



Mathematical Structures in Massive Operator Matrix Elements

Mathematical Structures in Feynman Integrals, Siegen, Germany

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DESY

Based on:

- A. Behring, J.B., and K. Schönwald, The inverse Mellin transform via analytic continuation, DESY 20–053.
- 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.

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- 1 Introduction
- 2 Solutions in Mellin Space
- 3 Inverse Mellin transform via analytic continuation
 - Harmonic polylogarithms
 - Cyclotomic harmonic polylogarithms
 - Generalized harmonic polylogarithms
 - Square root valued alphabets
 - Iterative non-iterative Integrals
 - Iterating on ${}_2F_1$ solutions
- 4 The massive OME $A_{gg,Q}^{(3)}$
 - Binomial Sums
 - Small and large x limits
 - Small and large x limits
 - Numerical results
- 5 Conclusions

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: $A_{qq,Q}^{NS}$, $A_{qg,Q}$, $A_{qq,Q}^{PS}$, $A_{gq,Q}$, A_{Qq}^{PS} , $A_{gg,Q}$, A_{Qg} .
- To 2-loop order $A_{qq,Q}^{NS}$, A_{Qq}^{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 $A_{qq,Q}^{NS}$, $A_{qg,Q}$, $A_{gq,Q}$, A_{Qq}^{PS} [2014] are also given by harmonic sums only. [Also all logarithmic terms of all OMEs.]
- For A_{Qq}^{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 $A_{qq,Q}^{NS}$, $A_{qg,Q}$, $A_{qq,Q}^{PS}$, A_{Qq}^{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.

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

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

gen. Harmonic Sums

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

Cycl. Harmonic Sums

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

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

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

gen. multiple zeta values

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

cycl. multiple zeta values

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

associated numbers

$$H_{8,w_3} = 2\text{arccot}(\sqrt{7})^2$$

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 \implies algebras

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

- Also the corresponding quantities in the **polarized case** were calculated.
 - **A very long tale:**
 - 42 physics and 26 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 ?**

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
- HarmonicSums, [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.

- 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 \$\zeta_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.

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

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

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



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

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

$$\mathfrak{A} = \{f_1(t), \dots, f_m(t)\}$$

$$G(b, \vec{a}; t) = \int_0^t dx_1 f_b(x_1) G(\vec{a}; x_1).$$

Regularization for $t \rightarrow 0$ needed.

$$\left[\frac{d}{dt} \frac{1}{f_{a_{k-1}}(t)} \frac{d}{dt} \dots \frac{1}{f_{a_1}(t)} \frac{d}{dt} \right] G(\vec{a}; t) = f_{a_k}(t).$$

$$F(x) = \frac{1}{\pi} \text{Im} \tilde{F} \left(t = \frac{1}{x} \right). \quad (1)$$

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.

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

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

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

Example:

$$\tilde{F}_1(t) = H_{0,0,1}(t)$$

$$F_1(x) = \frac{1}{2} H_0^2(x)$$

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

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

Cyclotomic harmonic polylogarithms



Also here the index set has to contain $f_1(t)$.

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

Example:

$$\tilde{F}_2(t) = H_{\{2,0\},\{1,0\},\{1,0\},\{6,0\}}(t)$$

$$\begin{aligned} F_2(x) = & -\frac{1}{3} \ln^2(2) \pi \frac{1}{\sqrt{3}} - \frac{1}{9} \pi^3 \frac{1}{\sqrt{3}} + \frac{1}{3} \left[-\psi^{(1)}\left(\frac{1}{3}\right) + 4\zeta_2 \right] H_0 + \frac{\pi}{3\sqrt{3}} H_0^2 \\ & + \left[-\frac{2}{3\sqrt{3}} \pi H_0 - \frac{4}{3} \zeta_2 + \frac{1}{3} \psi^{(1)}\left(\frac{1}{3}\right) \right] H_{-1} + \frac{2}{3\sqrt{3}} \pi \left[H_{0,1} + H_{0,-1} - H_{-1,1} \right] + \frac{4}{3} \ln(2) \zeta_2 \\ & - \frac{1}{3} \ln(2) \psi^{(1)}\left(\frac{1}{3}\right). \end{aligned}$$

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

$$F_3(x) = \frac{1}{\pi} \text{ImG} \left(\left\{ \frac{1}{2-y} \right\}; \frac{1}{t} \right) = \theta \left(\frac{1}{2} - x \right)$$

$$\gamma_1 = 1/(1-2x)$$

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

$$\left. \left. - 2 \ln(2) \pi^2 + 21 \zeta_3) - H_{2,0,0}(x) \right] - \theta(2-x) (4 \ln^3(2) - 2 \ln(2) \pi^2 + 21 \zeta_3) \right\},$$

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

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

Square root valued alphabets



$$\mathfrak{A}_{\text{sqrt}} = \left\{ f_4, f_5, f_6 \dots \right\}$$

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

Monodromy also through:

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

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

$$F_8(x) = \frac{1}{\pi} \text{Im} \frac{1}{t} G\left(4, 2; \frac{1}{t}\right) = -\frac{1}{\pi} \left[4 \frac{(1-x)^{3/2}}{\sqrt{x}} + 2(1-x)(1+2x) \sqrt{\frac{1-x}{x}} [H_0(x) + H_1(x)] \right. \\ \left. + 8[G(5, 2; x) + G(5, 1; x)] \right],$$

- 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, 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.

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

$$R_1(t, \varepsilon) = \frac{1}{t(1-t)\varepsilon^3} \left[16 - \frac{68}{3}\varepsilon + \left(\frac{59}{3} + 6\zeta_2 \right) \varepsilon^2 + \left(-\frac{65}{12} - \frac{17}{2}\zeta_2 + 2\zeta_3 \right) \varepsilon^3 \right] + O(\varepsilon),$$

$$R_2(t, \varepsilon) = \frac{1}{t(1-t)\varepsilon^3} \left[8 - \frac{16}{3}\varepsilon + \left(\frac{4}{3} + 3\zeta_2 \right) \varepsilon^2 + \left(\frac{14}{3} - 2\zeta_2 + \zeta_3 \right) \varepsilon^3 \right] + O(\varepsilon),$$

$$R_3(t, \varepsilon) = \frac{1}{12t(8+t)\varepsilon^3} \left[-192 + 8\varepsilon - 8(4 + 9\zeta_2)\varepsilon^2 + (68 + 3\zeta_2 - 24\zeta_3)\varepsilon^3 \right] + O(\varepsilon).$$

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

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

Iterative non-iterative Integrals



Alphabet:

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

$$F_1(t) = \frac{8}{\varepsilon^3} \left[1 + \frac{1}{t} H_1(t) \right] - \frac{1}{\varepsilon^2} \left[\frac{1}{6} (106 + t) + \frac{(9 + 2t)}{t} H_1(t) + \frac{4}{t} H_{0,1}(t) \right]$$

$$+ \frac{1}{\varepsilon} \left\{ \frac{1}{12} (271 + 9t) + \left[\frac{71 + 32t + 2t^2}{12t} + \frac{3\zeta_2}{t} \right] H_1(t) + \frac{(9 + 2t)}{2t} H_{0,1}(t) + \frac{2}{t} H_{0,0,1}(t) \right.$$

$$\left. + 3\zeta_2 \right\} + \frac{1}{t} \left\{ \frac{6696 - 22680t - 16278t^2 - 255t^3 - 62t^4}{864t} + (9 + 9t + t^2) g_1(t) \left[\frac{31 \ln(2)}{16} \right. \right.$$

$$\left. \left. + \frac{1}{144} (265 + 31\pi(-3i + \sqrt{3})) + \frac{3}{8} \ln(2)\zeta_2 + \frac{1}{24} (10 + \pi(-3i + \sqrt{3}))\zeta_2 - \frac{7}{4}\zeta_3 \right] \right\}$$

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

$$\begin{aligned}
F_2(t) = & \frac{8}{\varepsilon^3} + \frac{1}{\varepsilon^2} \left[-\frac{1}{3}(34 + t) + \frac{2(1-t)}{t} H_1(t) \right] + \frac{1}{\varepsilon} \left[\frac{116 + 15t}{12} + 3\zeta_2 - \frac{(1-t)(8+t)}{3t} H_1(t) \right. \\
& \left. - \frac{1-t}{t} H_{0,1}(t) \right] + \frac{992 - 368t + 75t^2 - 27t^3}{144t} + (1-t) \left(\frac{(43 + 10t + t^2)}{12t} H_1(t) + \frac{(4-t)}{4t} \right. \\
& \left. \times H_{0,1}(t) + \frac{3\zeta_2}{4t} H_1(t) \right) + (1-t)g_1(t) \left(\frac{31 \ln(2)}{16} + \frac{1}{144} (265 + 31\pi(-3i + \sqrt{3})) \dots \right)
\end{aligned}$$

$$\begin{aligned}
& + \frac{1}{4} [g_2(t)G(8, 1, 2; t) - g_1(t)G(14, 1, 2; t)] \Big\} + \zeta_3 + O(\varepsilon), \\
F_3(t) = & \frac{1}{\varepsilon^2} \left[\frac{10}{3} - \frac{t}{6} \right] + \frac{1}{\varepsilon} \left[-\frac{31}{6} + \frac{3t}{8} - \left(\frac{1}{3} - \frac{1}{6t} - \frac{t}{6} \right) H_1(t) \right] + \left[\frac{3}{4} \ln(2)g_1(t) \right. \\
& + \frac{1}{12} (10 + \pi(-3i + \sqrt{3}))g_1(t) - \frac{g_2(t)}{3} + \frac{25}{54} [g_1(t)G(13; t) - g_2(t)G(7; t)] \\
& + \frac{28}{27} [g_2(t)G(8; t) - g_1(t)G(14; t)] + \frac{1}{3} [g_1(t)G(16; t) - g_2(t)G(10; t)] \Big] \zeta_2 + \frac{31}{8} \ln(2)g_1(t) \\
& + \frac{1}{72} (265 + 31\pi(-3i + \sqrt{3}))g_1(t) - \frac{7}{2} \zeta_3 g_1(t) - \frac{31g_2(t)}{18} + \frac{31}{18} [g_1(t)G(16; t) \\
& - g_2(t)G(10; t)] + \frac{7}{12} [g_1(t)G(5; t) - g_2(t)G(4; t)] + \frac{655}{324} [g_1(t)G(13; t) - g_2(t)G(7; t)] \\
& + \frac{518}{81} [g_2(t)G(8; t) - g_1(t)G(14; t)] + \frac{1}{3} [g_1(t)G(5, 2; t) - g_2(t)G(4, 2; t)] \\
& + \frac{1}{12} [g_2(t)G(6, 2; t) - g_1(t)G(12, 2; t)] + \frac{7}{4} [g_2(t)G(8, 2; t) - g_1(t)G(14, 2; t)] \\
& + \frac{1}{2} [g_2(t)G(8, 1, 2; t) - g_1(t)G(14, 1, 2; t)] + O(\varepsilon).
\end{aligned}$$

$$\begin{aligned}
 F_1(x) &= \frac{8x}{\varepsilon^3} - \frac{1}{\varepsilon^2}(2 + 9x - 4xH_0) + \frac{1}{\varepsilon} \left[\frac{1}{12x} [2 + 32x + (71 + 36\zeta_2)x^2] - \frac{1}{2}(2 + 9x)H_0 + xH_0^2 \right] \\
 &\quad + F_1^{(0)}(x) + O(\varepsilon), \\
 F_2(x) &= -\frac{1}{\varepsilon^2}2(1-x) + \frac{1}{\varepsilon}(1-x) \left[\frac{(1+8x)}{3x} - H_0(x) \right] + F_2^{(0)}(x) + O(\varepsilon), \\
 F_3(x) &= \frac{1}{\varepsilon} \frac{(1-x)^2}{6x} + F_3^{(0)}(x) + O(\varepsilon).
 \end{aligned}$$

It is very essential to have no singularities in $x \in]0, 1[$ because of the analytic continuation.

This would have not been the case using the elliptic integral representations [Ablinger et al., (2017)]: discontinuity at $x = 1/3$.

Here: pole at $x = -1/8$; \implies convergence radius $r \leq 1/8$ around $x = 0$.

- The **alphabet** in x is obtained by $t \rightarrow 1/x$ and subsequent partial fractioning.
- **Three regions:** $x \in [0, 1/10]$, $x \in [1/10, 8/10]$, $x \in [8/10, 1]$, (overlapping choice).

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** $G(\dots; 1)$ are calculated numerically. [At most double integrals.]

Iterative non-iterative Integrals



One example:

Expansion around $x = 1$:

$$F_3^{(0),1}(x) = \sum_{k=2}^{\infty} c_{3,k}^1 (1-x)^k$$

Expansion around $x = 0$:

$$\begin{aligned} F_3^{(0),0}(x) = & -\frac{1}{6} \frac{\ln(x)}{x} - \frac{3}{8x} + \left(\frac{1}{2} - \frac{7}{6} \ln(x) \right) + x \left(\frac{9}{8} + \frac{7}{12} \ln(x) - \frac{3}{2} \ln^2(x) \right) \\ & + \frac{1}{3} x^2 [-13 + 18 \ln(x) + 9 \ln^2(x)] + \frac{1}{24} x^3 [259 - 720 \ln(x) - 252 \ln^2(x)] \\ & + \frac{1}{15} x^4 [-451 + 2295 \ln(x) + 720 \ln^2(x)] + \frac{3}{80} x^5 [2339 - 22460 \ln(x) - 6640 \ln^2(x)] \\ & + O(x^6) \quad \text{At higher orders also non-rational terms contribute.} \end{aligned}$$

$$a_{Qg}^{(3)} = \frac{64}{243} C_A^2 T_F (1312 + 135\zeta_2 - 189\zeta_3) \frac{\ln(x)}{x} \quad [\text{rescaled from PS}],$$

[Ablinger et al. Nucl. Phys. B **890** (2014) 48]; [Catani et al., Nucl. Phys. B **366** (1991) 135].

Expansion around $x = 1/2$:

$$F_3^{(0),1/2}(x) = \sum_{k=0}^{\infty} c_{3,k}^{1/2} \left(x - \frac{1}{2}\right)^k.$$

Similar results for $F_1(x)$ and $F_2(x)$.

Second ${}_2F_1$ -set:

$$F_k(x) = -F_{k-3}(1-x), \quad k \in \{4, 5, 6\}.$$

by using the above representations [expressed in G-functions].

- Check all representations against known Mellin moments numerically.

Iterating on ${}_2F_1$ solutions



- In $A_{Qg}^{(3)}$ only $2 \times 3 \times 3$ 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.

$$\begin{aligned} \hat{A}_{gg,Q}^{(1)} &= \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2} \left[\frac{\hat{\gamma}_{gg}^{(0)}}{\varepsilon} + a_{gg,Q}^{(1)} + \varepsilon \bar{a}_{gg,Q}^{(1)} + \varepsilon^2 \bar{\bar{a}}_{gg,Q}^{(1)} \right] + O(\varepsilon^3), \\ \hat{A}_{gg,Q}^{(2)} &= \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon} \left[\frac{1}{\varepsilon^2} c_{gg,Q,(2)}^{(-2)} + \frac{1}{\varepsilon} c_{gg,Q,(2)}^{(-1)} + c_{gg,Q,(2)}^{(0)} + \varepsilon c_{gg,Q,(2)}^{(1)} \right] + O(\varepsilon^2), \\ \hat{A}_{gg,Q}^{(3)} &= \left(\frac{\hat{m}^2}{\mu^2}\right)^{3\varepsilon/2} \left[\frac{1}{\varepsilon^3} c_{gg,Q,(3)}^{(-3)} + \frac{1}{\varepsilon^2} c_{gg,Q,(3)}^{(-2)} + \frac{1}{\varepsilon} c_{gg,Q,(3)}^{(-1)} + a_{gg,Q}^{(3)} \right] + O(\varepsilon). \end{aligned}$$

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



$$BS_0(N) = \frac{1}{2N - (2l + 1)}, \quad l \in \mathbb{N},$$

$$BS_2(N) = \frac{1}{4^N} \frac{(2N)!}{(N!)^2},$$

$$BS_4(N) = \sum_{\tau_1=1}^N \frac{4^{\tau_1} (\tau_1!)^2}{(2\tau_1)! \tau_1^2},$$

$$BS_6(N) = \sum_{\tau_1=1}^N \frac{4^{-\tau_1} (2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{4^{\tau_2} (\tau_2!)^2}{(2\tau_2)! \tau_2^2}}{(\tau_1!)^2 \tau_1},$$

$$BS_8(N) = \sum_{\tau_1=1}^N \frac{\sum_{\tau_2=1}^{\tau_1} \frac{4^{\tau_2} (\tau_2!)^2}{(2\tau_2)! \tau_2^2}}{\tau_1},$$

$$BS_{10}(N) = \sum_{\tau_1=1}^N \frac{4^{\tau_1}}{(2\tau_1)!} \frac{1}{\tau_1^2} S_1(\tau_1).$$

$$BS_1(N) = 4^N \frac{(N!)^2}{(2N)!},$$

$$BS_3(N) = \sum_{\tau_1=1}^N \frac{4^{-\tau_1} (2\tau_1)!}{(\tau_1!)^2 \tau_1},$$

$$BS_5(N) = \sum_{\tau_1=1}^N \frac{4^{\tau_1} (\tau_1!)^2}{(2\tau_1)! \tau_1^3},$$

$$BS_7(N) = \sum_{\tau_1=1}^N \frac{4^{-\tau_1} (2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{4^{\tau_2} (\tau_2!)^2}{(2\tau_2)! \tau_2^3}}{(\tau_1!)^2 \tau_1},$$

$$BS_9(N) = \sum_{\tau_1=1}^N \frac{4^{-\tau_1} (2\tau_1)! \sum_{\tau_2=1}^{\tau_1} \frac{4^{\tau_2} (\tau_2!)^2 \sum_{\tau_3=1}^{\tau_2} \frac{1}{\tau_3}}{(2\tau_2)! \tau_2^2}}{(\tau_1!)^2 \tau_1},$$

Recursions and Asymptotic Representation



$$BS_8(N) - BS_8(N-1) = \frac{1}{N} BS_4(N),$$

$$BS_9(N) - BS_9(N-1) = \frac{1}{N} BS_3(N) BS_{10}(N),$$

$$BS_{10}(N) - BS_{10}(N-1) = \frac{1}{N} BS_1(N) S_1.$$

$$BS_0(N) \propto \frac{1}{2N} \sum_{k=0}^{\infty} \left(\frac{2k+1}{2N} \right)^k,$$

$$BS_8(N) \propto -7\zeta_3 + \left[+3(\ln(N) + \gamma_E) + \frac{3}{2N} - \frac{1}{4N^2} + \frac{1}{40N^4} - \frac{1}{84N^6} + \frac{1}{80N^8} - \frac{1}{44N^{10}} \right] \zeta_2$$

$$+ \sqrt{\frac{\pi}{N}} \left[4 - \frac{23}{18N} + \frac{1163}{2400N^2} - \frac{64177}{564480N^3} - \frac{237829}{7741440N^4} + \frac{5982083}{166526976N^5} \right.$$

$$+ \frac{5577806159}{438593126400N^6} - \frac{12013850977}{377864847360N^7} - \frac{1042694885077}{90766080737280N^8}$$

$$\left. + \frac{6663445693908281}{127863697547722752N^9} + \frac{23651830282693133}{1363413316298342400N^{10}} \right],$$

Inverse Mellin Transform



$$\mathbf{M}^{-1}[\text{BS}_8(N)](x) = \left[-\frac{4(1-\sqrt{1-x})}{1-x} + \left(\frac{2(1-\ln(2))}{1-x} + \frac{H_0(x)}{\sqrt{1-x}} \right) H_1(x) - \frac{H_{0,1}(x)}{\sqrt{1-x}} + \frac{H_1(x)G(\{6,1\},x)}{2(1-x)} - \frac{G(\{6,1,2\},x)}{2(1-x)} \right]_+,$$

$$\mathbf{M}^{-1}[\text{BS}_{10}(N)](x) = \left[-\frac{1}{1-x} \left[-4 - 4\ln(2)(-1 + \sqrt{1-x}) + 4\sqrt{1-x} + \zeta_2 \right] + 2(-1 + \ln(2))(-1 + \sqrt{1-x} + x) \frac{H_0(x)}{(1-x)^{3/2}} - 2 \frac{H_1(x)}{\sqrt{1-x}} + \frac{H_{0,1}(x)}{\sqrt{1-x}} - \frac{(-2 + \ln(2))G(\{6,1\},x)}{1-x} + \frac{G(\{6,1,2\},x)}{2(1-x)} - \frac{G(\{1,6,1\},x)}{2(1-x)} \right]_+.$$

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



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

$$\begin{aligned} & \frac{1}{x} \left\{ \ln(x) \left[C_A^2 T_F \left(-\frac{11488}{81} + \frac{224\zeta_2}{27} + \frac{256\zeta_3}{3} \right) + C_A C_F T_F \left(-\frac{15040}{243} - \frac{1408\zeta_2}{27} \right. \right. \right. \\ & \left. \left. \left. - \frac{1088\zeta_3}{9} \right) \right] + C_A T_F^2 \left[\frac{112016}{729} + \frac{1288}{27}\zeta_2 + \frac{1120}{27}\zeta_3 + \left(\frac{108256}{729} + \frac{368\zeta_2}{27} - \frac{448\zeta_3}{27} \right) \right. \right. \\ & \left. \left. \times N_F \right] + C_F \left[T_F^2 \left(-\frac{107488}{729} - \frac{656}{27}\zeta_2 + \frac{3904}{27}\zeta_3 + \left(\frac{116800}{729} + \frac{224\zeta_2}{27} - \frac{1792\zeta_3}{27} \right) N_F \right) \right. \right. \\ & \left. \left. + C_A T_F \left(-\frac{5538448}{3645} + \frac{1664B_4}{3} - \frac{43024\zeta_4}{9} + \frac{12208}{27}\zeta_2 + \frac{211504}{45}\zeta_3 \right) \right] \right. \\ & \left. + C_A^2 T_F \left(-\frac{4849484}{3645} - \frac{352B_4}{3} + \frac{11056\zeta_4}{9} - \frac{1088}{81}\zeta_2 - \frac{84764}{135}\zeta_3 \right) \right. \\ & \left. + C_F^2 T_F \left(\frac{10048}{5} - 640B_4 + \frac{51104\zeta_4}{9} - \frac{10096}{9}\zeta_2 - \frac{280016}{45}\zeta_3 \right) \right\} \end{aligned}$$

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



$$\begin{aligned}
 & + \left[-\frac{4}{3} C_F C_A T_F + \frac{2}{15} C_F^2 T_F \right] \ln^5(x) + \left[-\frac{40}{27} C_A^2 T_F + \frac{4}{9} C_F^2 T_F + C_F \left(-\frac{296}{27} C_A T_F \right. \right. \\
 & \left. \left. + \left(\frac{28}{27} + \frac{56}{27} N_F \right) T_F^2 \right) \right] \ln^4(x) + \left[\frac{112}{81} C_A (1 + 2N_F) T_F^2 + C_F \left(\left(\frac{1016}{81} + \frac{496}{81} N_F \right) T_F^2 \right. \right. \\
 & \left. \left. + C_A T_F \left(-\frac{10372}{81} - \frac{328\zeta_2}{9} \right) \right) + C_F^2 T_F \left[-\frac{2}{3} + \frac{4\zeta_2}{9} \right] + C_A^2 T_F \left[-\frac{1672}{81} + 8\zeta_2 \right] \right] \ln^3(x) \\
 & + \left[\frac{8}{81} C_A (155 + 118N_F) T_F^2 + C_F \left[T_F^2 \left(-\frac{32}{81} + N_F \left(\frac{3872}{81} - \frac{16\zeta_2}{9} \right) + \frac{232\zeta_2}{9} \right) \right. \right. \\
 & \left. \left. + C_A T_F \left(-\frac{70304}{81} - \frac{680\zeta_2}{9} + \frac{80\zeta_3}{3} \right) \right) + C_A^2 T_F \left[\frac{4684}{81} + \frac{20\zeta_2}{3} \right] + C_F^2 T_F \left[56 \right. \right. \\
 & \left. \left. + \frac{8\zeta_2}{3} - 40\zeta_3 \right] \right] \ln^2(x) + \left[C_F \left[T_F^2 \left(\frac{140992}{243} + N_F \left(\frac{182528}{243} - \frac{400\zeta_2}{27} - \frac{640\zeta_3}{9} \right) \right) \right. \right.
 \end{aligned}$$

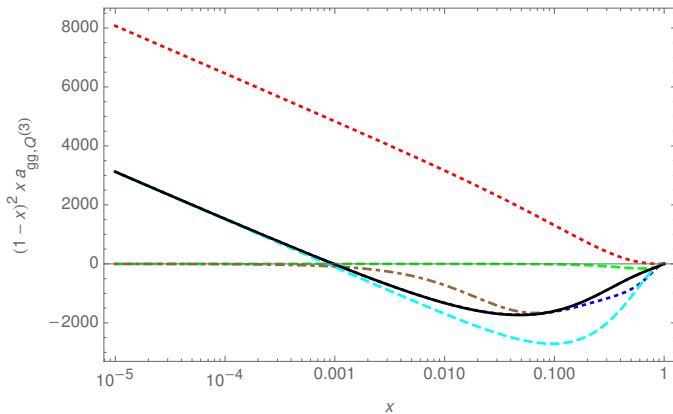
Small and large x limits of $a_{gg,Q}^{(3)}$



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

$$\begin{aligned}
 a_{gg,Q}^{(3),x \rightarrow 1}(x) & \propto a_{gg,Q,\delta}^{(3)} \delta(1-x) + a_{gg,Q,\text{plus}}^{(3)}(x) + \left[-\frac{32}{27} C_A T_F^2 (17 + 12N_F) + C_A C_F T_F \left(56 - \frac{32\zeta_2}{3} \right) \right. \\
 & \left. + C_A^2 T_F \left(\frac{9238}{81} - \frac{104\zeta_2}{9} + 16\zeta_3 \right) \right] \ln(1-x) + \left[-\frac{8}{27} C_A T_F^2 (7 + 8N_F) \right. \\
 & \left. + C_A^2 T_F \left(\frac{314}{27} - \frac{4\zeta_2}{3} \right) \right] \ln^2(1-x) + \frac{32}{27} C_A^2 T_F \ln^3(1-x).
 \end{aligned}$$

- 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: $N \rightarrow N + 1$.
 - 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 $t \rightarrow x$ 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 \pm -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.

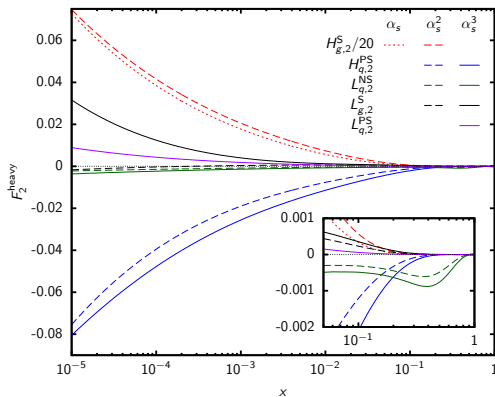


The non- N_F terms of $a_{gg,Q}^{(3)}(N)$ (rescaled) as a function of x . Full line (black): complete result; upper dotted line (red): term $\propto \ln(x)/x$, **BFKL limit**; lower dashed line (cyan): small x terms $\propto 1/x$; lower dotted line (blue): small x terms including all $\ln(x)$ terms up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

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 ...



- 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 through 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.

- 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.
 \implies QCD analysis.
- BFKL-like approaches are shown to utterly fail in describing these quantities.