set $\mathbb{S} \subset \mathbb{N}^{s+r+2}$ and degree bounds $B \in \mathbb{N}$, $\beta \in \mathbb{N}^s$, $b \in \mathbb{N}^{r+1}$.
Find, if possible, a recurrence of the form

$$\sum_{(u,v,w)\in\mathbb{S}} c_{u,v,w}(N, \sigma, j, \varepsilon)\, \mathcal{F}(N+u, \sigma+v, j+w, \varepsilon) = 0 \tag{46}$$

with polynomial coefficients $c_{u,v,w} \in \mathbb{K}[N, \sigma, j]$, not all zero, where the degrees of the variables N, j_i and σ_i are bounded by B, β_i and b_i, respectively.

Remark 3. **(1)** In all our computations we found such a summand recurrence by setting the degree bounds to 1, i.e., $B = \beta_i = b_i = 1$.
(2) To determine a small structure set $\mathbb{S} \subseteq \mathbb{Z}^{s+r+2}$ which provides a solution w.r.t. our fixed degree bounds, A. Riese and B. Zimmermann enhanced the package `MultiSum` by modular computations. In this way one can loop through possible choices in a cheap fashion until one succeeds to find such a recurrence (46).

Next, the algorithm successively divides the polynomial recurrence operator (46) by

all forward-shift difference operators

$$\Delta_{\sigma_i}\mathcal{F}(N,\sigma,j,\varepsilon) := \mathcal{F}\left(N,\sigma_1,\ldots,\sigma_i+1,\ldots,\sigma_s,j,\varepsilon\right) - \mathcal{F}(N,\sigma,j,\varepsilon)$$

for $1 \le i \le s$, as well as, by similar Δ-operators defined for the variables from j which have finite summation bounds.

At last we obtain an operator free of shifts in the summation variables (σ, j) called the principal part of the recurrence (46) which equals the sum of all delta parts in the summation variables from (σ, j), i.e.,

$$\sum_{m\in\mathbb{S}'} a_m(\varepsilon,N)\mathcal{F}(N+m,\sigma,j,\varepsilon) = \sum_{l=0}^{r}\Delta_{j_l}\left(\sum_{(m,n)\in\mathbb{S}'_l} d_{m,n}(N,\sigma,j,\varepsilon)\mathcal{F}(N+m,\sigma,j+n,\varepsilon)\right)$$
$$+\sum_{i=1}^{s}\Delta_{\sigma_i}\left(\sum_{(m,k,n)\in\mathbb{S}_i} b_{m,k,n}(N,\sigma,j,\varepsilon)\mathcal{F}(N+m,\sigma+k,j+n,\varepsilon)\right) \tag{47}$$

where the coefficients a_m, not all zero, $b_{m,k,n}$ and $d_{m,n}$ are polynomials and the sets $\mathbb{S}' \subset \mathbb{N}$, $\mathbb{S}_i \subset \mathbb{N}^{s+r+2}$ and $\mathbb{S}'_l \subset \mathbb{N}^{r+2}$ are finite.

Recurrences of the form (47) satisfied by the hypergeometric summand are called certificate recurrences and have polynomial coefficients $a_m(\varepsilon, N)$ free of the summation variables from (σ, j), while the coefficients of the delta-parts are polynomials involving all variables.

Remark 4. In principle, the degrees of the polynomials $b_{m,k,n}$ and $d_{m,n}$ arising in (47) can be chosen arbitrarily large w.r.t. σ_i and j_i. However, in Step 2 we will sum (47) over the input range and hence we have to guarantee that the resulting sums over (47) are well defined. As a consequence, the degrees of the $d_{m,n}$ and $b_{m,k,n}$ w.r.t. the variables σ_i have to be chosen carefully if in (21) one of the constants c_i is zero. As mentioned earlier, for such cases we restrict ourself to the case that $s = 1$. In this instance, the degree in the $b_{m,k,n}$ should be smaller than the constant d_1 from (21) and the degree in the $d_{m,n}$ should be not bigger than the constant e from (23). To control this total bound $b := \min(d_1 - 1, e)$, we exploit the following observation (Wegschaider, 1997, p. 43): While transforming (46) to (47) by dividing through the operators (4), one only has to perform a simple sequence of additions of the occurring coefficients in (46), and thus the degrees w.r.t. the variables do not increase. Summarizing, if we choose β_1 in our ansatz such that $\beta_1 < b$, the degrees in the $b_{m,k,n}$ and $d_{m,n}$ w.r.t. the variable σ_1 are smaller than b.
In some rare instances it might happen that the principal part gets 0. It has been shown in (Wegschaider, 1997, Thm. 3.2) that this unlucky case can be cured by some extra operations where the degrees of some of the variables might increase. If within this construction the degree w.r.t. σ_1 increases too much, manual adjustment is needed (e.g., force the structure set to be different or change the degree bounds manually); however, within our computations we never entered in such a situation.

We illustrate all these mechanisms by a concrete example. The package `MultiSum` 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
```

For $N \geq 3$ a discrete parameter and $\varepsilon > 0$ we introduce the sum

$$\mathcal{S}(\varepsilon, N) := \sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-3-j_0} (-1)^{j_1}(j_1+1)\binom{N-2-j_0}{j_1+1} \frac{\Gamma(j_0+j_1+1)\left(1-\frac{\varepsilon}{2}\right)_{j_0}\left(3-\frac{\varepsilon}{2}\right)_{j_1}}{(4-\varepsilon)_{j_0+j_1}\left(\frac{\varepsilon}{2}+4\right)_{j_0+j_1}}. \tag{48}$$

As it was mentioned above, we apply WZ-summation techniques included in the Mathematica package `MultiSum` to compute a certificate recurrence for its summand

```
In[2]:= termS = (-1)^j1 (j1 + 1) Binomial[N - 2 - j0, j1 + 1] Gamma[j0 + j1 + 1] Pochhammer[1 - e/2, j0] Pochhammer[3 - e/2, j1] / ((4 - e)_(j0 + j1) Pochhammer[e/2 + 4, j0 + j1])
```

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

```
In[3]:= FindStructureSet[termS, N, {j0, j1}, 1];
In[4]:= strSetS = %[[1]]
Out[4]= {{0, 0, 1}, {0, 1, 0}, {0, 1, 1}, {1, 1, 0}, {1, 1, 1}}
```

(the input 1 sets all degree bounds to 1) and calling further the `MultiSum` procedure

```
In[5]:= FindRecurrence[termS, N, {j1, j0}, strSetS, 1, WZ -> True];
In[6]:= certRecS = ShiftRecurrence[%[[1]], {N, 1}, {j0, 1}, {j1, 1}]
Out[6]= (e - 2N)NF[N, j0, j1] - (e - N - 3)(e + 2N + 2)F[N + 1, j0, j1] == Δ_j0[(e^2 + j0 e + e - 2j1 -
        2j0 N - 4j1 N - 12N - 6)F[N + 1, j0, j1]] + Δ_j1[(e - 2N)(j0 + j1 - N + 1)F[N, j0, j1] + (-2N^2 +
        eN + 2j0 N + 4j1 N + 4N - 2e - e j0 + 2j1)F[N + 1, j0, j1]]
```

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

Step 2: A recurrence for the sum. Taking as input the certificate recurrences (47) we algorithmically find the inhomogeneous part of the recurrence satisfied by the sum (19) which will contain special instances of the original multisum of lower nesting depth.

The recurrence for the multisum (19) is obtained by summing the certificate recurrence (47) over all variables from (σ, j) in the given summation range $\mathcal{R} \subseteq \mathbb{Z}^{s+r+1}$. Since it can be easily checked whether the summand $\mathcal{F}$ indeed satisfies the relation (47), the certificate recurrence also provides an algorithmic proof of the recurrence for the multisum $\mathcal{S}(N, \varepsilon)$. In particular, since we set up the degrees of the coefficients in (47) w.r.t. the variables accordingly, see Remark 4, it follows that the resulting sums are analytically well defined.

To pass from the certificate recurrence to a homogeneous or inhomogeneous recurrences for the sum we use the telescoping property of the Δ-operators. The finite summation bounds appearing in (19) lead to an inhomogeneous right hand side after summing over the recurrence satisfied by the summand $\mathcal{F}$.

A method to set up the inhomogeneous recurrences for the summation problems (19) was introduced in (Stan, 2010, Chapter 3). In the next paragraphs we summarize the steps of this approach implemented in the package

```
In[7]:= << FSums.m
        A package for nested sums with nonstandard summation bounds by Flavia Stan – © RISC Linz
```

In this context, we use tuples to denote multi-dimensional intervals. The range represented by the tuple interval $[i \dots k]$ is the Cartesian product of the intervals defined by

the components $i, k \in \mathbb{Z}^n$. More precisely,

$$[i \dots k] := [i_1 \dots k_1] \times [i_2 \dots k_2] \times \cdots \times [i_n \dots k_n].$$

Often when working with nested sums, 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. We will use a variant of the cartesian product notation to denote such a summation range. Namely, to refer to a variable associated to a range, we will specify it as a subscript at the corresponding interval and use $\ltimes$ signs instead of the $\times$ symbols. For example, the range for the sum (24) can be written as

$$[0 \dots \infty] \times [0 \dots N-3]_{j_0} \ltimes [0 \dots N-j_0-3] \ltimes [0 \dots j_0+1].$$

We also introduce this notation for the initial range of the sum (19) as

$$\mathcal{R} := \mathcal{R}_\sigma \times \mathcal{R}_j \tag{49}$$

where $\mathcal{R}_\sigma := [p \dots \infty)$ and $\mathcal{R}_j = [q_0 \dots N+c] \ltimes [q_1 \dots B_1] \ltimes \cdots \ltimes [q_r \dots B_r]$, are the infinite and the finite range, respectively.

Step 2.1: Refining the input sum. As indicated earlier, we consider the summands from (19) as well-defined only inside the initial input range $\mathcal{R} \subseteq D_{\mathcal{F}}$ where $D_{\mathcal{F}}$ denotes the set of well-defined values for the proper hypergeometric function $\mathcal{F}$. This restriction adds to the complexity of the method from (Stan, 2010, Chapter 3) since we need to determine a possible smaller summation range over which we are allowed to sum the certificate recurrences (47).

We illustrate this phenomenon by our concrete example (48). Let us start by summing over the initial summation range

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

over the delta parts on the right hand side of the recurrence `certRecS` (see Out[6]) which is of the form (47). For this we denote the polynomial coefficients inside the delta parts Δ_{j_0} and Δ_{j_1} with $e[N, j_0, j_1, \varepsilon]$ and $d_1[N, j_0, j_1, \varepsilon]$, $d_2[N, j_0, j_1, \varepsilon]$, respectively.

By summing over the first term inside the Δ_{j_1}-part and using the telescoping property, we have

$$\sum_{j_0=0}^{N-3} \sum_{j_1=0}^{N-3-j_0} \Delta_{j_1}[d_1[N, j_0, j_1, \varepsilon] F[N, j_0, j_1]] = \sum_{j_0=0}^{N-3} (d_1[N, j_0, j_1, \varepsilon] F[N, j_0, j_1]) \Big|_{j_1=0}^{j_1=N-2-j_0}$$
$$= \sum_{j_0=0}^{N-3} d_1[N, j_0, N-2-j_0, \varepsilon] F[N, j_0, N-2-j_0] - \sum_{j_0=0}^{N-3} d_1[N, j_0, 0, \varepsilon] F[N, j_0, 0]$$

where we introduce the following short-hand notation

$$\sum_{k=0}^{l} \mathcal{F}(k, l) \Big|_{l=A}^{l=B} := \sum_{k=0}^{A} \mathcal{F}(k, A) - \sum_{k=0}^{B} \mathcal{F}(k, B).$$

We observe that, after telescoping, the upper bound $N-2-j_0$ for j_1 translates into a term outside the original summation range. To work under the assumption that our summand `termS` is well-defined only inside its range $\mathcal{R}$, we need to adjust the range over

which we sum the certificate recurrence or shift this relation with respect to the free parameter N. As discussed in (Stan, 2010, Chapter 3), the approach based on computing a smaller admissible summation range is more efficient since it leads to less new sums in the inhomogeneous parts of the recurrences.

In the case of our example $\mathcal{S}(\varepsilon, N)$, we consider the new range

$$\mathcal{R}' = [0 \dots N-4]_{j_0} \ltimes [0 \dots N-j_0-4].$$

As a consequence we compute separately a single sum which was called in (Stan, 2010, Chapter 3) a sore spot,

$$\mathcal{S}(\varepsilon, N) = \sum_{j_0=0}^{N-4} \sum_{j_1=0}^{N-4-j_0} F[N, j_0, j_1] + \sum_{j_0=0}^{N-3} F[N, j_0, N-j_0-3]. \tag{50}$$

In general, the package `FSums` contains an algorithm that determines the admissible summation range and computes the necessary sore spots for sums of the form (19); these extra sums with lower nesting depth have to be considered separately (see also the DIVIDE step in our method described in Section 5). Subsequently, we denote the sum over the restricted range $\mathcal{R}'$ by $\mathcal{S}'(\varepsilon, N)$.

Step 2.2: Determining the inhomogeneous part of the recurrence. Summing a certificate recurrence of the form (47) over the restricted range $\mathcal{R}'$ determined in the previous step, leads to a recurrence for a new sum $\mathcal{S}'(\varepsilon, N)$. The inhomogeneous part contains special instances of this sum of lower nesting depth. Next, we introduce the types of sums appearing on the right hand side.

Step 2.2.1: The finite summation bounds. Subsequently, we will illustrate these aspects with our running example (48). As deduced from Step 2.1, we continue from now on with the new sum

$$\mathcal{S}'(\varepsilon, N) = \sum_{j_0=0}^{N-4} \sum_{j_1=0}^{N-4-j_0} F[N, j_0, j_1]. \tag{51}$$

Shift compensating sums are a first 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` (see Out[6]) summing over the restricted range $\mathcal{R}'$, we obtain

$$\sum_{j_0=0}^{N-4} \sum_{j_1=0}^{N-4-j_0} F[N+1, j_0, j_1] = \mathcal{S}'(\varepsilon, N+1) - \sum_{j=0}^{N-3} F[N+1, j, N-3-j]. \tag{52}$$

Compensating sums of this form appear only in the case of upper summation bounds depending on the free variable N. 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. Including the new shifted sum as the first term of the output, the following procedure delivers the right hand side of (52)

In[8]:= **ShiftCompensatingSums[$F[N, j_0, j_1]$, {{j_0, 0, $N-4$}, {j_1, 0, $N-4-j_0$}}, N, 1]**

Out[8]= $\mathrm{SUM}[N+1] + \mathrm{FSum}[-F[1+N, j_0, -3-j_0+N], \{\{j_0, 0, -3+N\}\}]$.

Note that we use the structure `FSum` to store sums with nonstandard boundary conditions

of the form (19). 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 (19), starting with the infinite sums and ending with the sums with finite summation bounds in the order of their dependence.

When summing over the Δ-parts we generate two type of sums on the right side of the recurrence, the Δ-boundary sums and so-called telescoping compensating sums. For example when summing over the Δ_{j_0}-part of the recurrence `certRecS` of `Out[6]`, we have

$$\sum_{j_0=0}^{N-3}\sum_{j_1=0}^{N-3-j_0}\Delta_{j_0}[e[N,j_0,j_1,\varepsilon]F[N+1,j_0,j_1]] = \tag{53}$$
$$= \sum_{j_1=0}^{N-3-j_0}(e[N,j_0,j_1,\varepsilon]F[N+1,j_0,j_1])\Big|_{j_0=0}^{j_0=N-2}$$
$$+\sum_{j_0=1}^{N-2} e[N,j_0,N-2-j_0,\varepsilon]F[N+1,j_0,N-2-j_0].$$

Because of the structure of the summation bounds for the nested sums (19) we can use again our procedure `ShiftCompensatingSums` to generate the shift and the telescoping compensating sums. This connection becomes more clear, when we consider the more involved sum (24) (with its restricted range $N-4$ instead of its original range $N-3$) and apply, e.g., the Δ_{j_0}-operator:

$$\sum_{\sigma_0=0}^{\infty}\sum_{j_0=0}^{N-4}\sum_{j_1=0}^{N-j_0-4}\sum_{j_2=0}^{j_0}\Delta_{j_0}[F[N,\sigma_0,j_0,j_1,j_2]] = \sum_{\sigma_0=0}^{\infty}\sum_{j_1=0}^{N-j_0-4}\sum_{j_2=0}^{j_0}F[N,\sigma_0,j_0,j_1,j_2]\Big|_{j_0=0}^{j_0=N-3}$$
$$+\sum_{\sigma_0=0}^{\infty}\sum_{j_0=1}^{N-3}\sum_{j_2=0}^{j_0-1}F[N,\sigma_0,j_0,N-j_0-3,j_2] - \sum_{\sigma_0=0}^{\infty}\sum_{j_0=1}^{N-3}\sum_{j_1=0}^{N-j_0-4}F[N,\sigma_0,j_0,j_1,j_0];$$

note that the first element on the right side of this identity produces the Δ-boundary sums while the last two are due to telescoping compensation. More precisely, with the following function call

```
In[9]:= ShiftCompensatingSums[F[N, σ0, j0 - 1, j1, j2], {{σ0, 0, ∞}, {j1, 0, N - j0 - 4},
          {j2, 0, j0}}/.j0 → (j0 - 1), j0, 1]

Out[9]= {FSum[F[N, σ0, j0, j1, j2], {{σ0, 0, ∞}, {j1, 0, N - 4 - j0}, {j2, 0, j0}}], FSum[F[N, σ0, j0, N - 3 -
          j0, j2], {{σ0, 0, ∞}, {j2, 0, j0 - 1}}], FSum[-F[N, σ0, j0, j1, j0], {{σ0, 0, ∞}, {j1, 0, N - 4 - j0}}]}
```

we obtain exactly this result: the delta boundary sums are obtained by evaluating the first entry of the output for $j_0 = 0$ and $j_0 = N-3$ and the compensating sums result by adding the shifted sum $[1 \dots N-3]_{j_0}$ to the range of the other terms in the output.

Step 2.2.2: The infinite summation bounds. To sum over the delta parts in (47) coming from the summation variables σ_i, e.g., $\Delta_{\sigma_i} b_{m,k,n}(N,\sigma,j,\varepsilon)\mathcal{F}(N+m,\sigma+k,j+n,\varepsilon)$ we have to ensure that

$$\lim_{\sigma_i\to\infty} b_{m,k,n}(N,\sigma,j,\varepsilon)\mathcal{F}(N+m,\sigma+k,j+n,\varepsilon)$$

exists. Looking at the asymptotic conditions (21) of the input sum (19), there will be no problem if $c_i > 0$. However, if the constant c_i is zero, we need to verify that the degrees of the polynomial coefficients $b_{m,k,n}$ appearing in the respective Δ_{σ_i}-part are smaller then the bound β_i. As worked out in Remark 4 this property is guaranteed by our ansatz.

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 (19) after summing over corresponding certificate recurrences (47). A procedure to generate these inhomogeneous recurrences is implemented in the package `FSums`. E.g., the recurrence satisfied by the sum $\mathcal{S}'(\varepsilon, N)$, which we denote by simply SUM$[N]$, is returned by

In[10]:= **finalRecS = InhomogenRec[certRecS, {{j_0, 0, −4 + N}, {j_1, 0, −4 − j_0 + N}}, N]**

Out[10]=
$$
\begin{aligned}
&(\varepsilon - 2N)N\mathrm{SUM}[N] + (3 - \varepsilon + N)(2 + \varepsilon + 2N)\mathrm{SUM}[1 + N] == \\
&\quad \mathrm{FSum}[(1 + j_0 - N)(-\varepsilon + 2N)F[N, j_0, 0], \{\{j_0, 0, -4 + N\}\}] + \\
&\quad \mathrm{FSum}[-2(\varepsilon - 2N)F[N, j_0, -3 - j_0 + N], \{\{j_0, 0, -4 + N\}\}] + \\
&\quad \mathrm{FSum}[(\varepsilon - 2N)(2 + j_0 - N)F[1 + N, j_0, 0], \{\{j_0, 0, -4 + N\}\}] + \\
&\quad \mathrm{FSum}[(6 - \varepsilon - \varepsilon^2 + 2j_1 + 12N + 4j_1N)F[1 + N, 0, j_1], \{\{j_1, 0, -4 + N\}\}] + \\
&\quad \mathrm{FSum}[(3 - \varepsilon + N)(2 + \varepsilon + 2N)F[1 + N, j_0, -3 - j_0 + N], \{\{j_0, 0, -3 + N\}\}] + \\
&\quad \mathrm{FSum}[(\varepsilon + \varepsilon^2 + 2j_0 + \varepsilon j_0 - 2N + 2j_0N - 4N^2)F[1 + N, j_0, -3 - j_0 + N], \{\{j_0, 1, -3 + N\}\}] + \\
&\quad \mathrm{FSum}[-((6 + 2\varepsilon + 2j_0 + \varepsilon j_0 + 6N - \varepsilon N + 2j_0N - 2N^2)F[1 + N, j_0, -3 - j_0 + N]), \{\{j_0, 0, -4 + N\}\}].
\end{aligned}
$$

5. An efficient approach to find ε-expansions for multi-sums

Let $\mathcal{S}(\varepsilon, N)$ be a multisum of the form (19) with the properties (1)–(6) from Assumption 1 and assume that $\mathcal{S}(\varepsilon, N)$ has a series expansion (20) for all $N \geq \lambda$ for some $\lambda \in \mathbb{N}$. Combining the methods of the previous sections we obtain the following general method to compute the first coefficients, say $F_t(N), \ldots, F_u(N)$ of (20).

Divide and conquer strategy

(1) BASE CASE: If $\mathcal{S}(\varepsilon, N)$ has no summation quantifiers, compute the expansion by formulas such as (14) and (15).

(2) DIVIDE: As worked out in Section 4, compute a recurrence relation

$$a_0(\varepsilon, N)\mathcal{S}(\varepsilon, N) + \cdots + a_d(\varepsilon, N)\mathcal{S}(\varepsilon, N + d) = h(\varepsilon, N) \tag{54}$$

with polynomial coefficients $a_i(\varepsilon, N) \in \mathbb{K}[\varepsilon, N]$, $a_m(\varepsilon, N) \neq 0$ and the right side $h(\varepsilon, N)$ containing a linear combination of hypergeometric multisums each with less than $s + r + 1$ summation quantifiers. Note: In some instances, the sum has to be refined and some "sore spots" (again with less summation quantifiers) have to be treated separately by calling our method again; see Step 2.1 in Section 4.

(3) CONQUER: Apply the strategy recursively to the simpler sums in $h(\varepsilon, N)$. This results in an expansion of the form

$$h(\varepsilon, N) = h_t(N) + h_1(N)\varepsilon + \cdots + h_u(N)\varepsilon^u + O(\varepsilon^{u+1}); \tag{55}$$

if the method fails to find the $h_t(N), \ldots, h_u(N)$ in terms of indefinite nested product-sum expressions, STOP.

(4) COMBINE: Given (54) with[5] (55), compute, if possible, the $F_t(N), \ldots, F_u(N)$ of (20) in terms of nested product-sum expressions by executing Algorithm FLSR.

We illustrate our method with the double sum (48) where the summand is denoted by $F[N, j_0, j_1]$; internally we transform all the objects in terms of $\Gamma(x)$-functions in order to apply expansion formulas such as (14) and (15). First, we compute the summand recurrence given in Out[6]. While computing a recurrence for the sum itself, it turns out that we have to refine the summation range, i.e., our computation splits into two problems as given in (50). We continue with the refined double sum (51) and obtain the inhomogeneous recurrence `finalRecS` given in Out[10]. Now we apply recursively our method and compute successively expansions for each of the single sums on the right hand side; see also Section 3.1 for a typical example. Adding all the expansions termwise gives the recurrence

$$
\begin{aligned}
&(\varepsilon-2N)N\mathcal{S}'(\varepsilon,N)-(\varepsilon-N-3)(\varepsilon+2N+2)\mathcal{S}'(\varepsilon,N+1)=\\
&\quad\tfrac{18(2N^6-3N^5-8N^4+13N^3-4N+8)}{(N-2)(N-1)N(N+1)(N+2)}-\tfrac{36(2N^4+N^3-9N^2-2N+4)(-1)^N}{(N-2)(N-1)N(N+1)(N+2)}\\
&\quad+\varepsilon\left[\tfrac{3(N^8-6N^7-32N^6+20N^5+151N^4+14N^3-200N^2-28N+56)}{(N-2)(N-1)N(N+1)^2(N+2)^2}\right.\\
&\quad\left.+\tfrac{6(2N^6+N^5-14N^4+9N^3+40N^2-22N-28)(-1)^N}{(N-2)(N-1)N(N+1)^2(N+2)^2}+\frac{36S_1(N)}{N+1}\right]\\
&\quad+\varepsilon^2\left[\frac{9S_1(N)^2}{N+1}-\frac{6(N-5)S_1(N)}{(N+1)^2}-\tfrac{N^6(5N^3+48N^2+246N+568)}{4(N^2-3N+2)(N^2+3N+2)^3}\right.\\
&\quad+\tfrac{363N^6+3720N^5+3672N^4-5280N^3-10712N^2-4592N-128}{4N(N^2-3N+2)(N^2+3N+2)^3}\\
&\quad\left.+\left(\tfrac{9\left(N^4-N^3-4N^2+4N+8\right)}{(N-2)(N-1)N(N+1)(N+2)}-\tfrac{18\left(2N^4+N^3-9N^2-2N+4\right)(-1)^N}{(N-2)(N-1)N(N+1)(N+2)}\right)S_2(N)\right]+O(\varepsilon^3).
\end{aligned}
$$

Using in addition its first initial value $\mathcal{S}'(\varepsilon,4)=\frac{27}{16}-\frac{1}{128}\varepsilon-\frac{11}{1024}\varepsilon^2$ we are ready to activate Algorithm FLSR and get the result

$$
\begin{aligned}
\mathcal{S}'(\varepsilon,N)=&\frac{9(N^5-3N^4-3N^3+15N^2-6N-12)+36(N^2-3)(-1)^N}{2N(N^4-5N^2+4)}\\
&+\varepsilon\left[\frac{3(N^8-12N^7-46N^6+201N^4+276N^3-36N^2-336N-288)}{8N^2(N^2-3N+2)(N^2+3N+2)^2}\right.\\
&\left.-\frac{3(N^4-3N^3-10N^2+12N+30)(-1)^N}{N(N^2-3N+2)(N^2+3N+2)^2}+\frac{9(N+3)S_1(N)}{N(N^2+3N+2)}\right]\\
&+\varepsilon^2\left[\frac{9(N+3)S_1(N)^2}{4N(N^2+3N+2)}-\frac{3(5N^3+36N^2+37N-18)S_1(N)}{4N(N^2+3N+2)^2}\right.\\
&\left.+\frac{9\left(N^3-3N+4(N^2-3)(-1)^N-6\right)S_2(N)}{4N(N^4-5N^2+4)}\right.\\
&\left.-\frac{(49N^6+306N^5+472N^4-474N^3-1769N^2-1092N+132)(-1)^N}{4N(N^2-3N+2)(N^2+3N+2)^3}\right.\\
&\left.+\frac{3\left(335N^6+1586N^5+3972N^4+4584N^3+352N^2-3072N-1152\right)}{32N^3\left(N^2-3N+2\right)\left(N^2+3N+2\right)^3}\right]
\end{aligned}
$$

[5] See Step 2 of Section 3.3 how we deal with the initial values.

$$- \frac{N^4\left(5N^4+27N^3+176N^2+414N+185\right)}{32\left(N^2-3N+2\right)\left(N^2+3N+2\right)^3}\Bigg] + O(\varepsilon^3).$$

Finally, we compute our extra sum $\sum_{j_0=0}^{N-3} F[N, j_0, N-3-j_0]$ with our method, and adding this result to our previous computation leads to the final result

$$\begin{aligned}
&\mathcal{S}(\varepsilon, N) = \frac{81(N^2-3N+2)}{4N^2} \\
&+ \varepsilon\left[\frac{3(N^4-13N^3-28N^2-32N+24)}{8N^3(N+2)} + \frac{9(N+3)S_1(N)}{N(N+1)(N+2)}\right] \\
&+ \varepsilon^2\left[\frac{9(N+3)S_1(N)^2}{4N(N+1)(N+2)} - \frac{3(5N^3+36N^2+37N-18)S_1(N)}{4N(N+1)^2(N+2)^2} + \frac{9(N^2+3N+4)S_2(N)}{4N^2(N+1)(N+2)}\right. \\
&\left. - \frac{5N^6+17N^5+162N^4+208N^3+592N^2+240N-288}{32N^4(N+2)^2}\right] + O(\varepsilon^3).
\end{aligned}$$

Similarly, we compute, e.g., the first two coefficients of the expansion of the sum (24):

$$\begin{aligned}
\mathcal{U}(\varepsilon, N) = N!\Big(&\frac{3(-1)^N\left(N^2+2N-1\right)S_1(N)}{N(N+1)} - 9(-1)^N + \frac{6\ (-1)^N S_2(N)}{N}\Big) + \\
&\varepsilon\Big[\zeta(2)N!\Big(-\frac{3(-1)^N(4N+3)}{2N} - \frac{3(-1)^N(3N+2)\ S_{-1}(N)}{N} + \frac{9}{2N}\Big) \\
&+ N!\Big(\frac{3(-1)^N S_1(N)^2}{2\ (N+1)} + \frac{(-1)^N\left(2N^4+34N^3+101N^2+89N+2\right)S_1(N)}{2N(N+1)^2\ (N+2)} \\
&+ \frac{3(-1)^N\left(4N^2+14N+13\right)}{(N+1)(N+2)} + \frac{(-1)^N\ \left(-30N^2-38N+1\right)S_2(N)}{2N(N+1)} \\
&- \frac{9(-1)^N(2N+1)\ S_3(N)}{N} - \frac{6(-1)^N(3N+2)S_{-2}(N)S_{-1}(N)}{N} \\
&+ \frac{9\ S_{-2}(N)}{N} + 9(-1)^N S_{2,1}(N) + \frac{6(-1)^N(3N+2)\ S_{-2,-1}(N)}{N}\Big)\Big] + O(\varepsilon^2)
\end{aligned}$$

where $\zeta(2) = \sum_{i=1}^{\infty} \frac{1}{i^2} = \pi^2/6$.

In the following we give further comments on our proposed method and provide strategies how it can be used in the context to evaluate Feynman integrals.

Remark 5. 1. A heuristic. The conquer step turns our procedure to a method and not to an algorithm. Knowing that there is an expansion of $\mathcal{S}(\varepsilon, N)$ in terms of indefinite nested sums and products and plugging this solution into the left hand side of (54) shows that also the right hand side of (54) can be written in terms of indefinite nested product-sum expressions. But, in our method the right hand side is split into various sub-sums and it is not guaranteed that each sum in its own is expressible in terms of indefinite nested product-sum expressions – only the combination has this particular form. However, for the input class of multi-sums arising from Feynman-integrals this method always worked. 2. A hybrid version for speed ups. As it turned out, the bottleneck in our computations is the task to compute a recurrence of the form (54) with the `MultiSum`-package. To be more precise, in several instances we succeeded in finding a structure set S with the corresponding degree bounds for the polynomial coefficients, but we failed to determine the summand recurrence (46) explicitly, since the underlying linear system was to

large to solve. For such instances, we dropped, e.g., the outermost summation quantifier, say $\sum_{\sigma_1=p_1}^{\infty}$ and searched for a recurrence in σ_1; in particular the variable N was put in the base field $\mathbb{K}$. In this simpler form, we succeeded in finding a recurrence. Next, we computed the initial values (in terms of N) by using another round of our method. With this input, Algorithm FLSR found an expansion with coefficients in terms of $F_t(N,\sigma), F_{t+1}(N,\sigma), \dots, F_u(N,\sigma)$. To this end, we applied the infinite sum

$$\sum_{\sigma_1=p_1}^{\infty} F_i(\sigma, N) \tag{56}$$

to the coefficients $F_i(N,\sigma)$ and simplified these expressions further by the techniques described in Ablinger et al. (2010b). In various instances, it turned out that this hybrid technique was preferable than computing a pure recurrence in N or just simplifying the expressions (18) by using the methods given in Ablinger et al. (2010b).

3. Asymptotic expansions for infinite expressions. As mentioned in Remark 2 we obtained also sums of the form (19) which could be defined only by considering a truncated version of the infinite sums. For such instances we computed the coefficients $F_i(\sigma, N)$ as above and considered –instead of (56)– the expressions $\sum_{\sigma=0}^{a} F_i(\sigma, N)$ for large values a. To be more precise, we computed asymptotic expansions for all these sums and combined them to one asymptotic expansion in a. In this final form all the expressions canceled which were not defined when performing $a \to \infty$ and we ended up with the correct coefficient for the expansion of $\mathcal{S}(\varepsilon, N)$.

4. Dealing with several infinite sums. In all our computations we considered the situation that only one infinite sum arose. In principle, our method works also for more such sums. However, in order to set up the recurrence in Section 4, we need additional properties such as (23) for the multivariate case. If such properties are not available, we propose two strategies: 4.1 Drop some (or all) of the infinite sums and proceeds as explained in point 2 of our remark. 4.2 Set up the recurrence with formal sums and expand the sums on the right hand side: here one can either use the strategies as described in Step 4 of Section 2 (in particular, if asymptotic expansions have to be computed), or one can proceed with the method of this section whenever the sum is analytically well defined.

6. Conclusion

We presented a general framework that enables one to compute the first coefficients $F_i(N)$ of the corresponding Laurent expansion of a given Feynman parameter integral, whenever the $F_i(N)$ are expressible in terms of indefinite nested product-sum expressions. Namely, starting from such integrals, we described a symbolic approach to obtain a multi-sum representation over hypergeometric terms. Given this representation, we developed symbolic summation tools to extract these coefficients from its sum representation. In order to tackle this problem, Wegschaider's `MultiSum` package has been enhanced with Stan's package `FSum` that handles sums which do not satisfy finite support conditions. Moreover, given a recurrence relation of the form (42) together with initial values, Schneider's `Sigma` package has been extended to decide constructively, if the first coefficients of the formal Laurent series solution is expressible in terms of indefinite nested product-sum expressions.

In order to fit the input class of hypergeometric multi-sum packages, we split the sums

with the price of possible divergencies. We overcame this situation by combining our new methods with other tools described, e.g., in Ablinger et al. (2010b); see Remark 5. Further analysis of the introduced method should lead to a uniform approach that can handle in one stroke also solutions in terms of asymptotic expansions.

The described summation tools assisted in the task to compute two- and simpler three-loop diagrams, which occurred in the calculation of the massive Wilson coefficients for deep-inelastic scattering in Ref. Ablinger et al. (2010b); Blümlein et al. (2006); Bierenbaum et al. (2007a, 2009a, 2008).

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