Mathematical Structures in Massive Operator Matrix Elements and Wilson Coefficients

Scattering Amplitudes across Germany, Akademiezentrum Raitenhaslach, Germany

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DESY

Based on:

- A. Behring, J.B., and K. Schönwald, The inverse Mellin transform via analytic continuation, JHEP **06** (2023) 62.
- J. Ablinger et al., The unpolarized and polarized single-mass three-loop heavy flavor operator matrix elements $A_{gg}^{(3)} and \Delta A_{gg}^{(3)}$, JHEP **12** (2022) 134.

In collaboration with:

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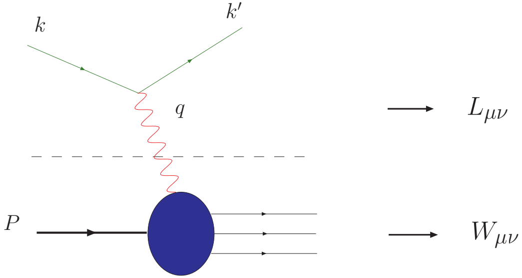
[2] Supported by TU München.

Outline

Unpolarized Deep–Inelastic Scattering (DIS):



$$Q^2 := -q^2, \quad x := \frac{Q^2}{2P.q} \quad \text{Bjorken–x}$$

$$\frac{d\sigma}{dQ^2\, dx} \sim W_{\mu\nu} L^{\mu\nu}$$

$$W_{\mu\nu}(q,P,s) = \frac{1}{4\pi} \int d^4\xi \exp(iq\xi) \langle P,s \mid [J_\mu^{em}(\xi), J_\nu^{em}(0)] \mid P,s\rangle =$$

$$\frac{1}{2x}\left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right) F_L(x,Q^2) + \frac{2x}{Q^2}\left(P_\mu P_\nu + \frac{q_\mu P_\nu + q_\nu P_\mu}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu}\right) F_2(x,Q^2)\,.$$

Structure Functions: $F_{2,L}$ contain light and heavy quark contributions.
At 3-Loop order also graphs with two heavy quarks of different mass contribute.
$\Longrightarrow$ Single and 2-mass contributions: c and b quarks in one graph.

Factorization of the Structure Functions

At leading twist the structure functions factorize in terms of a Mellin convolution

$$F_{(2,L)}(x, Q^2) = \sum_j \underbrace{\mathbb{C}_{j,(2,L)}\left(x, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right)}_{perturbative} \otimes \underbrace{f_j(x, \mu^2)}_{nonpert.}$$

into (pert.) Wilson coefficients and (nonpert.) parton distribution functions (PDFs).
$\otimes$ denotes the Mellin convolution

$$f(x) \otimes g(x) \equiv \int_0^1 dy \int_0^1 dz \, \delta(x - yz) f(y) g(z) \, .$$

The subsequent calculations are performed in Mellin space, where $\otimes$ reduces to a multiplication, due to the Mellin transformation

$$\hat{f}(N) = \int_0^1 dx \, x^{N-1} f(x) \, .$$

Wilson coefficients:

$$\mathbb{C}_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right) = C_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}\right) + H_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right) .$$

At $Q^2 \gg m^2$ the heavy flavor part

$$H_{j,(2,L)}\left(N, \frac{Q^2}{\mu^2}, \frac{m^2}{\mu^2}\right) = \sum_i C_{i,(2,L)}\left(N, \frac{Q^2}{\mu^2}\right) A_{ij}\left(\frac{m^2}{\mu^2}, N\right)$$

[Buza, Matiounine, Smith, van Neerven 1996]

factorizes into the light flavor Wilson coefficients C and the massive operator matrix elements (OMEs) of local operators O_i between partonic states j

$$A_{ij}\left(\frac{m^2}{\mu^2}, N\right) = \langle j \mid O_i \mid j \rangle .$$

$\rightarrow$ additional Feynman rules with local operator insertions for partonic matrix elements.
The unpolarized light flavor Wilson coefficients are known up to NNLO [Moch, Vermaseren, Vogt, 2005; JB, Marquard, Schneider, Schönwald, 2022].
For $F_2(x, Q^2)$: at $Q^2 \gtrsim 10 m^2$ the asymptotic representation holds at the 1% level.

Introduction

- Massive OMEs allow to describe the massive DIS Wilson coefficients for $Q^2 \gg m_Q^2$.
- Furthermore, they form the transition elements in the variable flavor number scheme (VFNS).
- The current state of art is 3-loop order, including two-mass corrections, because m_c/m_b is not small.
- After having calculated a series of moments in 2009 I. Bierenbaum, JB, S. Klein, Nucl. Phys B **820** (2009) 417, we started to calculate all OMEs for general values of the Mellin variable N.
- There are the following massive OMEs: $A_{qq,Q}^{\rm NS}, A_{qg,Q}, A_{qq,Q}^{\rm PS}, A_{gq,Q}, A_{Qq}^{\rm PS}, A_{gg,Q}, A_{Qg}$.
- To 2-loop order $A_{qq,Q}^{\rm NS}, A_{Qq}^{\rm PS}, A_{Qg}$, [2007] $A_{gq,Q}, A_{gg,Q}$ [2009] contribute. These quantities are represented by harmonic sums resp. harmonic polylogarithms. [Older work by van Neerven, et al.]
- The 3-loop contributions of $O(N_F)$ [2010] to all OMEs and the $A_{qq,Q}^{\rm NS}, A_{qg,Q}, A_{gq,Q}, A_{qq,Q}^{\rm PS}$ [2014] are also given by harmonic sums only. [Also all logarithmic terms of all OMEs.]
- For $A_{Qq}^{\rm PS}$ [2014] also generalized harmonic sums are necessary.
- $A_{gg,Q}$ [2022] requires finite binomial sums.
- Finally, A_{Qg} depends also on ${}_2F_1$-solutions [2017] (or modular forms).
- In the two-mass case to 3-loop order $A_{qq,Q}^{\rm NS}, A_{qg,Q}, A_{qq,Q}^{\rm PS}, A_{Qq}^{\rm PS}, A_{gq,Q}, A_{gg,Q}$ [2017-2020] can be solved analytically due to 1st order factorization of the respective differential equations. The solution for A_{Qg} is by far more involved.

Introduction

- Also the corresponding quantities in the polarized case were calculated.
- **A very long tale:**
  42 physics and 27 algorithmic and mathematical journal/book publications so far.
- All solved cases up to now could be calculated in the single mass case in Mellin space.
- In the two-mass PS-case one has to refer to x space, because in Mellin space there is no 1st order factorization.
- Massless 3-loop calculations: anomalous dimensions and Wilson coefficients (unpolarized/polarized), JB, P. Marquard, C. Schneider, K. Schönwald, Nucl. Phys B **971** (2021) 115542, JHEP **01** (2022) 193, Nucl. Phys. B **980** (2022) 115794, JHEP **11** (2022) 156 (extending and confirming earlier work by Moch, Vermaseren and Vogt, [2004,2005,2014])
- massive QED applications: JB, A. De Freitas, C. Raab, K. Schönwald, W.L. van Neerven, 2011, 2019/21.
- $A_{gg,Q}$: Also here one diagram is better computed in x-space first.
- A_{Qg}: ongoing: ${}_2F_1$ contributions; not yet implemented in N-space algorithms.
- Very large recurrences can be computed. However, their factorization beyond the first order factors is still not possible.
- Therefore, we will deal with the ${}_2F_1$-dependent master integrals in x space first.
- How to go from N-space to x-space analytically ?

Mathematical Structure of Feynman Integrals

- 1998: Harmonic Sums [Vermaseren; JB]. At this time Nielsen integrals were exhausted and something new had to be done for single scale quantities.

A new era in QFT started.

- 1997 More was known (or claimed to be) on numbers [zero scale quantities] [Broadhurst, Kreimer]
- 1999: Harmonic Polylogarithms [Remiddi, Vermaseren]
- 2000, 2003, 2009: Analytic continuation of harmonic sums, systematic algebraic reduction; structural relations [JB]
- 1999,2001: Generalized Harmonic Sums [Borwein, Bradley, Broadhurst, Lisonek], [Moch, Uwer, Weinzierl]
- 2004: Infinite harmonic (inverse) binomial sums [Davydychev, Kalmykov; Weinzierl]
- 2009: MZV data mine [JB, Broadhurst, Vermaseren]
- 2011: (generalized) Cyclotomic Harmonic Sums, polylogarithms and numbers [Ablinger, JB, Schneider]
- 2013: Systematic Theory of Generalized Harmonic Sums, polylogarithms and numbers [Ablinger, JB, Schneider]
- 2014: Finite nested Generalized Cyclotomic Harmonic Sums with (inverse) Binomial Weights [Ablinger, JB, Raab, Schneider]
- 2014-: Elliptic integrals with (involved) rational arguments.
- now: More-scale problem: Kummer-elliptic integrals

Particle Physics Generates NEW Mathematics & steadily needs new methods from Mathematics.

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

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

iterated integrals on ${}_2F_1$ *functions*

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

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

Except the last line integrals, all other ones stem from 1st order factorizable equations $\Longrightarrow$ modular forms.

Principal computation steps

Chains of packages are used to perform the calculation:

- `QGRAF`, Nogueira, 1993 Diagram generation
- `FORM`, Vermaseren, 2001; Tentyukov, Vermaseren, 2010 Lorentz algebra
- `Color`, van Ritbergen, Schellekens and Vermaseren, 1999 Color algebra
- `Reduze 2` Studerus, von Manteuffel, 2009/12, `Crusher`, Marquard, Seidel IBPs
- Method of arbitrary high moments, JB, Schneider, 2017 Computing large numbers of Mellin moments
- `Guess`, Kauers et al. 2009/2015; JB, Kauers, Schneider, 2009 Computing the recurrences
- `Sigma, EvaluateMultiSums, SolveCoupledSystems`, Schneider, 2007/14 Solving the recurrences
- `OreSys`, Zürcher, 1994; Gerhold, 2002; Bostan et al., 2013 Decoupling differential and difference equations
- `Diffeq`, Ablinger et al, 2015, JB, Marquard, Rana, Schneider, 2018 Solving differential equations
- `HarmoncisSums`, Ablinger and Ablinger et al. 2010-2019 Simplifying nested sums and iterated integrals to basic building blocks, performing series and asymptotic expansions, Almkvist-Zeilberger algorithm etc.

Solutions in Mellin Space

- Use IBP relations to obtain large sets of Mellin moments JB, Schneider, 2017
- Compute the corresponding recurrences for all color-ζ factors.
- Solve all 1st order factorizing cases by using the package `Sigma`.
- Inverse Mellin transform by using the tools of the package `HarmonicSums`.
- Numerical implementations in N- and x space.
- Remaining: Non-first order factorizable cases.
  - $A_{Qg}^{(3)}$: color coefficients $\propto T_F^2$: 8000 moments allow to get all recurrences.
  - $A_{Qg}^{(3)}$: color coefficients $\propto T_F \zeta_3$: 15000 moments allow to get all recurrences.
  - Many more moments needed to obtain the recurrences for the rational terms $\propto T_F$.
  - the solutions for $\propto T_F^2$ and $\propto T_F^2 \zeta_3$ each do diverge for $N \rightarrow \infty$, while their sum converges to 0.
  - Observe the dynamical creation of a ζ_3 term in the large N limit.
- One may try to compute the asymptotic behaviour of these recurrences, but this needs much more work.
- Usually it is important here to know the associated x space solution.
- More work is needed here.

Conjugation

$$f_2(N,\varepsilon) \equiv f_1^C(N,\varepsilon) = -\sum_{k=0}^{N}(-1)^k \binom{N}{k} f_1(k,\varepsilon)$$

$$\tilde{f}_1^C(x,\varepsilon) = -\tilde{f}_1(1-x), x \in]0,1[.$$

Example: Vermaseren, 1998

$$S_1^C(N) = \frac{1}{N}$$

$$\left(-\frac{1}{1-x}\right)^C = \frac{1}{x}$$

- Relates many master integrals, which need not to be calculated individually.
- Can be easily traced by inspecting their (known) Mellin moments.
- Holds for general ε.
- Saves us one ${}_2F_1$ dependent 3×3 system, since conjugation holds irrespectively of 1st order factorization.

Inverse Mellin transform via analytic continuation: $a_{Qg}^{(3)}$

Resumming Mellin N into a continuous variable t, observing crossing relations. Ablinger et al. 2014

$$\sum_{k=0}^{\infty} t^k (\Delta.p)^k \frac{1}{2}[1 \pm (-1)^k] = \frac{1}{2}\left[\frac{1}{1 - t\Delta.p} \pm \frac{1}{1 + t\Delta.p}\right]$$

$$\mathfrak{A} = \{f_1(t), ..., f_m(t)\}, \quad \mathrm{G}(b, \vec{a}; t) = \int_0^t dx_1 f_b(x_1)\mathrm{G}(\vec{a}; x_1), \quad \left[\frac{d}{dt}\frac{1}{f_{a_{k-1}}(t)}\frac{d}{dt}\cdots\frac{1}{f_{a_1}(t)}\frac{d}{dt}\right]\mathrm{G}(\vec{a}; t) = f_{a_k}(t).$$

Regularization for $t \to 0$ needed.

$$\begin{aligned} F(N) &= \int_0^1 dx x^{N-1}[f(x) + (-1)^{N-1} g(x)] \\ \tilde{F}(t) &= \sum_{N=1}^{\infty} t^N F(N) \\ f(x) + (-1)^{N-1} g(x) &= \frac{1}{2\pi i}\left[\mathrm{Disc}_x \tilde{F}\left(\frac{1}{x}\right) + (-1)^{N-1}\mathrm{Disc}_x \tilde{F}\left(-\frac{1}{x}\right)\right]. \end{aligned} \quad (1)$$

t-space is still Mellin space. One needs closed expressions to perform the analytic continuation (1). Continuation is needed to calculate the small x behaviour analytically.

Harmonic polylogarithms

$$\mathfrak{A}_{\rm HPL} = \{f_0, f_1, f_{-1}\} \left\{\frac{1}{t}, \frac{1}{1-t}, \frac{1}{1+t}\right\}$$

$$\mathrm{H}_{b,\vec{a}}(x) = \int_0^x dy f_b(y) \mathrm{H}_{\vec{a}}(y), \quad f_c \in \mathfrak{A}_{\rm HPL}, \quad \mathrm{H}_{\underbrace{0,\ldots,0}_{k}}(x) := \frac{1}{k!} \ln^k(x).$$

A finite monodromy at $x = 1$ requires at least one letter $f_1(t)$.

Example:

$$\tilde{F}_1(t) = \mathrm{H}_{0,0,1}(t)$$

$$F_1(x) = \frac{1}{2} \mathrm{H}_0^2(x)$$

$$\mathbf{M}[F_1(x)](n-1) = \frac{1}{n^3}$$

$$\tilde{F}_1(t) = t + \frac{t^2}{8} + \frac{t^3}{27} + \frac{t^4}{64} + \frac{t^5}{125} + \frac{t^6}{216} + \frac{t^7}{343} + \frac{t^8}{512} + \frac{t^9}{729} + \frac{t^{10}}{1000} + O(t^{11})$$

Cyclotomic harmonic polylogarithms

Also here the index set has to contain $f_{\pm}1(t)$.

$$\mathfrak{A}_{\rm cycl} = \left\{\frac{1}{x}\right\} \cup \left\{\frac{1}{1-x}, \frac{1}{1+x}, \frac{1}{1+x+x^2}, \frac{x}{1+x+x^2} \frac{1}{1+x^2}, \frac{x}{1+x^2}, \frac{1}{1-x+x^2}, \frac{x}{1-x+x^2}, \dots \right\}.$$

Example:

$$\begin{aligned}\tilde{F}_3(t) &= \frac{1}{3(1-t)t^{1/3}} \mathrm{G}\left[\frac{\xi^{1/3}}{1-\xi}; t\right] \\ &= \frac{1}{1-t}\left(-1 + \frac{t^{-1/3}}{3}\left(\mathrm{H}_1(t^{1/3}) + 2\mathrm{H}_{\{3,0\}}(t^{1/3}) + \mathrm{H}_{\{3,1\}}(t^{1/3})\right)\right).\end{aligned}$$

$$F_3(x) = -\frac{1}{3}\left[\frac{1}{1-x}\right]_+ + \frac{1}{18}\left[\sqrt{3}\pi + 9(-2+\ln(3))\right]\delta(1-x) + \frac{1-x^{4/3}}{3(1-x)}$$

Generalized harmonic polylogarithms

$$\mathfrak{A}_{\rm gHPL} = \left\{\frac{1}{x-a}\right\}, \quad a \in \mathbb{C}.$$

$$F_5(x) = \frac{1}{\pi}\mathrm{Im}\frac{t}{t-1}\left[\mathrm{H}_{0,0,0,1}(t) + 2\mathrm{G}(\gamma_1,0,0,1;t)\right] = -\frac{1}{1-x}\left\{\theta(1-x)\left[\frac{1}{24}\left(4\ln^3(2) - 2\ln(2)\pi^2 + 21\zeta_3\right)\right.\right.$$
$$\left.\left. -\mathrm{H}_{2,0,0}(x)\right] - \theta(2-x)\frac{1}{24}\left(4\ln^3(2) - 2\ln(2)\pi^2 + 21\zeta_3\right)\right\},$$

In intermediary steps Heaviside functions occur and the support of the x-space functions is here [0,2].

$$\tilde{\mathbf{M}}_a^{+,b}[g(x)](N) = \int_0^a dx(x^N - b^N)f(x), \quad a, b \in \mathbb{R},$$

$$\tilde{\mathbf{M}}_2^{+,1}[F_5(x)](N) = -S_{1,3}\left(2, \frac{1}{2}\right)(N-1),$$

$$S_{b,\vec{a}}(c,\vec{d})(N) = \sum_{k=1}^{N}\frac{c^k}{k^b}S_{\vec{a}}(\vec{d})(k), \quad b, a_i \in \mathbb{N}\backslash\{0\}, \quad c, d_i \in \mathbb{C}\backslash\{0\}.$$

Square root valued alphabets

$$\mathfrak{A}_{\rm sqrt} = \left\{ f_4, f_5, f_6 \ldots \right\}$$

$$= \left\{ \frac{\sqrt{1-x}}{x}, \sqrt{x(1-x)}, \frac{1}{\sqrt{1-x}}, \frac{1}{\sqrt{x}\sqrt{1\pm x}}, \frac{1}{x\sqrt{1\pm x}}, \frac{1}{\sqrt{1\pm x}\sqrt{2\pm x}}, \frac{1}{x\sqrt{1\pm x/4}}, \ldots \right\},$$

Monodromy also through:

$$(1-t)^\alpha, \quad \alpha \in \mathbb{R},$$

$$F_7(x) = \frac{1}{\pi} \mathrm{Im} \frac{1}{t} \mathrm{G}\left(4; \frac{1}{t}\right) = 1 - \frac{2(1-x)(1+2x)}{\pi}\sqrt{\frac{1-x}{x}} - \frac{8}{\pi}\mathrm{G}(5;x),$$

$$F_8(x) = \frac{1}{\pi} \mathrm{Im} \frac{1}{t} \mathrm{G}\left(4,2; \frac{1}{t}\right) = -\frac{1}{\pi}\left[4\frac{(1-x)^{3/2}}{\sqrt{x}} + 2(1-x)(1+2x)\sqrt{\frac{1-x}{x}}[\mathrm{H}_0(x)+\mathrm{H}_1(x)] \right.$$

$$\left. +8[\mathrm{G}(5,2;x) + \mathrm{G}(5,1;x)] \right],$$

Iterative non-iterative Integrals

- Master integrals, solving differential equations not factorizing to 1st order
- ${}_2F_1$ solutions Ablinger et al. [2017]
- Mapping to complete elliptic integrals: duplication of the higher transcendental letters.
- Complete elliptic integrals, modular forms Sabry, Broadhurst, Weinzierl, Remiddi, Tancredi, Duhr, Broedel et al. and many more
- Abel integrals
- K3 surfaces Brown, Schnetz [2012]
- Calabi-Yau motives Klemm, Duhr, Weinzierl et al. [2022]

Refer to as few as possible higher transcendental functions, the properties of which are known in full detail.

- $A_{Qg}^{(3)}$: effectively only one 3×3 system of this kind.
- The system is connected to that occurring in the case of ρ parameter. Ablinger et al. [2017], JB et al. [2018], Abreu et al. [2019]
- Most simple solution: two ${}_2F_1$ functions.

Iterative non-iterative Integrals

$$\frac{d}{dt}\begin{bmatrix} F_1(t) \\ F_2(t) \\ F_3(t) \end{bmatrix} = \begin{bmatrix} -\frac{1}{t} & -\frac{1}{1-t} & 0 \\ 0 & -\frac{1}{t(1-t)} & -\frac{2}{1-t} \\ 0 & \frac{2}{t(8+t)} & \frac{1}{8+t} \end{bmatrix} \begin{bmatrix} F_1(t) \\ F_2(t) \\ F_3(t) \end{bmatrix} + \begin{bmatrix} R_1(t,\varepsilon) \\ R_2(t,\varepsilon) \\ R_3(t,\varepsilon) \end{bmatrix} + O(\varepsilon),$$

It is very important to which function $F_i(t)$ the system is decoupled.

Iterative non-iterative Integrals

- Decoupling for F_1 first leads to a very involved solution: ${}_2F_1$-terms seemingly enter at $O(1/\varepsilon)$ already.
- However, these terms are actually not there.
- Furthermore, there is also a singularity at $x = 1/4$.
- All this can be seen, when decoupling for F_3 first.

Homogeneous solutions:

$$F_3'(t) + \frac{1}{t}F_3(t) = 0, \quad g_0 = \frac{1}{t}$$

$$F_1''(t) + \frac{(2-t)}{(1-t)t}F_1'(t) + \frac{2+t}{(1-t)t(8+t)}F_1(t) = 0,$$

with

$$\begin{aligned} g_1(t) &= \frac{2}{(1-t)^{2/3}(8+t)^{1/3}}\,{}_2F_1\left[\begin{matrix}\frac{1}{3},\frac{4}{3}\\ 2\end{matrix};-\frac{27t}{(1-t)^2(8+t)}\right], \\ g_2(t) &= \frac{2}{(1-t)^{2/3}(8+t)^{1/3}}\,{}_2F_1\left[\begin{matrix}\frac{1}{3},\frac{4}{3}\\ \frac{2}{3}\end{matrix};1+\frac{27t}{(1-t)^2(8+t)}\right], \end{aligned}$$

Iterative non-iterative Integrals

Alphabet:

$$\mathfrak{A}_2 = \Biggl\{\frac{1}{t}, \frac{1}{1-t}, \frac{1}{8+t}, g_1, g_2, \frac{g_1}{t}, \frac{g_1}{1-t}, \frac{g_1}{8+t}, \frac{g_1'}{t}, \frac{g_1'}{1-t}, \frac{g_1'}{8+t}, \frac{g_2}{t}, \frac{g_2}{1-t}, \frac{g_2}{8+t}, \frac{g_2'}{t}, \frac{g_2'}{1-t}, \frac{g_2'}{8+t}, tg_1, tg_2\Biggr\}$$

$$\begin{aligned}
F_1(t) = {} & \frac{8}{\varepsilon^3}\left[1+\frac{1}{t}\mathrm{H}_1(t)\right] - \frac{1}{\varepsilon^2}\left[\frac{1}{6}(106+t) + \frac{(9+2t)}{t}\mathrm{H}_1(t) + \frac{4}{t}\mathrm{H}_{0,1}(t)\right] \\
& + \frac{1}{\varepsilon}\left\{\frac{1}{12}(271+9t) + \left[\frac{71+32t+2t^2}{12t} + \frac{3\zeta_2}{t}\right]\mathrm{H}_1(t) + \frac{(9+2t)}{2t}\mathrm{H}_{0,1}(t) + \frac{2}{t}\mathrm{H}_{0,0,1}(t)\right. \\
& \left. + 3\zeta_2\right\} + \frac{1}{t}\left\{\frac{6696-22680t-16278t^2-255t^3-62t^4}{864t} + (9+9t+t^2)g_1(t)\left[\frac{31\ln(2)}{16}\right.\right. \\
& \left. + \frac{1}{144}(265+31\pi(-3i+\sqrt{3})) + \frac{3}{8}\ln(2)\zeta_2 + \frac{1}{24}(10+\pi(-3i+\sqrt{3}))\zeta_2 - \frac{7}{4}\zeta_3\right]
\end{aligned}$$

$$
\begin{aligned}
&+\mathrm{G}(18,t)\Biggl[-\frac{93\ln(2)}{16}+\frac{1}{48}\bigl(-265-31\pi(-3i+\sqrt{3})\bigr)+\Biggl(-\frac{9\ln(2)}{8}\\
&+\frac{1}{8}\bigl(-10-\pi\bigl(-3i+\sqrt{3}\bigr)\bigr)\Biggr)\zeta_2+\frac{21}{4}\zeta_3\Biggr]\ldots\\
&+\frac{5}{2}[\mathrm{G}(4,14,1,2;t)-\mathrm{G}(5,8,1,2;t)]+\frac{1}{4}[\mathrm{G}(13,8,1,2;t)-\mathrm{G}(7,14,1,2;t)]\\
&+\frac{9}{4}[\mathrm{G}(10,14,1,2;t)-\mathrm{G}(16,8,1,2;t)]+\frac{3}{4}[\mathrm{G}(19,14,1,2;t)-\mathrm{G}(19,8,1,2;t)]\Biggr\}+O(\varepsilon),
\end{aligned}
$$

$$
\begin{aligned}
F_2(t) \;=\;& \frac{8}{\varepsilon^3}+\frac{1}{\varepsilon^2}\Biggl[-\frac{1}{3}(34+t)+\frac{2(1-t)}{t}\mathrm{H}_1(t)\Biggr]+\frac{1}{\varepsilon}\Biggl[\frac{116+15t}{12}+3\zeta_2-\frac{(1-t)(8+t)}{3t}\mathrm{H}_1(t)\\
&-\frac{1-t}{t}\mathrm{H}_{0,1}(t)\Biggr]+\frac{992-368t+75t^2-27t^3}{144t}+(1-t)\Biggl(\frac{\left(43+10t+t^2\right)}{12t}\mathrm{H}_1(t)+\frac{(4-t)}{4t}\\
&\times\mathrm{H}_{0,1}(t)+\frac{3\zeta_2}{4t}\mathrm{H}_1(t)\Biggr)+(1-t)g_1(t)\Biggl(\frac{31\ln(2)}{16}+\frac{1}{144}\bigl(265+31\pi\bigl(-3i+\sqrt{3}\bigr)\bigr)\ldots
\end{aligned}
$$

Structure in x space

Expansion around $x = 1$:

$$\sum_{k=0}^{\infty} \sum_{l=0}^{L} \hat{a}_{k,l} (1-x)^k \ln^l(1-x).$$

Expansion around $x = 0$:

$$\frac{1}{x} \sum_{k=0}^{\infty} \sum_{l=0}^{S} \hat{b}_{k,l} x^k \ln^l(x).$$

Expansion around $x = 1/2$:

$$\sum_{k=0}^{\infty} \hat{c}_k \left(x - \frac{1}{2}\right)^k .$$

The occurring constants $\mathrm{G}(...;1)$ are calculated numerically. [At most double integrals.]

Iterating on ${}_2F_1$ solutions

- In $A_{Qg}^{(3)}$ only 2 3×3 systems contribute, which are not factorizing at 1st order & they are conjugate to each other.
- Both form seeds on which only 1st order factorizing factors have to be iterated to obtain all ${}_2F_1$-dependent master integrals.
- The corresponding differential equations read

$$y'(x) + \frac{A}{x-b} y(x) = h(x)$$

$$y(x) = (b-x)^{-A} \left[C\, b^A + \int_0^x dy (b-y)^A h(y) \right].$$

- $h(x)$ is a G-functions containing ${}_2F_1$-dependent letters.
- The occurring G-functions containing ${}_2F_1$-dependent letters have a rather simple structure, which helps in expansions and the calculation of constants.
- In this way we compute all ${}_2F_1$-dependent master integrals contributing to

$a_{Qg}^{(3)}$. All types of other letters up to root-valued letters contribute here too.

The massive OME $A_{gg,Q}^{(3)}$

A 1st order factorizing, but involved case.

$$\hat{\hat{A}}_{gg,Q}^{(1)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2} \left[\frac{\hat{\gamma}_{gg}^{(0)}}{\varepsilon} + a_{gg,Q}^{(1)} + \varepsilon \overline{a}_{gg,Q}^{(1)} + \varepsilon^2 \overline{\overline{a}}_{gg,Q}^{(1)}\right] + O(\varepsilon^3),$$

$$\hat{\hat{A}}_{gg,Q}^{(2)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon} \left[\frac{1}{\varepsilon^2} c_{gg,Q,(2)}^{(-2)} + \frac{1}{\varepsilon} c_{gg,Q,(2)}^{(-1)} + c_{gg,Q,(2)}^{(0)} + \varepsilon c_{gg,Q,(2)}^{(1)}\right] + O(\varepsilon^2),$$

$$\hat{\hat{A}}_{gg,Q}^{(3)} = \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2} \left[\frac{1}{\varepsilon^3} c_{gg,Q,(3)}^{(-3)} + \frac{1}{\varepsilon^2} c_{gg,Q,(3)}^{(-2)} + \frac{1}{\varepsilon} c_{gg,Q,(3)}^{(-1)} + a_{gg,Q}^{(3)}\right] + O(\varepsilon) \,.$$

The alphabet:

$$\mathfrak{A} = \{f_k(x)\}|_{k=1..6} = \left\{\frac{1}{x}, \frac{1}{1-x}, \frac{1}{1+x}, \frac{\sqrt{1-x}}{x}, \sqrt{x(1-x)}, \frac{1}{\sqrt{1-x}}\right\}.$$

Binomial Sums

$$\mathrm{BS}_0(N) = \frac{1}{2N-(2l+1)}, \quad l \in \mathbb{N}, \qquad \mathrm{BS}_1(N) = 4^N \frac{(N!)^2}{(2N)!},$$

$$\mathrm{BS}_2(N) = \frac{1}{4^N}\frac{(2N)!}{(N!)^2}, \qquad \mathrm{BS}_3(N) = \sum_{\tau_1=1}^{N} \frac{4^{-\tau_1}(2\tau_1)!}{(\tau_1!)^2\tau_1},$$

$$\mathrm{BS}_4(N) = \sum_{\tau_1=1}^{N} \frac{4^{\tau_1}(\tau_1!)^2}{(2\tau_1)!\tau_1^2}, \qquad \mathrm{BS}_5(N) = \sum_{\tau_1=1}^{N} \frac{4^{\tau_1}(\tau_1!)^2}{(2\tau_1)!\tau_1^3},$$

$$\mathrm{BS}_6(N) = \sum_{\tau_1=1}^{N} \frac{4^{-\tau_1}(2\tau_1)!\sum_{\tau_2=1}^{\tau_1}\frac{4^{\tau_2}(\tau_2!)^2}{(2\tau_2)!\tau_2^2}}{(\tau_1!)^2\tau_1}, \qquad \mathrm{BS}_7(N) = \sum_{\tau_1=1}^{N} \frac{4^{-\tau_1}(2\tau_1)!\sum_{\tau_2=1}^{\tau_1}\frac{4^{\tau_2}(\tau_2!)^2}{(2\tau_2)!\tau_2^3}}{(\tau_1!)^2\tau_1},$$

$$\mathrm{BS}_8(N) = \sum_{\tau_1=1}^{N} \frac{\sum_{\tau_2=1}^{\tau_1}\frac{4^{\tau_2}(\tau_2!)^2}{(2\tau_2)!\tau_2^2}}{\tau_1}, \qquad \mathrm{BS}_9(N) = \sum_{\tau_1=1}^{N} \frac{4^{-\tau_1}(2\tau_1)!\sum_{\tau_2=1}^{\tau_1}\frac{4^{\tau_2}(\tau_2!)^2\sum_{\tau_3=1}^{\tau_2}\frac{1}{\tau_3}}{(2\tau_2)!\tau_2^2}}{(\tau_1!)^2\tau_1},$$

$$\mathrm{BS}_{10}(N) = \sum_{\tau_1=1}^{N} \frac{4^{\tau_1}}{\binom{2\tau_1}{\tau_1}}\frac{1}{\tau_1^2}S_1(\tau_1).$$

Recursions and Asymptotic Representation

$$\mathrm{BS}_8(N) - \mathrm{BS}_8(N-1) = \frac{1}{N}\mathrm{BS}_4(N),$$

$$\mathrm{BS}_9(N) - \mathrm{BS}_9(N-1) = \frac{1}{N}\mathrm{BS}_3(N)\mathrm{BS}_{10}(N),$$

$$\mathrm{BS}_{10}(N) - \mathrm{BS}_{10}(N-1) = \frac{1}{N}\mathrm{BS}_1(N) S_1 .$$

$$\mathrm{BS}_0(N) \propto \frac{1}{2N}\sum_{k=0}^{\infty}\left(\frac{2l+1}{2N}\right)^k,$$

$$\mathrm{BS}_8(N) \propto -7\zeta_3 + \left[+3(\ln(N)+\gamma_E) + \frac{3}{2N} - \frac{1}{4N^2} + \frac{1}{40N^4} - \frac{1}{84N^6} + \frac{1}{80N^8} - \frac{1}{44N^{10}}\right]\zeta_2$$
$$+\sqrt{\frac{\pi}{N}}\left[4 - \frac{23}{18N} + \frac{1163}{2400N^2} - \frac{64177}{564480N^3} - \frac{237829}{7741440N^4} + \frac{5982083}{166526976N^5}\right.$$
$$+\frac{5577806159}{438593126400N^6} - \frac{12013850977}{377864847360N^7} - \frac{1042694885077}{90766080737280N^8}$$
$$\left.+\frac{6663445693908281}{127863697547722752N^9} + \frac{23651830282693133}{1363413316298342400N^{10}}\right],$$

Inverse Mellin Transform

$$\mathbf{M}^{-1}[\mathrm{BS}_8(N)](x) = \Biggl[-\frac{4\left(1-\sqrt{1-x}\right)}{1-x} + \left(\frac{2(1-\ln(2))}{1-x} + \frac{\mathrm{H}_0(x)}{\sqrt{1-x}}\right)\mathrm{H}_1(x) - \frac{\mathrm{H}_{0,1}(x)}{\sqrt{1-x}} + \frac{\mathrm{H}_1(x)\mathrm{G}(\{6,1\},x)}{2(1-x)} - \frac{\mathrm{G}(\{6,1,2\},x)}{2(1-x)}\Biggr]_+,$$

$$\mathbf{M}^{-1}[\mathrm{BS}_{10}(N)](x) = \Biggl[-\frac{1}{1-x}\left[-4-4\ln(2)\left(-1+\sqrt{1-x}\right)+4\sqrt{1-x}+\zeta_2\right] + 2(-1+\ln(2))\left(-1+\sqrt{1-x}+x\right)\frac{\mathrm{H}_0(x)}{(1-x)^{3/2}} - 2\frac{\mathrm{H}_1(x)}{\sqrt{1-x}} + \frac{\mathrm{H}_{0,1}(x)}{\sqrt{1-x}} - \frac{(-2+\ln(2))\mathrm{G}(\{6,1\},x)}{1-x} + \frac{\mathrm{G}(\{6,1,2\},x)}{2(1-x)} - \frac{\mathrm{G}(\{1,6,1\},x)}{2(1-x)}\Biggr]_+.$$

Small x limits of $a_{gg,Q}^{(3)}$

$$a_{gg,Q}^{x\to 0}(x) \propto$$

$$\frac{1}{x}\Biggl\{\ln(x)\Biggl[C_A^2 T_F\left(-\frac{11488}{81}+\frac{224\zeta_2}{27}+\frac{256\zeta_3}{3}\right)+C_A C_F T_F\left(-\frac{15040}{243}-\frac{1408\zeta_2}{27}\right.$$

$$\left.\left.-\frac{1088\zeta_3}{9}\right)\right]+C_A T_F^2\Biggl[\frac{112016}{729}+\frac{1288}{27}\zeta_2+\frac{1120}{27}\zeta_3+\left(\frac{108256}{729}+\frac{368\zeta_2}{27}-\frac{448\zeta_3}{27}\right)$$

$$\times N_F\Biggr]+C_F\Biggl[T_F^2\left(-\frac{107488}{729}-\frac{656}{27}\zeta_2+\frac{3904}{27}\zeta_3+\left(\frac{116800}{729}+\frac{224\zeta_2}{27}-\frac{1792\zeta_3}{27}\right)N_F\right)$$

$$+C_A T_F\left(-\frac{5538448}{3645}+\frac{1664\mathrm{B}_4}{3}-\frac{43024\zeta_4}{9}+\frac{12208}{27}\zeta_2+\frac{211504}{45}\zeta_3\right)\Biggr]$$

$$+C_A^2 T_F\left(-\frac{4849484}{3645}-\frac{352\mathrm{B}_4}{3}+\frac{11056\zeta_4}{9}-\frac{1088}{81}\zeta_2-\frac{84764}{135}\zeta_3\right)$$

$$+C_F^2 T_F\left(\frac{10048}{5}-640\mathrm{B}_4+\frac{51104\zeta_4}{9}-\frac{10096}{9}\zeta_2-\frac{280016}{45}\zeta_3\right)\Biggr\}$$

Small x limits of $a_{gg,Q}^{(3)}$

$$+\Big[-\frac{4}{3}C_F C_A T_F+\frac{2}{15}C_F^2 T_F\Big]\ln^5(x)+\Big[-\frac{40}{27}C_A^2 T_F+\frac{4}{9}C_F^2 T_F+C_F\Big(-\frac{296}{27}C_A T_F$$

$$+\Big(\frac{28}{27}+\frac{56}{27}N_F\Big)T_F^2\Big)\Big]\ln^4(x)+\Big[\frac{112}{81}C_A(1+2N_F)T_F^2+C_F\Big(\Big(\frac{1016}{81}+\frac{496}{81}N_F\Big)T_F^2$$

$$+C_A T_F\Big(-\frac{10372}{81}-\frac{328\zeta_2}{9}\Big)\Big)+C_F^2 T_F\Big[-\frac{2}{3}+\frac{4\zeta_2}{9}\Big]+C_A^2 T_F\Big[-\frac{1672}{81}+8\zeta_2\Big]\Big]\ln^3(x)$$

$$+\Big[\frac{8}{81}C_A(155+118N_F)T_F^2+C_F\Big[T_F^2\Big(-\frac{32}{81}+N_F\Big(\frac{3872}{81}-\frac{16\zeta_2}{9}\Big)\Big)+\frac{232\zeta_2}{9}\Big]$$

$$+C_A T_F\Big(-\frac{70304}{81}-\frac{680\zeta_2}{9}+\frac{80\zeta_3}{3}\Big)\Big)+C_A^2 T_F\Big[\frac{4684}{81}+\frac{20\zeta_2}{3}\Big]+C_F^2 T_F\Big[56$$

$$+\frac{8\zeta_2}{3}-40\zeta_3\Big]\Big]\ln^2(x)+\Big[C_F\Big[T_F^2\Big(\frac{140992}{243}+N_F\Big(\frac{182528}{243}-\frac{400\zeta_2}{27}-\frac{640\zeta_3}{9}\Big)$$

Small and large x limits of $a_{gg,Q}^{(3)}$

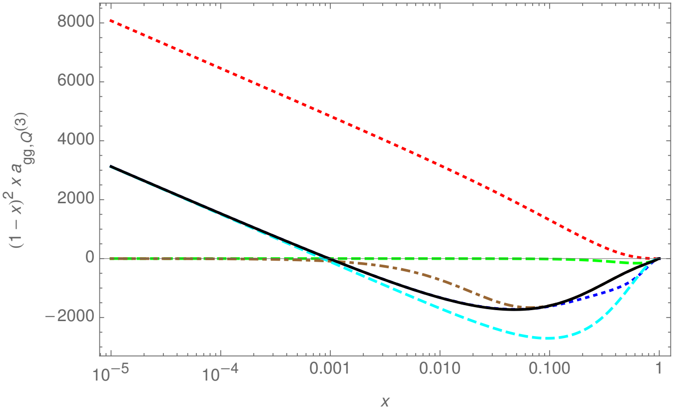
$$
-\frac{728}{27}\zeta_2-\frac{224}{9}\zeta_3\Bigg)+C_AT_F\left(-\frac{514952}{243}+\frac{152\zeta_4}{3}-\frac{21140\zeta_2}{27}-\frac{2576\zeta_3}{9}\right)\Bigg]
+C_AT_F^2\left[\frac{184}{27}+N_F\left(\frac{656}{27}-\frac{32\zeta_2}{27}\right)+\frac{464\zeta_2}{27}\right]+C_A^2T_F\left[-\frac{42476}{81}-92\zeta_4+\frac{4504\zeta_2}{27}
+\frac{64\zeta_3}{3}\right]+C_F^2T_F\left[-\frac{1036}{3}-\frac{976\zeta_4}{3}-\frac{58\zeta_2}{3}+\frac{416\zeta_3}{3}\right]\Bigg]\ln(x),
$$

$$
a_{gg,Q}^{(3),x\to 1}(x) \propto a_{gg,Q,\delta}^{(3)}\delta(1-x)+a_{gg,Q,\mathrm{plus}}^{(3)}(x)+\Bigg[-\frac{32}{27}C_AT_F^2(17+12N_F)+C_AC_FT_F\left(56-\frac{32\zeta_2}{3}\right)
+C_A^2T_F\left(\frac{9238}{81}-\frac{104\zeta_2}{9}+16\zeta_3\right)\Bigg]\ln(1-x)+\Bigg[-\frac{8}{27}C_AT_F^2(7+8N_F)
+C_A^2T_F\left(\frac{314}{27}-\frac{4\zeta_2}{3}\right)\Bigg]\ln^2(1-x)+\frac{32}{27}C_A^2T_F\ln^3(1-x).
$$

Representations of the OME

- The logarithmic parts of $(\Delta)A_{Qg}^{(3)}$ were computed in [Behring et al., (2014)], [JB et al. (2021)].
- We did not spent efforts to choose the MI basis such that the needed ε-expansion is minimal, which we could afford in all first order factorizing cases.
- N space
  - Recursions available for all building blocks: $N \to N + 1$.
  - Asymptotic representations available.
  - Contour integral around the singularities of the problem at the non-positive real axis.
- x space
  - All constants occurring in the transition $t \to x$ can be calculated in terms of ζ-values.
  - This can be proven analytically by first rationalizing and then calculating the obtained cyclotomic G-functions.
  - Separate the $\delta(1 - x)$ and $+$-function terms first.
  - Series representations to 50 terms around $x = 0$ and $x = 1$ can be derived for the regular part analytically (12 digits).
  - The accuracy can be easily enlarged, if needed.

$a_{gg,Q}^{(3)}$



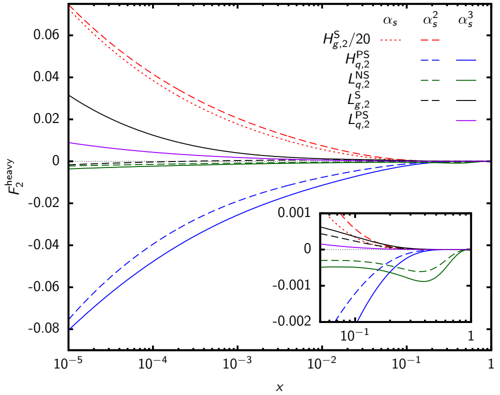
The non–N_F terms of $a_{gg,Q}^{(3)}(N)$ (rescaled) as a function of x. Full line (black): complete result; upper dotted line (red): term $\propto \ln(x)/x$, BFKL limit; lower dashed line (cyan): small x terms $\propto 1/x$; lower dotted line (blue): small x terms including all $\ln(x)$ terms up to the constant term; upper dashed line (green): large x contribution up to the constant term; dash-dotted line (brown): complete large x contribution.

1st order factorizing contributions: $a_{Qg}^{(3)}$

- 1009 of 1233 contributing Feynman diagrams
- Solved: N_F-terms, ζ_2, ζ_4 and B_4 terms, unpolarized and polarized.
- Contributions to the rational and ζ_3 terms:
  - The sum of the contributions vanishes for $N \to \infty$, while the individual terms $\propto 1$ and $\propto \zeta_3$ do strongly diverge.
  - Dynamical generation of a factor of ζ_3.
  - Calculated asymptotic expansions in N space: harmonic sums, generalized harmonic sums, binomial sums
  - Appearance of a large set of special numbers given as G-functions at $x = 1$
  - individually divergent contributions for $N \to \infty$: $\propto 2^N, 4^N$ cancel between the different terms
- Calculated inverse Mellin transforms: requires the use of the t-variable method in the most involved cases for nested binomial sums.

Current summary on F_2^{charm}

An example to show numerical effects: the charm quark contributions to the structure function $F_2(x, Q^2)$



Allows to strongly reduce the current theory error on m_c.

Started $\sim$ 2009; might be completed this year.

Lots of new algorithms had to be designed; different new function spaces; new analytic calculation techniques ...

Conclusions

- Contributions to massless & massive OMEs and Wilson coefficients factorizing at 1st order can be computed in Mellin N space using difference ring techniques as implemented in the package `Sigma`.
- N-space methods also applicable in the case of non-1st order factorization are more involved and need further study.
- x-space representations are needed also to determine the small x behaviour, since it cannot be obtained by the N-space methods, because they are related to integer values in N not covered.
- The t-resummation of the original N-space expressions is already necessary to perform the IBP reduction.
- The transformation from the continuous variable t to the continuous variable x is possible trough the optical theorem.
- This applies to all 1st order factorizing cases and also to non-1st order factorizing situations, provided one can derive a closed form solution of the respective equations and perform the analytic continuation.
- This includes also the calculation of various new constants, which might open up a new field for special numbers, unless these quantities finally reduce to what is known already.
- The moments of the master integrals depend on ζ-values only.

Conclusions

- It is most efficient to work with ${}_2F_1$-solutions in the present examples, because they are most compact and since everything is known about them.
- For numerical representations analytic expansions around $x = 0$, $x = 1/2$ and $x = 1$ suffice, with ~ 50 terms, (Example: $a_{Qg}^{(3)}$). In some cases further overlapping series expansions have to be performed.
- $A_{gg,Q}^{(3)}$ has contributions from finite central binomial sums or square-root valued alphabets, factorizing at 1st order.
- Both efficient N- and x-space solutions can be derived which are very fast numerically. $\Longrightarrow$ QCD analysis.
- BFKL-like approaches are shown to utterly fail in describing these quantities. Various sub-leading terms are needed in addition.