Perturbative calculations with shuffle algebras and polylogs

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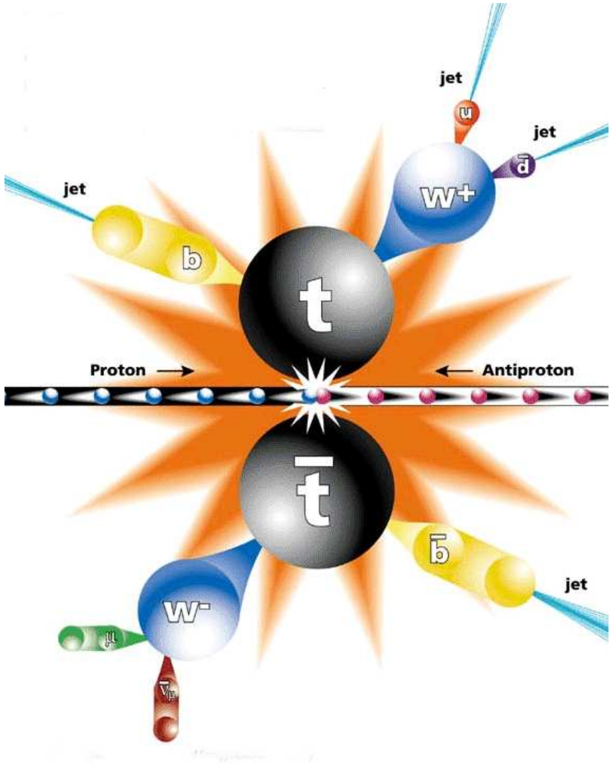
I. **Motivation**

II. **Nested sums and iterated integrals**

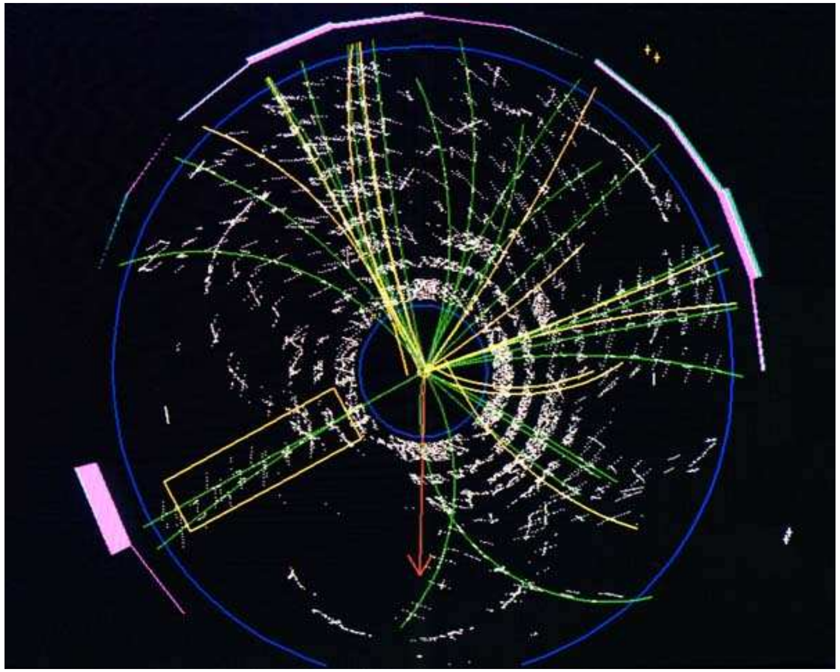
III. **Multiple Polylogarithms**

IV. **Applications**

LHC physics



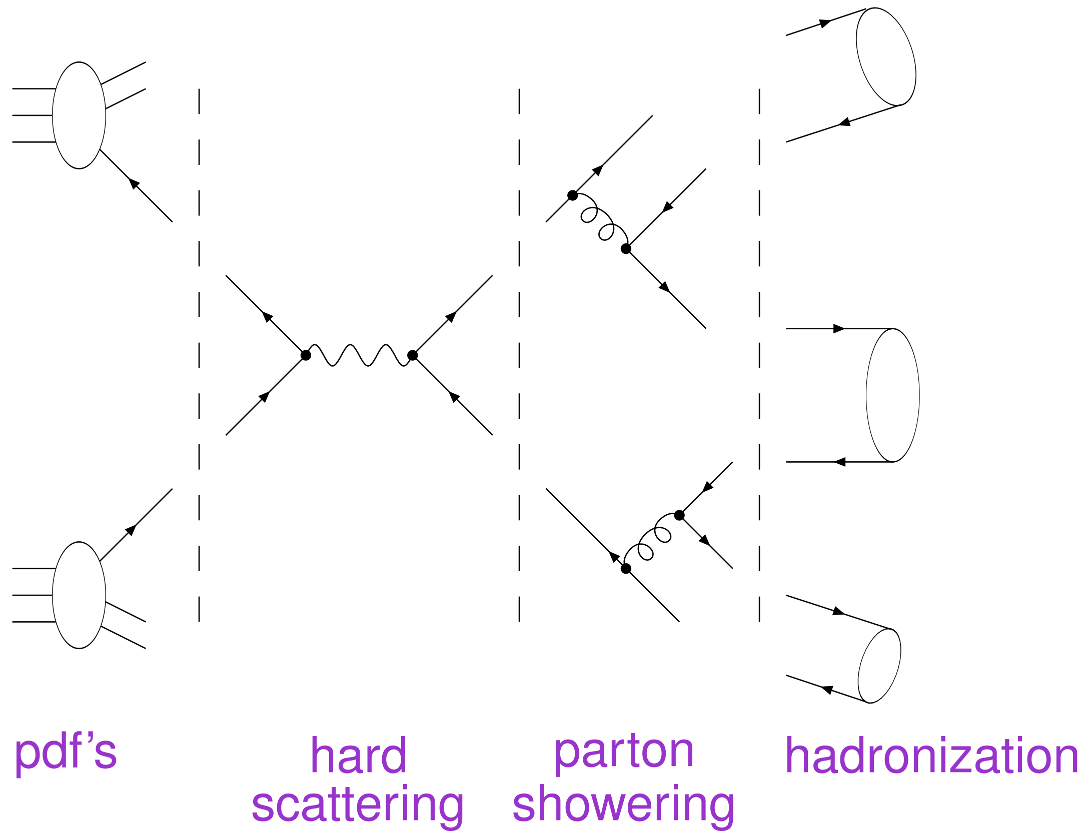
A schematic view of a top-pair event.



A $t\bar{t}$ event from CDF.

Jets: A bunch of particles moving in the same direction

Theoretical understanding



Parton distribution functions are extracted from experiments.
Hard scattering calculated in perturbation theory.
Showering and hadronization depends on approximations and/or models.

Infrared-safe observables depend only mildly on showering and hadronization.

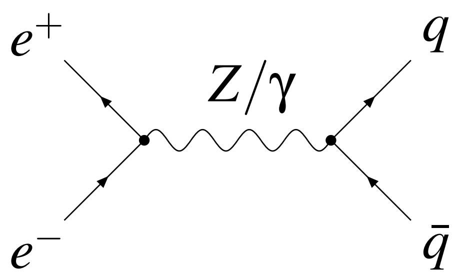
Perturbation theory

Due to the smallness of the coupling constants α and α_s, we may compute the hard scattering at high energies reliable in perturbation theory,

$$\sigma = \sigma_{LO} + \frac{\alpha_s}{2\pi}\sigma_{NLO} + \left(\frac{\alpha_s}{2\pi}\right)^2 \sigma_{NNLO} + \dots$$

At each order, the contribution is given as a sum of Feynman diagrams.

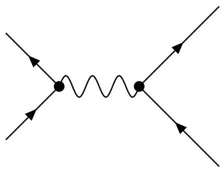
A Feynman diagram for electron-positron annihilation:



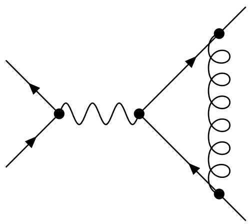
Diagrams

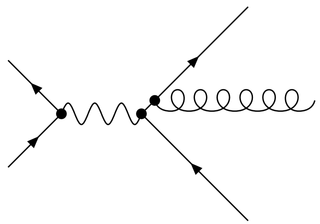
Some examples of diagrams contributing to the various orders in perturbation theory:

LO:

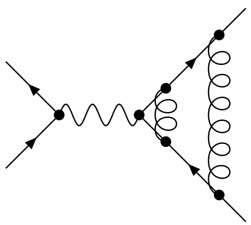


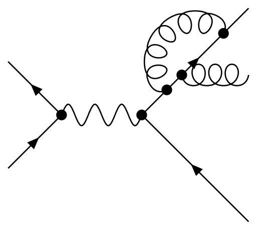
NLO:

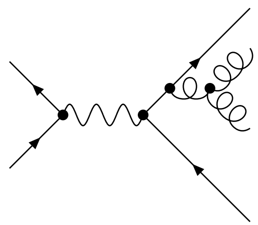


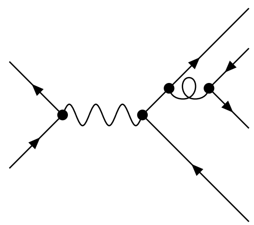


NNLO:



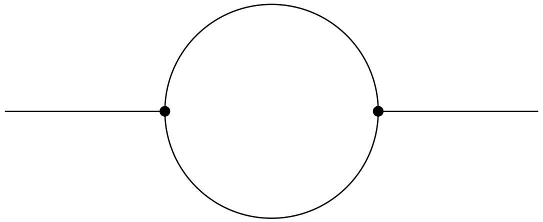






Quantum loop corrections

Loop diagrams are divergent !



$$\int \frac{d^4k}{(2\pi)^4}\frac{1}{(k^2)^2} = \frac{1}{(4\pi)^2}\int_0^\infty dk^2\frac{1}{k^2} = \frac{1}{(4\pi)^2}\int_0^\infty \frac{dx}{x}$$

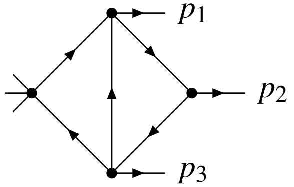
This integral diverges at

- $k^2 \longrightarrow \infty$ (UV-divergence) and at
- $k^2 \longrightarrow 0$ (IR-divergence).

Use dimensional regularization to regulate UV- and IR-divergences.

The two-loop C-topology

The result for the C-topology in arbitrary dimensions and with arbitrary powers of the propagators:



$$
= \frac{\Gamma(2m-2\varepsilon-\nu_{1235})\Gamma(1+\nu_{1235}-2m+2\varepsilon)\Gamma(2m-2\varepsilon-\nu_{2345})\Gamma(1+\nu_{2345}-2m+2\varepsilon)}{\Gamma(\nu_1)\Gamma(\nu_2)\Gamma(\nu_3)\Gamma(\nu_4)\Gamma(\nu_5)\Gamma(3m-3\varepsilon-\nu_{12345})} \frac{\Gamma(m-\varepsilon-\nu_5)\Gamma(m-\varepsilon-\nu_{23})}{\Gamma(2m-2\varepsilon-\nu_{235})}
$$

$$
\cdot(-s_{123})^{2m-2\varepsilon-\nu_{12345}} \sum_{i_1=0}^{\infty}\sum_{i_2=0}^{\infty} \frac{x_1^{i_1}}{i_1!}\frac{x_2^{i_2}}{i_2!} \left[\frac{\Gamma(i_1+\nu_3)\Gamma(i_2+\nu_2)\Gamma(i_1+i_2-2m+2\varepsilon+\nu_{12345})\Gamma(i_1+i_2-m+\varepsilon+\nu_{235})}{\Gamma(i_1+1-2m+2\varepsilon+\nu_{1235})\Gamma(i_2+1-2m+2\varepsilon+\nu_{2345})\Gamma(i_1+i_2+\nu_{23})} \right.
$$

$$
-x_1^{2m-2\varepsilon-\nu_{1235}} \frac{\Gamma(i_1+2m-2\varepsilon-\nu_{125})\Gamma(i_2+\nu_2)\Gamma(i_1+i_2+\nu_4)\Gamma(i_1+i_2+m-\varepsilon-\nu_1)}{\Gamma(i_1+1+2m-2\varepsilon-\nu_{1235})\Gamma(i_2+1-2m+2\varepsilon+\nu_{2345})\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{15})}
$$

$$
-x_2^{2m-2\varepsilon-\nu_{2345}} \frac{\Gamma(i_1+\nu_3)\Gamma(i_2+2m-2\varepsilon-\nu_{345})\Gamma(i_1+i_2+\nu_1)\Gamma(i_1+i_2+m-\varepsilon-\nu_4)}{\Gamma(i_1+1-2m+2\varepsilon+\nu_{1235})\Gamma(i_2+1+2m-2\varepsilon-\nu_{2345})\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{45})}
$$

$$
+x_1^{2m-2\varepsilon-\nu_{1235}} x_2^{2m-2\varepsilon-\nu_{2345}}
$$

$$
\left. \times \frac{\Gamma(i_1+2m-2\varepsilon-\nu_{125})\Gamma(i_2+2m-2\varepsilon-\nu_{345})}{\Gamma(i_1+1+2m-2\varepsilon-\nu_{1235})\Gamma(i_2+1+2m-2\varepsilon-\nu_{2345})} \frac{\Gamma(i_1+i_2+2m-2\varepsilon-\nu_{235})\Gamma(i_1+i_2+3m-3\varepsilon-\nu_{12345})}{\Gamma(i_1+i_2+4m-4\varepsilon-\nu_{12345}-\nu_5)} \right],
$$

with $D = 2m-2\varepsilon$, $x_1 = (-s_{12})/(-s_{123})$ and $x_2 = (-s_{23})/(-s_{123})$.

This sum can be expanded systematically in ε.

Higher transcendental functions

More generally, we get the following types of infinite sums:

- Type A:
$$\sum_{i=0}^{\infty} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a_1')...\Gamma(i+a_k')}\, x^i$$

  Example: Hypergeometric functions ${}_{J+1}F_J$ (up to prefactors).

- Type B:
$$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a_1')...\Gamma(i+a_k')} \frac{\Gamma(j+b_1)...\Gamma(j+b_l)}{\Gamma(j+b_1')...\Gamma(j+b_l')} \frac{\Gamma(i+j+c_1)...\Gamma(i+j+c_m)}{\Gamma(i+j+c_1')...\Gamma(i+j+c_m')}\, x^i y^j$$

  Example: First Appell function F_1.

- Type C:
$$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} \binom{i+j}{j} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a_1')...\Gamma(i+a_k')} \frac{\Gamma(i+j+c_1)...\Gamma(i+j+c_m)}{\Gamma(i+j+c_1')...\Gamma(i+j+c_m')}\, x^i y^j$$

  Example: Kampé de Fériet function S_1.

- Type D:
$$\sum_{i=0}^{\infty}\sum_{j=0}^{\infty} \binom{i+j}{j} \frac{\Gamma(i+a_1)...\Gamma(i+a_k)}{\Gamma(i+a_1')...\Gamma(i+a_k')} \frac{\Gamma(j+b_1)...\Gamma(j+b_l)}{\Gamma(j+b_1')...\Gamma(j+b_l')} \frac{\Gamma(i+j+c_1)...\Gamma(i+j+c_m)}{\Gamma(i+j+c_1')...\Gamma(i+j+c_m')}\, x^i y^j$$

  Example: Second Appell function F_2.

All a, b, c's are of the form “integer $+$ const $\cdot\, \varepsilon$”.

Introducing nested sums

- Definition of Z-sums:

$$Z(n; m_1, \ldots, m_k; x_1, \ldots, x_k) = \sum_{n \geq i_1 > i_2 > \ldots > i_k > 0} \frac{x_1^{i_1}}{i_1^{m_1}} \frac{x_2^{i_2}}{i_2^{m_2}} \ldots \frac{x_k^{i_k}}{i_k^{m_k}}.$$

- Multiple polylogarithms $(n = \infty)$ are a special subset
- Euler-Zagier sums $(x_1 = \ldots = x_k = 1)$ are a special subset
- The nested sums form a Hopf algebra

Z-sums interpolate between multiple polylogarithms and Euler-Zagier sums.

Special cases

For $n=\infty$ the Z-sums are the multiple polylogarithms of Goncharov:

$$\text{Li}_{m_1,...,m_k}(x_1,...,x_k) \quad = \quad Z(\infty;m_1,...,m_k;x_1,...,x_k) = \sum_{i_1>i_2>...>i_k>0}^{\infty} \frac{x_1^{i_1}}{i_1^{m_1}} \frac{x_2^{i_2}}{i_2^{m_2}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}$$

For $x_1 = ... = x_k = 1$ the definition reduces to the Euler-Zagier sums:

$$Z_{m_1,...,m_k}(n) \quad = \quad Z(n;m_1,...,m_k;1,...,1) = \sum_{i_1>i_2>...>i_k>0}^{n} \frac{1}{i_1^{m_1}} \frac{1}{i_2^{m_2}} \cdots \frac{1}{i_k^{m_k}}$$

For $n=\infty$ and $x_1 = ... = x_k = 1$ the sum is a multiple ζ-value:

$$\zeta_{m_1,...,m_k} \quad = \quad Z(\infty;m_1,...,m_k;1,...,1) = \sum_{i_1>i_2>...>i_k>0}^{\infty} \frac{1}{i_1^{m_1}} \frac{1}{i_2^{m_2}} \cdots \frac{1}{i_k^{m_k}}$$

Closely related to Euler-Zagier sums: Harmonic sums

$$S_{m_1,...,m_k}(n) \quad = \quad \sum_{i_1 \geq i_2 \geq ... \geq i_k \geq 1}^{n} \frac{1}{i_1^{m_1}} \frac{1}{i_2^{m_2}} \cdots \frac{1}{i_k^{m_k}}.$$

(Gonzale-Arroyo, Lopez, Yndurain ’79, Vermaseren ’98, Blümlein, Kurth ’98)

Expansion of Gamma functions

Euler-Zagier sums (or harmonic sums) occur in the expansion for Γ functions: For positive integers n we have

$$\Gamma(n+\varepsilon) = \Gamma(1+\varepsilon)\Gamma(n) \cdot \left(1+\varepsilon Z_1(n-1)+\varepsilon^2 Z_{11}(n-1)+\varepsilon^3 Z_{111}(n-1)+...+\varepsilon^{n-1} Z_{11...1}(n-1)\right).$$

Z-sums interpolate between Goncharov's multiple polylogarithms and Euler-Zagier sums.

Multiplication

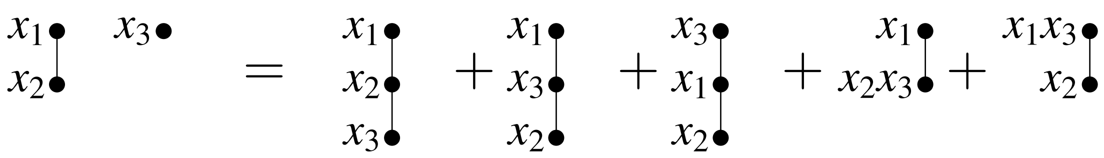
Z-sums obey an algebra:

$$Z(n;m_1,m_2;x_1,x_2)\cdot Z(n;m_3;x_3) =$$

$$= \quad Z(n;m_1,m_2,m_3;x_1,x_2,x_3)+Z(n;m_1,m_3,m_2;x_1,x_3,x_2)+Z(n;m_3,m_1,m_2;x_3,x_1,x_2)$$

$$+Z(n;m_1,m_2+m_3;x_1,x_2x_3)+Z(n;m_1+m_3,m_2;x_1x_3,x_2)$$

Pictorial representation:



The multiplication law corresponds to a quasi-shuffle algebra (Hoffman ‘99), also called stuffle algebra (Broadhurst)) or mixed shuffle algebra (Guo).

Hopf algebras

The Z-sums form actually a Hopf algebra.

- An algebra has a multiplication $\cdot$ and a unit e.
- A coalgebra has a comultiplication Δ and a counit $\bar{e}$.
- A Hopf algebra is an algebra and a coalgebra at the same time, such that the two structures are compatible with each other.

  In addition, there is an antipode S.

Algorithms

Multiplication:

$$Z(n;m_1,...;x_1,...)\cdot Z(n;m'_1,...;x'_1,...)$$

Convolution: Sums involving i and $n-i$

$$\sum_{i=1}^{n-1}\frac{x_1^i}{i^{m_1}}Z(i-1;m_2...;x_2,...)\frac{{x'_1}^{n-i}}{(n-i)^{m'_1}}Z(n-i-1;m'_2,...;x'_2,...)$$

Conjugations:

$$-\sum_{i=1}^{n}\left(\begin{array}{c} n \\ i \end{array}\right)(-1)^i\frac{x_0^i}{i^{m_0}}Z(i;m_1,...,m_k;x_1,...,x_k)$$

Conjugation and convolution: Sums involving binomials and $n-i$

$$-\sum_{i=1}^{n-1}\left(\begin{array}{c} n \\ i \end{array}\right)(-1)^i\frac{x_1^i}{i^{m_1}}Z(i;m_2...;x_2,...)\frac{{x'_1}^{n-i}}{(n-i)^{m'_1}}Z(n-i;m'_2,...;x'_2,...)$$

(Moch, Uwer, S.W., '01)

Multiple polylogarithms

$$\mathrm{Li}_{m_1,...,m_k}(x_1,...,x_k) = \sum_{i_1>i_2>...>i_k>0} \frac{x_1^{i_1}}{i_1^{m_1}} \frac{x_2^{i_2}}{i_2^{m_2}} \cdots \frac{x_k^{i_k}}{i_k^{m_k}}.$$

- Special subsets: Harmonic polylogs, Nielsen polylogs, classical polylogs

  (Remiddi and Vermaseren, Gehrmann and Remiddi).

- Have also an integral representation.

- Fulfill two Hopf algebras.

- Can be evaluated numerically for all complex values of the arguments

  (Gehrmann and Remiddi, Vollinga and S.W.).

Multiple polylogarithms

The multiple polylogarithms have extensively been studied by Borwein, Bradley, Broadhurst and Lisonek. The multiple polylogarihms contain as subsets the classical polylogarithms

$$\text{Li}_n(x),$$

Nielsen's generalized polylogarithms

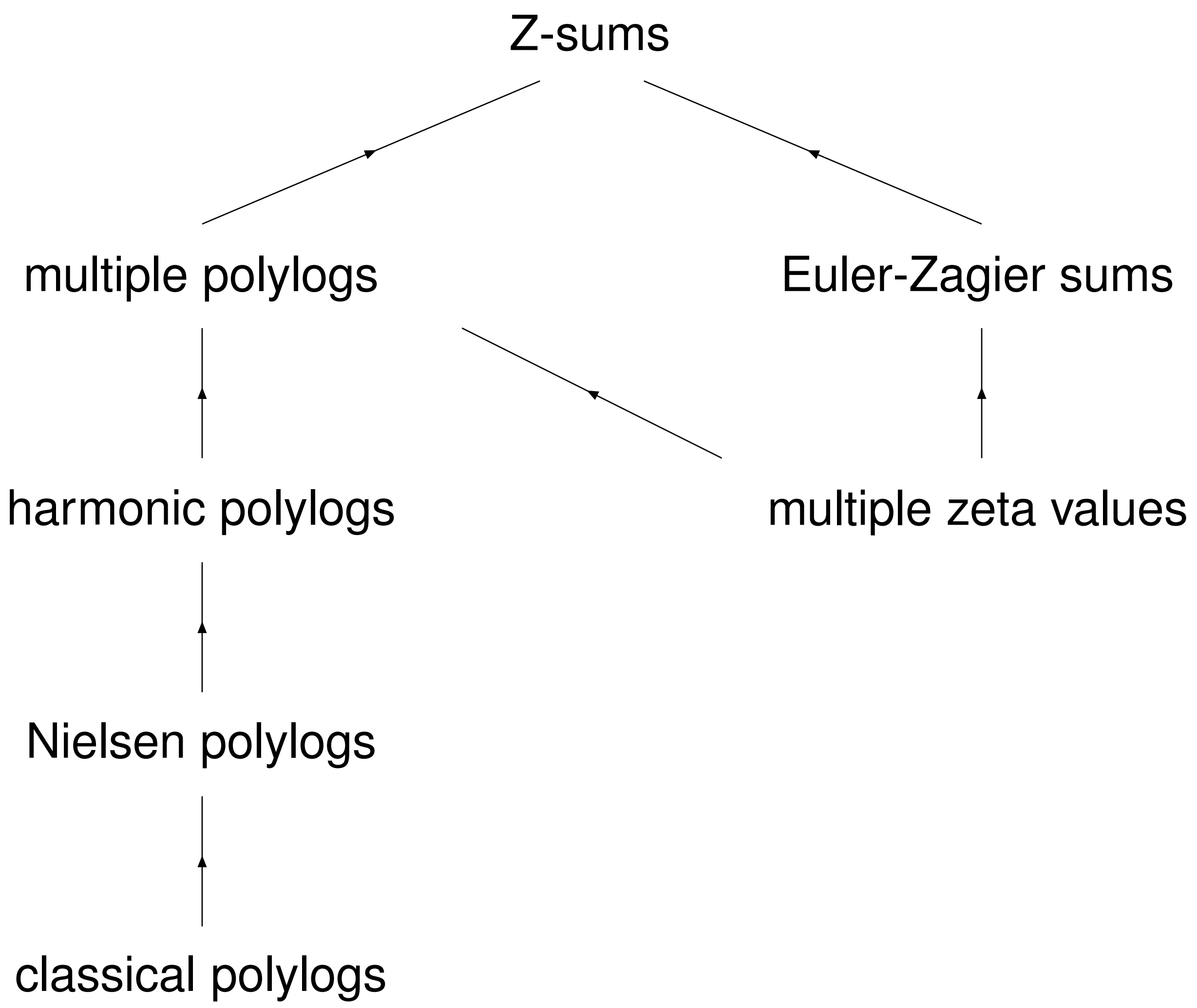
$$S_{n,p}(x) = \text{Li}_{n+1,1,...,1}(x,\underbrace{1,...,1}_{p-1}),$$

the harmonic polylogarithms of Remiddi and Vermaseren

$$H_{m_1,...,m_k}(x) = \text{Li}_{m_1,...,m_k}(x,\underbrace{1,...,1}_{k-1})$$

and the two-dimensional harmonic polylogarithms introduced by Gehrmann and Remiddi.

Inheritance



Iterated integrals

Define the functions G by

$$G(z_1,...,z_k;y) \quad = \quad \int\limits_0^y \frac{dt_1}{t_1-z_1} \int\limits_0^{t_1} \frac{dt_2}{t_2-z_2} ... \int\limits_0^{t_{k-1}} \frac{dt_k}{t_k-z_k}.$$

Scaling relation:

$$G(z_1,...,z_k;y) \quad = \quad G(xz_1,...,xz_k;xy)$$

Short hand notation:

$$G_{m_1,...,m_k}(z_1,...,z_k;y) \quad = \quad G(\underbrace{0,...,0}_{m_1-1},z_1,...,z_{k-1},\underbrace{0...,0}_{m_k-1},z_k;y)$$

Conversion to multiple polylogarithms:

$$\mathrm{Li}_{m_1,...,m_k}(x_1,...,x_k) \quad = \quad (-1)^k G_{m_1,...,m_k}\left(\frac{1}{x_1},\frac{1}{x_1 x_2},...,\frac{1}{x_1...x_k};1\right).$$

Shuffle algebra

The functions $G(z_1, ..., z_k; y)$ fulfill a shuffle algebra.

Example:

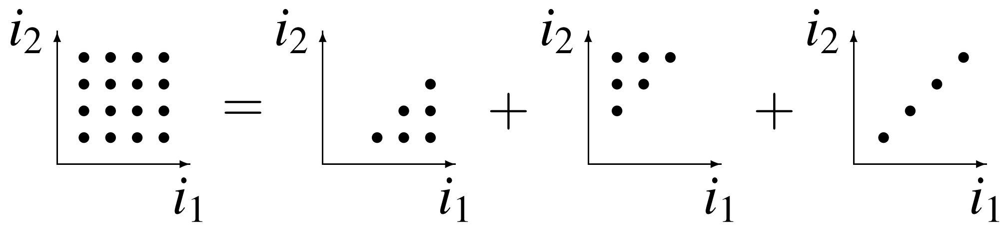
$$G(z_1, z_2; y) G(z_3; y) \quad = \quad G(z_1, z_2, z_3; y) + G(z_1, z_3 z_2; y) + G(z_3, z_1, z_2; y)$$

This algebra is different from the quasi-algebra already encountered and provides the second Hopf algebra for multiple polylogarithms.

Shuffle algebra versus quasi-shuffle algebra

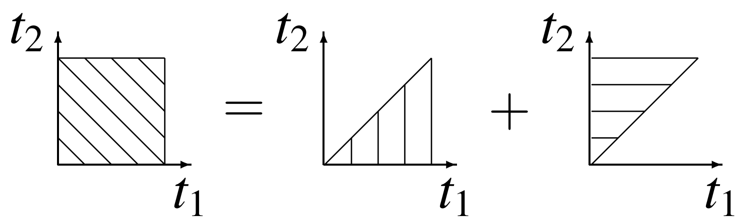
Quasi-shuffle algebra for Z-sums:

$$Z(n;m_1;x_1)Z(n;m_2;x_2) = Z(n;m_1,m_2;x_1,x_2) + Z(n;m_2,m_1;x_2,x_1) + Z(n;m_1+m_2;x_1x_2).$$



Shuffle algebra for G-functions:

$$G(z_1;y)G(z_2;y) = G(z_1,z_2;y) + G(z_2,z_1;y)$$



Partial integration and the antipode

Integration-by-parts identity:

$$G(z_1,...,z_k;y)+(-1)^k G(z_k,...,z_1;y)$$
$$= \quad G(z_1;y)G(z_2,...,z_k;y) - G(z_2,z_1;y)G(z_3,...,z_k;y) + ... - (-1)^{k-1} G(z_{k-1},...,z_1;y)G(z_k;y)$$

From the Hopf algebra we have the antipode

$$SG(z_1,...,z_k;y) \quad = \quad (-1)^k G(z_k,...,z_1;y)$$

Working out the identity for the antipode

$$\sum_{(G)} S\left(G^{(1)}\right) \cdot G^{(2)} \quad = \quad 0$$

one recovers the integration-by-parts identity.

The antipode

From the shuffle algebra of the iterated integrals we had:

$$G(z_1,...,z_k;y) + (-1)^k G(z_k,...,z_1;y)$$
$$= \text{simpler terms}$$

Using the equation for the antipode for Z-sums in the quasi-shuffle algebra:

$$Z(n;m_1,...,m_k;x_1,...,x_k) + (-1)^k Z(n;m_k,..,m_1;x_k,...,x_1)$$
$$= \text{simpler terms}$$

The equation for the antipode generalizes integration-by-parts identities to cases where no integral representation exists !

Numerical evaluations of multiple polylogarithms

Example: Numerical evaluation of the dilogarithm ('t Hooft, Veltman, Nucl. Phys. B153, (1979), 365)

$$\mathrm{Li}_2(x) = -\int_0^x dt \frac{\ln(1-t)}{t} = \sum_{n=1}^{\infty} \frac{x^n}{n^2}$$

Map into region $-1 \leq \mathrm{Re}(x) \leq 1/2$, using

$$\mathrm{Li}_2(x) = -\mathrm{Li}_2\left(\frac{1}{x}\right) - \frac{\pi^2}{6} - \frac{1}{2}\left(\ln(-x)\right)^2, \qquad \mathrm{Li}_2(x) = -\mathrm{Li}_2(1-x) + \frac{\pi^2}{6} - \ln(x)\ln(1-x).$$

Accelaration using Bernoulli numbers:

$$\mathrm{Li}_2(x) = \sum_{i=0}^{\infty} \frac{B_i}{(i+1)!}\left(-\ln(1-x)\right)^{i+1},$$

Generalization to multiple polylogarithms, using arbitrary precision arithmetic in C++.

J. Vollinga, S.W., (2004)

Numerical evaluations of multiple polylogarithms

Use the integral representation

$$G_{m_1,...,m_k}(z_1,z_2,...,z_k;y) \quad = \quad \int\limits_0^y \left(\frac{dt}{t}\circ\right)^{m_1-1} \frac{dt}{t-z_1} \left(\frac{dt}{t}\circ\right)^{m_2-1} \frac{dt}{t-z_2} ... \left(\frac{dt}{t}\circ\right)^{m_k-1} \frac{dt}{t-z_k}$$

to transform all arguments into a region, where we have a converging power series expansion:

$$G_{m_1,...,m_k}(z_1,...,z_k;y) =$$
$$\sum_{j_1=1}^{\infty} ... \sum_{j_k=1}^{\infty} \frac{1}{(j_1+...+j_k)^{m_1}} \left(\frac{y}{z_1}\right)^{j_1} \frac{1}{(j_2+...+j_k)^{m_2}} \left(\frac{y}{z_2}\right)^{j_2} ... \frac{1}{(j_k)^{m_k}} \left(\frac{y}{z_k}\right)^{j_k}.$$

Use the Hölder convolution to accelerate the convergent series.

(Borwein, Bradley, Broadhurst and Lisonek)

Computer algebra systems and packages

GiNaC was written in 1999-2004 by Ch. Bauer, A. Frink, R. Kreckel and J. Vollinga at the University of Mainz.

Despite it's name, it is a computer algebra system. Allows symbolic calculations in C++.

Available at `http://www.ginac.de`.

FORM

Written by J.A.M. Vermaseren.
Available at `http://www.nikhef.nl/~form`.

Nestedsums: S.W., '02
XSummer: S. Moch, P. Uwer, '05

The amplitudes for $e^+e^- \longrightarrow 3$ jets at NNLO

A NNLO calculation of $e^+e^- \longrightarrow 3$ jets requires the following amplitudes:

- Born amplitudes for $e^+e^- \longrightarrow 5$ jets:

  F. Berends, W. Giele and H. Kuijf.

- One-loop amplitudes for $e^+e^- \longrightarrow 4$ jets:

  Z. Bern, L. Dixon, D.A. Kosower and S.W.;

  J. Campbell, N. Glover and D. Miller.

- Two-loop amplitudes for $e^+e^- \longrightarrow 3$ jets:

  L. Garland, T. Gehrmann, N. Glover, A. Koukoutsakis and E. Remiddi;

  S. Moch, P. Uwer and S.W.

Results for the two-loop amplitude

The finite part of the coefficient of a spinor structure:

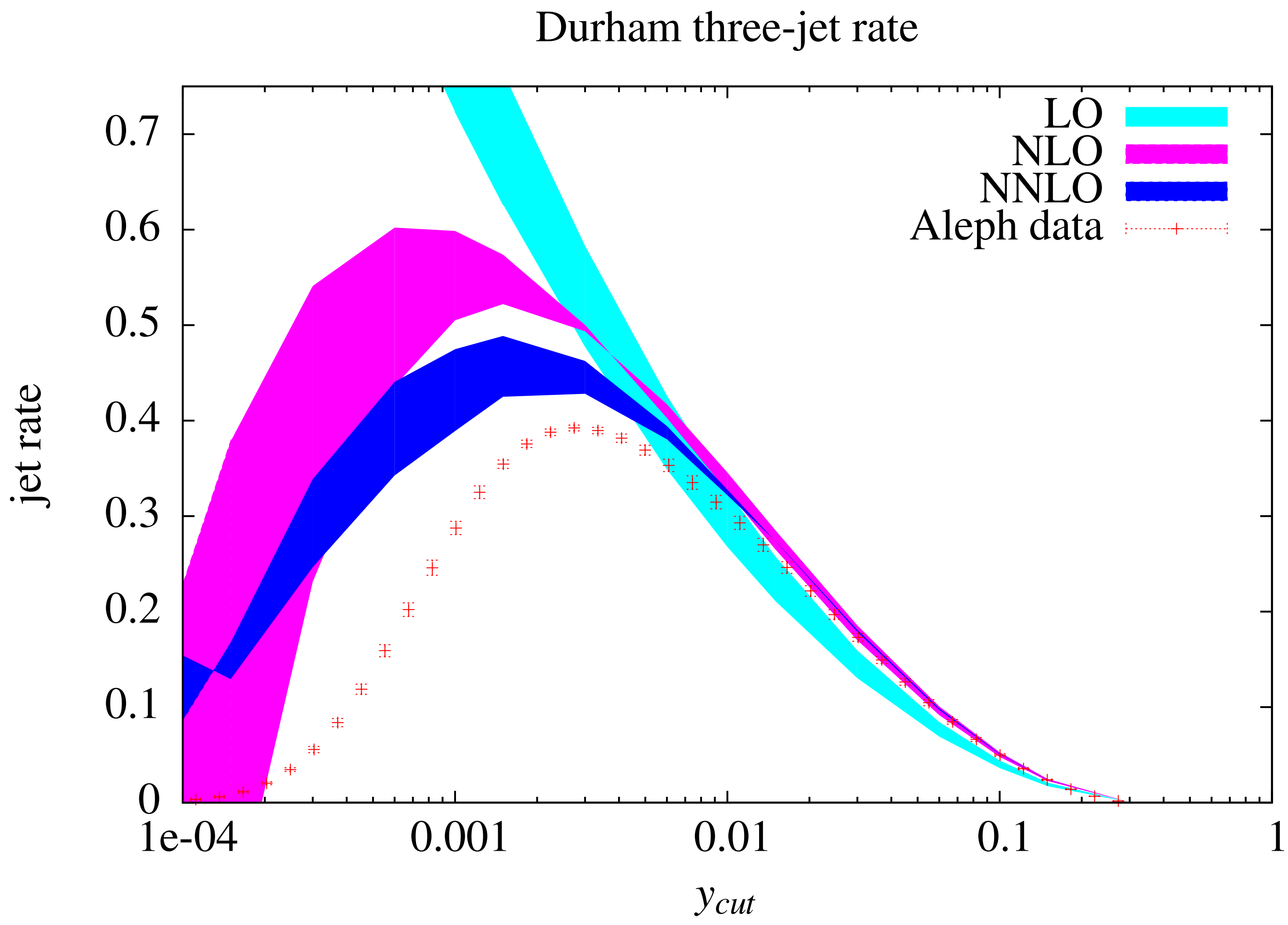
$$c_{12}^{(2),\mathrm{fin}}(x_1,x_2) = N_f N \Bigg(3\frac{\ln(x_1)}{(x_1+x_2)^2} + \frac{1}{4}\frac{\ln(x_2)^2 - 2\mathrm{Li}_2(1-x_2)}{x_1(1-x_2)} + \frac{1}{12}\frac{\zeta(2)}{(1-x_2)x_1} - \frac{1}{18}\frac{13x_1{}^2+36x_1-10x_1x_2-18x_2+31x_2{}^2}{(x_1+x_2)^2x_1(1-x_2)}\ln(x_2)$$
$$+\frac{x_1{}^2-x_2{}^2-2x_1+4x_2}{(x_1+x_2)^4}\mathrm{R}_1(x_1,x_2) - \frac{1}{12}\frac{\mathrm{R}(x_1,x_2)}{x_1(x_1+x_2)^2}\left[5x_2+42x_1+5-\frac{(1+x_1)^2}{1-x_2}-4\frac{1-3x_1+3x_1{}^2}{1-x_1-x_2}-72\frac{x_1{}^2}{x_1+x_2}\right] + \left[\frac{1}{12}\frac{1}{x_1(1-x_2)}+\frac{6}{(x_1+x_2)^3}\right.$$
$$\left.-\frac{1+2x_1}{x_1(x_1+x_2)^2}\right](\mathrm{Li}_2(1-x_2)-\mathrm{Li}_2(1-x_1)) - \frac{1}{(x_1+x_2)x_1}\Bigg) - \frac{1}{2}I\pi N_f N\frac{\ln(x_2)}{x_1(1-x_2)}\,.$$

where $\mathrm{R}(x_1,x_2)$ and $\mathrm{R}_1(x_1,x_2)$ are defined by

$$\mathrm{R}(x_1,x_2) = \left(\frac{1}{2}\ln(x_1)\ln(x_2) - \ln(x_1)\ln(1-x_1) + \frac{1}{2}\zeta(2) - \mathrm{Li}_2(x_1)\right) + (x_1 \leftrightarrow x_2)\,.$$

$$\mathrm{R}_1(x_1,x_2) = \Bigg(\ln(x_1)\mathrm{Li}_{1,1}\left(\frac{x_1}{x_1+x_2},x_1+x_2\right) - \frac{1}{2}\zeta(2)\ln(1-x_1-x_2) + \mathrm{Li}_3(x_1+x_2) - \ln(x_1)\mathrm{Li}_2(x_1+x_2) - \frac{1}{2}\ln(x_1)\ln(x_2)\ln(1-x_1-x_2)$$
$$-\mathrm{Li}_{1,2}\left(\frac{x_1}{x_1+x_2},x_1+x_2\right) - \mathrm{Li}_{2,1}\left(\frac{x_1}{x_1+x_2},x_1+x_2\right)\Bigg) + (x_1 \leftrightarrow x_2)\,.$$

Results for the three-jet rate in electron-positron annihilation



S.W., arXiv:0807.3241

Summary

- Systematic algorithms for the calculation of loop integrals based on:
  - nested sums,
  - iterated integrals

- These iterated objects exhibit a rich algebraic structure

- Multiple polylogarithms appear in loop integrals