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Symbolic Summation for Particle Physics

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A warm up example: Simplify

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} \right. \\ \left. + \frac{j!k!(j+k+n)!(-S_1(j) + S_1(j+k) + S_1(j+n) - S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} \right) \\ \underbrace{\hspace{15em}}_{f(j)}$$

where

$$S_1(n) = \sum_{i=1}^n \frac{1}{i} (= H_n)$$

Arose in the context of

I. Bierenbaum, J. Blümlein, and S. Klein, *Evaluating two-loop massive operator matrix elements with Mellin-Barnes integrals*. 2006

A warm up example: Simplify

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} \right. \\ \left. + \frac{j!k!(j+k+n)!(-S_1(j) + S_1(j+k) + S_1(j+n) - S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} \right) \\ \underbrace{\hspace{15em}}_{f(j)}$$

FIND $g(j)$:

$$f(j) = g(j+1) - g(j)$$

A warm up example: Simplify

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} \right. \\ \left. + \frac{j!k!(j+k+n)!(-S_1(j) + S_1(j+k) + S_1(j+n) - S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} \right) \\ \underbrace{\hspace{15em}}_{f(j)}$$

FIND $g(j)$:

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The summation package Sigma computes

$$g(j) = \frac{(j+k+1)(j+n+1)j!k!(j+k+n)!(S_1(j) - S_1(j+k) - S_1(j+n) + S_1(j+k+n))}{kn(j+k+1)!(j+n+1)!(k+n+1)!}$$

(based on a refined version of Karr's algorithm (1981))

A warm up example: Simplify

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} \right. \\ \left. + \frac{j!k!(j+k+n)!(-S_1(j) + S_1(j+k) + S_1(j+n) - S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} \right) \\ \underbrace{\hspace{15em}}_{f(j)}$$

FIND $g(j)$:

$$f(j) = g(j+1) - g(j)$$

Summing the telescoping equation over j from 0 to a gives

$$\sum_{j=0}^a f(n, k, j) = g(a+1) - g(0) \\ = \frac{(a+1)!(k-1)!(a+k+n+1)!(S_1(a) - S_1(a+k) - S_1(a+n) + S_1(a+k+n))}{n(a+k+1)!(a+n+1)!(k+n+1)!} \\ + \frac{S_1(k) + S_1(n) - S_1(k+n)}{kn(k+n+1)n!} + \frac{(2a+k+n+2)a!k!(a+k+n)!}{(a+k+1)(a+n+1)(a+k+1)!(a+n+1)!(k+n+1)!}$$

 $a \rightarrow \infty$

A warm up example: Simplify

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} \right. \\ \left. + \frac{j!k!(j+k+n)!(-S_1(j) + S_1(j+k) + S_1(j+n) - S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} \right) \\ \underbrace{\hspace{15em}}_{f(j)}$$

$$\sum_{j=0}^{\infty} f(n, k, j) = \frac{S_1(k) + S_1(n) - S_1(k+n)}{kn(k+n+1)n!}$$

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n) + 1}{(n+1)^3}$$

recurrence finder

$$A(n) = \sum_{k=1}^{\infty} \frac{S_1(k) + S_1(n) - S_1(k+n)}{kn(k+n+1)}$$

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n) + 1}{(n+1)^3}$$

recurrence solver

$$A(n) = \sum_{k=1}^{\infty} \frac{S_1(k) + S_1(n) - S_1(k+n)}{kn(k+n+1)}$$

\in

$$\left\{ c \times \frac{1}{n(n+1)} + \frac{S_1(n)^2 + S_2(n)}{2n(n+1)} \mid c \in \mathbb{R} \right\}$$

where

$$S_1(n) = \sum_{i=1}^n \frac{1}{i}$$

$$S_2(n) = \sum_{i=1}^n \frac{1}{i^2}$$

$$(n+2)\mathbf{A}(n+1) - n\mathbf{A}(n) = \frac{(n+1)S_1(n) + 1}{(n+1)^3}$$

$$A(n) = \sum_{k=1}^{\infty} \frac{S_1(k) + S_1(n) - S_1(k+n)}{kn(k+n+1)} = \frac{1}{2} \times \frac{1}{n(n+1)} + \frac{S_1(n)^2 + S_2(n)}{2n(n+1)}$$

where

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A warm up example: Simplify

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} \left(\frac{(2j+k+n+2)j!k!(j+k+n)!}{(j+k+1)(j+n+1)(j+k+1)!(j+n+1)!(k+n+1)!} \right. \\ \left. + \frac{j!k!(j+k+n)!(-S_1(j) + S_1(j+k) + S_1(j+n) - S_1(j+k+n))}{(j+k+1)!(j+n+1)!(k+n+1)!} \right) \\ \underbrace{\hspace{15em}}_{f(j)}$$

$$\sum_{k=1}^{\infty} \sum_{j=0}^{\infty} f(n, k, j) = \sum_{k=1}^{\infty} \frac{S_1(k) + S_1(n) - S_1(k+n)}{kn(k+n+1)n!} \\ = \frac{S_1(n)^2 + S_2(n)}{2n(n+1)!}$$

where

$$S_1(n) = \sum_{i=1}^n \frac{1}{i} \qquad S_2(n) = \sum_{i=1}^n \frac{1}{i^2}$$

Sigma's summation spiral:

1. Creative telescoping (for the special case of hypergeometric terms see Zeilberger's algorithm (1991))

GIVEN a **definite** sum

$$A(n) = \sum_{k=0}^n f(n, k);$$

$f(n, k)$: indefinite nested product-sum in k ;
 n : extra parameter

FIND a **recurrence** for $A(n)$

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2. Recurrence solving

GIVEN a recurrence

$a_0(n), \dots, a_d(n), h(n)$:
 indefinite nested product-sum expressions.

$$a_0(n)A(n) + \dots + a_d(n)A(n+d) = h(n);$$

FIND **all solutions** expressible by indefinite nested products and sums
 (Abramov/Bronstein/Petkovšek/Schneider, in preparation)

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3. Find a "closed form"

$A(n)$ =combined solutions.

“Background of our 3-loop computations”

- ▶ The following examples arise in the context of 2- and 3-loop massive single scale Feynman diagrams with operator insertion.
- ▶ These are related to the QCD anomalous dimensions and massive operator matrix elements.
- ▶ At 2-loop order all respective calculations are finished:

M. Buza, Y. Matiounine, J. Smith, R. Migneron, W.L. van Neerven, Nucl. Phys. **B472** (1996) 611;

I. Bierenbaum, J. Blümlein, S. Klein, Nucl. Phys. **B780** (2007) 40;

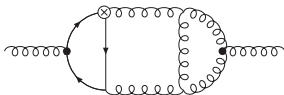
I. Bierenbaum, J. Blümlein, S. Klein, C. Schneider, Nucl.Phys. **B803** (2008)

and lead to representations in terms of harmonic sums.

Example 1: All n -Results for 3-Loop Ladder Graphs

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

In total around 50 diagrams (for this class) have been calculated, like e.g.



(containing three massive fermion propagators)



Around 1000 sums have to be calculated for this diagram

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

Simple sum

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

||

$$\sum_{j=0}^{n-2} \sum_{r=0}^{j+1} \boxed{\sum_{s=0}^{n-j+r-2} \frac{(-1)^{r+s} \binom{j+1}{r} \binom{-j+n+r-2}{s} (-j+n-2)! r!}{(n-s)(s+1)(-j+n+r)!}}$$

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

||

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

||

$$\left(\binom{j+1}{r} \left(\frac{(-1)^r (-j+n-2)! r!}{(n+1)(-j+n+r-1)(-j+n+r)!} + \frac{(-1)^{n+r} (j+1)! (-j+n-2)! (-j+n-1)_r r!}{(n-1)n(n+1)(-j+n+r)! (-j-1)_r (2-n)_j} \right) \right)$$

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

$$\parallel$$

$$\sum_{j=0}^{n-2} \left(\sum_{r=0}^{j+1} \binom{j+1}{r} \left(\frac{(-1)^r (-j+n-2)! r!}{(n+1)(-j+n+r-1)(-j+n+r)!} + \frac{(-1)^{n+r} (j+1)! (-j+n-2)! (-j+n-1)_r r!}{(n-1)n(n+1)(-j+n+r)! (-j-1)_r (2-n)_j} \right) \right)$$

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

||

$$\sum_{j=0}^{n-2} \left(\sum_{r=0}^{j+1} \binom{j+1}{r} \left(\frac{(-1)^r (-j+n-2)! r!}{(n+1)(-j+n+r-1)(-j+n+r)!} + \frac{(-1)^{n+r} (j+1)! (-j+n-2)! (-j+n-1)_r r!}{(n-1)n(n+1)(-j+n+r)! (-j-1)_r (2-n)_j} \right) \right)$$

||

$$\left(\frac{n^2 - n + 1}{(n-1)^2 n^2 (n+1) (2-n)_j} + \frac{\sum_{i=1}^j \frac{(2-n)_i}{(-i+n-1)^2 (i+1)!}}{(n+1) (2-n)_j} + \frac{(-1)^{j+n} (-j-2) (-j+n-2)!}{(j-n+1) (n+1)^2 n!} \right) (j+1)! - \frac{1}{(n+1)^2 (-j+n-1)}$$

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

||

$$\sum_{j=0}^{n-2} \left(\left(\frac{n^2 - n + 1}{(n-1)^2 n^2 (n+1)(2-n)_j} + \frac{\sum_{i=1}^j \frac{(2-n)_i}{(-i+n-1)^2 (i+1)!}}{(n+1)(2-n)_j} + \frac{(-1)^{j+n} (-j-2)(-j+n-2)!}{(j-n+1)(n+1)^2 n!} \right) (j+1)! - \frac{1}{(n+1)^2 (-j+n-1)} \right)$$

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

||

$$\sum_{j=0}^{n-2} \left(\left(\frac{n^2 - n + 1}{(n-1)^2 n^2 (n+1)(2-n)_j} + \frac{\sum_{i=1}^j \frac{(2-n)_i}{(-i+n-1)^2 (i+1)!}}{(n+1)(2-n)_j} + \frac{(-1)^{j+n} (-j-2)(-j+n-2)!}{(j-n+1)(n+1)^2 n!} \right) (j+1)! - \frac{1}{(n+1)^2 (-j+n-1)} \right)$$

||

$$\frac{-n^2 - n - 1}{n^2 (n+1)^3} + \frac{(-1)^n (n^2 + n + 1)}{n^2 (n+1)^3} - \frac{2S_{-2}(n)}{n+1} + \frac{S_1(n)}{(n+1)^2} + \frac{S_2(n)}{-n-1}$$

Note: $S_a(n) = \sum_{i=1}^N \frac{\text{sign}(a)^i}{i^{|a|}}$, $a \in \mathbb{Z} \setminus \{0\}$.

Sigma

Mathematica Session:

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

Sigma - A summation package by Carsten Schneider © RISC-Linz

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

HarmonicSums by Jakob Ablinger © RISC-Linz

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

EvaluateMultiSums by Carsten Schneider © RISC-Linz

In[4]:= **EvaluateMultiSum** $\left[\frac{(-1)^{r+s} \binom{j+1}{r} \binom{-j+n+r-2}{s} (-j+n-2)! r!}{(n-s)(s+1)(-j+n+r)!}, \{ \{s, 0, n-j+r-2\}, \{r, 0, j+1\}, \{j, 0, n-2\} \} \right]$

Out[4]= $\frac{-n^2 - n - 1}{n^2(n+1)^3} + \frac{(-1)^n (n^2 + n + 1)}{n^2(n+1)^3} - \frac{2S_{-2}(n)}{n+1} + \frac{S_1(n)}{(n+1)^2} + \frac{S_2(n)}{-n-1}$

A typical sum

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

A typical sum

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

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

$$+ \dots$$

where, e.g.,

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

Vermaseren 98/Blümlein/Kurth 99

A typical sum

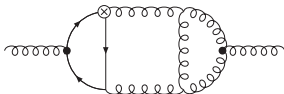
$$\begin{aligned}
& \sum_{j=0}^{n-2} \sum_{s=1}^{j+1} \sum_{r=0}^{n+s-j-2} \sum_{\sigma=0}^{\infty} \frac{-2(-1)^{s+r} \binom{j+1}{s} \binom{-j+n+s-2}{r} (n-j)!(s-1)! \sigma! S_1(r+2)}{(n-r)(r+1)(r+2)(-j+n+\sigma+1)(-j+n+\sigma+2)(-j+n+s+\sigma)!} \\
&= \frac{(2n^2 + 6n + 5) S_{-2}(n)^2}{2(n+1)(n+2)} + S_{-2,-1,2}(n) + S_{-2,1,-2}(n) \\
&+ \dots - S_{2,1,1,1}(-1, 2, \frac{1}{2}, -1; n) + S_{2,1,1,1}(1, \frac{1}{2}, 1, 2; n) \\
&+ \dots
\end{aligned}$$

where, e.g.,

145 S -sums occur

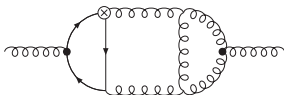
$$S_{2,1,1,1}(1, \frac{1}{2}, 1, 2; n) = \sum_{i=1}^n \frac{\sum_{j=1}^i \frac{\left(\frac{1}{2}\right)^j \sum_{k=1}^j \frac{\sum_{l=1}^k \frac{2^l}{l}}{k}}{j}}{i^2}$$

S. Moch, P. Uwer, S. Weinzierl 02



Sigma.m

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



Sigma.m

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

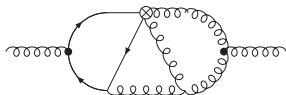


J. Ablinger's HarmonicSum.m

After elimination the following sums remain:

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

So far, the most complicated 3-loop ladder graph:



$$= F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \boxed{F_0(n)}$$

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$$= F_{-3}(n)\varepsilon^{-3} + F_{-2}(n)\varepsilon^{-2} + F_{-1}(n)\varepsilon^{-1} + \boxed{F_0(n)}$$

||

$$\sum_{j=0}^{n-3} \sum_{k=0}^j \sum_{l=0}^k \sum_{q=0}^{-j+n-3-l+n-q-3} \sum_{s=1}^{-l+n-q-3} \sum_{r=0}^{-l+n-q-s-3} (-1)^{-j+k-l+n-q-3} \times$$

$$\times \frac{\binom{j+1}{k+1} \binom{k}{l} \binom{n-1}{j+2} \binom{-j+n-3}{q} \binom{-l+n-q-3}{s} \binom{-l+n-q-s-3}{r} r! (-l+n-q-r-s-3)! (s-1)!}{(-l+n-q-2)! (-j+n-1) (n-q-r-s-2) (q+s+1)}$$

$$\left[4S_1(-j+n-1) - 4S_1(-j+n-2) - 2S_1(k) \right.$$

$$\left. - (S_1(-l+n-q-2) + S_1(-l+n-q-r-s-3) - 2S_1(r+s)) \right.$$

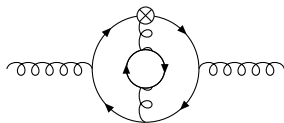
$$\left. + 2S_1(s-1) - 2S_1(r+s) \right] + \mathbf{3 \text{ further 6-fold sums}}$$

$$\begin{aligned}
\boxed{F_0(n)} = & \\
& \frac{7}{12} S_1(n)^4 + \frac{(17n+5)S_1(n)^3}{3n(n+1)} + \left(\frac{35n^2-2n-5}{2n^2(n+1)^2} + \frac{13S_2(n)}{2} + \frac{5(-1)^n}{2n^2} \right) S_1(n)^2 \\
& + \left(-\frac{4(13n+5)}{n^2(n+1)^2} + \left(\frac{4(-1)^n(2n+1)}{n(n+1)} - \frac{13}{n} \right) S_2(n) + \left(\frac{29}{3} - (-1)^n \right) S_3(n) \right. \\
& + \left(2 + 2(-1)^n \right) S_{2,1}(n) - 28S_{-2,1}(n) + \frac{20(-1)^n}{n^2(n+1)} \left. \right) S_1(n) + \left(\frac{3}{4} + (-1)^n \right) S_2(n)^2 \\
& - 2(-1)^n S_{-2}(n)^2 + S_{-3}(n) \left(\frac{2(3n-5)}{n(n+1)} + (26 + 4(-1)^n) S_1(n) + \frac{4(-1)^n}{n+1} \right) \\
& + \left(\frac{(-1)^n(5-3n)}{2n^2(n+1)} - \frac{5}{2n^2} \right) S_2(n) + S_{-2}(n) (10S_1(n)^2 + \left(\frac{8(-1)^n(2n+1)}{n(n+1)} \right. \\
& + \left. \frac{4(3n-1)}{n(n+1)} \right) S_1(n) + \frac{8(-1)^n(3n+1)}{n(n+1)^2} + \left(-22 + 6(-1)^n \right) S_2(n) - \frac{16}{n(n+1)} \\
& + \left(\frac{(-1)^n(9n+5)}{n(n+1)} - \frac{29}{3n} \right) S_3(n) + \left(\frac{19}{2} - 2(-1)^n \right) S_4(n) + \left(-6 + 5(-1)^n \right) S_{-4}(n) \\
& + \left(-\frac{2(-1)^n(9n+5)}{n(n+1)} - \frac{2}{n} \right) S_{2,1}(n) + (20 + 2(-1)^n) S_{2,-2}(n) + \left(-17 + 13(-1)^n \right) S_{3,1}(n) \\
& - \frac{8(-1)^n(2n+1) + 4(9n+1)}{n(n+1)} S_{-2,1}(n) - (24 + 4(-1)^n) S_{-3,1}(n) + (3 - 5(-1)^n) S_{2,1,1}(n) \\
& + 32S_{-2,1,1}(n) + \left(\frac{3}{2} S_1(n)^2 - \frac{3S_1(n)}{n} + \frac{3}{2} (-1)^n S_{-2}(n) \right) \zeta(2)
\end{aligned}$$

Example 2: 3-Loop All N-Results for the N_f Contributions

Joint work with J. Ablinger (RISC), J. Blümlein (DESY),
F. Wißbrock (DESY), S. Klein (RWTH)

E.g., for the diagram



768 sums are simplified.

Simple example:

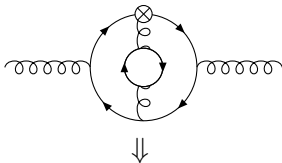
$$\begin{aligned}
& \sum_{j=1}^{n-2} \frac{j(j+1)(j+2)(n-j)(j-1)!^2(-j+n-1)!^2}{-j+n-1} \\
&= \frac{(-n^3 - 5n^2 - 4n + 6)(n!)^2}{(n-1)^2 n^2} \\
&+ \frac{3}{2} \frac{(n!)^2 (n^3 + 6n^2 + 11n + 6)}{(n-1)n(2n+1) \binom{2n}{n}} \sum_{i=1}^n \frac{\binom{2i}{i}}{i}.
\end{aligned}$$

Not expressible in terms of harmonic sums or S -sums!

The final expression is given in terms of 703 indefinite nested sums and products. Typical examples are:

$$\sum_{i=1}^n \frac{\sum_{j=1}^i \frac{\binom{2j}{j}}{j}}{\binom{2i}{i}}, \quad \sum_{i=1}^n \frac{S_1(i) \sum_{j=1}^i \frac{\binom{2j}{j}}{j}}{\binom{2i}{i}};$$

Sigma finds all algebraic relations among them. We get:



$$\begin{aligned}
 & - \frac{20S(1,n)^4}{27(n+1)(n+2)} + \frac{32(6n^3+61n^2-21n+24)S_1(n)^3}{81n^2(n+1)(n+2)} - \frac{16(48n^5+746n^4+2697n^3+2746n^2+1104n+240)S_1(n)^2}{81n^2(n+1)^2(n+2)^2} \\
 & + \frac{32(264n^7+4046n^6+21591n^5+52844n^4+74856n^3+66812n^2+30576n+2640)S_1(n)}{243n^2(n+1)^3(n+2)^3} \\
 & - \frac{4(48n^2+101n+96)S_2(n)^2}{9n(n+1)(n+2)} - \frac{32(363n^7+6758n^6+41285n^5+121235n^4+190235n^3+150758n^2+46964n+2904)}{243n(n+1)^4(n+2)^3} \\
 & + \left(-\frac{40S_1(n)^2}{9(n+1)(n+2)} + \frac{32(6n^3+61n^2-21n+24)S_1(n)}{27n^2(n+1)(n+2)} \right. \\
 & \left. - \frac{16(124n^5+198n^4-2387n^3-6162n^2-3632n-480)}{81n^2(n+1)^2(n+2)^2} \right) S_2(n) + \\
 & + \left(-\frac{32(9n^3-623n^2+894n+276)}{81n^2(n+1)(n+2)} - \frac{160S_1(n)}{27(n+1)(n+2)} \right) S_3(n) - \frac{8(56n^2+169n+112)S_4(n)}{9n(n+1)(n+2)} \\
 & + \left(\frac{64S_1(n)}{3(n+1)(n+2)} - \frac{128(n^3+9n^2-10n-6)}{9n^2(n+1)(n+2)} \right) S_{2,1}(n) + \frac{64S_{3,1}(n)}{3(n+1)(n+2)} + \frac{64(3n^2+7n+6)}{3n(n+1)(n+2)} S_{2,1,1}(n) \\
 & + \zeta(2) \left(\frac{8S_1(n)^2}{3(n+1)(n+2)} + \frac{16(3n^3-n^2+30n+12)S_1(n)}{9n^2(n+1)(n+2)} - \frac{16(3n^3+2n^2+17n+6)}{9n(n+1)^2(n+2)} - \frac{8(4n^2+9n+8)S_2(n)}{3n(n+1)(n+2)} \right) + \\
 & + \zeta(3) \left(\frac{448}{9(n+1)(n+2)} - \frac{448S_1(n)}{9(n+1)(n+2)} \right)
 \end{aligned}$$

Note: for our computations we used properties of

Harmonic sums (J. Vermaseren, J. Blümlein)

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

Note: for our computations we used properties of
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$$S_{2,1}(n) = \boxed{\sum_{i=1}^n \frac{1}{i^2} \sum_{j=1}^i \frac{1}{j}}$$

Integral representation:

$$= \int_0^1 \frac{x^n - 1}{1 - x} \left(\int_0^x \frac{\int_0^y \frac{1}{1-z} dz}{y} dy - \zeta(2) \right) dx,$$

$$\zeta(z) := \sum_{i=1}^{\infty} 1/i^z$$

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Asymptotic expansion:

$$= \left(\frac{1}{30n^5} - \frac{1}{6n^3} + \frac{1}{2n^2} - \frac{1}{n} \right) \ln(n) \\ - \frac{1}{100n^5} - \frac{1}{6n^4} + \frac{13}{36n^3} - \frac{1}{4n^2} - \frac{1}{n} + 2\zeta(3) + O\left(\frac{\ln(n)}{n^6}\right).$$

limit computations

numerical evaluation

Note: for our computations we used properties of

Generalization to cyclotomic harmonic sums (J. Ablinger, J. Blümlein, CS)

$$\boxed{\sum_{k=1}^n \frac{(-1)^k}{2k+1}} =$$

Integral representation:

$$= -(-1)^n \int_0^1 \frac{x^{2n}}{x^2+1} dx + \frac{(-1)^n}{2n+1} - 1 + \frac{\pi}{4},$$

Asymptotic expansion:

$$= (-1)^n \left(-\frac{3}{64n^5} - \frac{1}{16n^4} + \frac{3}{16n^3} - \frac{1}{4n^2} + \frac{1}{4n} \right) + \frac{\pi}{4} - 1 + O\left(\frac{1}{n^6}\right)$$

limit computations

numerical evaluation

Discovering algebraic relations (J. Ablinger, J. Blümlein, CS)

multiple ζ -values

$$\sum_{i=1}^{\infty} \frac{1}{i^3} \sum_{j=1}^i \frac{(-1)^j}{j^2} \sum_{k=1}^j \frac{1}{k}$$

(Tremendous literature: M.E. Hoffman, D. Zagier, P. Cartier, D.J. Broadhurst, D. Kreimer, M. Waldschmidt, D.M. Bradley, J. Vermaseren, J. Blümlein, etc.)

computer algebra

cyclotomic ζ -values

$$\sum_{i=1}^{\infty} \frac{1}{i^3} \sum_{j=1}^i \frac{(-1)^j}{(2j+1)^2} \sum_{k=1}^j \frac{1}{k}$$

(up to weight 6)

\longleftrightarrow

ζ -values with roots of unity

$$\sum_{i=1}^{\infty} \frac{1}{i^3} \sum_{j=1}^i \frac{(-1)^{\frac{j}{3}}}{j^2} \sum_{k=1}^j \frac{1}{k}$$

(up weight 2, up to 20th root of unity)
(siehe auch P. Deligne/A. Goncharov, D.J. Broadhurst)

Concluding remarks

- ▶ Symbolic summation is ready for many classes of 3-loop problems
- ▶ Relies on complex analysis assisted by computer algebra: e.g., asymptotic expansions of nested sums and products

Algorithms are implemented in J. Ablinger's HarmonicSums package

- ▶ Alternative summation methods are available (see, e.g., J. Blümlein, S. Klein, C.S., F. Stan; 2010)