Computer Algebra Algorithms for Special Functions in Particle Physics.

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joint work with
J. Blümlein (DESY) and C. Schneider (RISC)

7. Mai 2012

Definition (Harmonic Sums (H-Sums))

For $c_i \in \mathbb{Z}^*$ and $n \in \mathbb{N}$ we define

$$S_{c_1,\ldots,c_k}(n) = \sum_{n \geq i_1 \geq i_2 \geq \cdots \geq i_k \geq 1} \frac{\text{sign}(c_1)^{i_1}}{i_1^{|c_1|}} \cdots \frac{\text{sign}(c_k)^{i_k}}{i_k^{|c_k|}}$$

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Blümlein, Hoffman, Moch, Vermaseren, ...

Definition (S-Sums)

For $c_i \in \mathbb{N}$ and $x_i \in \mathbb{R}^*$ we define

$$\mathrm{S}_{c_1,\ldots,c_k}(x_1,\ldots,x_k;n) = \sum_{n \geq i_1 \geq i_2 \geq \cdots \geq i_k \geq 1} \frac{x_1^{i_1}}{i_1^{c_1}} \cdots \frac{x_k^{i_k}}{i_k^{c_k}}.$$

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Definition (Cyclotomic Harmonic Sums (C-Sums))

Let $a_i, k \in \mathbb{N}^*$, $b_i, n \in \mathbb{N}$ and $c_i \in \mathbb{Z}^*$ we define

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$$S_{(2,1,2),(3,2,1)}(4, 5, n) = \sum_{i=1}^{n} \frac{i^4 \sum_{j=1}^{i} \frac{j^5}{3j+2}}{(2i+1)^2}$$

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Connection between these nested sums

Harmonic Sums

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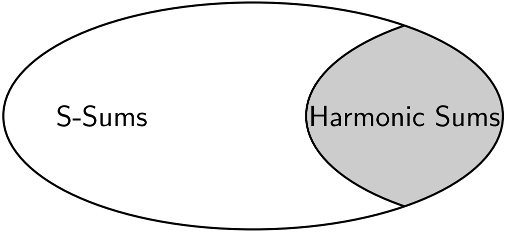

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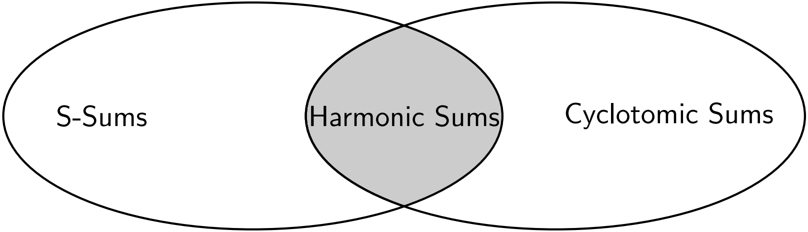

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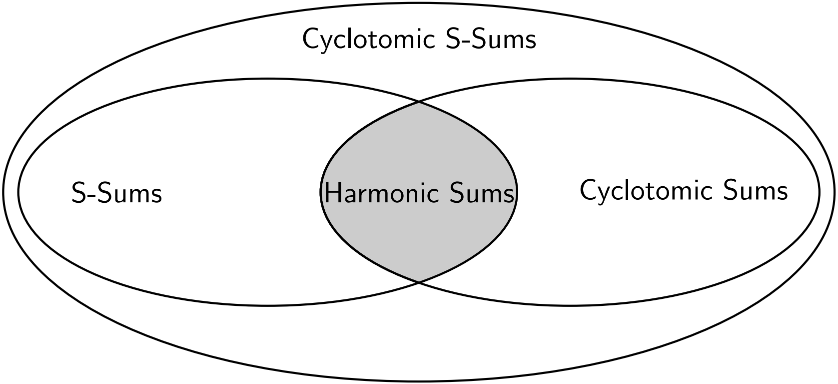
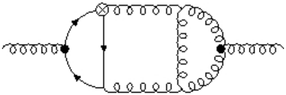


Example: All N-Results for 3–Loop Ladder Graphs

Joint work with J. Blümlein (DESY), C. Schneider (RISC)
A. Hasselhuhn (DESY), S. Klein (RWTH)

Consider, e.g., the diagram



(containing three massive fermion propagators)

$$\Downarrow$$

Around 1000 sums have to be calculated

A typical sum

$$\sum_{j=0}^{N-2}\sum_{s=1}^{j+1}\sum_{r=0}^{N+s-j-2}\sum_{\sigma=0}^{\infty}\frac{-2(-1)^{s+r}\binom{j+1}{s}\binom{-j+N+s-2}{r}(N-j)!(s-1)!\sigma!S_1(r+2)}{(N-r)(r+1)(r+2)(-j+N+\sigma+1)(-j+N+\sigma+2)(-j+N+s+\sigma)!}$$

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$$=\frac{\left(2N^2+6N+5\right)S_{-2}(N)^2}{2(N+1)(N+2)}+S_{-2,-1,2}(N)+S_{-2,1,-2}(N)$$

$$+\cdots-S_{2,1,1,1}(-1,2,\frac{1}{2},-1;N)+S_{2,1,1,1}(1,\frac{1}{2},1,2;N)$$

$$+\dots$$

mit, z.B.,

145 S–sums occur

$$S_{2,1,1,1}(1,\frac{1}{2},1,2;N)=\sum_{i=1}^{N}\frac{\sum_{j=1}^{i}\frac{\left(\frac{1}{2}\right)^j\sum_{k=1}^{j}\frac{\sum_{l=1}^{k}\frac{2^l}{l}}{k}}{j}}{i^2}$$

Algebraic Relations

Harmonic Sums, S-sums, cyclotomic harmonic sums und cyclotomic S-sums form a **quasi-shuffle algebra**.

There are relations of the form:

$$S_{1,1,2}(n) = \frac{1}{2}\left(2S_1(n)\left(S_3(n) - S_{2,1}(n)\right) - 2S_{3,1}(n) + 2S_{2,1,1}(n) + S_2(n)S_1(n)^2 + S_4(n)\right)$$

$$\begin{aligned}S_{a_1,a_1,a_2}(x_1,x_2,x_3;n) = {} & S_{a_2}(x_3;n)\,S_{a_1,a_1}(x_1,x_2;n) + S_{a_1,a_1+a_2}(x_1,x_2x_3;n)\\ & - S_{a_1}(x_1;n)\,S_{a_2,a_1}(x_3,x_2;n) - S_{a_2,2a_1}(x_3,x_1x_2;n) + S_{a_2,a_1,a_1}(x_3,x_2,x_1;n)\end{aligned}$$

$$\begin{aligned}S_{(2,1,2),(3,2,1),(2,1,2)}(n) = {} & -6S_{(2,1,1),(2,1,2)}(n) - 6S_{(2,1,2),(2,1,1)}(n) + S_{(3,2,1)}(n)S_{(2,1,2),(2,1,2)}(n)\\ & + 4S_{(2,1,2),(2,1,2)}(n) + 9S_{(2,1,2),(3,2,1)}(n) + 9S_{(3,2,1),(2,1,2)}(n) - S_{(2,1,2),(2,1,2),(3,2,1)}(n)\\ & - S_{(3,2,1),(2,1,2),(2,1,2)}(n),\end{aligned}$$

$$\begin{aligned}S_{(3,2,1),(2,1,2),(2,1,2)}(x_2,x_1,x_1;n) = {} & -6S_{(2,1,1),(2,1,2)}(x_1x_2,x_1;n) - 6S_{(2,1,2),(2,1,1)}(x_1,x_1x_2;n)\\ & + S_{(3,2,1)}(x_2;n)\,S_{(2,1,2),(2,1,2)}(x_1,x_1;n) + 2S_{(2,1,2),(2,1,2)}(x_1,x_1x_2;n)\\ & + 2S_{(2,1,2),(2,1,2)}(x_1x_2,x_1;n) + 9S_{(2,1,2),(3,2,1)}(x_1,x_1x_2;n) + 9S_{(3,2,1),(2,1,2)}(x_1x_2,x_1;n)\\ & - S_{(2,1,2),(2,1,2),(3,2,1)}(x_1,x_1,x_2;n) - S_{(2,1,2),(3,2,1),(2,1,2)}(x_1,x_2,x_1;n)\end{aligned}$$

Differential Relations

- integral representation

$$S_{1,2,1}\left(2,\frac{1}{2},1;n\right) = \int_0^1 \frac{1}{x_1-1}\int_1^{x_1}\frac{1}{x_2}\int_0^{x_2}\frac{1}{x_3-2}\int_2^{x_3}\frac{x_4^n-1}{x_4-1}dx_4dx_3dx_2dx_1$$

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- differentiation

$$\frac{\partial \mathrm{S}_{1,2,1}\left(2,\frac{1}{2},1;n\right)}{\partial n} = \int_0^1 \frac{1}{x_1-1}\int_1^{x_1}\frac{1}{x_2}\int_0^{x_2}\frac{1}{x_3-2}\int_2^{x_3}\frac{x_4^n\log(x_4)}{x_4-1}dx_4dx_3dx_2dx_1$$

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- integration of right hand side

$$\begin{aligned}\frac{\partial \mathrm{S}_{1,2,1}\left(2,\frac{1}{2},1;n\right)}{\partial n} = & -2\mathrm{H}_{0,0,1,2,1}(1)-4\mathrm{H}_{0,0,2,1,1}(1)-\mathrm{H}_{0,1,0,2,1}(1)-\mathrm{H}_{0,1,2,0,1}(1)-2\mathrm{H}_{0,2,0,1,1}(1)\\ & -\mathrm{H}_{0,2,1,0,1}(1)+(\mathrm{H}_2(1)(\mathrm{H}_{0,1,2}(1)+\mathrm{H}_{0,2,1}(1))+2\mathrm{H}_{0,0,1,2}(1)+2\mathrm{H}_{0,0,2,1}(1)\\ & +\mathrm{H}_{0,1,0,2}(1))\mathrm{S}_1(2;n)+\mathrm{S}_2(\infty)\left(\frac{3(\mathrm{H}_{0,1,2}(1)+\mathrm{H}_{0,2,1}(1))}{2}+\mathrm{S}_{1,2}\left(2,\frac{1}{2};n\right)\right)\\ & -\mathrm{H}_2(1)\mathrm{S}_{1,2,1}\left(2,\frac{1}{2},1;n\right)-\mathrm{S}_{-1}(\infty)\,\mathrm{S}_{1,2,1}\left(2,\frac{1}{2},1;n\right)-\mathrm{S}_{1,2,2}\left(2,\frac{1}{2},1;n\right)\\ & -2\mathrm{S}_{1,3,1}\left(2,\frac{1}{2},1;n\right)-\mathrm{S}_{2,2,1}\left(2,\frac{1}{2},1;n\right)\end{aligned}$$

Number of Basis Sums

Example (Harmonic sums)

w	Number of							
	N_S	N_A	N_D	N_H	N_{AD}	N_{AH}	N_{DH}	N_{ADH}
1	2	2	2	1	2	1	1	1
2	6	3	4	4	1	2	3	1
3	18	8	12	14	5	6	10	4
4	54	18	36	46	10	15	32	9
5	162	48	108	146	30	42	100	27
6	486	116	324	454	68	107	308	65
7	1458	312	972	1394	196	294	940	187
8	4374	810	2916	4246	498	780	2852	486

Number of Basis Sums

For $w \geq 2$ we have

$$
\begin{aligned}
N_S(w) &= 2 \cdot 3^{w-1} \\
N_A(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d \\
N_D(w) &= 4 \cdot 3^{w-2} \\
N_H(w) &= 2 \cdot 3^{w-1} - 2^{w-1} \\
N_{AD}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) 3^d - \frac{1}{w-1} \sum_{d|w-1} \mu\left(\frac{w-1}{d}\right) 3^d \\
N_{AH}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) \left[3^d - 2^d\right] \\
N_{DH}(w) &= 4 \cdot 3^{w-2} - 2^{w-2} \\
N_{ADH}(w) &= \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) \left[3^d - 2^d\right] - \frac{1}{w-1} \sum_{d|w-1} \mu\left(\frac{w-1}{d}\right) \left[3^d - 2^d\right]
\end{aligned}
$$

Number of Basis Sums

We consider

$$S_{(a_1,b_1,c_1),\ldots,(a_k,b_k,c_k)}(n)$$

with $a_i \in \{1,2\}$, $b_i \in \{0,1\}$, $a_i > b_i$ and $c_i \in \mathbb{Z}^*$.

Example (Cyclotomic harmonic sums)

w	N_S	N_A	N_D	N_{H_1}	$N_{H_1H_2}$	N_{H_1M}	$N_{H_1H_2M}$	N_{AD}	$N_{AH_1H_2M}$	$N_{DH_1H_2M}$	$N_{ADH_1H_2M}$
1	4	4	4	3	3	2	2	4	2	2	2
2	20	10	16	18	17	16	15	6	8	13	6
3	100	40	80	96	93	92	89	30	35	74	27
4	500	150	400	492	485	484	477	110	142	388	107
5	2500	624	2000	2484	2469	2468	2453	474	607	1976	465

Number of Basis Sums

$$
\begin{aligned}
N_S(w) &= 4\cdot 5^{w-1}\\
N_A(w) &\overset{w\geq 1}{=} \frac{1}{w}\sum_{d|w}\mu\left(\frac{w}{d}\right)5^d\\
N_D(w) &= N_S(w)-N_S(w-1)\overset{w\geq 1}{=}16\cdot 5^{w-2}\\
N_{H_1}(w)=N_{H_2}(w)=N_M(w) &= N_S(w)-2^{w-1}=4\cdot 5^{w-1}-2^{w-1}\\
N_{H_1H_2}(w) &= N_S(w)-(2\cdot 2^{w-1}-1)=4\cdot 5^{w-1}-(2\cdot 2^{w-1}-1)\\
N_{H_1M}(w)=N_{H_2M}(w) &= N_S(w)-2\cdot 2^{w-1}=4\cdot 5^{w-1}-2\cdot 2^{w-1}\\
N_{H_1H_2M}(w) &= N_S(w)-(3\cdot 2^{w-1}-1)=4\cdot 5^{w-1}-(3\cdot 2^{w-1}-1)\\
N_{AD}(w) &= N_A(w)-N_A(w-1)\\
&\overset{w\geq 2}{=} \frac{1}{w}\sum_{d|w}\mu\left(\frac{w}{d}\right)5^d-\frac{1}{w-1}\sum_{d|(w-1)}\mu\left(\frac{w-1}{d}\right)5^d\\
N_{AH_1H_2M}(w) &\overset{w\geq 1}{=} \frac{1}{w}\sum_{d|w}\mu\left(\frac{w}{d}\right)5^d-\left(3\cdot\frac{1}{w}\sum_{d|w}\mu\left(\frac{w}{d}\right)2^d-1\right)\\
N_{DH_1H_2M}(w) &= N_{H_1H_2M}(w)-N_{H_1H_2M}(w-1)\\
&\overset{w\geq 1}{=} 16\cdot 5^{w-2}-3\cdot 2^{w-2}\\
N_{ADH_1H_2M}(w) &= N_{AH_1H_2M}(w)-N_{AH_1H_2M}(w-1)\\
&\overset{w\geq 2}{=} \frac{1}{w}\sum_{d|w}\mu\left(\frac{w}{d}\right)(5^d-3\cdot 2^d)\\
&\quad -\frac{1}{w-1}\sum_{d|(w-1)}\mu\left(\frac{w-1}{d}\right)(5^d-3\cdot 2^d)
\end{aligned}
$$

Number of Basis Sums

We consider

$$S_{a_1,\ldots,a_k}(x_1,\ldots,x_k;n)$$

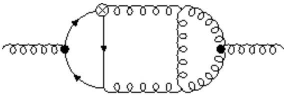
with $x_i \in \{1,-1,1/2,-1/2,2,-2\}$.

Example (S-Sums)

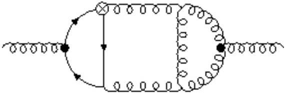
Each of the indices $\{1/2,-1/2,2,-2\}$ is allowed to appear just once in each sum.

Weight	Number of			
	N_S	N_A	N_D	N_{AD}
1	6	6	6	6
2	38	23	32	17
3	222	120	184	97
4	1206	654	984	543
5	6150	3536	4944	2882
6	29718	18280	23568	14744

Example: continued



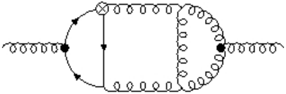
Example: continued



$$\Downarrow$$

C. Schneider's Sigma.m

Around 1000 sums are calculated containing in total 533 S–sums



$$\Downarrow$$ C. Schneider's Sigma.m

Around 1000 sums are calculated containing in total 533 S–sums

$$\Downarrow$$ HarmonicSums.m

After elimination the following sums remain:

$$S_{-4}(N), S_{-3}(N), S_{-2}(N), S_1(N), S_2(N), S_3(N), S_4(N), S_{-3,1}(N),$$
$$S_{-2,1}(N), S_{2,-2}(N), S_{2,1}(N), S_{3,1}(N), S_{-2,1,1}(N), S_{2,1,1}(N)$$

Harmonic Polylogarithms (H-Logs)

We define $f : \{0, 1, -1\} \times (0, 1) \mapsto \mathbb{R}$ by

$$\begin{aligned} f(0,x) &= \frac{1}{x}, \\ f(1,x) &= \frac{1}{1-x}, \\ f(-1,x) &= \frac{1}{1+x}. \end{aligned}$$

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Definition (Harmonic Polylogarithms (H-Logs))

Let $m_i \in \{-1, 0, 1\}$ we define for $x \in (0, 1)$:

$$\begin{aligned} \mathrm{H}(x) &= 1, \\ \mathrm{H}_{m_1,m_2,\ldots,m_k}(x) &= \begin{cases} \frac{1}{k!}(\log x)^k, & \text{if } (m_1,\ldots,m_k) = \mathbf{0} \\ \int_0^x f_{m_1}(y)\mathrm{H}_{m_2,\ldots,m_k}(y)dy, & \text{otherwise.} \end{cases} \end{aligned}$$

Multiple Polylogarithms (M-Logs)

Let $a \in \mathbb{R}$ and

$$q = \begin{cases} a, & \text{if } a > 0 \\ \infty, & \text{otherwise} \end{cases}$$

We define f as follows:

$$f_a : (0, q) \mapsto \mathbb{R}$$
$$f_a(x) = \begin{cases} \frac{1}{x}, & \text{if } a = 0 \\ \frac{1}{|a| - \text{sign}(a)\, x}, & \text{otherwise.} \end{cases}$$

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Let $m_i \in \mathbb{R}$ and let $q = \min_{m_i > 0} m_i$ we define for $x \in (0, q)$:

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The first cyclotomic polynomials are given by

$$\begin{aligned}
\Phi_1(x) &= x-1\\
\Phi_2(x) &= x+1\\
\Phi_3(x) &= x^2+x+1\\
\Phi_4(x) &= x^2+1\\
\Phi_5(x) &= x^4+x^3+x^2+x+1\\
\Phi_6(x) &= x^2-x+1\\
\Phi_7(x) &= x^6+x^5+x^4+x^3+x^2+x+1\\
\Phi_8(x) &= x^4+1\\
\Phi_9(x) &= x^6+x^3+1\\
\Phi_{10}(x) &= x^4-x^3+x^2-x+1\\
\Phi_{11}(x) &= x^{10}+x^9+x^8+x^7+x^6+x^5+x^4+x^3+x^2+x+1\\
\Phi_{12}(x) &= x^4-x^2+1, \quad \text{etc.}
\end{aligned}$$

Cyclotomic Harmonic Polylogarithms (C-Logs)

We now define the alphabet

$$\mathfrak{A} := \left\{\frac{1}{x}\right\} \cup \left\{ \frac{x^l}{\Phi_k(x)} \middle| k \in \mathbb{N}^*, 0 \leq l < \varphi(k) \right\},$$

where $\Phi_k(x)$ denotes the kth cyclotomic polynomial and φ is Euler's totient function.

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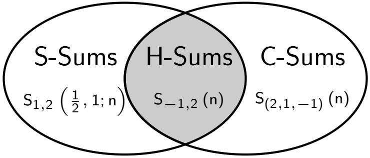
k is called the depth of $\mathrm{H}_{\mathbf{m}}(x)$.

Connection between these structures



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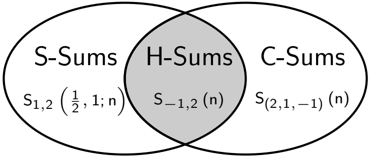

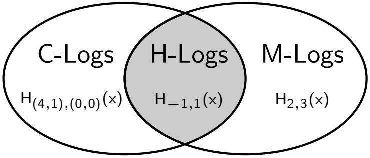

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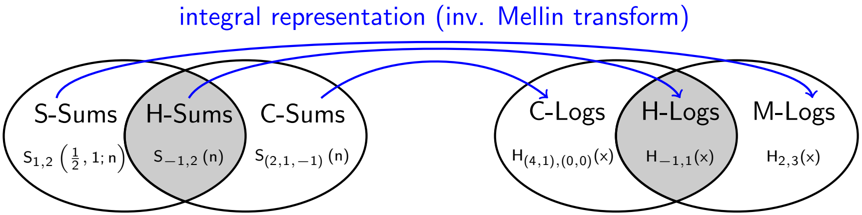

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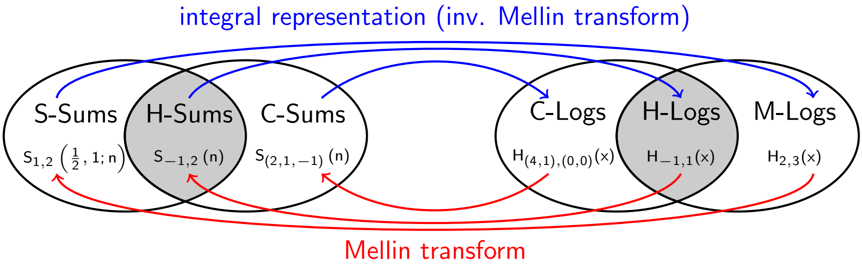

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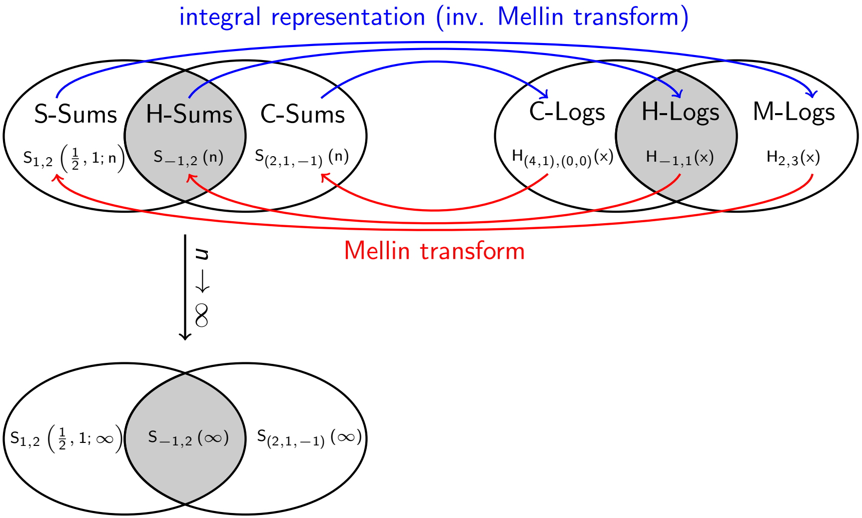

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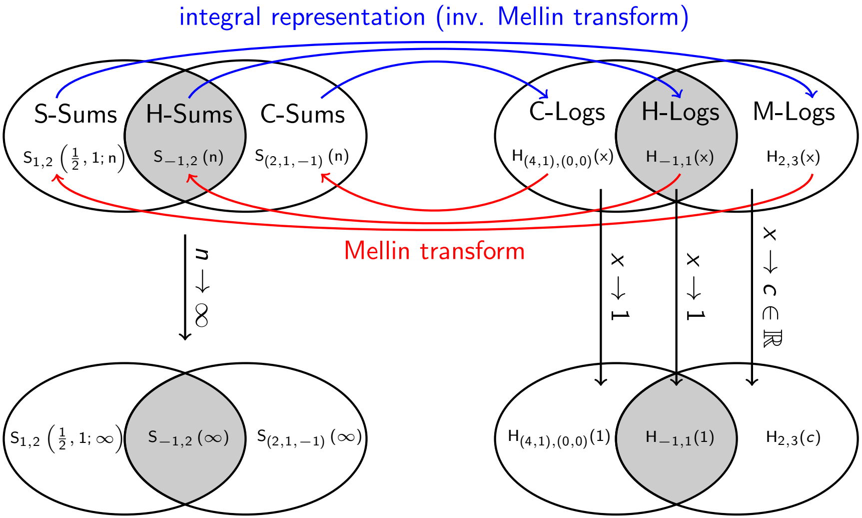

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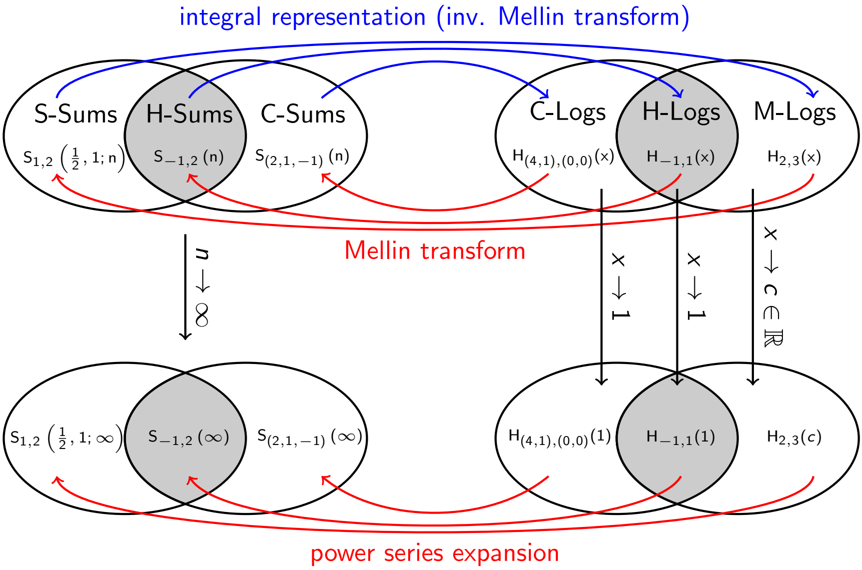

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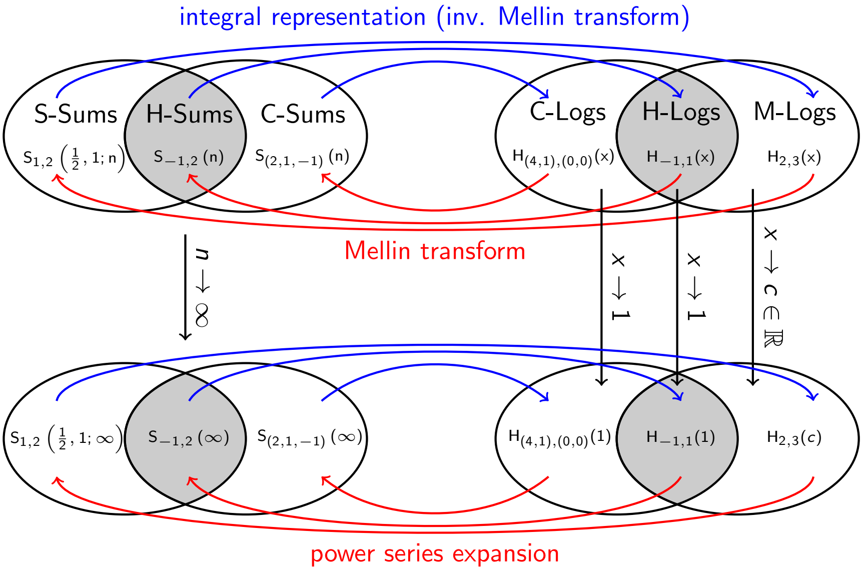

Asymptotic Expansion of Harmonic Sums

We say that the function $f : \mathbb{R} \to \mathbb{R}$ is expanded in an asymptotic series

$$f(x) \sim \sum_{k=0}^{\infty} \frac{a_k}{x^k},\ x \to \infty,$$

where a_k are constants, if for all $K \geq 0$

$$R_K(x) = f(x) - \sum_{k=0}^{K} \frac{a_k}{x^k} = o\left(\frac{1}{x^K}\right),\ x \to \infty.$$

Why do we need these expansions of harmonic sums?

E.g.,

- for limits of the form

$$\lim_{n\to\infty} n\left(S_2(n)-\zeta_2-S_{2,2}(n)+\frac{7\,\zeta_2^2}{10}\right)$$

- for the approximation of the values of analytic continued harmonic sums at the complex plane

$$S_{2,-3}(-20+10i)$$

Basic Idea

$$S_{-1,3}(n) \;=\; (-1)^n \int_0^1 x^n \frac{\mathrm{H}_{1,0,0}(x)}{1+x} dx + const$$

Basic Idea

$$S_{-1,3}(n) = (-1)^n \int_0^1 x^n \frac{\overbrace{\mathrm{H}_{1,0,0}(x)}^{\varphi(x)}}{1+x} dx + const$$

Basic Idea

$$\varphi(x) \longrightarrow \varphi(1-x) = \sum_{k=0}^{\infty} a_k x^k$$

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$$b_1 = a_1$$

$$b_k = \sum_{l=0}^{k-2} (-1)^l S_{k-l}^l a_{k-l} (k-l)!$$

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$$S_{-1,3}(n) \sim (-1)^n \left(-\frac{1}{4n^3} + \frac{5}{8n^4} - \frac{5}{8n^5} - \frac{5}{16n^6}\right) + \frac{3 \ \log(2) \ \zeta_3}{4}$$
$$+(-1)^n \left(\frac{1}{2n} - \frac{1}{4n^2} + \frac{1}{8n^4} - \frac{1}{4n^6}\right) \zeta_3 - \frac{19 \ \zeta_2^2}{40}$$

Asymptotic Expansions

- this basic idea can be turned into an algorithm:

$$S_{-1,3}(n) \sim (-1)^n \left(-\frac{1}{4n^3}+\frac{5}{8n^4}-\frac{5}{8n^5}-\frac{5}{16n^6}\right)+\frac{3\ \log(2)\,\zeta_3}{4}+(-1)^n\left(\frac{1}{2n}-\frac{1}{4n^2}+\frac{1}{8n^4}-\frac{1}{4n^6}\right)\zeta_3-\frac{19\,\zeta_2^2}{40}$$

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- extension to cyclotomic sums:

$$\begin{aligned} S_{(2,1,2),(1,0,1)}(n) \sim\ & -4\log(2) S_{(2,1,-1)}(\infty)^2 - 8\log(2) S_{(2,1,-1)}(\infty) - 4\log(2) + \frac{1}{9n^3} - \frac{1}{4n} + \frac{7\zeta_3}{4} \\ & + \left(-\frac{11}{48n^3} + \frac{1}{4n^2} - \frac{1}{4n}\right)(\log(n) + \gamma) \end{aligned}$$

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- extension to a subset of the S-Sums:

$$\begin{aligned}S_{2,1}(1,\tfrac{1}{3})(n) \sim\ & -S_{1,2}\left(\frac{1}{3},1;\infty\right)+3^{-n}\left(\frac{3}{2n^3}-\frac{3}{4n^2}+\frac{1}{2n}\right)H_{0,3}(1)+3^{-n}\left(-\frac{3}{2n^3}+\frac{3}{4n^2}-\frac{1}{2n}\right)S_2\left(\frac{1}{3};\infty\right)\\ &+\left(3^{-n}\left(-\frac{3}{2n^3}+\frac{1}{2n^2}+3^n\left(-\frac{1}{6n^3}+\frac{1}{2n^2}-\frac{1}{n}\right)\right)+\zeta_2\right)S_1\left(\frac{1}{3};\infty\right)\\ &+S_3\left(\frac{1}{3};\infty\right)+H_3(1)3^{-n}\left(\frac{3}{2n^3}-\frac{1}{2n^2}\right)+\frac{3^{-n}}{4n^3}\end{aligned}$$

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- extension to a subset of the cyclotomic S-Sums:

$$S_{(2,1,2)}\left(\frac{1}{2};n\right) \sim -\frac{\pi^2-6\left(8H_{0,1}\left(\frac{1}{\sqrt{2}}\right)+\log^2(2)\right)}{24\sqrt{2}}-2^{-n}\left(-\frac{293}{8n^5}+\frac{99}{16n^4}-\frac{5}{4n^3}+\frac{1}{4n^2}+2^n\right)$$

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- calculate the asymptotic expansion of harmonic sums and their generalizations
- perform several other tasks not mentioned in this talk (see, e.g., my PhD thesis, April 2012)

Almkvist Zeilberger Algorithm

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 structure

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

are of relevance for many physical processes at high energy colliders, such as the Large Hadron Collider, LHC, and others.

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are of relevance for many physical processes at high energy colliders, such as the Large Hadron Collider, LHC, and others.

These integrals can be transformed to integrals of the form

$$\int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(N; x_1, \dots, x_d, \varepsilon) dx_1 \dots dx_d$$

Recurrence for the Integrand

$$F(n; x_1, \ldots, x_d) = q(n; x_1, \ldots, x_d) \cdot e^{\frac{a(x_1,\ldots,x_d)}{b(x_1,\ldots,x_d)}} \cdot \left(\prod_{p=1}^{P} S_p(x_1, \ldots, x_d)^{\alpha_p} \right) \cdot \left(\frac{s(x_1, \ldots, x_d)}{t(x_1, \ldots, x_d)} \right)^n,$$

where

$a(x_1, \ldots, x_d), b(x_1, \ldots, x_d), s(x_1, \ldots, x_d), t(x_1, \ldots, x_d), q(n; x_1, \ldots, x_d) \in \mathbb{K}[x_1, \ldots, x_d]$ and $S_p(x_1, \ldots, x_d) \in \mathbb{K}[x_1, \ldots, x_d], \alpha_p \in \mathbb{K}$ for $1 \leq p \leq P$. With e.g., $\mathbb{K} = \mathbb{Q}(\varepsilon, n)$.

Recurrence for the Integrand

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Then there exist

$L\in\mathbb{N}, e_0(n), e_1(n),\dots,e_L(n)\in\mathbb{K}[n]$, *not all zero*, and $R_i(n;x_1,\dots,x_d)\in\mathbb{K}(n,x_1,\dots,x_d)$

such that

$$G_i(n;x_1,\dots,x_d):=R_i(n;x_1,\dots,x_d)F(n;x_1,\dots,x_d)$$

satisfy

$$\sum_{i=0}^{L}e_i(n)F(n+i;x_1,\dots,x_d)=\sum_{i=1}^{d}D_{x_i}G_i(n;x_1,\dots,x_d).$$

Recurrence for the Integrand

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$$F(n; x_1, \dots, x_d) = q(n; x_1, \dots, x_d) \cdot e^{\frac{a(x_1,\dots,x_d)}{b(x_1,\dots,x_d)}} \cdot \left(\prod_{p=1}^{P} S_p(x_1, \dots, x_d)^{\alpha_p} \right) \cdot \left(\frac{s(x_1, \dots, x_d)}{t(x_1, \dots, x_d)} \right)^n,$$

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Recurrence for the Integral 1

We now consider the integral

$$a(n) := \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d) dx_1 \dots dx_d,$$

where for $F(n; x_1, \dots, x_d)$ we have

$$\sum_{i=0}^{L} e_i(n) F(n+i; x_1, \dots, x_d) = \sum_{i=1}^{d} D_{x_i} G_i(n; x_1, \dots, x_d).$$

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If

$$F(n; \dots, x_{i-1}, u_i, x_{i+1}, \dots) = F(n; \dots, x_{i-1}, o_i, x_{i+1}, \dots) = 0,$$

we also have

$$G_i(n; \dots, x_{i-1}, u_i, x_{i+1}, \dots) = G_i(n; \dots, x_{i-1}, o_i, x_{i+1}, \dots) = 0$$

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and hence $a(n)$ satisfies the homogenous linear recurrence

$$\sum_{i=0}^{L} e_i(n) a(n+i) = 0.$$

Recurrence for the Integral 2

We again consider the integral

$$a(n) := \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d) dx_1 \dots dx_d,$$

- suppose $F(n; x_1, \dots, x_d)$ does not vanish at the bounds

Recurrence for the Integral 2

We again consider the integral

$$a(n) := \int_{u_d}^{o_d} \dots \int_{u_1}^{o_1} F(n; x_1, \dots, x_d) dx_1 \dots dx_d,$$

- suppose $F(n; x_1, \dots, x_d)$ does not vanish at the bounds
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- then force the G_i to vanish at the integration bounds by modifying the ansatz, and look for G_i of the form

$$G_i(n; x_1, \dots, x_d) = \overline{G}_i(n; x_1, \dots, x_d)(x_i - u_i)(x_i - o_i),$$

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- hence $a(n)$ satisfies again a homogenous linear recurrence of the form

$$\sum_{i=0}^{L} e_i(n) a(n+i) = 0.$$

Example

$$I(\varepsilon, n) = \int_0^1 \int_0^1 \underbrace{\frac{(1 + x_1 \cdot x_2)^n}{(1 + x_1)^\varepsilon}}_{F(n):=} dx_1 dx_2.$$

Note that the integrand does not vanish at the integration bounds.

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Note that the integrand does not vanish at the integration bounds.
Using our ansatz we find

$$\begin{aligned}
&2(n+1)(\varepsilon - n - 2)F(n) - (n+2)(5\varepsilon - 5n - 13)F(n+1) \\
&+(n+3)(4\varepsilon - 4n - 13)F(n+2) - (n+4)(\varepsilon - n - 4)F(n+3) \\
&= D_{x_1} F(n)(x_1 - 1)\, x_1\, (x_1 + 1)\, x_2\, ((n+3)x_1 x_2 + 2) \\
&+D_{x_2} F(n)(x_2 - 1)\, x_2\, \left(x_2^2 x_1^3(-\varepsilon + n + 4) - (\varepsilon - 3)x_2 x_1^2 + (n+2)x_2 x_1 + 1\right).
\end{aligned}$$

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&+(n+3)(4\varepsilon-4n-13)F(n+2)-(n+4)(\varepsilon-n-4)F(n+3)\\
&=D_{x_1}F(n)(x_1-1)\,x_1\,(x_1+1)\,x_2\,((n+3)x_1x_2+2)\\
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Integration of this reccurence yields

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Solving the recurrence leads to

$$I(\varepsilon,n)=\frac{1}{n+1}\left(\sum_{i=1}^n\frac{1}{-i+\varepsilon-1}-2^{1-\varepsilon}\sum_{i=1}^n\frac{2^i}{-i+\varepsilon-1}+\frac{2^{-\varepsilon}\left(2^\varepsilon-2\right)}{\varepsilon-1}\right)$$

Recurrence for the Integral 3

We look again at the integral

$$a(n) := \int_{u_d}^{o_d} \cdots \int_{u_1}^{o_1} F(n; x_1, \ldots, x_d) dx_1 \ldots dx_d.$$

Suppose that we found

$$\sum_{i=0}^{L} e_i(n) F(n+i; x_1, \ldots, x_d) = \sum_{i=1}^{d} D_{x_i} G_i(n; x_1, \ldots, x_d)$$

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By integration with respect to $x_1, \ldots, x_d$ we get

$$\begin{aligned}\sum_{i=0}^{L} e_i(n) a(n+i) &= \sum_{i=1}^{d} \int_{u_d}^{o_d} \cdots \int_{u_{i-1}}^{o_{i-1}} \int_{u_{i+1}}^{o_{i+1}} \cdots \int_{u_1}^{o_1} O_i(n) dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_d \\ &\quad - \sum_{i=1}^{d} \int_{u_d}^{o_d} \cdots \int_{u_{i-1}}^{o_{i-1}} \int_{u_{i+1}}^{o_{i+1}} \cdots \int_{u_1}^{o_1} U_i(n) dx_1 \ldots dx_{i-1} dx_{i+1} \ldots dx_d\end{aligned}$$

with

$$\begin{aligned}U_i(n) &:= G_i(n; x_1, \ldots, x_{i-1}, o_i, x_{i+1} \ldots, x_d)\\ O_i(n) &:= G_i(n; x_1, \ldots, x_{i-1}, u_i, x_{i+1} \ldots, x_d).\end{aligned}$$

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Note that there are $2 \cdot d$ integrals of dimension $d-1$, to compute.

Example

$$I(\varepsilon,n)=\int_0^1\int_0^1 \underbrace{\frac{(1+x_1\cdot x_2)^n}{(1+x_1)^\varepsilon}}_{F(n;x_1,x_2):=} dx_1 dx_2,$$

Applying the algorithm leads to

$$-(n+1)F(n;x_1,x_2)+(n+2)F(n+1;x_1,x_2)=D_{x_1}0+D_{x_2}\frac{x_2(x_1\cdot x_2+1)^{n+1}}{(1+x_1)^\varepsilon}$$

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In the next step apply the algorithm to $I_1(n)$; we find

$$I_1(\varepsilon,n)=\frac{4\cdot 2^n-2^\varepsilon}{2^\varepsilon(n+2-\varepsilon)}.$$

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$$I(\varepsilon,n)=\frac{1}{n+1}\left(\sum_{i=1}^n\frac{1}{-i+\varepsilon-1}-2^{1-\varepsilon}\sum_{i=1}^n\frac{2^i}{-i+\varepsilon-1}+\frac{2^{-\varepsilon}\left(2^\varepsilon-2\right)}{\varepsilon-1}\right).$$

Laurent Series Expansion of the Integral

- we look again at the integral

$$\mathcal{I}(\varepsilon, n) := \int_{u_d}^{o_d} \cdots \int_{u_1}^{o_1} F(n; x_1, \ldots, x_d) dx_1 \ldots dx_d.$$

- assume that we can write it in the form

$$\mathcal{I}(\varepsilon, n) = \sum_{l=-L}^{\infty} \varepsilon^l I_l(n).$$

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- find $I_{-L}(n), I_{-L+1}(n), \ldots, I_u(n)$ in terms of indefinite nested product-sum expressions.

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- compute a recurrence for $\mathcal{I}(\varepsilon, n)$ in the form

$$a_0(\varepsilon, n) T(\varepsilon, n) + \cdots + a_d(\varepsilon, n) T(\varepsilon, n+d) = h_0(n) + \cdots + h_u(n)\varepsilon^u + O(\varepsilon^{u+1});$$

  use one of the methods presented above

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  use one of the methods presented above
- use algorithm FLSR implemented in Sigma.

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$$-(n+1)I(\varepsilon,n)+(n+2)I(\varepsilon,n+1)=\underbrace{\int_0^1 (x_1+1)^{n+1-\varepsilon}dx_1}_{I_1(n)}-\int_0^1 0 dx_1.$$

In the next step apply the method to $I_1(n)$; we find

$$\begin{aligned}I_1(\varepsilon,n) &= \frac{2^{n+2}-1}{n+2}+\frac{\varepsilon\left(-2^{n+2}\left(\mathrm{H}_{-1}(1)(n+2)-1\right)-1\right)}{(n+2)^2}\\ &+\frac{\varepsilon^2\left(2^{n+1}\left(\mathrm{H}_{-1}(1)^2(n+2)^2-2\mathrm{H}_{-1}(1)(n+2)+2\right)-1\right)}{(n+2)^3}+O\left(\varepsilon^3\right).\end{aligned}$$

Plugging in and solving the resulting recurrence by means of FLSR and combining the solution with the initial values of the integral yields the result.

$$
\begin{aligned}
I(\varepsilon, n) \;=\; & \frac{\mathrm{S}_1(2;n)}{n+1} - \frac{\mathrm{S}_1(n)}{n+1} + \frac{2(n+1)^3 + 4\left(-n+2^n-1\right)(n+1)^2 + 2n(n+1)^2}{2(n+1)^4} \\
& + \varepsilon \Bigg(\mathrm{H}_{-1}(1) \left(\frac{-2^{n+2}(n+1) - 2^{n+2}n(n+1)}{2(n+1)^4} - \frac{\mathrm{S}_1(2;n)}{n+1} \right) \\
& + \frac{\left(2(n+1)n^2 + 4(n+1)n + 2(n+1)\right)\mathrm{S}_2(2;n)}{2(n+1)^4} - \frac{\mathrm{S}_2(n)}{n+1} \\
& + \frac{2^{n+2}(n+1) - 2(n+1)}{2(n+1)^4} \Bigg) + \varepsilon^2 \Bigg(\mathrm{H}_{-1}(1)^2 \left(\frac{\mathrm{S}_1(2;n)}{2(n+1)} + \frac{2^{n+1}(n^2+2n+1)}{2(n+1)^4} \right) \\
& + \mathrm{H}_{-1}(1) \left(\frac{-2^{n+2}n - 2^{n+2}}{2(n+1)^4} - \frac{\mathrm{S}_2(2;n)}{n+1} \right) + \frac{\mathrm{S}_3(2;n)}{n+1} - \frac{\mathrm{S}_3(n)}{n+1} + \frac{2^{n+2}-2}{2(n+1)^4} \Bigg) \\
& + O\left(\varepsilon^3\right).
\end{aligned}
$$

The Package MultiIntegrate

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

In[2]:= << **HarmonicSums.m**

In[3]:= << **EvaluateMultiSums.m**

In[4]:= << **MultiIntegrate.m**

Sigma - A summation package by Carsten Schneider -RISC Linz- V 1.0 (7/7/11)

HarmonicSums by Jakob Ablinger -RISC Linz- Version 1.0 (1/3/12)

EvaluateMultiSums by Carsten Schneider -RISC Linz- Version 1.0 (11/8/11)

MultiIntegrate by Jakob Ablinger -RISC Linz- Version 1.0 (1/3/12)

In[5]:= **mAZIntegrate[(1 + x1 * x2)^n/(1 + x1)^ε, {n}, {{x1, 0, 1}, {x2, 0, 1}}]**

Out[5]= $$\frac{\sum_{\iota_1=1}^{n}\frac{1}{\iota_1-\epsilon+1}}{-n-1}-\frac{2\sum_{\iota_1=1}^{n}\frac{2^{\iota_1}}{-\iota_1+\epsilon-1}}{(n+1)2^{\epsilon}}+\frac{2^{\epsilon}-2}{(n+1)(\epsilon-1)2^{\epsilon}}$$

The Package `MultiIntegrate`

The following integral occurs in the direct computation of a 3-loop diagram of the ladder-type:

$$\int_0^1 \int_0^1 \Bigg(\frac{(s(x-1)+t(u-1)+1)^n}{(w-1)(z-1)(sx-s+tu-t-u+1)(sx-s+tu-t-x+1)}$$
$$+\frac{1}{(z-1)(sx-s+tu-t-x+1)} \frac{(z(-s+tu-t+1)+x((s-1)z+1))^n}{-swx+sw+sxz-sz-tuw+tuz+tw-tz+uw-u-w-xz+x+z}$$
$$+\frac{1}{(w-1)(sx-s+tu-t-u+1)} \frac{(u((t-1)w+1)-w(s(-x)+s+t-1))^n}{swx-sw-sxz+sz+tuw-tuz-tw+tz-uw+u+w+xz-x-z} \Bigg) dudx$$

The Package `MultiIntegrate`

The following integral occurs in the direct computation of a 3-loop diagram of the ladder-type:

$$\int_0^1\int_0^1\Bigg(\frac{(s(x-1)+t(u-1)+1)^n}{(w-1)(z-1)(sx-s+tu-t-u+1)(sx-s+tu-t-x+1)}$$
$$+\frac{1}{(z-1)(sx-s+tu-t-x+1)}\frac{(z(-s+tu-t+1)+x((s-1)z+1))^n}{-swx+sw+sxz-sz-tuw+tuz+tw-tz+uw-u-w-xz+x+z}$$
$$+\frac{1}{(w-1)(sx-s+tu-t-u+1)}\frac{(u((t-1)w+1)-w(s(-x)+s+t-1))^n}{swx-sw-sxz+sz+tuw-tuz-tw+tz-uw+u+w+xz-x-z}\Bigg)\,dudx$$

$$=\frac{1}{(w-1)(z-1)(s+t-1)}\Bigg(S_{1,1}\left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1},\frac{sw-sz+z-1}{z-1};n\right)-S_{1,1}\left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1},\frac{z(sw-sz+z-1)}{w(z-1)};n\right)$$
$$-S_{1,1}\left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1},\frac{(t-1)(sw-sz+z-1)}{(s+t-1)(z-1)};n\right)+S_{1,1}\left(\frac{s+t-1}{t-1},(1-t)w;n\right)+S_{1,1}\left(\frac{s+t-1}{t-1},-\frac{(s-1)(t-1)}{s+t-1};n\right)$$
$$+S_{1,1}\left(-\frac{(s+t-1)w(z-1)}{sw-sz+z-1},\frac{(sw-sz+z-1)(tz-1)}{(s+t-1)w(z-1)};n\right)-S_{1,1}\left(\frac{s+t-1}{t-1},1-t;n\right)+S_{1,1}\left(\frac{s+t-1}{s-1},-\frac{(s-1)(t-1)}{s+t-1};n\right)$$
$$+S_{1,1}\left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1},\frac{-tw+w+tz-1}{w-1};n\right)-S_{1,1}\left(\frac{s+t-1}{t-1},-\frac{(t-1)(sw-1)}{s+t-1};n\right)+S_{1,1}\left(\frac{s+t-1}{s-1},(1-s)z;n\right)$$
$$-S_{1,1}\left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1},\frac{(s-1)(-tw+w+tz-1)}{(s+t-1)(w-1)};n\right)-S_{1,1}\left(\frac{s+t-1}{s-1},1-s;n\right)-S_{1,1}\left(\frac{s+t-1}{s-1},-\frac{(s-1)(tz-1)}{s+t-1};n\right)$$
$$-S_{1,1}\left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1},-\frac{w((t-1)w-tz+1)}{(w-1)z};n\right)+S_{1,1}\left(\frac{(s+t-1)(w-1)z}{(t-1)w-tz+1},-\frac{(sw-1)((t-1)w-tz+1)}{(s+t-1)(w-1)z};n\right)$$
$$-S_{1,1}(1,(1-s)z;n)+S_{1,1}(1,z-sz;n)+S_2((1-s)z;n)-S_{1,1}(1,(1-t)w;n)+S_{1,1}(1,w-tw;n)-S_2((-s-t+1)w;n)$$
$$-S_2((-s-t+1)z;n)+2S_2(-s-t+1;n)-S_2(1-s;n)+S_2((1-t)w;n)-S_2(1-t;n)\Bigg)$$