Mathematical Structures in Higher Order Calculations

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DESY

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1. Introduction

Let us consider massless Quantum Field Theories as QED or QCD.

Integral cross sections are no scale quantities

Single differential distributions are single scale quantities

Anomalous dimensions and coefficient functions belong to the latter class.

- What are the classes of basic objects, through which these objects are built order by order in perturbation theory ?

- How can the multiple, nested integrals be expressed and simplified?

- Equivalently: Which are the basic building blocks of the above quantities in QFT ?

No Scale Quantities : $\Longrightarrow$ Basic ζ-Values

Single Scale Quantities : $\Longrightarrow$ Basic Mellin Transforms

Consider:

- polylogarithms and Nielsen integrals of one scale
- multiple polylogarithms of one and more scales
- (multiple) harmonic polylogarithms
- multiple finite harmonic sums and their representation as integer valued Mellin transforms
- multiple infinite harmonic sums $\equiv$ multiple ζ-values and their relations
- Study the algebras of these quantities
- Continue the above Mellin transforms to rational, real, and complex values of the Mellin variable to obtain more relations

No Scale Quantities : $\lim_{N \to \infty}$ Mellin transforms of Single scale quantities.

Mellin transform :

$$\int_0^1 dx x^N f(x) = \mathbf{M}[f(x)](N)$$

Mellin convolution :

$$[f_1 \otimes f_2](x) = \int_0^1 dx_1 \int_0^1 dx_2 \delta(x - x_1 x_2) f_1(x_1) f_2(x_2)$$

$$\mathbf{M}[f_1 \otimes f_2](N) = \mathbf{M}[f_1](N) \cdot \mathbf{M}[f_2](N)$$

$\Longrightarrow$ **Essential Structural Simplification**

2. Polylogarithms and Nielsen Integrals

Feynman parameter integrals :

$$\frac{1}{ab} = \int_0^1 dx \frac{1}{(ax + b(1-x))^2}, \quad \text{and more involved}$$

One obtains integrals like

$$\int_0^x \frac{dz}{z} = \ln(x), \quad \int_0^x \frac{dz}{z-1} = \ln(1-x), \ldots$$

$\Longrightarrow$ LOGARITHMS

A 2nd integral (Euler, 1768) :

$$\int_0^x \frac{dz}{z} \ln(1-z) = -\mathrm{Li}_2(x), \quad \int_x^1 \frac{dz}{z-1} \ln(z) = \mathrm{Li}_2(1-x),$$

$\Longrightarrow$ DILOGARITHMS

Iterate integrals (J. Landen, ≥ 1760; W. Spence, 1809):

$$\mathrm{Li}_n(x) = \int_0^x \frac{dz}{z} \mathrm{Li}_{n-1}(z)$$

$\Longrightarrow$ POLYLOGARITHMS

The denominators x^{-1} and $(1-x)^{-1}$ do in general iterate in a wider class, in which the NIELSEN INTEGRALS occur:

$$S_{p,n}(x) = \frac{(-1)^{n+p-1}}{(n-1)!p!} \int_0^1 \frac{dz}{z} \ln^{n-1}(z) \ln^p(1-xz)$$

N. Nielsen, 1909

courtesy C. Berg, Copenhagen

Serial representations :

$$\mathrm{Li}_n(x) = \sum_{k=1}^{\infty} \frac{x^k}{k^n}$$

$$S_{1,2}(x) = \sum_{k=2}^{\infty} \frac{x^k}{k^2} S_1(k-1), \qquad S_{2,2}(x) = \sum_{k=2}^{\infty} \frac{x^k}{k^3} S_1(k-1)$$

Harmonic Sum :

$$S_1(k) = \sum_{l=1}^{k} \frac{1}{l}$$

$$\frac{d}{dx} S_{n,p}(x) = S_{n-1,p}(x)$$

(some) Relations :

$$\mathrm{Li}_2(1-x) = -\mathrm{Li}_2(x) - \ln(x)\ln(1-x) + \zeta_2$$

$$\mathrm{Li}_2\left(-\frac{1}{x}\right) = -\mathrm{Li}_2(-x) - \frac{1}{2}\ln^2(x) - \zeta_2$$

$$\mathrm{Li}_3(1-x) = -S_{1,2}(x)-\ln(1-x)\mathrm{Li}_2(x)-\frac{1}{2}\ln(x)\ln^2(1-x)+\zeta_2\ln(1-x)+\zeta_3$$

$$\begin{aligned}\mathrm{Li}_4\left(-\frac{x}{1-x}\right) &= \ln(1-x)[\mathrm{Li}_3(x) - S_{1,2}(x)] + S_{2,2}(x) - \mathrm{Li}_4(x) - S_{1,3}(x) \\ &- \frac{1}{2}\ln^2(1-x)\mathrm{Li}_2(x) - \frac{1}{24}\ln^4(1-x)\end{aligned}$$

$$\mathrm{Li}_n(x^2) = 2^{n-1}\left[\mathrm{Li}_n(x) + \mathrm{Li}_n(-x)\right]$$

Some values of Nielsen Integrals :

$$\mathrm{Li}_n(1) = \zeta_n = \sum_{k=1}^{\infty} \frac{1}{k^n},$$

Riemann
ζ-function

$$\mathrm{Li}_n(-1) = \left(1 - \frac{1}{2^{n-1}}\right)\zeta_n$$

$$\mathrm{Li}_2\left(\frac{1}{2}\right) = \frac{1}{2}\left[\zeta_2 - \ln^2(2)\right], \quad \mathrm{Li}_3\left(\frac{1}{2}\right) = \frac{7}{8}\zeta_3 - \frac{1}{2}\zeta_2 \ln(2) + \frac{1}{6}\ln^3(2)$$

These relations hold because of the above $x \leftrightarrow (1-x)$ relations.

Some values of Nielsen Integrals :

$$S_{1,p}(1) = \zeta_{p+1}$$

$$S_{2,2}(1) = \frac{1}{10}\zeta_2^2$$

$$S_{2,2}(-1) = -\frac{3}{4}\zeta_2^2 + 2\mathrm{Li}_4\left(\frac{1}{2}\right) + \frac{7}{4}\zeta_3 \ln(2) - \frac{1}{2}\zeta_2 \ln^2(2) + \frac{1}{12}\ln^4(2)$$

$$S_{1,3}(-1) = -\frac{2}{5}\zeta_2^2 + \mathrm{Li}_4\left(\frac{1}{2}\right) + \frac{7}{8}\zeta_3 \ln(2) - \frac{1}{4}\zeta_2 \ln^2(2) + \frac{1}{24}\ln^4(2)$$

Due to this $\mathrm{Li}_4(1/2)$ cannot be expressed by other constants in use.

Basic Numbers :

$$\Big\{(\sigma_1(\infty),\ \ln(2));\ \zeta_2;\ \zeta_3;\ \mathrm{Li}_4(1/2);\ (\zeta_5,\ \mathrm{Li}_5(1/2));$$
$$(\mathrm{Li}_6(1/2),\ \sigma_{-5,-1});(\zeta_7,\ \mathrm{Li}_7(1/2),\ \sigma_{-5,1,1},\ \sigma_{5,-1,-1});\ldots\Big\}$$

J. Vermaseren;

J.B., D. Broadhurst, J. Vermaseren (2009): w=12 (altern.), w=24 (non-altern.)

$$\sigma_1(\infty) = \sum_{k=1}^{\infty}\frac{1}{k}$$

3. Poincaré iterated Integrals

Poincaré–Lappo-Danilevsky–Chen Iteration:

Let $\varphi_i \,\epsilon \{\omega_{-1}; \omega_0; \omega_1\}$ be differential forms

$$\omega_k = \frac{dz}{z-k}(-1)^{\theta(k)}$$

$$P\left(\{\varphi\}_k; x\right) := \int_0^z \varphi_1 \dots \varphi_k := \int_0^z \varphi_1(t) \int_0^t \varphi_2 \dots \varphi_k$$

Examples :

$$\mathrm{Li}_n(x) = \int_0^x \omega_0^{n-1}\omega_1, \quad S_{p,n}(x) = \int_0^x \omega_0^p \omega_1^n, \quad H_{\vec{m}_w}(x) = \int_0^x \prod_{l=1}^{\vec{k}} \omega_{m_l}$$

cf. M. Waldschmidt, 2003

4. Shuffle Algebra and Theory of Words

Harmonic Sums :

$$S_{k_1,\dots,k_m}(N) = \sum_{l_1=1}^{N} \frac{[\mathrm{sign}(k_1)]^{l_1}}{l_1^{|k_1|}} S_{k_2,\dots,k_m}(l_1)$$

We will explain details of the shuffle algebra for the case of harmonic sums and use this structure for other quantities later.

First relation: L. Euler, 1775

$$S_{m,n} + S_{n,m} = S_m \cdot S_n + S_{m+n}, \qquad m, n > 0$$

Generalized to alternating sums:

$$\begin{aligned} S_{m,n} + S_{n,m} &= S_m \cdot S_n + S_{m \wedge n}, \\ m \wedge n &= [|m| + |n|]\, \mathrm{sign}(m)\mathrm{sign}(n) \end{aligned}$$

Determinant relation:

$$S_{\underbrace{-1,\dots,-1}_{k}} = \frac{1}{k!}\begin{vmatrix} S_{-1} & 1 & 0 & \dots & 0 \\ -S_2 & S_{-1} & 2 & \dots & 0 \\ S_{-3} & -S_2 & S_{-1} & \dots & 0 \\ \vdots & & & & \vdots \\ (-1)^{k+1}S_{(-1)^k k} & (-1)^k S_{(-1)^{k-1}(k-1)} & \dots & \dots & S_{-1} \end{vmatrix}$$

$$S_{\underbrace{a,\dots,a}_{k}}(N) = \frac{1}{k}\sum_{l=0}^{k} S_{\underbrace{a,\dots,a}_{l}}(N)\, S_{\wedge_{m=1}^{k-l} a}(N)$$

These & other relations hold widely independent of their **Value** and **Type.**

Determined by : • Index Structure
• Multiplication Relation

Ramanujan:
integer sums

Faa di Bruno:
roots of multivar. algebraic equations

The Formalism applies as well to the Harmonic Polylogarithms.
Remiddi, Vermaseren, 1999.

Linear Representations of Mellin Transform by Harmonic Sums:

$$\mathbf{M}[F_w(x)](N) = S^w_{k_1,\ldots,k_m}(N) + P\left(S^{\tau'}_{k_1,\ldots,k_r}, \sigma^{\tau''}_{k_1,\ldots,k_p}\right)$$

$w = \sum_{i=1}^m |k_i|$ weight, $\tau', \tau'' < w$ P is a polynomial.

w	#	Σ	
1	2	2	
2	6	8	
3	18	26	2 Loop anom. Dimensions
4	54	80	2 Loop Wilson Coefficients
5	162	242	3 Loop anom. Dimensions
6	486	728	3 Loop Wilson Coefficients
	$2 \cdot 3^{w-1}$	$3^w - 1$	

Shuffle Products

Depth 2:

$$S_{a_1}(N) ⧢ S_{a_2}(N) \quad = \quad S_{a_1,a_2}(N) + S_{a_2,a_1}(N)$$

Depth 3:

$$S_{a_1}(N) ⧢ S_{a_2,a_3}(N) \quad = \quad S_{a_1,a_2,a_3}(N) + S_{a_2,a_1,a_3}(N) + S_{a_2,a_3,a_1}(N)$$

Depth 4: .....

Algebraic Equations

Depth 2:

$$S_{a_1}(N) ⧢ S_{a_2}(N) - S_{a_1}(N)S_{a_2}(N) - S_{a_1 \wedge a_2}(N) = 0$$

Depth 3:

$$S_{a_1}(N) ⧢ S_{a_2,a_3}(N) \quad - \quad S_{a_1}(N)S_{a_2,a_3}(N) - S_{a_1 \wedge a_2,a_3}(N) - S_{a_2,a_1 \wedge a_3}(N) = 0$$

Depth 4: ....

 # Basic Sums = # Permutations - # Independent Equations

$$
\begin{aligned}
&S_{a,a,a,b,b,b} = \\
&\frac{1}{3}S_aS_{b,a,b,a,b} - \frac{1}{6}S_{b,a\wedge a,b,b,a} - \frac{1}{6}S_{a,b,b,b,a\wedge a} + \frac{1}{3}S_{b,a\wedge a,b,a,b} - \frac{1}{6}S_{a\wedge a,b,b,b,a} \\
&+\frac{1}{3}S_{a\wedge a,b,a,b,b} + \frac{1}{3}S_{a\wedge a,b,b,a,b} + \frac{1}{3}S_{a,b,b,a\wedge a,b} + \frac{1}{3}S_{a\wedge a,a,b,b,b} + \frac{1}{3}S_{a,b,a\wedge a,b,b} \\
&-\frac{1}{6}S_{a,b,a,a\wedge b,b} - \frac{1}{6}S_{b,a\wedge b,a,b,a} - \frac{1}{6}S_{a\wedge b,b,a,a,b} - \frac{1}{6}S_{b,a\wedge b,a,a,b} + \frac{1}{3}S_{a\wedge b,b,b,a,a} \\
&+\frac{1}{3}S_{a,a\wedge b,a,b,b} - \frac{1}{6}S_{a,a,b,a\wedge b,b} + \frac{1}{3}S_{a,a,b,b,a\wedge b} + \frac{1}{3}S_{b,a,a\wedge a,b,b} + \frac{1}{3}S_aS_{a,a,b,b,b} \\
&+\frac{1}{3}S_{b,b,a\wedge b,a,a} + \frac{1}{3}S_{b,a\wedge b,b,a,a} - \frac{1}{6}S_{a,b,b,a\wedge b,a} + \frac{1}{3}S_{b,a,b,a,a\wedge b} - \frac{1}{6}S_{a,a\wedge b,b,b,a} \\
&-\frac{1}{6}S_{a,b,a\wedge b,b,a} - \frac{1}{6}S_{b,a,a\wedge b,a,b} - \frac{1}{6}S_{a,a\wedge b,b,a,b} - \frac{1}{6}S_{a,b,a\wedge b,a,b} - \frac{1}{6}S_{a\wedge b,a,b,a,b} \\
&+\frac{1}{3}S_{a,b,b,a,a\wedge b} - \frac{1}{2}S_{a,b\wedge b,a,a,b} - \frac{1}{2}S_{b\wedge b,a,a,a,b} - \frac{1}{2}S_{a,b,a,a,b\wedge b} - \frac{1}{2}S_{a,a,b\wedge b,a,b} \\
&-\frac{1}{6}S_{b,a,a\wedge b,b,a} + \frac{1}{3}S_{b,a,a,b,a\wedge b} + \frac{1}{3}S_{a,a,a\wedge b,b,b} + \frac{1}{3}S_{a,b,a,b,a\wedge b} - \frac{1}{6}S_{b,b,a,a\wedge b,a} \\
&-\frac{1}{6}S_{a\wedge b,b,a,b,a} + \frac{1}{3}S_{b,b,a,a,a\wedge b} - \frac{1}{6}S_{b,a,a,a\wedge b,b} - \frac{1}{6}S_{b,a,b,a\wedge b,a} - \frac{1}{6}S_{b,b,a,b,a\wedge a} \\
&-\frac{1}{2}S_{b,a,a,a,b\wedge b} - \frac{1}{6}S_{a\wedge b,a,b,b,a} + \frac{1}{3}S_{b,b,a,a\wedge a,b} + \frac{1}{3}S_{b,b,b,a\wedge a,a} + \frac{1}{3}S_{b,b,b,a,a\wedge a}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{1}{6}S_{b,b,a\wedge a,b,a}+\frac{1}{3}S_{b,a,b,a\wedge a,b}+\frac{1}{3}S_{a,a\wedge a,b,b,b}+\frac{1}{3}S_{b,b,a\wedge a,a,b}+\frac{1}{3}S_{b,a\wedge a,a,b,b}\\
&-\frac{1}{2}S_{a,a,b,a,b\wedge b}-\frac{1}{6}S_{b,a,b,b,a\wedge a}-\underline{S_{b,b,b,a,a,a}}+\frac{1}{3}S_{a\wedge b,a,a,b,b}+\frac{1}{3}S_{a}S_{b,b,a,a,b}\\
&-\frac{1}{6}S_{a}S_{a,b,b,b,a}-\frac{1}{6}S_{a}S_{b,b,a,b,a}+\frac{1}{3}S_{a}S_{b,a,a,b,b}+\frac{1}{3}S_{a}S_{a,b,a,b,b}-\frac{1}{6}S_{a}S_{b,a,b,b,a}\\
&-\frac{1}{2}S_{b}S_{a,a,b,a,b}-\frac{1}{2}S_{b}S_{a,b,a,a,b}+\frac{1}{3}S_{a}S_{b,b,b,a,a}-\frac{1}{2}S_{b}S_{b,a,a,a,b}+\frac{1}{3}S_{a}S_{a,b,b,a,b}
\end{aligned}
$$

Theory of Words

Can we count the basis in simpler way ? $\Longrightarrow$ YES.

Free Algebras and Elements of the Theory of Codes

$\Longrightarrow$ **Particle Physics**

Only the multiplication relation

and the Index structure matters

$\mathfrak{A} = \{a, b, c, d, \ldots\}$ Alphabet

$a < b < c < d < \ldots$ ordered

$\mathfrak{A}^* (\mathfrak{A})$ Set of all words W

$$W = a_1 \cdot a_2 \cdot a_{27} \ldots a_{532} \equiv \text{concatenation product (nc)}$$

$$W = p \cdot x \cdot s$$

p = prefix; s = suffix

Definition:

A Lyndon word is smaller than any of its suffixes.

$\Rightarrow$ lexicographic ordering

Examples

- $\{a, a, \dots, a, b\} \Longrightarrow aaa \dots ab$ 1 Lyndon word for these sets
- $(n-1)$ $a's$: $n_{basic}/n_{all} = 1/n$ $n \equiv$ depth of the sums
- $\{a, a, a, b, b, b\} \Longrightarrow aaabbb, aababb, aabbab$ 3 Lyndon words $\rightarrow$

Symmetries lead to a smaller fraction. $n_{\text{Lyndon}}/n_{\text{all}} = 3/20 < 1/6$

$\{a_1, a_2, \dots a_k\}, a_i \neq a_j, \Longrightarrow$ 1/(k-1)! Lyndon words

Homework:

construct all Lyndon words for $\{a, a, a, a, a, a, b, b, b, b, b, b\}$ using lexicographic ordering.

Theorem: (Radford, 1979)

The shuffle algebra $K\langle\mathfrak{A}\rangle$ is freely generated by the Lyndon words.

I.e. the number of Lyndon words yields the number of basic elements.

Is there a general counting relation ?

E. Witt, 1937

$$l_n(n_1,\dots,n_q) = \frac{1}{n}\sum_{d|n_i}\mu(d)\frac{(n/d)!}{(n_1/d)!\dots(n_q/d)!}, \qquad \sum_i n_i = n$$

$\mu(k)$ = Möbius function

(2nd Witt formula.)

$\mu(1) = 1$

$\mu(p_1p_2\dots p_k) = 0,$ if one prime occurs twice

$\mu(p_1p_2\dots p_k) = (-1)^k$, if no prime occurs twice

The Length of the Basis is a function mainly of the Depth.

5. Harmonic and Multiple Polylogaritms

Definition: Harmonic Polylogarithms

Remiddi & Vermaseren, 1999

$$f(0;x) = x^{-1}, \qquad f(1,x) = (1-x)^{-1} \qquad f(-1,x) = (1+x)^{-1}$$

$$\frac{d}{dx} H(a,x) = f(a;x)$$

$$\vec{m}_w = (a, \vec{m}_{w-1}), \qquad H(\vec{m}_w;x) = \int_0^x dz f(a;z) H(\vec{m}_{w-1};z)$$

$$H(\vec{0}_w;x) = \frac{1}{w!} \ln^w(x) \qquad H(\vec{1}_w;x) = \frac{(-1)^w}{w!} \ln^w(1-x) \qquad H(\vec{-1}_w;x) = \frac{1}{w!} \ln^w(1+x)$$

Examples

$$H(0,0,1,1;x) = S_{2,2}(x); \qquad H(-1,0,0,1;x) = \int_0^x \frac{dz}{1+z} \mathrm{Li}_3(z)$$

Properties:

$$H(\vec{m}_w;x) = (-1)^w H(-\vec{m}_w;x)$$

$$H(\vec{m}_p;x) \cdot H(\vec{n}_q;x) = H(\vec{n}_q;x) \sqcup\!\sqcup\, H(\vec{n}_q;x)$$

shuffle algebra $\Longrightarrow$ algebraic relations   cf. sect. 4

Counting of basic HPL's vs weight:

1st Witt formula over 3 elements

$$N_{\rm basic}(w) = \frac{1}{w+1} \sum_{d|w+1} \mu\left(\frac{w+1}{d}\right) 3^d$$

(3; 8; 18; 48; 116; 312; 810;...)

$H(\vec{m}_w;1-x)$ is a polynomial of HPL's of highest weight (w-1)

non-negative indices

$H(\vec{m}_w; x^2)$ can be represented in terms of $\sum H(\vec{n}_q; x)$
non-negative indices

Mappings: $y \rightarrow 1/x - i\epsilon; \qquad y \rightarrow (1-x)/(1+x)$

Mellin Transforms:

Consider :

$$\int_0^1 dx\, x^N \left(\frac{H_{\vec{m}_w}(x)}{1 \pm x}\right)_{(+)} \quad \rightarrow \quad S_{\vec{n}_{w+1}}(N) + \dots$$

$$\int_0^1 dx\, x^N \left(\frac{H_{0,1}(x)}{1-x}\right)_+ = S_{2,1}(N) - \zeta_2 S_1(N)$$

$$\begin{aligned}(-1)^{N+1} \int_0^1 dx\, x^N \frac{H_{0,1,1}(x)}{1+x} \quad &= \quad S_{-2,1,1}(N) - \zeta_3 S_{-1}(N) + \mathrm{Li}_4\left(\frac{1}{2}\right) \\ &\quad -\frac{1}{8}\zeta_2^2 - \frac{1}{8}\zeta_3 \ln(2) - \frac{1}{4}\zeta_2 \ln^2(2) + \frac{1}{24}\ln^4(2)\end{aligned}$$

Shuffling of letters :

$$\begin{cases} \forall w \in \mathfrak{A}^* & 1 \sqcup\!\sqcup\, w = w \sqcup\!\sqcup\, 1 = w, \\ \forall x, y \in A, \forall\, u, v, \in \mathfrak{A}^*, & xu \sqcup\!\sqcup\, yv = x(u \sqcup\!\sqcup\, yv) + y(xu \sqcup\!\sqcup\, v) \end{cases}$$

Generalized Maurer–Cartan

(Knizhnik–Zamolodchikov) Equation :

$$\begin{aligned} dL(z) &= \left[\omega_{-1}x_{-1} + \omega_0 x_0 + \omega_1 x_1\right] L(z) \\ L(\varepsilon) &= \exp[x_0 \ln(\varepsilon)] + o(\sqrt{\varepsilon}), \\ & \varepsilon \rightarrow 0^+, \varepsilon \in \boldsymbol{R} \end{aligned}$$

Drinfeld :

$$\begin{aligned} \mathfrak{A} &= \{x_{-1}, x_0, x_1\} \\ L(z) &= \sum_{w \in \mathfrak{A}^*} L_w(z) w, \quad \forall z \boldsymbol{C} \setminus \{-1, 1\} \end{aligned}$$

⇒ Monodromy around $\{-1,0,1\}$: Lille Group (Hoang, Petitot et al.)

Examples :

$$\begin{aligned}
p &= 2\pi i \\
\mathcal{M}_1 \mathrm{Li}_{x_0} &= \mathrm{Li}_{x_0} = \ln(x) \\
\mathcal{M}_1 \mathrm{Li}_{x_1} &= \mathrm{Li}_{x_1} - p = -\ln(1-x) - p \\
\mathcal{M}_1 \mathrm{Li}_{x_{-1}} &= \mathrm{Li}_{x_{-1}} = \ln(1+x) \\
\mathcal{M}_1 \mathrm{Li}_{x_0^2 x_1^2} &= \mathrm{Li}_{x_0^2 x_1^2} - p\mathrm{Li}_{x_0^2 x_1} + \frac{p^2}{4}\mathrm{Li}^2_{x_0} + p\zeta_{x_0 x_1}\mathrm{Li}_{x_0} + p\zeta_{x_0^2 x_1}
\end{aligned}$$

One may derive directly relations between different arguments, such as :

$$\begin{aligned}
\mathrm{Li}_4(1-x) &= -\mathrm{Li}_{2,1,1}(x) + \mathrm{Li}_1(x)\mathrm{Li}_{2,1}(x) - \frac{1}{2}\mathrm{Li}_1^2(x)\mathrm{Li}_2(x) \\
&\quad + \frac{1}{6}\ln(x)\mathrm{Li}_1^3(x) + \frac{\zeta_2}{2}\mathrm{Li}_1^2(x) - \zeta_3\mathrm{Li}_1(x) + \frac{2}{5}\zeta_2^2 \\
\mathrm{Li}_{2,1}\left(1-\frac{1}{x}\right) &= -\mathrm{Li}_3(x) + \ln(x)\mathrm{Li}_2(x) - \frac{1}{2}\ln^2(x)\mathrm{Li}_1(x) - \frac{1}{6}\ln^3(x) + \zeta_3
\end{aligned}$$

$$\mathrm{Li}_{2,1}(x) \equiv S_{1,2}(x); \quad \mathrm{Li}_{2,1}(x) = S_{2,2}(x); \quad \mathrm{Li}_{2,1,1}(x) = S_{1,3}(x)$$

Definition: Multiple Polylogarithms

A. Goncharov, 1998

$$\begin{aligned}
\mathrm{Li}_{s_k,\dots,s_1}(x_k,\dots,x_1) &= \lambda\begin{pmatrix} s_1, & \dots, & s_k \\ y_1, & \dots, & y_k \end{pmatrix}, \qquad y_j := \prod_{i=1}^{j} x_i^{-1} \\
&= \sum_{n_1 > \dots > n_k > 0} \prod_{j=1}^{k} n_j^{-s_j} x_j^{n_j}
\end{aligned}$$

Equivalent expression:

Borwein, Bradley, Broadhurst, Lisonek, 1999

$$\lambda\begin{pmatrix} s_1, & \dots, & s_k \\ b_1, & \dots, & b_k \end{pmatrix} := \sum_{\nu_1,\dots,\nu_k=1}^{\infty} \prod_{j=1}^{k} b_j^{-\nu_j} \left(\sum_{i=j}^{k} \nu_j\right)^{-s_j}$$

Z–Sums

(Moch, Uwer, Weinzierl, 2001)

$$Z(n;\vec{m}_k;\vec{x}_k) = \sum_{i=1}^{n} \frac{x_1^l}{l^{m_1}} Z(l-1,\vec{m}|_2^k;\vec{x}|_2^k)$$

classical polylogs $\Longrightarrow$ Nielsen integrals $\Longrightarrow$ harmonic polylogs

$\Longrightarrow$ multiple polylogs $\Longrightarrow$ Z–sums

multiple ζ–values $\Longrightarrow$ multiple harmonic sums $\Longrightarrow$ Z–sums

PROGRAMS : nestedsums Weinzierl
xsummer Moch, Uwer

(M.E. Hoffman, 1999) $\Longrightarrow$ Hopf–algebra structure

6. Harmonic Sums and Mellin Transforms

Apply the shuffle algebra to reduce the number of sums.

Find basic Mellin transforms for Harmonic Sums

$\Longrightarrow$ One-dimensional integral representations :

$$S_{1,2}(N) = \mathbf{M}\left[\frac{\mathrm{Li}_2(1-x)}{1-x}\right](N) + \zeta_2 S_1(N) - \zeta_3$$

$$\mathrm{Li}_2(1-x) = -\mathrm{Li}_2(x) - \ln(x)\ln(1-x) + \zeta_2$$

not yet minimal $\Longrightarrow$

$$S_{2,1}(N) = \mathbf{M}\left[\left(\frac{\mathrm{Li}_2(x)}{1-x}\right)_+\right](N) + \zeta_2 S_1(N)$$

$$S_{3,1,1}(N) = -\mathbf{M}\left[\left(\frac{S_{2,2}(x)}{1-x}\right)_+\right](N) + \zeta_3 S_2(N) - \frac{\zeta_2^2}{10} S_1(N)$$

$$
\begin{aligned}
S_{-1,-1,-2}(N) &= (-1)^{N+1}\mathbf{M}\left[\frac{F_1(x)+\ln(1-x)\mathrm{Li}_2(-x)}{x+1}\right](N) \\
&= +(-1)^{N+1}\mathbf{M}\left[\frac{S_{1,2}(x^2)/2-S_{1,2}(x)-S_{1,2}(-x)}{x+1}\right](N) \\
&\quad +\frac{\zeta_2}{2}\left[S_{-1,1}(N)-S_{-1,-1}(N)\right] \\
&\quad +\left[\frac{9}{8}\zeta_3-\frac{3}{2}\zeta_2\ln(2)-\frac{1}{6}\ln^3(2)\right]S_{-1}(N) \\
&\quad -\frac{1}{10}\zeta_2^2+\frac{17}{8}\zeta_3\ln(2)-\frac{7}{4}\zeta_2\ln^2(2)0\frac{1}{6}\ln^4(2)
\end{aligned}
$$

with

$$
\begin{aligned}
F_1(x) &= S_{12}\left(\frac{1-x}{2}\right)+S_{1,2}(1-x)-S_{1,2}\left(\frac{1-x}{1+x}\right)+S_{1,2}\left(\frac{1}{1+x}\right) \\
&\quad -\ln(2)\mathrm{Li}_2\left(\frac{1-x}{2}\right)+\frac{1}{2}\ln^2(2)\ln\left(\frac{1+x}{2}\right)-\ln(2)\mathrm{Li}_2\left(\frac{1-x}{1+x}\right)
\end{aligned}
$$

$\Longrightarrow$ can always be reduced algebraically.

Hidden, nasty Mellin convolutions.

7. Multiple Zeta–Values

Euler-Zagier Values :

$$\zeta(a,\vec{m}_w) = \sum_{k=1}^{\infty} \frac{(\pm 1)^{\mathrm{sign}(a)}}{k^{|a|}} S(\vec{m}_w; k-1)$$

$S(\vec{m}_w; N)$ denotes a multiple harmonic sum of weight w.

If $\forall m_i > 0$: Multiple ζ-values

Otherwise : Colored ζ-values

The numerators are ($\sqrt[n]{1})^{\mathrm{sign}(m_i)}$. Here we consider: n = 2 only.

Building blocks : Basic numbers introduced before.

What is known about these numbers ?

$\ln(2)$ is transcendental	Lindemann, 1882: ζ_2 is transcendental
Apery, 1979: ζ_3 is irrational	Zudilin, 2000: one out of $\{\zeta_5, \zeta_7, \zeta_9, \zeta_{11}\}$ is irrational
unknown whether γ_E is irrational	Rivoal, 2000: infinitely many ζ_{2n+1} values are irrational

G.H. Hardy offered his Cambridge Chair to anyone who would proof that γ_E is irrational.

Basic Numbers :

$$\Big\{(\sigma_1(\infty),\ \ln(2));\ \zeta_2;\ \zeta_3;\ \mathrm{Li}_4(1/2);\ (\zeta_5,\ \mathrm{Li}_5(1/2));$$

$$(\mathrm{Li}_6(1/2),\ \sigma_{-5,-1});(\zeta_7,\ \mathrm{Li}_7(1/2),\ \sigma_{-5,1,1},\ \sigma_{5,-1,-1});\ldots\Big\}$$

$$\sigma_1(\infty) = \sum_{k=1}^{\infty} \frac{1}{k}$$

Relations :

(i) Shuffle relation ⧢ :(HPL's(x=1))

$$\zeta_{w_1} \cdot \zeta_{w_2} = \zeta(w_1 ⧢ w_2)$$

(ii) Stuffle relation $\star$ (M. Hoffman, 1997):

(HSUMS's(N$\rightarrow \infty$))

$$\zeta_{w_1} \cdot \zeta_{w_2} = \zeta(w_1 \star w_2); \quad \star : \mathfrak{A}^* \times \mathfrak{A}^* \rightarrow \mathfrak{H}$$

$$e \star w = w \star e = w$$

$$y_s u \star y_t v = y_s(u \star y_t v) + y_t(y_s u \star v) + y_{s+t}(u \star v),$$

$$s, t \,\epsilon\, N; \quad s, t > 0$$

$$\Longrightarrow \zeta(w_1 ⧢ w_2 - w_1 \star w_2) = 0$$

Examples :

Shuffle: $\zeta_{2,1}\zeta_2 = 6\zeta_{3,1,1} + 3\zeta_{2,2,1} + \zeta_{2,1,2}$

Stuffle: $\zeta_{2,1}\zeta_2 = 2\zeta_{2,2,1} + \zeta_{4,1} + \zeta_{2,3} + \zeta_{2,1,2}$

$\Longrightarrow$: $6\zeta_{3,1,1} + \zeta_{2,2,1} - \zeta_{4,1} - \zeta_{2,3} = 0$

(iii) Duality :

$$(-1)^r \int_0^1 \prod_{j=1}^m \omega_0^{s_j+1}\omega_1^{r_j+1} = (-1)^s \int_0^1 \prod_{j=1}^m \omega_0^{r_j+1}\omega_1^{s_j+1}$$

Examples : $\zeta(\{2,1\}_n) = \zeta(\{3\}_n)$; $\zeta(2,\{1\}_n) = \zeta(n+2)$

(iv) Sum Theorem :

(Granville, Zagier, 1997);

$$\sum_{\substack{s_1 > 1,\, s_i|_{i=2}^l \geq 1 \\ s_1 + \ldots + s_l = s}} \zeta(s_1, \ldots, s_l) = \zeta(s)$$

(v) Hoffman's relation (1992) :

$$\sum_{k=1}^{l} \zeta(\vec{s}|_1^{k-1}, s_k+1, \vec{s}|_{k+1}^{l}) = \sum_{k=1}^{l} \sum_{j=0}^{s_k-2} \zeta(\vec{s}_1^{k-1}, s_k - j, j+1, \vec{s}|_{k+1}^{l})$$

Euler : $\zeta_s = \sum_{j=1}^{s-2} \zeta_{s-j,j}, \quad s \geq 3$

Other Theorems more :

- Le-Murakami Theorem;
- Cyclic sum Theorem;
- Derivation Theorem; and others.

Alternating Sums: Generalized duplication formulae are of instrumental importance, (JB, D. Broadhurst, J. Vermaseren, 2009)

Which infinite nested harmonic sums are reducible ?

Examples :

$$\zeta_{2,1} = \zeta_3, \quad \zeta_{4,1} = 2\zeta_4 - \zeta_2^2 = -\frac{1}{5}\zeta_2^2 = -\frac{\pi^4}{180}$$

$$2\zeta_{m,1} = m\zeta_{m+1} - \sum_{k=1}^{m-2} \zeta_{m-k}\zeta_{k+1}, \quad 2 \leq m$$

$$\zeta(\{2\}_n) = \frac{2(2\pi)^{2n}}{(2n+1)!}\left(\frac{1}{2}\right)^{2n+1}$$

$$\zeta(\{10\}_n) = \frac{10(2\pi)^{2n}}{(10n+5)!}\left[1 + \left(\frac{1+\sqrt{5}}{2}\right)^{10n+5} + \left(\frac{1-\sqrt{5}}{2}\right)^{10n+5}\right]$$

$$\zeta(\{3,1\}_n) = \frac{1}{4^n}\zeta(\{4\}_n) = \frac{2\pi^{4n}}{(4n+2)!)}$$

Evaluated to :

multiple ζ-values:

Bigotte et al.,	1998	rank 12
Broadhurst,	2000	rank 9
Vermaseren,	2000	rank 9
Minh, Petitot,	2000	rank 10
Vermaseren,	2003	rank 16
Minh, Petitot,	2003	rank 16
J.B., Broadhurst, Vermaseren	2009	rank 24 (26)

$N = 2$ colored multiple ζ-values:

Gastmans & Troost,	1981	rank 4
J.B. & S. Kurth,	1998	rank 4 completed
Vermaseren,	2000	rank 9
Bigotte et al.,	2002	rank 7
J.B., Broadhurst, Vermaseren	2009	rank 12

Examples: (Petitot et al.)

rank 12 multiple ζ-value:

$$\zeta(2,1,1,5,1,2) = -\frac{19}{4}\zeta_3^4 + \frac{511}{4}\zeta_2\zeta_5^2 - \frac{26907}{16}\zeta_5\zeta_7 + \frac{6639743}{63000}\zeta_2^6$$
$$+\frac{1377}{20}\zeta_5\zeta_3\zeta_2^2 - \frac{3740}{3}\zeta_3\zeta_9 + \frac{7723}{210}\zeta_2^3\zeta_3^2 + \frac{1943}{8}\zeta_7\zeta_2\zeta_3$$
$$+\frac{1107}{8}\zeta_2\zeta_{8,2} + \frac{1943}{40}\zeta_2^2\zeta_{6,2} + \frac{123}{2}\zeta_{8,2,1,1} - \frac{7045}{32}\zeta_{10,2}$$

rank 7 (± 1)-colored multiple ζ-value:

$$\zeta(-1,1,1,1,-1,2) = \frac{295}{256}\zeta_2\zeta_5 + \frac{1469}{13440}\zeta_3\zeta_2^2 + \frac{3}{8}\zeta_{-1}\zeta_{-5,1} - \frac{23}{192}\zeta_{-1}^4\zeta_3$$
$$+\frac{85}{84}\zeta_{5,1,-1} - \frac{1}{2}\zeta_{-1}\zeta_3^2 \quad \ldots\ldots \quad - \frac{5}{6}\zeta_{-1}\zeta_{3,1,1,1,-1} - \frac{5}{12}\zeta_{-1}^2\zeta_{3,1,-1}$$

Counting basic elements :

multiple ζ-value:

Zagier; Broadhurst & Kreimer conjecture,similar to the 1st Witt relation.

$$N(w) = \frac{1}{w} \sum_{d|w} \mu\left(\frac{w}{d}\right) P_d,$$

$$P_1 = 0,\ P_2 = 2,\ P_3 = 3; \quad P_d = P_{d-2} + P_{d-3},\ d \geq 3$$

P_d - Perrin numbers.

$$\{0;\ 1;\ 1;\ 0;\ 1;\ 0;\ 1;\ 0; \ldots\}$$

$(\pm)$-colored multiple ζ-value:

$$\{2;\ 1;\ 1;\ 1;\ 2;\ 2;\ 4; \ldots\}$$

8. Structural Relations

To consider the Mellin variable N to be integer is not necessary.

We need analytic continuation to $N \epsilon \mathbf{C}$.

Proceed as follows:

$$N \ \epsilon \ \mathbf{N} \Rightarrow N \ \epsilon \ \mathbf{Q} \Rightarrow N \ \epsilon \ \mathbf{R} \Rightarrow N \ \epsilon \ \mathbf{C}$$

(i) N, rational:

$$\frac{1}{2^{n-2}} \frac{\mathrm{Li}_n(x^2)}{1-x^2} = \frac{\mathrm{Li}_n(x)}{1-x} + \frac{\mathrm{Li}_n(x)}{1+x} + \frac{\mathrm{Li}_n(-x)}{1-x} + \frac{\mathrm{Li}_n(-x)}{1+x}$$

Express one Mellin transform knowing $\mathbf{M}[(\mathrm{Li}_n(x)/(1-x)](N)$ for N and $N/2$.

(ii) N, real:

One may introduce differential operators d/dN.

$$\frac{d^k}{dN^k}\mathbf{M}\left[f(x)\right](N) = \mathbf{M}\left[\ln^k(x)f(x)\right](N)$$

Example :

$$\begin{aligned} S_{-2,-3}(N) \quad &= \quad \mathbf{M}\left\{\left[\frac{1}{1-x}\left(\frac{1}{2}\ln^2(x)\mathrm{Li}_2(-x) - 2\ln(x)\mathrm{Li}_3(-x) - 3\mathrm{Li}_4(-x)\right)\right]_+\right\}(N) \\ &\quad +\frac{3}{4}\zeta_3\left[S_2(N) - S_{-2}(N)\right] + \frac{21}{8}\zeta_4 S_1(N) \end{aligned}$$

is no basic function, neither is any of its contributions.

Map back to $\mathrm{Li}_4/(1 \pm x)$ and functions of lower weight.

9. The Basic Functions to w = 5,6

Here we list all basic function contributing up to the level of the 3-loop anomalous dimensions.

Weight w=1,2 :

Only weighted logarithms contribute ⇒ single sums

Representative : $S_1(N) = \psi(N+1) + \gamma_E$ and its derivatives.

$$F_1(N) = \mathbf{M}\left[\left(\frac{1}{1-x}\right)_+\right](N)$$

Remark on the only irreducible function at w=2

$$F_2(N) = \mathbf{M}\left[\frac{\ln(1+x)}{1+x}\right](N)$$

This function does not occur in physical quantities genuinely. However, it is useful in reductions of large classes of functions.

Weight w=3 :

$$F_3(N) = \mathbf{M}\left[\frac{\mathrm{Li}_2(x)}{1+x}\right](N), \qquad F_4(N) = \mathbf{M}\left[\left(\frac{\mathrm{Li}_2(x)}{1-x}\right)_+\right](N)$$

Ynduarin et al., 1981: $F_2(N)$

Weight w=4 :

$$F_5(N) := \mathbf{M}\left[\frac{\mathrm{Li}_3(x)}{1+x}\right](N), \quad F_{6,7}(N) := \mathbf{M}\left[\frac{S_{1,2}(x)}{1 \pm x}\right](N),$$

$F_4(N) - F_7(N)$: J.B., S. Moch, 2003; J.B., V. Ravindran ,2004

Weight w = 5,6 :

$$F_{8,9}(N) = \mathbf{M}\left[\left(\frac{\mathrm{Li}_4(x)}{1 \pm x}\right)_{(+)}\right](N), \qquad F_{10}(N) = \mathbf{M}\left[\frac{S_{1,3}(x)}{1+x}\right](N),$$

$$F_{11,12}(N) = \mathbf{M}\left[\left(\frac{S_{2,2}(x)}{1 \pm x}\right)_{(+)}\right](N), \qquad F_{13}(N) = \mathbf{M}\left[\frac{\mathrm{Li}_2^2(x)}{1+x}\right](N),$$

$$F_{14,15}(N) := \mathbf{M}\left[\left(\frac{\ln(x)S_{1,2}(-x) - \mathrm{Li}_2^2(-x)/2}{1 \pm x}\right)_{(+)}\right](N)$$

$F_8(N) - F_{15}(N)$: J.B., S. Moch, 2004.
20 new functions for w=6 J.B., 2009

11. Summary

- Harmonic polylogarithms are a tool to organize the results of integration for single scale quantities in z space.
- Harmonic polylogarithms are generated by a generalized Knizhnik-Zamolodchikov-Drinfeld DEQ.
- Special cases are usual polylogarithms and usual Nielsen integrals
- A high degree of simplification can be achieved expressing the results in terms of harmonic sums.
- Harmonic sums of the variable N are associated to Mellin transforms of weighted harmonic polylogarithms.
- Harmonic sums can be simplified through algebraic and structural relations.
- The number of basic functions contributing to
  1 loop anomalous dimensions and coefficient functions is 1,
  2 loop anomalous dimensions is 2,
  2 loop coefficient functions is 6,
  3 loop anomalous dimensions is 15.
  3 loop coefficient functions is 35.

- All numerator functions are polynomials of Nielsen integrals up to w=5.
- The analytic continuation of the basic Mellin transforms are known exactly and in form of highly accurate numerical representations.
- Multiple Zeta-values are related by shuffle- and stuffle-algebra relations, duality, an others.
- The conjecture that these are all relations was checked up to weight w=26 for numerators $\nu = 1$. The number of basis elements is connected to the Perrin numbers.
- A larger basis is obtained for the case of numerators $\nu = \pm$, with counting relation based on Padovan numbers. It was checked up to weight w=12; exotic relations are still possible.