

## The package HarmonicSums: Computer Algebra and Analytic aspects of Nested Sums

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This paper summarizes the essential functionality of the computer algebra package `HarmonicSums`. On the one hand `HarmonicSums` can work with nested sums such as harmonic sums and their generalizations and on the other hand it can treat iterated integrals of the Poincaré and Chen-type, such as harmonic polylogarithms and their generalizations. The interplay of these representations and the analytic aspects are illustrated by concrete examples.

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## 1. Introduction

This paper is dedicated to the presentation of the basic features of the computer algebra package `HarmonicSums` which was developed in [2] and [1] and which was afterwards extended and generalized. The package `HarmonicSums` was designed to support calculations with special nested objects arising in massive higher order perturbative calculations in renormalizable quantum field theories. On the one hand `HarmonicSums` can work with nested sums such as harmonic sums [15, 26] and their generalizations (S-sums [4, 22], cyclotomic harmonic sums [3], cyclotomic S-sums [1], binomial sums [5, 6, 7, 21, 27]) and on the other hand it can treat iterated integrals of the Poincaré and Chen-type, such as harmonic polylogarithms [23] and their generalizations (multiple polylogarithms [4], cyclotomic harmonic polylogarithms [3]). `HarmonicSums` provides functions to compute (generalizations of) the Mellin-transformation of these iterated integrals which leads to the nested sums and on the other hand inverse Mellin transforms of the nested sums can be computed. `HarmonicSums` offers commands that rewrite certain types of nested sums into expressions in terms of generalized S-sums and it can be used to derive algebraic and structural relations between the nested sums (compare [1, 2, 16, 17, 18, 19]) as well as relations between the values of the sums at infinity and connected to it the values of the iterated integrals evaluated at special constants (compare [1, 3, 4, 20]). In addition algorithms to compute series expansions (especially asymptotic expansions) of these nested objects are implemented. The package has already been used extensively, for example during the work on [10, 11, 12, 13, 14].

## 2. The package `HarmonicSums`

Note that this section contains a whole Mathematica session that runs throughout the sections. The inputs are given in the way how one has to type them into Mathematica and the outputs are displayed as Mathematica gives them back. We start the session by loading the package `HarmonicSums`:

```
In[1]:= << HarmonicSums.m
```

```
HarmonicSums by Jakob Ablinger -RISC Linz- Version 1.0 (15/05/04)
```

### Definition of the Nested Sums

In the package `HarmonicSums` harmonic sums, S-sums, cyclotomic harmonic sums and cyclotomic S-sums are denoted by the letter `S` as we can see in the following examples.

The command `ToHarmonicSumsSum` yields the definition of the sums.

```
In[2]:= {S[1, 2, 3, 4, n], S[1, 2, 3, {2, 1/3, 4}, n]}/ToHarmonicSumsSum
```

$$\text{Out[2]} = \left\{ \sum_{\tau_1=1}^n \frac{\sum_{\tau_2=1}^{\tau_1} \frac{\sum_{\tau_3=1}^{\tau_2} \frac{\sum_{\tau_4=1}^{\tau_3} \frac{1}{\tau_4}}{\tau_3}}{\tau_2}}{\tau_1}, \sum_{\tau_1=1}^n \frac{2^{\tau_1} \sum_{\tau_2=1}^{\tau_1} \frac{3^{-\tau_2} \sum_{\tau_3=1}^{\tau_2} \frac{4^{\tau_3}}{\tau_3}}{\tau_2}}{\tau_1} \right\}$$

```
In[3]:= {S[{{3, 2, 1}, {4, 1, 2}, {2, 0, -2}}, n], S[{{3, 2, 1}, {4, 1, 2}, {2, 0, 2}}, {2, 1/3, -4}, n]}/ToHarmonicSumsSum
```

$$\text{Out[3]} = \left\{ \sum_{\tau_1=1}^n \frac{\sum_{\tau_2=1}^{\tau_1} \frac{\sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3}}{4\tau_3^2}}{(1+4\tau_2)^2}}{2+3\tau_1}, \sum_{\tau_1=1}^n \frac{2^{\tau_1} \sum_{\tau_2=1}^{\tau_1} \frac{3^{-\tau_2} \sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3} 4^{-1+\tau_3}}{\tau_3^2}}{(1+4\tau_2)^2}}{2+3\tau_1} \right\}$$

Note that for internal reasons, sometimes the name CS is used to denote cyclotomic harmonic sums and cyclotomic S-sums.

`In[4]:= {CS[{{3, 2, 1}, {4, 1, 2}, {2, 0, -2}}, n], CS[{{3, 2, 1}, {4, 1, 2}, {2, 0, 2}}, {2, 1/3, -4}, n]}//ToHarmonicSumsSum`

$$\text{Out[4]} = \left\{ \sum_{\tau_1=1}^n \frac{\sum_{\tau_2=1}^{\tau_1} \frac{\sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3}}{4\tau_3^2}}{(1+4\tau_2)^2}}{2+3\tau_1}, \sum_{\tau_1=1}^n \frac{2^{\tau_1} \sum_{\tau_2=1}^{\tau_1} \frac{3^{-\tau_2} \sum_{\tau_3=1}^{\tau_2} \frac{(-1)^{\tau_3} 4^{-1+\tau_3}}{\tau_3^2}}{(1+4\tau_2)^2}}{2+3\tau_1} \right\}$$

In addition `HarmonicSums` can deal with binomial sums, which are denoted by BS:

`In[5]:= BS[{{2, 1, 3}, {1, 0, 1}}, {4, 3}, {{{2}, {1, 1}}, {{1, 1}, {2}}}, n]//ToHarmonicSumsSum`

$$\text{Out[5]} = \sum_{\tau_1=1}^n \frac{4^{\tau_1} (2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{3^{\tau_2} (\tau_2!)^2}{(2\tau_2)! \tau_2}}{(\tau_1!)^2 (1+2\tau_1)^3}$$

Hence a summand of the form  $\frac{x^{\tau_i}}{(a\tau_i+b)^c} \frac{(f_1 \tau_i)! \dots (f_j \tau_i)!}{(g_1 \tau_i)! \dots (g_k \tau_i)!}$  is represented by  $\{a, b, c\}$  in the first,  $x$  in the second and  $\{\{f_1, \dots, f_j\}, \{g_1, \dots, g_k\}\}$  in the third index set.

### Transformation to Nested Sums

Using the command `TransformToSSums` an extension [8] of the algorithm described in [1] is performed to rewrite nested sum expressions in terms of harmonic sums, S-sums, cyclotomic harmonic sums and cyclotomic S-sums.

`In[6]:= \sum_{i=1}^n \frac{2(5+2i) \sum_{j=1}^i \frac{1}{j^2}}{(2+3i+i^2)(12+7i+i^2)} //TransformToSSums`

$$\text{Out[6]} = \frac{1}{(n+1)(n+2)(n+3)(n+4)} \frac{1}{54} (-n(43n^3 + 394n^2 + 1163n + 1100) + 36(n+1)^2(n^2 + 8n + 15)S_2(n))$$

### Definition of the Nested Integrals

Harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms are denoted by the letter H as we can see in the following examples. The command `ToHarmonicSumsIntegrate` yields the definition of the nested integrals.

`In[7]:= {H[1,2,-3,4,x], H[{{3,1},{5,1},{2,0},x]}//ToHarmonicSumsIntegrate`

$$\text{Out[7]} = \left\{ \int_0^x \int_0^{\tau_1} \int_0^{\tau_2} \frac{\int_0^{\tau_3} \frac{1}{\tau_4-4} d\tau_4}{\tau_2-2} d\tau_3, \int_0^x \frac{\tau_1 \left( \int_0^{\tau_1} \frac{\tau_2 \left( \int_0^{\tau_2} \frac{1}{\tau_3+1} d\tau_3 \right)}{\tau_2^4 + \tau_2^3 + \tau_2^2 + \tau_2 + 1} d\tau_2 \right)}{\tau_1^2 + \tau_1 + 1} d\tau_1 \right\}$$

Note that an index  $a \in \mathbb{R}$  yields an iteration over  $\frac{1}{\text{sign}(a)\tau_i - a}$ , while an index  $\{l, k\}$   $l, k \in \mathbb{N}$  indicates an iteration over  $\frac{\tau_i^k}{\Phi_l(\tau_i)}$ , where  $\Phi_l$  is the  $l$ -th cyclotomic polynomial. For iterations over more general functions the name GL is reserved. The functions can then be defined using `VarGL`:

`In[8]:= GL[{\sqrt{1 - VarGL}, \frac{1}{VarGL+1}}, x]//ToHarmonicSumsIntegrate`

$$\text{Out[8]} = \int_0^x \left( \int_0^{\tau_1} \frac{1}{1 + \tau_2} d\tau_2 \right) \sqrt{1 - \tau_1} d\tau_1$$

### Shuffle and Quasi-Shuffle Product

The functions `LinearExpand` and `LinearHExpand` are provided to expand products of harmonic sum, S-sums, cyclotomic harmonic sums and cyclotomic S-sums and products of harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms, respectively.

`In[9]:= S[{{3, 2, 1}, {2, 0, -2}}, {1, 4}, n] S[{{3, 1, 1}}, {-3}, n]//LinearExpand`

$$\begin{aligned} \text{Out[9]} = & -S[{{3, 1, 1}, {2, 0, -2}}, \{-3, 4\}, n] + S[{{3, 2, 1}, {2, 0, -2}}, \{-3, 4\}, n] + \\ & S[{{3, 1, 1}, {3, 2, 1}, {2, 0, -2}}, \{-3, 1, 4\}, n] + S[{{3, 2, 1}, {2, 0, -2}, {3, 1, 1}}, \{1, 4, -3\}, n] + \\ & S[{{3, 2, 1}, {3, 1, 1}, {2, 0, -2}}, \{1, -3, 4\}, n] \end{aligned}$$

`In[10]:= H[1, 2, x] H[3, 4, x]//LinearHExpand`

$$\text{Out[10]} = H[1, 2, 3, 4, x] + H[1, 3, 2, 4, x] + H[1, 3, 4, 2, x] + H[3, 1, 2, 4, x] + H[3, 1, 4, 2, x] + H[3, 4, 1, 2, x]$$

### Differentiation of Nested Sums

In order to differentiate expressions involving harmonic sums, S-sums or cyclotomic harmonic sums the Mathematica function `D` is extended. Note that here we actually work with the analytic continuation of these sums; for details see e.g., [1, 4, 18, 19].

`In[11]:= D[S[3, 1, n] + n S[3, {2}, n] - S[{{2, 1, 1}}, n], n]`

$$\begin{aligned} \text{Out[11]} = & 1 + (1 + 2n)^{-2} - (3 + 2n)^{-2} + (1 + 2(1 + n))^{-2} + S[{{2, 1, 2}}, n] + H[\{0, 0\}, \{1, 0\}, 1] - \frac{S[2, n]}{4} \\ & + H[\{2, 0\}, \{0, 0\}, 1] + S[2, 2n] + S[2, \infty] S[3, n] - S[2, \infty] S[3, \infty] + 9 \frac{S[5, \infty]}{2} - S[3, 2, n] + S[3, \{2\}, n] - 3 S[4, 1, n] + \\ & n ((H[0, 0, 1] - H[0, 0, 2]) H[1, 0, 1] + (-H[0, 0, 1] + H[0, 0, 2]) H[1, 0, 1] - H[0, 0, 1, 0, 2] + H[0, 2] S[3, \{2\}, n] - \\ & 3 S[4, \{2\}, n]) \end{aligned}$$

### Basis Representations

For computing basis representations of harmonic sums, S-sums, cyclotomic harmonic sums, harmonic polylogarithms, cyclotomic polylogarithms or multiple polylogarithms `HarmonicSums` provides the functions `ComputeHSumBasis`, `ComputeSSumBasis`, `ComputeCSumBasis` and `ComputeHLogBasis` are provided.

- `ComputeHSumBasis[w, n]` computes a basis and the corresponding relations for harmonic sums at weight  $w$ . With the options `UseDifferentiation` and `UseHalfInteger` it can be specified whether relations due to differentiation and argument duplication should be used.
- `ComputeSSumBasis[w, x, n]` computes a basis and the corresponding relations for S-sums at weight  $w$  where the allowed “ $x$ ”-indices are defined in the list  $x$ . With the options `UseDifferentiation` and `UseHalfInteger` it can be specified whether relations due to differentiation and argument duplication should be used.
- `ComputeCSumBasis[w, let, n]` computes a basis and the corresponding relations for cyclotomic harmonic sums at weight  $w$  with letters  $let$ . With the options `UseDifferentiation`, `UseMultipleInteger` and `UseHalfInteger` it can be specified whether relations due to differentiation and argument multiplication should be used.
- `ComputeHLogBasis[w, n]` computes a basis and the corresponding relations for multiple polylogarithms at weight  $w$ . The option `Alphabet->a` and `IndexStructure->i` can be used to specify an alphabet or a special index structure respectively.

In[12]:= **ComputeCSumBasis[2, {{2, 1}}, n, UseDifferentiation -> False,  
UseMultipleInteger -> False, UseHalfInteger -> False**

$$\text{Out[12]= } \left\{ \begin{aligned} & \{S[\{\{2, 1, -2\}\}, n], S[\{\{2, 1, 2\}\}, n], S[\{\{2, 1, -1\}, \{2, 1, 1\}\}, n]\}, \\ & \{S[\{\{2, 1, 1\}, \{2, 1, 1\}\}, n] \rightarrow \frac{1}{2}S[\{\{2, 1, 1\}\}, n]^2 + \frac{1}{2}S[\{\{2, 1, 2\}\}, n], \\ & S[\{\{2, 1, 1\}, \{2, 1, -1\}\}, n] \rightarrow S[\{\{2, 1, -2\}\}, n] + S[\{\{2, 1, -1\}\}, n]S[\{\{2, 1, 1\}\}, n] \\ & - S[\{\{2, 1, -1\}, \{2, 1, 1\}\}, n], S[\{\{2, 1, -1\}, \{2, 1, -1\}\}, n] \rightarrow \frac{1}{2}S[\{\{2, 1, -1\}\}, n]^2 + \\ & \frac{1}{2}S[\{\{2, 1, 2\}\}, n] \} \end{aligned} \right.$$

In order to look for relations for harmonic sums, S-sums and cyclotomic harmonic sums at infinity we can use the functions `ComputeHSumInfBasis`, `ComputeSSumInfBasis` and `ComputeCSumInfBasis` while for looking for relations between multiple polylogarithms and cyclotomic polylogarithms at 1 the functions `ComputeGeneralizedH1Basis` and `ComputeCyclotomicH1Basis` are provided.

In[13]:= **ComputeCSumInfBasis[2, {{2, 1}}]**

$$\text{Out[13]= } \left\{ \begin{aligned} & \{S[\{\{2, 1, -2\}\}, \infty], S[\{\{2, 1, 2\}\}, \infty], S[\{\{2, 1, -1\}, \{2, 1, 1\}\}, \infty]\}, \\ & \{S[\{\{2, 1, 1\}, \{2, 1, 1\}\}, \infty] \rightarrow \frac{1}{2}S[\{\{2, 1, 1\}\}, \infty]^2 + \frac{1}{2}S[\{\{2, 1, 2\}\}, \infty], \\ & S[\{\{2, 1, 1\}, \{2, 1, -1\}\}, \infty] \rightarrow S[\{\{2, 1, -2\}\}, \infty] + S[\{\{2, 1, -1\}\}, \infty]S[\{\{2, 1, 1\}\}, \infty] \\ & - S[\{\{2, 1, -1\}, \{2, 1, 1\}\}, \infty], S[\{\{2, 1, -1\}, \{2, 1, -1\}\}, \infty] \rightarrow \frac{1}{2}S[\{\{2, 1, -1\}\}, \infty]^2 + \\ & \frac{1}{2}S[\{\{2, 1, 2\}\}, \infty] \} \end{aligned} \right.$$

For harmonic sums and cyclotomic harmonic sums tables with relations are provided [3, 9]. These tables can be applied using the command `ReduceToBasis`. With the options `UseDiff-`

erentiation and `UseHalfInteger` it is possible to specify whether relations due to differentiation and argument duplication should be used.

`ReduceToBasis[expr, n, Dynamic->True]` computes relations for harmonic sums, S-sums and cyclotomic harmonic sums in `expr` from scratch and applies them while `ReduceToBasis[expr, n, Dynamic->Automatic]` uses the precomputed tables and computes relations that exceed the tables from scratch.

`ReduceToHBasis` uses precomputed tables with relations between harmonic polylogarithms and applies them to expressions involving harmonic polylogarithms similar as for `ReduceToBasis` the options `Dynamic->Automatic/True` can be set.

`ReduceConstants` uses precomputed tables with relations between harmonic polylogarithms at argument 1 and harmonic sums at infinity to reduce the appearing constants as far as possible again the options `Dynamic->Automatic/True` can be set.

In[14]:= **ReduceToBasis[S[2, 1, n] + S[1, 2, n], n]**

Out[14]=  $S[1, n]S[2, n] + S[3, n]$

In[15]:= **ReduceToBasis[S[5, 5, {3, 3}, n], n, Dynamic -> True]**

Out[15]=  $\frac{1}{2} \left( S[5, \{3\}, n]^2 + S[10, \{9\}, n] \right)$

In[16]:= **ReduceToHBasis[H[1, 0, x] + H[0, 1, x]]**

Out[16]=  $H[0, x]H[1, x]$

In[17]:= **ReduceConstants[S[1,1,1,1,1,1,1,1, ∞] + 2 H[1, 0, 1] + H[0, 1, -1, 1], Dynamic -> Automatic]**

Out[17]= 
$$\begin{aligned} & \frac{5}{201600} \left( S[1, \infty]^8 + 140S[2, \infty]S[1, \infty]^6 + 560S[3, \infty]S[1, \infty]^5 + 1890S[2, \infty]^2S[1, \infty]^4 \right. \\ & + 1120(5S[2, \infty]S[3, \infty] + 6S[5, \infty])S[1, \infty]^3 + 20 \left( 549S[2, \infty]^3 + 280S[3, \infty]^2 \right) S[1, \infty]^2 \\ & + 720 \left( 21S[3, \infty]S[2, \infty]^2 + 28S[5, \infty]S[2, \infty] + 40S[7, \infty] \right) S[1, \infty] + 7893S[2, \infty]^4 \\ & \left. - 5600S[2, \infty] \left( -S[3, \infty]^2 + 54S[-1, \infty] + 72 \right) + 1680(8S[3, \infty](S[5, \infty] - 15) + 15S[8, \infty]) \right) \end{aligned}$$

## Series Expansions

The function `HarmonicSumsSeries[expr, {n, p, ord}]` can be used to compute series expansions about the point `n=p` of expressions `expr` involving harmonic sums, S-sums, cyclotomic harmonic sums, harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms up to a specified order `ord`.

In[18]:= **HarmonicSumsSeries[n\*S[2, n] + n\*H[-2, n], {n, 0, 4}] // ReduceConstants**

Out[18]=  $n^4 \left( 4z5 + \frac{1}{24} \right) + n^3 \left( -\frac{6z2^2}{5} - \frac{1}{8} \right) + n^2 \left( 2z3 + \frac{1}{2} \right)$

In[19]:= **HarmonicSumsSeries[n\*S[2, n] + n\*H[-2, n], {n, ∞, 4}] // ReduceConstants**

Out[19]=  $-n H[0, 2] + n H[0, n] - \frac{4}{n^3} + \frac{5}{2n^2} + n z2 - \frac{3}{2n} + 1$

In[20]:= **HarmonicSumsSeries[S[3, 1, {1/2, 1/3}, n], {n, ∞, 3}]**

$$\begin{aligned} \text{Out[20]}= & S\left[1, \left\{\frac{1}{3}\right\}, \infty\right] \left(-S\left[3, \left\{\frac{1}{6}\right\}, \infty\right] + S\left[3, \left\{\frac{1}{2}\right\}, \infty\right] + 6^{-n} \left(\frac{1}{5n^3} - \frac{3^n}{n^3}\right)\right) + \\ & 6^{-n} \left(\frac{12}{25n^3} - \frac{1}{5n^2}\right) S\left[2, \left\{\frac{1}{3}\right\}, \infty\right] + 6^{-n} \left(\frac{42}{125n^3} - \frac{6}{25n^2} + \frac{1}{5n}\right) S\left[3, \left\{\frac{1}{3}\right\}, \infty\right] + \\ & S\left[2, \left\{\frac{1}{6}\right\}, \infty\right] S\left[2, \left\{\frac{1}{3}\right\}, \infty\right] - S\left[1, \left\{\frac{1}{6}\right\}, \infty\right] S\left[3, \left\{\frac{1}{3}\right\}, \infty\right] - S\left[4, \left\{\frac{1}{3}\right\}, \infty\right] + S\left[1, 3, \left\{\frac{1}{6}, 2\right\}, \infty\right] + \\ & 6^{-n} \left(\frac{1}{5n^2} - \frac{12}{25n^3}\right) H[0, 3, 1] + 6^{-n} \left(-\frac{42}{125n^3} + \frac{6}{25n^2} - \frac{1}{5n}\right) H[0, 0, 3, 1] - \frac{H[3, 1] 6^{-n}}{5n^3} \end{aligned}$$

Note that  $z_2, z_3, \dots$  are used as abbreviations for  $S[2, \infty], S[3, \infty], \dots$  respectively. In order to compute asymptotic expansions of an S-sums  $S[a_1, a_2, \dots, \{x_1, x_2, \dots\}, n]$  with  $|x_i| > 1$  for at least one  $i$  the option `PrincipalValue -> True` has to be set:

In[21]:= **HarmonicSumsSeries[S[1, 1, {2, 1}, n], {n, ∞, 3}]**

$$\text{Out[21]}= S[1, 1, \{2, 1\}, n]$$

In[22]:= **HarmonicSumsSeries[S[1, 1, {2, 1}, n], {n, ∞, 3}, PrincipalValue->True]**

$$\text{Out[22]}= \frac{1}{2} \left( 2^n \left( -\frac{2}{n^2} - \frac{43}{3n^3} \right) - \frac{\pi^2}{2} + 2^n \left( \frac{4}{n} + \frac{4}{n^2} + \frac{12}{n^3} \right) \text{LG}[n] \right)$$

Note that the function `LG` is defined as  $\text{LG}[n] := \log(n) + \gamma$ , where  $\gamma$  is the Euler-Mascheroni constant. For computing asymptotic expansions of expressions of the form  $\int_0^1 x^n \text{GL}[a, x] dx$  for  $n \rightarrow \infty$  the command `GLExpansion` is provided:

In[23]:= **GLExpansion[GL[{\sqrt{1 + VarGL}}, x], x, n, ord]**

$$\text{Out[23]}= -\frac{2}{3n^5} + \frac{4225}{96\sqrt{2}n^5} + \frac{2}{3n^4} - \frac{469}{24\sqrt{2}n^4} - \frac{2}{3n^3} + \frac{55}{6\sqrt{2}n^3} + \frac{2}{3n^2} - \frac{7\sqrt{2}}{3n^2} - \frac{2}{3n} + \frac{4\sqrt{2}}{3n}$$

The function `HToS` can be used to compute the full power series expansions of harmonic polylogarithms, multiple polylogarithms and cyclotomic harmonic polylogarithms about 0. `SToSH` is used to perform the reverse direction.

In[24]:= **HToS[{H[-1, 0, -1, x], H[-3, 0, -1/2, x]}]**

$$\text{Out[24]}= \left\{ \sum_{l_1=1}^{\infty} \frac{S[2, l_1] (-x)^{l_1}}{l_1} - \sum_{l_1=1}^{\infty} \frac{(-x)^{l_1}}{l_1^3}, \sum_{l_1=1}^{\infty} \frac{3^{-l_1} (-x)^{l_1} S[2, \{6\}, l_1]}{l_1} - \sum_{l_1=1}^{\infty} \frac{2^{l_1} (-x)^{l_1}}{l_1^3} \right\}$$

In[25]:= **SToSH[{\sum\_{l\_1=1}^{\infty} \frac{(-x)^{l\_1} S[6, l\_1]}{l\_1}, \sum\_{l\_1=1}^{\infty} \frac{3^{-l\_1} (-x)^{l\_1} S[2, \{6\}, l\_1]}{l\_1}}]**

$$\text{Out[25]}= \left\{ H[-1, 0, -1, x] - H[0, 0, -1, x], H[-3, 0, -\frac{1}{2}, x] - H[0, 0, -\frac{1}{2}, x] \right\}$$

For the more general iterated integrals `GL` the command `GLToS` has to be used, note that this command internally relies on the recurrence solver of the package `Sigma` [24, 25].

In[26]:= **GLToS[GL[{\sqrt{4 - VarGL}\sqrt{VarGL}}, x]]**

$$\text{Out[26]} = \sum_{o_1=2}^{\infty} \frac{256x^{\frac{1}{2}(-1+2o_1)} \left(\prod_{t_1=1}^{o_1} \frac{-1+2t_1}{8t_1}\right) (-1+o_1)o_1}{(-5+2o_1)(-3+2o_1)(-1+2o_1)^2}$$

### Mellin Transformation and Inverse Mellin Transformation

To compute the Mellin transform of a possibly weighted harmonic polylogarithm, multiple polylogarithm (with indices in  $\mathbb{R} \setminus (-1, 1) \cup \{0\}$ ) and cyclotomic polylogarithm  $\text{hlog}[x]$  we can use the command `Mellin[hlog[x], x, n]`.

In[27]:= `Mellin[H[1, 0, x]/(1+x)+H[3,x]/(3-x), x, n]`

$$\text{Out[27]} = -2(-1)^n S[3, \infty] + (-1)^n S[-2, -1, \infty] + (-1)^n S[-1, -2, \infty] - (-1)^n S[-1, 2, n] + 3^n S[1, n] S[1, \{1/3\}, \infty] - 3^n S[1, \{1/3\}, n] S[1, \{1/3\}, \infty] - 3^n S[2, \{1/3\}, \infty] + 3^n S[1, 1, \{1/3, 1\}, \infty] - 3^n S[1, 1, \{1, 1/3\}, n]$$

For computing the Mellin transform of more general input `expr` the command `GeneralMellin[expr, x, n]` is provided. Note that this command internally relies on the recurrence solver of the package `Sigma`.

In[28]:= `GeneralMellin[InvMellGen[S[1, 2, {2, 1/2}, n] + S[1, n], n, x], n, x]`

$$\begin{aligned} \text{Out[28]} = & \frac{4(-1)^n \sqrt{2\pi} n!}{(2n+1)(2n+3)(2n+5)(n-\frac{1}{2})!} \text{BS}[\{\{1, 0, 0\}, \{-(1/4)\}, \{\{2\}, \{1, 1\}\}, n\} \\ & + \frac{2(3(-5+6\sqrt{2})+2(-8+13\sqrt{2})n+(-4+8\sqrt{2})n^2)}{3(n+1)(2n+3)(2n+5)} \\ & + \frac{(-1)^n \sqrt{\pi} n!}{(2n+1)(2n+3)(2n+5)(n-\frac{1}{2})!} (8\sqrt{2} - 15 \text{GL}[\{\{\text{VarGL}\sqrt{1+\text{VarGL}}\}, 1\}) \\ & + \frac{-(-1+3^{n+1})(n+1)\text{GL}[\{\{\frac{1}{3-\text{VarGL}}\}, 1\}] + 3^{n+1}(n+1)S_1(\frac{1}{3}, n) + 1}{(n+1)^2} \end{aligned}$$

To compute the inverse Mellin transform of a harmonic sum or a S-sum denoted by `sum` we can use the command `InvMellin[sum, n, x]`. For a definition of S-sum we refer to [1]. Note that  $\delta_{1-x}$  denotes the Dirac- $\delta$ -distribution  $\delta(1-x) \in \mathcal{D}'[0, 1]$ . For cyclotomic harmonic sums and S-sums which are not S-sums `InvMellin` yields an integral representations, where  $\text{Mellin}[a[x, n]] := \int_0^1 a(x, n) dx$  and  $\text{Mellin}[a[x, n], \{x, c, d\}] := \int_c^d a(x, n) dx$ .

In[29]:= `InvMellin[S[1, 2, n], n, x]`

$$\text{Out[29]} = \frac{H[1, 0, x]}{1-x}$$

In[30]:= `InvMellin[S[1, 2, {1, 1/3}, n], n, x]`

$$\begin{aligned} \text{Out[30]} = & \delta_{1-x} \left( -S[1, \{1/3\}, \infty] S[2, \{1/3\}, \infty] - 2S[3, \{1/3\}, \infty] + S[1, 2, \{1/3, 1\}, \infty] + \right. \\ & \left. S[2, 1, \{1/3, 1\}, \infty] \right) + \frac{3^{-n} S[2, \{1/3\}, \infty]}{3-x} - \frac{S[2, \{1/3\}, \infty]}{1-x} - \frac{3^{-n} H[3, 0, x]}{x-3} \end{aligned}$$

In[31]:= `InvMellin[S[\{3, 1, 2\}], n, n, x]`

$$\begin{aligned} \text{Out[31]} = & -\text{Mellin}\left[x^{3n} H[0, x]\right] - \frac{1}{3} \text{Mellin}\left[\frac{(x^{3n}-1)H[0, x]}{x-1}\right] + \frac{1}{3} \left( 2 \text{Mellin}\left[\frac{(x^{3n}-1)H[0, x]}{x^2+x+1}\right] + \right. \\ & \left. \text{Mellin}\left[\frac{x(x^{3n}-1)H[0, x]}{x^2+x+1}\right] \right) - 1 \end{aligned}$$



In order to compute an integral representation of an expression `expr` containing general S-sums together with harmonic sums and cyclotomic sums the command `InvMellGen[expr, n, x]` can be used:

In[32]:= `CollectMellinGen[InvMellGen[S[1, 2, {2, 1/2}, n] + S[1, n], n, x], n, x]`

Out[32]=  $\text{MellinGen}\left[-\frac{\text{H}[2, 0, 1](x^n - 1)}{x - 1}, \{x, 1, 2\}\right] + \text{MellinGen}\left[\frac{(x^n - 1)(1 - \text{H}[2, 0, x])}{x - 1}, \{x, 0, 1\}\right]$

Note that here we use the notation  $\text{MellinGen}[a[x, n], \{x, c, d\}] := \int_c^d a(x, n) dx$ .

### 3. Conclusion

In this paper we summarized some features of the computer algebra package `HarmonicSums`. Due to space limitations we had to restrict to the presentation of the main commands, while there are many more commands implemented. For more information we refer to [1, 2, 4]. The package together with several precomputed tables and a more detailed description can be downloaded at <http://www.risc.jku.at/research/combinat/software/HarmonicSums>.

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