Computer Algebra Methods in Probing the Physics at Shortest Distances of the Microcosm

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1. Introduction

Loops and Legs:

Feynman diagrams describe elementary scattering processes between bosons and fermions in Quantum Field Theory (QFT). Here we will thoroughly refer to renormalizable QFTs.

Where are these techniques important?

1. Perturbation Theory of the Standard Model and its renormalizable extensions.
2. String amplitude calculations
3. Perturbative calculations in Gravity
4. non-relativistic field theories in vacuum and at finite temperature and/or density

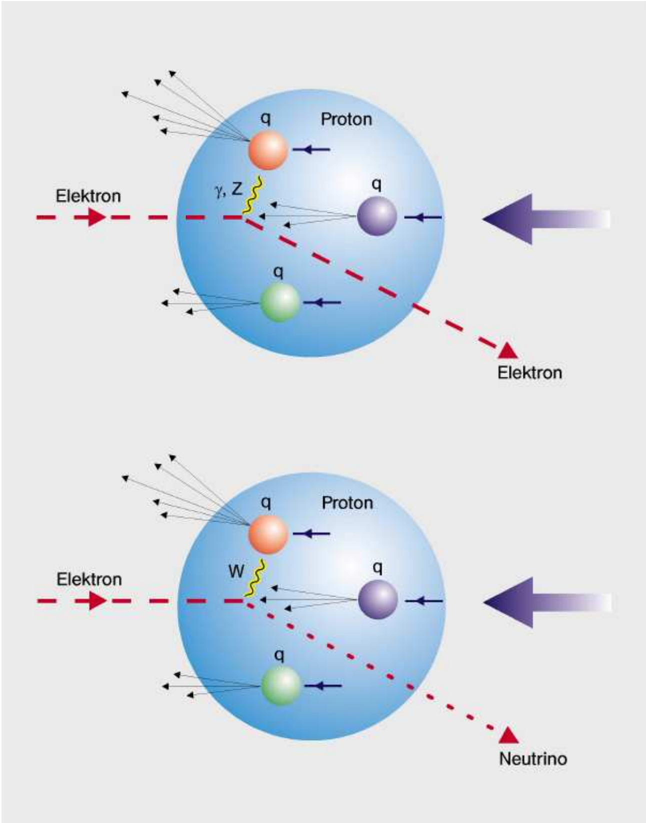
We will calculate Feynman diagrams. These are skeletons according to Feynman rules, connecting vertices with propagators.

They possess external lines: The Legs.

They possess internal closed lines: The Loops.

The machines, for which we perform the calculations:

LHC, Geneva/CH



HERA, Hamburg/D

microscopy of the proton

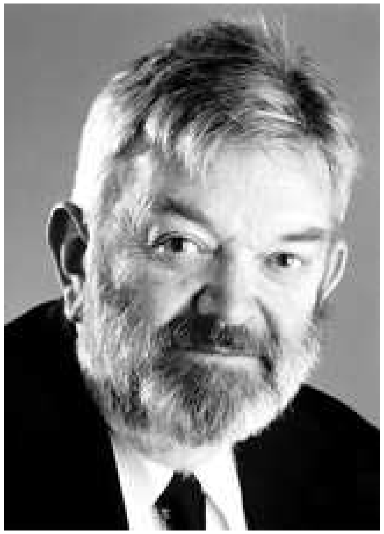
Why are these calculations important ?

1. Precision extraction of coupling constants: $\alpha_s(M_Z)@1\%$
2. Do couplings unite at high scales and in which field theories?
3. Precision measurements of m_c, m_b, m_t at LHC and a future ILC
4. Precision understanding of the Higgs and top sector (at the LHC, ILC and possibly other machines)
5. Unravel the mathematical structure of microscopic processes analytically: get further with the Stueckelberg-Feynman programme as far as you can.

$\Longrightarrow$ Genetic Code of the Micro Cosmos

2. The Computer Algebra Landscape in Quantum Field Theory

The pioneers:



M. Veltman
Schoonschip

A.C. Hearn
Reduce

(1999)

both started 1963

1. Almost all calculations in QFT were performed using these packages $\lesssim 1989$.
2. The renormalizibility proof of the SM needed Schoonschip to be verified in its details.
3. Level: 1- and 2-loop calculations mostly; first 3-loop calculations.

The Computer Algebra Landscape in Quantum Field Theory

Many symbolic systems and packages written using various languages are in use and will be in use in the future.

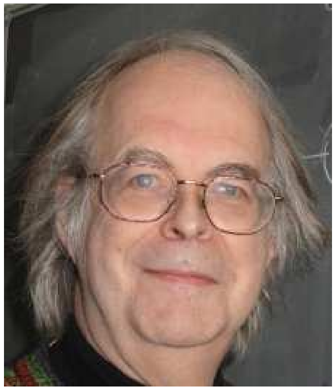
1. Fortran, C
2. Mathematica
3. Maple
4. FORM
5. GiNac
6. Sage
7. Pari, and others

- Many calculations bind different packages by shell-scripts to a general computer-algebraic work-flow to solve large-scale problems.
- Condition: the average time used in the parts is not tiny.
- Allows for natural checkpoints; in- and output pattern has to be provided in an automated form.

Our computer-algebra cluster currently consists of more than 10 units with $\sim$ 16 Tbyte RAM and $\sim$ 230 Tbyte fast disc together; we use hundreds of Mathematica licenses.

The main steps of a typical large scale calculation

1. Generate the Feynman diagrams: $O(100 - 100.000)$ package QGRAF [Fortran]
   P. Nogueira
2. Calculate all group theoretic structures: package COLOR [FORM]
   T. van Ritbergen et al.
3. Perform all tensor and Dirac-matrix calculations in $4 + \varepsilon$ dimensions, perform all radial momentum integrals: package FORM; J. Vermaseren
   remaining: Feynman parameter integrals.



J. Vermaseren

1. FORM (since the late 80ies) became the most powerful C-programme to perform particle physics calculations. It is a specialized package.
2. Efficient treatment of giant number of terms, very good memory management, several parallelization possibilities
3. Several additional packages: e.g. special numbers, harmonic sums, harmonic polylogarithms
4. Implementation of 4-loop master integrals, R^* renormalization operation; allows for several 5-loop calculations.

The main steps of a typical large scale calculation

4. Alternatively: reduce to a small number of scalar master integrals, to be calculated by other methods.
5. All accessible Gauß-Stokes integrals are used to reduce millions of scalar integrals often to $O(100 - 5000)$ master integrals; different codes. Examples: S. Laporta, Anastasiou, Studerus/Manteuffel: Reduze2, Marquard, Lee, and many more.

Example: 3-loop heavy flavor corrections to DIS

[S. Wolfram computed the 1-loop correction in 1978, after E. Witten 1976]

The reduction to master integrals produces 1.6 Tbyte C-output of relations to determine the master integrals.

100.000ds of scalar integrals $\Longrightarrow$ 687 3-loop master integrals.

In the calculation of the master integrals Mathematica plays a key-role.

Cooperation with the Research Institute of Symbolic Computation

1. Symbolic summation and integration in difference field theory
2. Symbolic solution of large differential equation systems
3. Special functions and numbers in QFT
4. Modular forms and functions, q-series

C. Schneider

J. Ablinger

P. Paule, chairman of RISC

Mathematica packages :

1. Sigma (C.S.)
2. EvaluateMultSums, Sumproduction, SolveCoupledSystems (C.S)
3. HarmonicSums, MultiIntegrate (J.A.)
4. RhoSum (M. Round)

3. Symbolic Integration of Feynman Integrals

1. Integration by parts technique
2. Mellin-Barnes techniques
3. PSLQ: zero-dimensional integrals
4. Guessing: one-dimensional integrals
5. Generalized hypergeometric functions (and extensions)
6. Risch algorithms [C.G. Raab]
7. Solution of master-integrals using difference and differential equations
8. Summation techniques: construction of difference rings and fields
9. (multivalued) Almkvist-Zeilberger algorithm ... and others.
10. The method of arbitrary high moments

Function Spaces

Sums

Harmonic Sums

$$\sum_{k=1}^{N} \frac{1}{k} \sum_{l=1}^{k} \frac{(-1)^l}{l^3}$$

gen. Harmonic Sums

$$\sum_{k=1}^{N} \frac{(1/2)^k}{k} \sum_{l=1}^{k} \frac{(-1)^l}{l^3}$$

Cycl. Harmonic Sums

$$\sum_{k=1}^{N} \frac{1}{(2k+1)} \sum_{l=1}^{k} \frac{(-1)^l}{l^3}$$

Binomial Sums

$$\sum_{k=1}^{N} \frac{1}{k^2} \binom{2k}{k} (-1)^k$$

Integrals

Harmonic Polylogarithms

$$\int_0^x \frac{dy}{y} \int_0^y \frac{dz}{1+z}$$

gen. Harmonic Polylogarithms

$$\int_0^x \frac{dy}{y} \int_0^y \frac{dz}{z-3}$$

Cycl. Harmonic Polylogarithms

$$\int_0^x \frac{dy}{1+y^2} \int_0^y \frac{dz}{1-z+z^2}$$

root-valued iterated integrals

$$\int_0^x \frac{dy}{y} \int_0^y \frac{dz}{z\sqrt{1+z}}$$

non-iterating integrals.

$$\int_0^z dx \frac{\ln(x)}{1+x} \, {}_2F_1\left[\begin{matrix} \frac{4}{3}, \frac{5}{3} \\ 2 \end{matrix}; \frac{x^2(x^2-9)^2}{(x^2+3)^3}\right]$$

Special Numbers

multiple zeta values

$$\int_0^1 dx \frac{\mathrm{Li}_3(x)}{1+x} = -2\mathrm{Li}_4(1/2) + \ldots$$

gen. multiple zeta values

$$\int_0^1 dx \frac{\ln(x+2)}{x-3/2} = \mathrm{Li}_2(1/3) + \ldots$$

cycl. multiple zeta values

$$\mathbf{C} = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)^2}$$

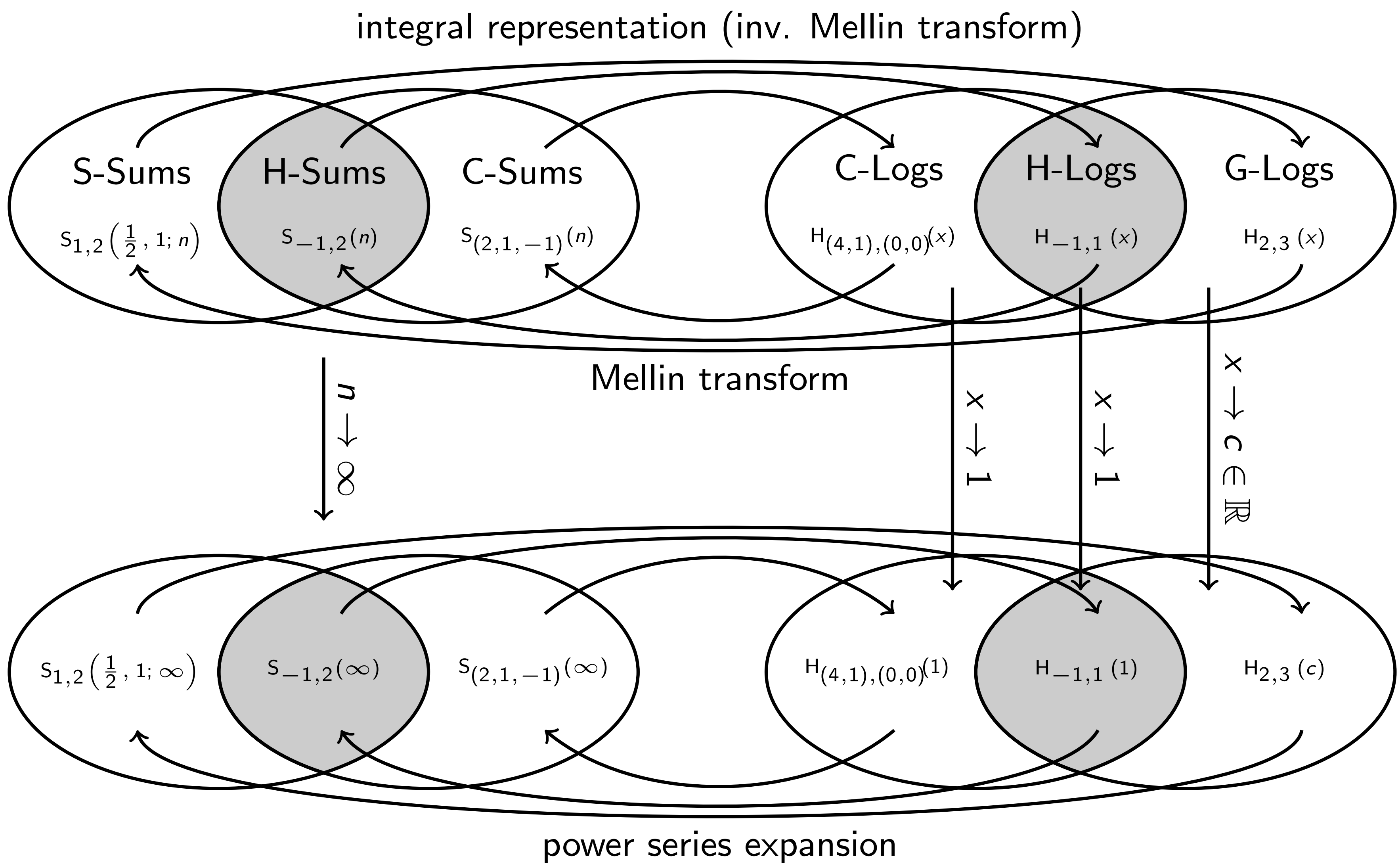
associated numbers

$$\mathrm{H}_{8,w_3} = 2\mathrm{arccot}(\sqrt{7})^2$$

associated numbers

$$\int_0^1 dx \, {}_2F_1\left[\begin{matrix} \frac{4}{3}, \frac{5}{3} \\ 2 \end{matrix}; \frac{x^2(x^2-9)^2}{(x^2+3)^3}\right]$$

shuffle, stuffle, and various structural relations $\Longrightarrow$ algebras



square-root valued letters $\Longleftrightarrow$ nested binomial sums $\binom{2i}{i}$

non-iterative iterative integrals $\Longrightarrow$ Iterate on non-it. integrals with rat. argument (complete elliptic integrals) (arXiv:1706.01299)

The PSLQ-Method

Seek an Integer Relation over a basis of special numbers out of a special class.

Example:

$$I = \int_0^1 dx \frac{\mathrm{Li}_3(x)}{1+x}$$

The integral is of "transcendentality" $\tau = 4$.

The expected HPL(1) basis is spanned by:

$\ln^4(2),\ \ln(2)\zeta_3,\ \ln^2(2)\zeta_2,\ \zeta_2^2,\ \mathrm{Li}_4(1/2)$.

Calculate this integral numerically to high number of digits, e.g. 40 digits.

$$I \approx 0.3395454690873598695906678484608602061388$$

The PSLQ algorithm yields:

$$\begin{aligned} I &= -\frac{1}{12}\ln^4(2) + \frac{\pi^4}{60} + \frac{3}{4}\ln(2)\zeta_3 + \frac{1}{12}\ln^2(2)\pi^2 - 2\mathrm{Li}_4\left(\frac{1}{2}\right) \\ \zeta_{2k} &= (-1)^{k-1}\frac{(2\pi)^{2k}B_{2k}}{2(2k)!}; \quad B_n \quad \text{[Bernoulli number]} \end{aligned}$$

Guessing Difference Equations

It is often easier to calculate Mellin moments for a quantity for fixed values of N than to derive the relation for general values of N in the first place. If the quantity under consideration is known to be recurrent than its difference equation is of finite order and degree.

$$\exists \quad \sum_{k=0}^{O} P_k^{(l)}(N) F(k+N) = 0; \qquad \text{max}\{l\} \text{ - degree; } O \text{ - order}$$

Example:

$$-(N+1)^3 F(N) - (3N^2 - 9N - 7) F(N+1) + (N+2)^3 F(N+2) = 0$$

$$F(1) = 1; \quad F(2) = \frac{1}{8}$$

Solution: $$F(N) = \sum_{k=1}^{N} \frac{1}{k^3} = S_3(N)$$

Guessing Difference Equations

Solution of large problems

Assume you would like to calculate the massless 3-loop Wilson coefficients in deep-inelastic scattering using this method. How many moments would you need and how do they look like ?

About 5200 moments are needed. The largest ones are ratios of #13000/#13000 digits. They can be calculated within 15 min.

After 3 weeks you weree needed in 2009 find a difference equation of degree ~ 1000 and order 35, if you have a reasonable computer (100 Gbyte RAM). After another week you have the solution as function of N. [Now all times are much smaller: a few days only.]

Problem: It is sophisticated to obtain the input a priori. Combined solution-methods do work, however, to $O(1500)$ moments.

Recent results: 3-loop anomalous dimension computed from scratch.
[arXiv:1701.04614, 1705.01508, 1908.03779, 2107.06267, 2111.12401].

Generalized Hypergeometric Functions

At lower number of legs and/or loops Feynman integrals happen to be represented by these functions.

After suitable mappings these functions have compact representations in infinite (multiple) absolutely convergent sums.

This allows for the Laurent-expansion in ε under the summation operator.

Important Examples:

1. $B(a, b)$
2. ${}_pF_q(a_i; b_j; x)$; always single sums
3. Appell functions; double sums
4. Kampé de Feriet functions, Horn functions and higher; more sums [cf. 2111.15501]

The sums may be expanded and summed using algorithms like nestedsums, xsummer, HarmonicSums, Sigma, EvaluateMultiSums

Generalized Hypergeometric Functions

Example:

Integrals of the following type emerge:

$$\begin{aligned} I_1(z) &= \int_0^1 dy y^\delta (1-y)^\eta \int_0^1 dx x^{\beta-1} (1-x)^{\gamma-\beta-1} (1-xyz)^{-\alpha} \\ &= B(\beta, \gamma-\beta) \int_0^1 dy y^\delta (1-y)^\eta \; {}_2F_1(\alpha, \beta; \gamma; yz) \\ &= B(\beta, \gamma-\beta) B(\delta, \eta-\delta) \; {}_3F_2(\delta, \alpha, \beta; \eta, \gamma; z) \end{aligned}$$

All ${}_pF_q$'s have single series representations. One series counts as one integral.

$${}_pF_q(a_1, ..., a_p; b_1...b_q; z) = \sum_{k=0}^{\infty} \frac{(a_1)_k ... (a_p)_k}{(b_1)_k ... (b_q)_k} \frac{z^k}{k!}$$

Summation Techniques

The integrals can usually be traded for a lower number of sums (finite or infinite).

Solve these sums for N and/or in terms of special constants.

Principal Idea:

1. Sums may be represented in vector spaces, algebras, and finally fields/rings
2. Rephrase the sums in the setting of difference fields and rings
3. Apply telescoping, creative telescoping, and other principles in this setting to compute recurrences
4. Try to solve the recurrences; possible for most sums occurring from Feynman integrals
5. In addition, use nested sums algebras to speed up calculations

Telescoping: Find a function $g(k)$ such

$$\begin{aligned} f(k) &= g(k+1) - g(k) \\ F(N) &= \sum_{k=1}^{N} f(k) = g(N+1) - g(1) \end{aligned}$$

$\Longrightarrow$ nested sums algebras $\Longrightarrow$ bases

Sigma solves large scale problems running over months and using several hundred Gb RAM.

Differential Equations

The IBPs deliver a vast amount of differential equations forming systems, which are nested hierarchically.

Provide boundary conditions [usually using other methods]

Perform uncoupling of these systems

• In case of complete 1st order uncoupling: $\exists$ complete solution algorithm in case of any basis choice for 1 parameter systems
All solutions are iterative integrals over whatsoever alphabet:
$\int_0^x dy f_a(y) H_{\vec{b}}(y)$

• Irreducible nth order systems $(n \geq 2)$: present target of research even in mathematics; good prospects in case of 2nd order systems [convergent near integer power series (CIS)]
At least one function is given by a definite integral, others iterate on.

$\Longrightarrow$ iterated integral algebras $\Longrightarrow$ bases

The Almkvist-Zeilberger Algorithm

- Given a multiple integral over hyperexponential terms:

$F(n) = \int_0^1 dx_1 ... dx_j \prod_{k=1}^{l} (P(x_i, n))^{r_k, \epsilon}$, $r_k \in \mathbb{R}$ and $n \in \mathbb{N}$ a parameter.

- Find a recurrence: $\sum_{k=0}^{m} p_k(n, \epsilon) F(n+k) = H(n, \epsilon)$ with some inhomogeneity $H(n, \epsilon)$.
- Correspondingly $n \to x$, a differential equation:

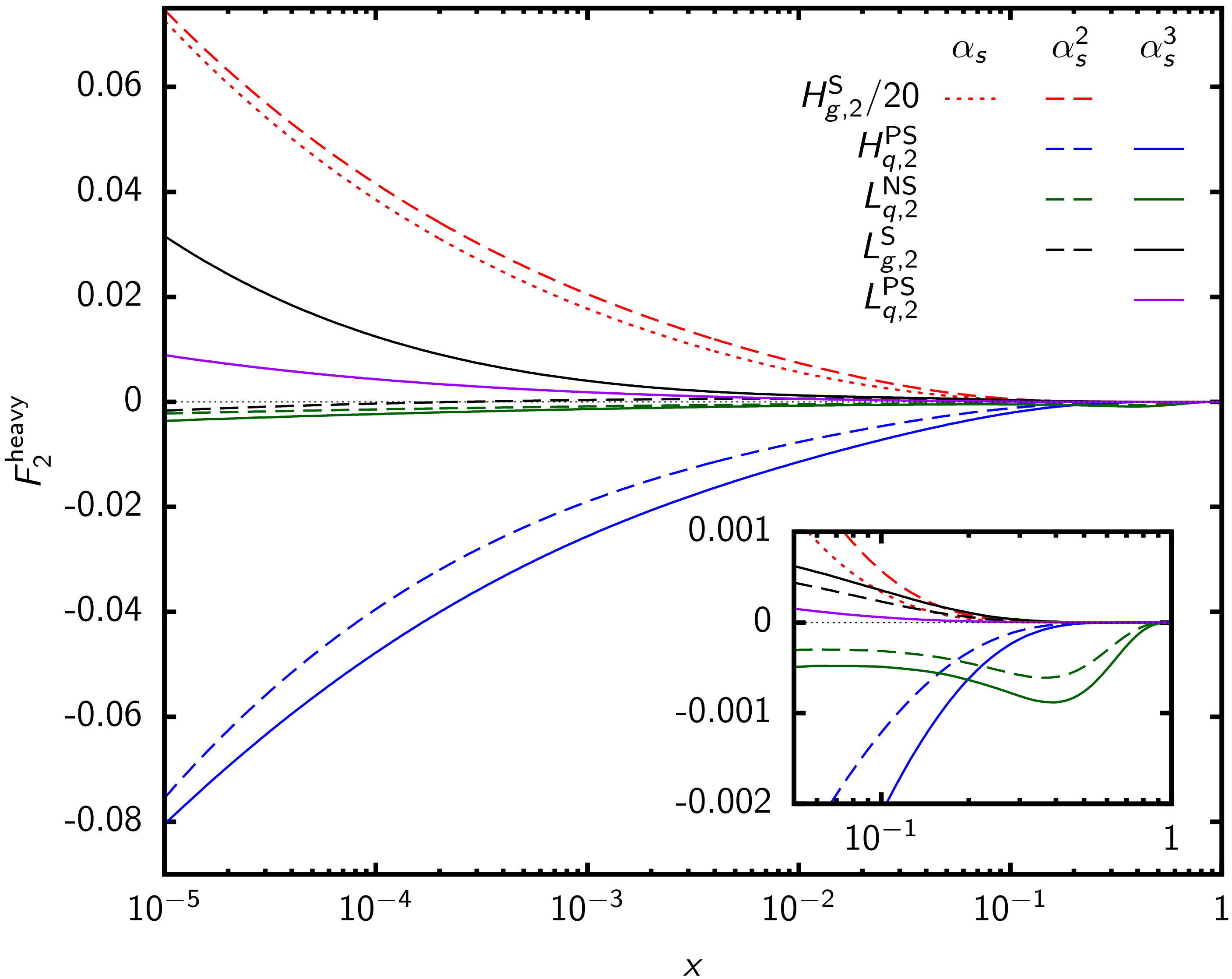
$\sum_{k=0}^{m} p_k(x, \epsilon) \frac{d^k}{dx^k} F(x) = K(x, \epsilon)$ with some inhomogeneity $K(x, \epsilon)$.

Either the inhomogeneities can be forced to vanish, or a hierarchy of equations has to be solved using summation techniques and DEQ-solvers (which may also be summation techniques).

The method of arbitrary high moments

- 0–scale problems are simpler to solve than 1–scale problems
- Mellin moments can be obtained for fixed values of $N \in \mathbb{N}$ and satisfy the difference equations, obtained from the differential equations due to the IBP relations for the master integrals.
- One generates large enough sets of moments for master integrals (at the moment up to 8000.)
- The master integrals are inserted into the final amplitude. Here lots of potential non-first order factorizing terms cancel.
- Guessing is used to obtain corresponding recurrences.
- In quite a series of cases these recurrences factorize to first order and Sigma can solve these recurrences.
- Otherwise non-first order factorizing terms can all be split off. Other technologies are needed to proceed, which are currently developed. [1701.04614]

The present NC corrections to $F_2(x, Q^2)$



$Q^2 = 100$ GeV^2, $H_{g,2}^S$ scaled down by a factor 20.

The Strength of Mathematica and Possible Improvements

All our symbolic integration codes are written in Mathematica.

- Over the years they were steadily improved and extended.
- Mathematica's rich special function implementations and the strong integrator are most helpful.
- This also applies to the math world's pages and detailed on-line tabulations of other kind.
- Freeing memory in Mathematica which is no longer used would be instrumental in some cases. We operate jobs with a RAM request of up to $\sim$ 500 Gbyte and sometimes face difficulties.
- Dynamic outsourcing to fast disc, like available in FORM, would be very helpful.
- In some cases relying heavily on very fast integer arithmetics we had to use Sage because of the size and run time requests of our current problems.

4. What can be achieved by all that ?

- A lot of integration technology has been created for many analytic precision calculations for the Large Hadron Collider and the planned International Linear Collider.
- The results allow also for many advanced solutions in combinatorics and number theory.
- Within elementary particle physics the present results allow to improve the precision of two fundamental constants of the Standard Model:

$$\frac{\delta\alpha_s(M_Z)}{\alpha_s(M_Z)} < 1\% \qquad\qquad \delta m_c < 20\mathrm{MeV}$$

which may have consequences for various proposed extensions of the SM.

4. What can be achieved by all that ?

- Detailed exploration of the $t\bar{t}$ sector for new physics
- QCD background predictions in the search of unexpected signals by new particles
- At the theory side: 4–loop calculations of the scaling violations of parton distribution functions in the future
- Also: crucial tests for small x predictions.
- Computer algebra calculations in the 10-100 Gbyte region, lasting various CPU years.
- Still analytic solutions are possible.

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