



The 3-Loop Heavy Flavor Corrections to Deep-Inelastic Scattering

Seminar University of Zurich, May 16, 2024

Johannes Blümlein | May 17, 2024

DESY AND TU DORTMUND

- J. Ablinger et al., The unpolarized and polarized single-mass three-loop heavy flavor operator matrix elements $A_{gg,Q}$ and $\Delta A_{gg,Q}$, *JHEP* **12** (2022) 134.
- A. Behring, J.B., and K. Schönwald, The inverse Mellin transform via analytic continuation, *JHEP* **06** (2023) 62.
- J. Ablinger et al., The first-order factorizable contributions to the three-loop massive operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, *Nucl. Phys.B* 999 (2024) 116427.
- J. Ablinger et al., The non-first-order-factorizable contributions to the three-loop single-mass operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, 2403.00513 [hep-ph].



The Collaboration

[DESY-JKU Linz & younger colleagues]

- 2007-2009:

2-loop general N -results and 3-loop moments
I. Bierenbaum, JB. S. Klein

- 2010-now:

Individual 3-loop OMEs and HQ Wilson-coefficients at general N and x

J. Ablinger, A. Behring, JB, A. De Freitas, A. Hasselhuhn, S. Klein, A. von Manteuffel, M. Round, M. Saragnese, C. Schneider, K. Schönwald, F. Wißbrock

- Some special 2-loop applications (including massive QED)

also: G. Falcioni, W. van Neerven, T. Pfoh, C. Raab

Earlier calculations

- 1976-1982; 1991: Analytic 1-loop results

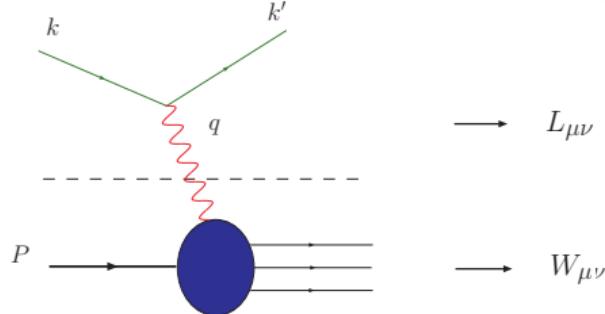
E. Witten; J. Babcock, D. W. Sivers, S. Wolfram; M.A. Shifman, A.I. Vainshtein, V.I. Zakharov; J.P. Leveille, T.J. Weiler; M. Glück, E. Hoffmann, E. Reya; C. Watson, W. Vogelsang

- 1995-1998: Analytic 2-loop results

M. Buza, Y. Matiounine, R. Migneron, W. van Neerven, J. Smith

1992-1995: Numeric 2-loop results E. Laenen, W. van Neerven, S. Riemersma, J. Smith

Deep-Inelastic Scattering (DIS):



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

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

$$\begin{aligned}
 W_{\mu\nu}(q, P, s) &= \frac{1}{4\pi} \int d^4\xi \exp(iq\xi) \langle P, s | [J_\mu^{em}(\xi), J_\nu^{em}(0)] | P, s \rangle = \\
 &\frac{1}{2x} \left(g_{\mu\nu} - \frac{q_\mu q_\nu}{q^2} \right) F_L(x, Q^2) + \frac{2x}{Q^2} \left(P_\mu P_\nu + \frac{q_\mu P_\nu + q_\nu P_\mu}{2x} - \frac{Q^2}{4x^2} g_{\mu\nu} \right) F_2(x, Q^2) \\
 &+ i\varepsilon_{\mu\nu\lambda\sigma} \frac{q^\lambda S^\sigma}{P \cdot q} g_1(x, Q^2) + i\varepsilon_{\mu\nu\lambda\sigma} \frac{q^\lambda (P \cdot q S^\sigma - S \cdot q P^\sigma)}{(P \cdot q)^2} g_2(x, Q^2).
 \end{aligned}$$

The structure functions $F_{2,L}$ and $g_{1,2}$ contain light and heavy quark contributions.
At 3-loop order also graphs with two heavy quarks of different mass contribute.
 \Rightarrow 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

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

into (pert.) **Wilson coefficients** and (nonpert.) **parton distribution functions (PDFs)**.

\otimes denotes the Mellin convolution

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

Many of 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:

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

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

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

→ additional Feynman rules with local operator insertions for partonic matrix elements.

The unpolarized light flavor Wilson coefficients are known up to NNLO

[Vermaseren, Moch, Vogt, 2005; JB, Marquard, Schneider, Schönwald, 2022].

For $F_2(x, Q^2)$: at $Q^2 \gtrsim 10m^2$ the asymptotic representation holds at the 1% level.



Why take large projects rather long ?

Examples:

- unpolarized anomalous dimensions and massless DIS Wilson coefficients
[Vermaseren, Larin, Nogueira, van Ritbergen, Moch, Vogt] **1990-2005: 15 years**
function space: harmonic sums
- unpolarized and polarized massive OMEs and asymptotic Wilson coefficients
[DESY-Linz collaboration] **2009 - 2024: 15 years**
function spaces: harmonic sums, generalized harmonic sums, finite cyclotomic sums, finite binomial sums, elliptic integrals, higher transcendental ${}_pF_q$ structures
- Initially the function spaces contributing were unknown.
- How to solve the systems of difference equations for the contributing topologies ?
- How to process the differential equations of the master integrals to provide large numbers of moments ?
- How to deal with all first order factorizing difference equations ?
- How to solve the elliptic-affected part ?
- How to tackle 2-mass problems analytically ?
- Are N-space solutions providing the right framework ? [Non-first order factorizable recurrences.]
- Do the computer resources suffice [in space and time] to establish all contributing recurrences ?

Why take large projects rather long ?



- At present, massless 3-loop problems are no problem anymore.
 - Typical computation times $O(1\text{year})$; pole-terms: $O(\text{month})$.
 - Basically all technologies needed are available in (private) codes.
 - **Example:** Polarized massless 3-loop Wilson coefficients for DIS.

These calculations are modern adventures.

One enters a terra incognita with rough ideas but insufficient means and one has to develop new technologies all the way along to get through. In this way one lifts the whole field to new levels, which allows to perform many more calculations.

One has to pass many intermediate stops (no-goes) to arrive at the final complete solution: the strategic goal.

Copernican turns:



[J. Reinhardt scan & Deutsche Bundespost]

I. Kant, Vorwort zu Kritik der Reinen Vernunft:

Es ist hiermit ebenso, als mit den ersten Gedanken des Kopernikus bewandt, der, nachdem es mit der Erklärung der Himmelsbewegungen nicht gut fort wollte, wenn er annahm, das ganze Sternenheer drehe sich um den Zuschauer, versuchte, ob es nicht besser gelingen möchte, wenn er den Zuschauer sich drehen, und dagegen die Sterne in Ruhe ließ. In der Metaphysik kann man nun, was die Anschauung der Gegenstände betrifft, es auf ähnliche Weise versuchen.

If one view [method] does not solve (a part of) a problem, try the adjoint view.

The solution to any problem is simple, after the correct Meta-Language has been found.

Copernican turns:

- Change from N -space methods to x -space methods (and probably back).
- Use local information (simpler equations), if the solution of global equations are too difficult or even impossible at the time.
- Don't forget about the **Principle of Simplicity**.



[BWV 846, from Wikipedia]



Copernican turns:

- All information counts. Try to access it and not to bury it.
- General methods are sometimes easier for the user. But they are also more costly and can get stuck.
- → One has to design problem-oriented new methods.

Don't follow any dogma!
Every problem determines its way of solution.

[These thoughts are thoughts a posteriori.]



The main time-line for the 3-loop corrections

- 2005 F_L [no massive 3-loop OMEs needed]
- 2010 All unpolarized N_F terms and $A_{qg,Q}^{(3)}, A_{qg,Q}^{(3),PS}$
- 2014 unpolarized logarithmic 3-loop contributions and $A_{qg,Q}^{(3)}, (\Delta)A_{qg,Q}^{(3),NS}, A_{Qq}^{(3),PS}$
- 2017 two-mass corrections $A_{qg,Q}^{(3)}, (\Delta)A_{qg,Q}^{(3),NS}, A_{Qq}^{(3),PS}$
- 2018 two-mass corrections $A_{qg,Q}^{(3)}$
- 2019 2-loop correction: $(\Delta)A_{Qq}^{(2),PS}$ whole kinematic region and $\Delta A_{Qq}^{(3),PS}$
- 2019 two-mass corrections $\Delta A_{Qq}^{(3),PS}$
- 2020 two-mass corrections $\Delta A_{gg,Q}^{(3)}$
- 2021 polarized logarithmic 3-loop contributions and $\Delta A_{qg,Q}^{(3)}, \Delta A_{qg,Q}^{(3),PS}, \Delta A_{gq}^{(3)}$
- 2022 3-loop polarized massless Wilson coefficients [JB, Marquard, Schneider, Schönwald]
- 2022 corrected the polarized 2-loop contributions
- 2022 $(\Delta)A_{gg,Q}^{(3)}$
- 2023 $(\Delta)A_{Qg}^{(3)}$: 1st order factorizing parts
- 2024 $(\Delta)A_{Qg}^{(3)}$, [two-mass corrections $(\Delta)A_{Qg}^{(3)}$]

- [45 physics papers \(journals\)](#)
- [26 mathematical papers](#)
 - 1998 Harmonic sums [[Vermaseren; JB](#)]
 - 2000,2005 Analytic continuations of harmonic sums to $N \in \mathbb{C}$ [[JB; JB, S. Moch](#)]
 - 2003 Concrete shuffle algebras [[JB](#)]
 - 2009 Guessing large recurrences [[JB, M. Kauers, S. Klein, C. Schneider](#)]
 - 2009 Structural relations of harmonic sums [[JB](#)]
 - 2009 MZV Data mine [[JB, D. Broadhurst, J. Vermaseren](#)]
 - 2011 Cyclotomic harmonic sums and harmonic polylogarithms [[Ablinger, JB, Schneider](#)]
 - 2013 Generalized harmonic sums and harmonic polylogarithms [[Ablinger, JB, Schneider](#)]; 2001 [[Moch, Uwer, Weinzierl](#)]
 - 2014 Finite binomial sums and root-valued iterated integrals [[Ablinger, JB, Raab, Schneider](#)]
 - 2017 ${}_2F_1$ solutions (iterated non-iterative integrals) [[J. Ablinger, JB, A. De Freitas, M. van Hoeij, E. Imamoglu, C. Raab, C.S. Radu, C. Schneider](#)]
 - 2017 Methods of arbitrary high moments [[JB, Schneider](#)]
 - 2018 Automated solution of first-order factorizing differential equation systems in an arbitrary basis [[J. Ablinger, JB, P. Marquard, N. Rana, C. Schneider](#)]
 - 2023 Analytic continuation form t to x -space [[JB, Behring, Schönwald](#)]

Important Computer-Algebra Packages

C. Schneider: Sigma, EvaluateMultiSums, SumProduction, SolveCoupledSystem

J. Ablinger: HarmonicSums

The Wilson Coefficients at large Q^2



$$L_{q,(2,L)}^{\text{NS}}(N_F + 1) = a_s^2 [A_{qq,Q}^{(2),\text{NS}}(N_F + 1)\delta_2 + \hat{C}_{q,(2,L)}^{(2),\text{NS}}(N_F)] + a_s^3 [A_{qq,Q}^{(3),\text{NS}}(N_F + 1)\delta_2 + A_{qq,Q}^{(2),\text{NS}}(N_F + 1)C_{q,(2,L)}^{(1),\text{NS}}(N_F + 1) + \hat{C}_{q,(2,L)}^{(3),\text{NS}}(N_F)]$$

$$L_{q,(2,L)}^{\text{PS}}(N_F + 1) = a_s^3 [A_{qq,Q}^{(3),\text{PS}}(N_F + 1)\delta_2 + N_F A_{gg,Q}^{(2),\text{NS}}(N_F) \tilde{C}_{g,(2,L)}^{(1),\text{NS}}(N_F + 1) + N_F \hat{C}_{g,(2,L)}^{(3),\text{PS}}(N_F)]$$

$$\begin{aligned} L_{g,(2,L)}^{\text{S}}(N_F + 1) = & a_s^2 A_{gg,Q}^{(1)}(N_F + 1) N_F \tilde{C}_{g,(2,L)}^{(2)}(N_F + 1) + a_s^3 [A_{gg,Q}^{(3)}(N_F + 1)\delta_2 + A_{gg,Q}^{(1)}(N_F + 1) N_F \tilde{C}_{g,(2,L)}^{(2)}(N_F + 1) \\ & + A_{gg,Q}^{(2)}(N_F + 1) N_F \tilde{C}_{g,(2,L)}^{(1)}(N_F + 1) + A_{Qg}^{(1)}(N_F + 1) N_F \tilde{C}_{q,(2,L)}^{(2),\text{PS}}(N_F + 1) + N_F \hat{C}_{g,(2,L)}^{(3)}(N_F)] \end{aligned}$$

$$\begin{aligned} H_{q,(2,L)}^{\text{PS}}(N_F + 1) = & a_s^2 [A_{Qq}^{(2),\text{PS}}(N_F + 1)\delta_2 + \tilde{C}_{q,(2,L)}^{(2),\text{PS}}(N_F + 1)] \\ & + a_s^3 [A_{Qq}^{(3),\text{PS}}(N_F + 1)\delta_2 + A_{gg,Q}^{(2)}(N_F + 1) \tilde{C}_{g,(1,L)}^{(2)}(N_F + 1) + A_{Qq}^{(2),\text{PS}}(N_F + 1) \tilde{C}_{q,(2,L)}^{(1),\text{NS}}(N_F + 1) + \tilde{C}_{q,(2,L)}^{(3),\text{PS}}(N_F + 1)] \end{aligned}$$

$$\begin{aligned} H_{g,(2,L)}^{\text{S}}(N_F + 1) = & a_s [A_{Qg}^{(1)}(N_F + 1)\delta_2 + \tilde{C}_{g,(2,L)}^{(1)}(N_F + 1)] \\ & + a_s^2 [A_{Qg}^{(2)}(N_F + 1)\delta_2 + A_{Qg}^{(1)}(N_F + 1) \tilde{C}_{q,(2,L)}^{(1)}(N_F + 1) + A_{gg,Q}^{(1)}(N_F + 1) \tilde{C}_{g,(2,L)}^{(1)}(N_F + 1) + \tilde{C}_{g,(2,L)}^{(2)}(N_F + 1)] \\ & + a_s^3 [A_{Qg}^{(3)}(N_F + 1)\delta_2 + A_{Qg}^{(2)}(N_F + 1) \tilde{C}_{q,(2,L)}^{(1)}(N_F + 1) + A_{gg,Q}^{(2)}(N_F + 1) \tilde{C}_{g,(2,L)}^{(1)}(N_F + 1) \\ & + A_{Qg}^{(1)}(N_F + 1) \tilde{C}_{q,(2,L)}^{(2),\text{S}}(N_F + 1) + A_{gg,Q}^{(1)}(N_F + 1) \tilde{C}_{g,(2,L)}^{(1)}(N_F + 1) + \tilde{C}_{g,(2,L)}^{(3)}(N_F + 1)] \end{aligned}$$

- The case for two different masses obeys an analogous representation.
- Note the contributions of the massless Wilson coefficients.



The variable flavor number scheme

- Matching conditions for parton distribution functions:

$$f_k(N_F + 2) + f_{\bar{k}}(N_F + 2) = A_{qq,Q}^{\text{NS}} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot [f_k(N_F) + f_{\bar{k}}(N_F)] + \frac{1}{N_F} A_{qq,Q}^{\text{PS}} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F)$$

$$+ \frac{1}{N_F} A_{qg,Q} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F),$$

$$f_Q(N_F + 2) + f_{\bar{Q}}(N_F + 2) = A_{Qq}^{\text{PS}} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F) + A_{Qg} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F),$$

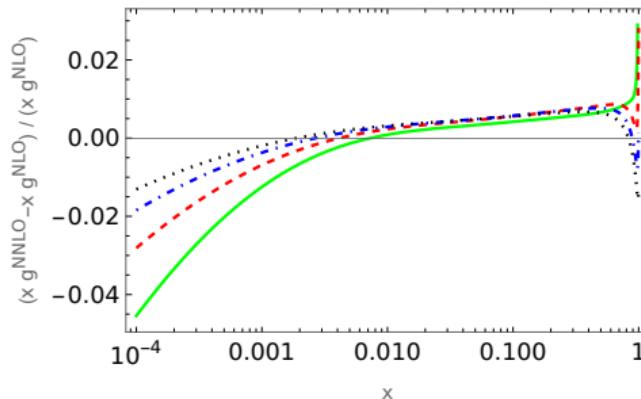
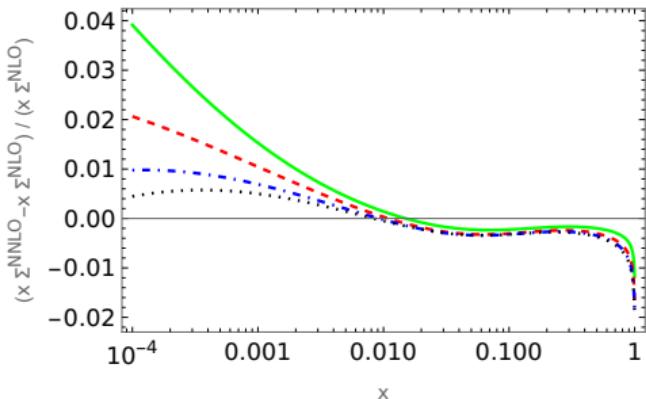
$$\Sigma(N_F + 2) = \left[A_{qq,Q}^{\text{NS}} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + A_{qq,Q}^{\text{PS}} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + A_{Qq}^{\text{PS}} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right] \cdot \Sigma(N_F)$$

$$+ \left[A_{qg,Q} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + A_{Qg} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right] \cdot G(N_F),$$

$$G(N_F + 2) = A_{gg,Q} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot \Sigma(N_F) + A_{gg,Q} \left(N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \cdot G(N_F).$$

The charm and bottom quark masses are not that much different.

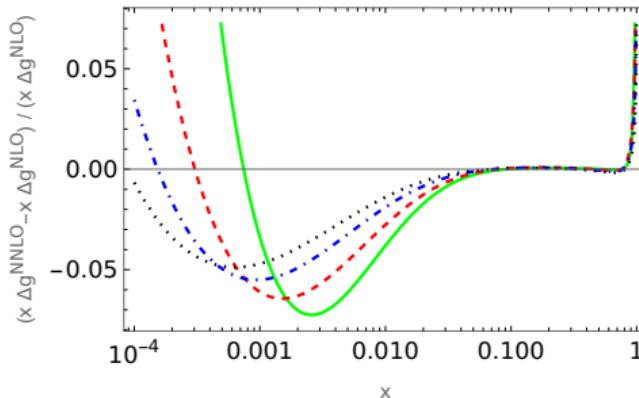
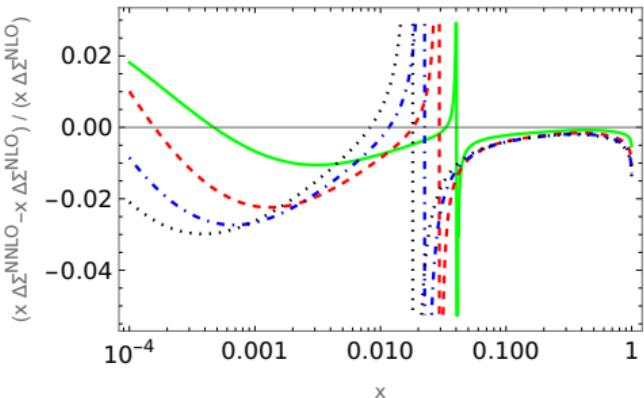
Relative effect in unpolarized NNLO evolution



$Q^2 = 10, 10^2, 10^3, 10^4 \text{ GeV}^2$ dotted, dash-dotted, dashed, full lines. [M. Saragnese, 2022]

The unpolarized world deep-inelastic data have a precision of $O(1\%)$.

Relative effect in polarized NNLO evolution



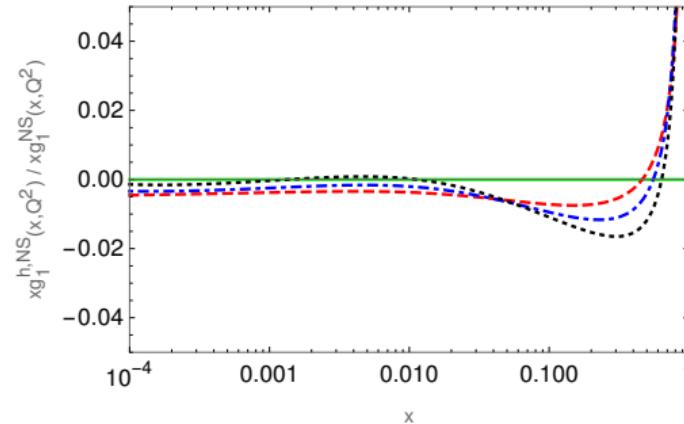
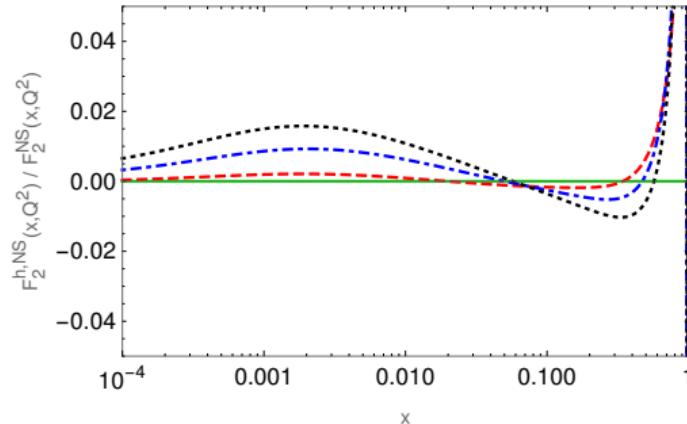
$Q^2 = 10, 10^2, 10^3, 10^4 \text{ GeV}^2$ dotted, dash-dotted, dashed, full lines. [M. Saragnese, 2022]

The future polarized data at the EIC will reach a precision of $O(1\%)$.

The relative contribution of HQ to non-singlet structure functions at N³LO



Scheme-invariant evolution



Left: The relative contribution of the heavy flavor contributions due to c and b quarks to the structure function F_2^{NS} at N³LO; dashed lines: 100 GeV^2 ; dashed-dotted lines: 1000 GeV^2 ; dotted lines: 10000 GeV^2 . Right: The same for the structure function xg_1^{NS} at N³LO. [JB, M. Saragnese, 2021].

Calculation of the 3-loop operator matrix elements



The OMEs are calculated using the QCD Feynman rules together with the following operator insertion Feynman rules:

$$p, i \quad p, j$$

$$\delta^{ij} \Delta \gamma_+ (\Delta \cdot p)^{N-1}, \quad N \geq 1$$

$$\begin{array}{c} \text{---} \nearrow \otimes \searrow \text{---} \\ p_1, i \qquad \qquad \qquad p_2, j \\ | \\ \textcircled{a} \end{array}$$

$$q t_{ii}^{\alpha} \Delta^{\mu} \Delta \gamma_+ \sum_{j=0}^{N-2} (\Delta \cdot p_1)^j (\Delta \cdot p_2)^{N-j-2}, \quad N \geq 2$$

$$g^2 \Delta^\mu \Delta^\nu \Delta \gamma_\pm \sum_{j=0}^{N-3} \sum_{l=j+1}^{N-2} (\Delta p_2)^j (\Delta p_1)^{N-l-2} \\ \left[(t^a t^b)_{ji} (\Delta p_1 + \Delta p_4)^{l-j-1} + (t^b t^a)_{ji} (\Delta p_1 + \Delta p_3)^{l-j-1} \right], \\ N > 2$$

N > 3

$$\begin{aligned}
& g^3 \Delta_{\mu} \Delta_{\nu} \Delta_{\rho} \delta_{\theta} \tau = \sum_{N=0}^{\infty} \sum_{m=1}^{N-1} \sum_{l=0}^{N-m} \sum_{j=1}^{m+l+1} (\Delta_2)^j (\Delta_1)^{N-m-2} \\
& \quad \left[\left(t^{ab} t^{bc} \right)_{ji} (\Delta_4 + \Delta_5 + \Delta_1)^{l-j-1} (\Delta_5 + \Delta_1)^{m-l-1} \right. \\
& \quad + \left(t^{ab} t^{cd} \right)_{ji} (\Delta_4 + \Delta_5 + \Delta_1)^{l-j-1} (\Delta_4 + \Delta_1)^{m-l-1} \\
& \quad + \left(t^{bd} t^{ca} \right)_{ji} (\Delta_3 + \Delta_5 + \Delta_1)^{l-j-1} (\Delta_5 + \Delta_1)^{m-l-1} \\
& \quad + \left(t^{bd} t^{cd} \right)_{ji} (\Delta_3 + \Delta_5 + \Delta_1)^{l-j-1} (\Delta_3 + \Delta_1)^{m-l-1} \\
& \quad + \left. \left(t^{cd} t^{ab} \right)_{ji} (\Delta_3 + \Delta_4 + \Delta_1)^{l-j-1} (\Delta_3 + \Delta_1)^{m-l-1} \right] ,
\end{aligned}$$

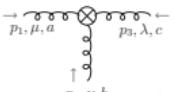
$$N > 4$$

$$\gamma_+ = 1, \quad \gamma_- = 2\pi.$$



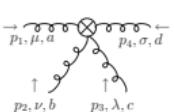
$$\frac{1+(-1)^N}{2} \delta^{ab} (\Delta \cdot p)^{N-2}$$

$$\left[g_{\mu\nu}(\Delta \cdot p)^2 - (\Delta_\mu p_\nu + \Delta_\nu p_\mu)\Delta \cdot p + p^2 \Delta_\mu \Delta_\nu \right], \quad N \geq 2$$



$$-ig\frac{1+(-1)^N}{2}f^{abc}\left(p_1+\Delta_\mu(p_{1,\nu}\Delta_\lambda-p_{1,\lambda}\Delta_\nu)\right)(\Delta\cdot p_1)^{N-2}$$

$$+ \sum_{\mu-\nu=\lambda-\mu}^{\infty} \left(\begin{array}{c} p_1 \rightarrow p_2 \rightarrow p_3 \rightarrow p_1 \\ \mu \rightarrow \nu \rightarrow \lambda \rightarrow \mu \end{array} \right) + \left(\begin{array}{c} p_1 \rightarrow p_3 \rightarrow p_2 \rightarrow p_1 \\ \mu \rightarrow \lambda \rightarrow \nu \rightarrow \mu \end{array} \right), \quad N \geq 2$$



$$g^{\frac{n+1+(-1)^N}{2}} \left(f^{abc} f^{cde} O_{\mu\nu\lambda\tau}(p_1, p_2, p_3, p_4) \right. \\ \left. + f^{bdc} O_{\mu\lambda\nu\tau}(p_1, p_3, p_2, p_4) + f^{ade} f^{bce} O_{\mu\alpha\nu\lambda}(p_1, p_4, p_2, p_3) \right), \\ (p_1, p_2, p_3, p_4) = \Delta_\alpha \Delta_\lambda - g_{\alpha\tau} (\Delta \cdot p_3 + \Delta \cdot p_4)^{N-2}$$

$$+ [p_{4,\mu} \Delta_\sigma - \Delta \cdot p_4 g_{\mu\sigma}] \sum_{i=0}^{N-3} (\Delta \cdot p_3 + \Delta \cdot p_4)^i (\Delta \cdot p_4)^{N-3-i}$$

$$-[p_{1,\sigma}\Delta_\mu - \Delta \cdot p_1 g_{\mu\sigma}] \sum_{i=0}^{N-3} (-\Delta \cdot p_1)^i (\Delta \cdot p_3 + \Delta \cdot p_4)^{N-3-i}$$

$$+ [\Delta \cdot p_1 \Delta \cdot p_4 g_{\mu\sigma} + p_1 \cdot p_4 \Delta_\mu \Delta_\sigma - \Delta \cdot p_4 p_{1,\sigma} \Delta_\mu - \Delta \cdot p_1 p_{4,\mu} \Delta_\sigma] \\ \times \sum_{i=0}^{N-4} \sum_{j=0}^i (-\Delta \cdot p_1)^{N-4-i} (\Delta \cdot p_3 + \Delta \cdot p_4)^{i-j} (\Delta \cdot p_4)^j \Big\}$$

$$-\left\{ \begin{smallmatrix} p_1 \leftrightarrow p_2 \\ \dots \\ p_{m-1} \leftrightarrow p_m \end{smallmatrix} \right\} - \left\{ \begin{smallmatrix} p_3 \leftrightarrow p_4 \\ \dots \\ p_{N-m} \leftrightarrow p_N \end{smallmatrix} \right\} + \left\{ \begin{smallmatrix} p_1 \leftrightarrow p_2, & p_3 \leftrightarrow p_4 \\ \dots \\ p_{m-1} \leftrightarrow p_m, & p_{N-m} \leftrightarrow p_N \end{smallmatrix} \right\}, \quad N \geq 2$$



Calculation methods

- Diagram generation: QGRAF [Nogueira, 1993]
- Lorentz and Dirac algebra: Form [Vermaseren, 2000]
- Color algebra: Color [van Ritbergen, Schellekens, Vermaseren, 1999]
- IBP reduction: Reduze 2 [von Manteuffel, Studerus 2009, 2012]
- N space calculations:
 - Method of arbitrary large moments [JB, Schneider, 2017]
 - Summation theory and solving first-order factorizing recurrences: Sigma [Schneider, 2007, 2013]
 - Reduce the results in the respective function spaces: HarmonicSums [Ablinger, 2009, 2012, etc.]
- x space calculations
 - solve 1st order factorizing differential equations
 - transform from $N \rightarrow t$ -space, solve the respective systems of differential equations (not necessarily factorizing to first order) [Behring, JB, Schönwald, 2023]
 - Reduce the results in the respective function spaces; iterated integrals over alphabets containing also higher transcendental letters [Ablinger et al. 2017]
 - The higher transcendental letters have to be known in analytic form for $z \in \mathbb{C}$.
- Both N and x space techniques are needed to solve the present problem. The recurrences for $A_{Qg}^{(3)}$ need far more than 15000 moments to be found & there are no technologies yet to solve non-first order factorizing recurrences analytically.
- Final numerical representation: In the most complicated cases: local series expansions in x at high precision.



Mathematical Background

- massless and massive contributions to two-loops: harmonic sums
- all pole terms to three-loops: harmonic sums
- all massless Wilson coefficients to three-loops: harmonic sums

Single-mass OMEs

- all N_F of the massive OMEs three-loops: harmonic sums
- $(\Delta)A_{qg,Q}^{(3),NS}, (\Delta)A_{gq,Q}^{(3)}, (\Delta)A_{gg,Q}^{(3)}, (\Delta)A_{qq,Q}^{(3),PS}$ to three-loops: harmonic sums
- $(\Delta)A_{Qq}^{(3),PS}$ to three-loops: generalized harmonic sums and also $H_{\bar{a}}(1 - 2x)$
- $(\Delta)A_{gg,Q}^{(3)}$ to three-loops: finite binomial sums and square-root valued iterated integrals
- $(\Delta)A_{Qg}^{(3)}$ to three-loops:
 - first-order factorizing contributions: finite binomial sums; all iterated integrals in x -space can be rationalized
 - non-first-order factorizing contributions: ${}_2F_1$ letters in iterated integrals in x -space

Two-mass OMEs

- $(\Delta)A_{qg,Q}^{(3),NS}, (\Delta)A_{gq,Q}^{(3)}$: harmonic sums
- $(\Delta)A_{Qq}^{(3),PS}$: analytic solutions in x -space only; different supports; root-values letters
- $(\Delta)A_{gg,Q}^{(3)}$: root-valued iterated integrals

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



Resumming Mellin N into a continuous variable t , observing crossing relations. Ablinger et al. 2012

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

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

The $f_i(t)$ include higher transcendental letters. Regularization for $t \rightarrow 0$ needed.

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

t-space is still Mellin space. One needs closed expressions to perform the analytic continuation (1). Analytic continuation is needed to calculate the small x behaviour. The final expansion maps the problem into a very large number of G -constants, including those with higher transcendental letters.



Harmonic polylogarithms

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

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

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

Example:

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

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

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

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



Square root valued alphabets

$$\begin{aligned}\mathfrak{A}_{\text{sqrt}} &= \left\{ f_4, f_5, f_6 \dots \right\} \\ &= \left\{ \frac{\sqrt{1-x}}{x}, \sqrt{x(1-x)}, \frac{1}{\sqrt{1-x}}, \frac{1}{\sqrt{x}\sqrt{1\pm x}}, \frac{1}{x\sqrt{1\pm x}}, \frac{1}{\sqrt{1\pm x}\sqrt{2\pm x}}, \frac{1}{x\sqrt{1\pm x/4}}, \dots \right\},\end{aligned}$$

Monodromy also through:

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

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

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

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

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

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



Iterative non-iterative Integrals

Alphabet:

$$\mathfrak{A}_2 = \left\{ \frac{1}{t}, \frac{1}{1-t}, \frac{1}{8+t}, g_1, g_2, \frac{g_1}{t}, \frac{g_1}{1-t}, \frac{g_1}{8+t}, \frac{g'_1}{t}, \frac{g'_1}{1-t}, \frac{g'_1}{8+t}, \frac{g_2}{t}, \frac{g_2}{1-t}, \frac{g_2}{8+t}, \frac{g'_2}{t}, \frac{g'_2}{1-t}, \frac{g'_2}{8+t}, tg_1, tg_2 \right\}$$

$$\begin{aligned} F_1(t) = & \frac{8}{\varepsilon^3} \left[1 + \frac{1}{t} H_1(t) \right] - \frac{1}{\varepsilon^2} \left[\frac{1}{6} (106 + t) + \frac{(9 + 2t)}{t} H_1(t) + \frac{4}{t} H_{0,1}(t) \right] \\ & + \frac{1}{\varepsilon} \left\{ \frac{1}{12} (271 + 9t) + \left[\frac{71 + 32t + 2t^2}{12t} + \frac{3\zeta_2}{t} \right] H_1(t) + \frac{(9 + 2t)}{2t} H_{0,1}(t) + \frac{2}{t} H_{0,0,1}(t) \right. \\ & \left. + 3\zeta_2 \right\} + \frac{1}{t} \left\{ \frac{6696 - 22680t - 16278t^2 - 255t^3 - 62t^4}{864t} + (9 + 9t + t^2) g_1(t) \left[\frac{31 \ln(2)}{16} \right. \right. \\ & \left. \left. + \frac{1}{144} (265 + 31\pi(-3i + \sqrt{3})) + \frac{3}{8} \ln(2) \zeta_2 + \frac{1}{24} (10 + \pi(-3i + \sqrt{3})) \zeta_2 - \frac{7}{4} \zeta_3 \right] \right\} \end{aligned}$$

$$\begin{aligned}
& + G(18, t) \left[-\frac{93 \ln(2)}{16} + \frac{1}{48} (-265 - 31\pi(-3i + \sqrt{3})) + \left(-\frac{9 \ln(2)}{8} \right. \right. \\
& \quad \left. \left. + \frac{1}{8} (-10 - \pi(-3i + \sqrt{3})) \right) \zeta_2 + \frac{21}{4} \zeta_3 \right] \dots \\
& + \frac{5}{2} [G(4, 14, 1, 2; t) - G(5, 8, 1, 2; t)] + \frac{1}{4} [G(13, 8, 1, 2; t) - G(7, 14, 1, 2; t)] \\
& \quad \left. + \frac{9}{4} [G(10, 14, 1, 2; t) - G(16, 8, 1, 2; t)] + \frac{3}{4} [G(19, 14, 1, 2; t) - G(19, 8, 1, 2; t)] \right\} + O(\varepsilon), \\
F_2(t) &= \frac{8}{\varepsilon^3} + \frac{1}{\varepsilon^2} \left[-\frac{1}{3}(34+t) + \frac{2(1-t)}{t} H_1(t) \right] + \frac{1}{\varepsilon} \left[\frac{116+15t}{12} + 3\zeta_2 - \frac{(1-t)(8+t)}{3t} H_1(t) \right. \\
& \quad \left. - \frac{1-t}{t} H_{0,1}(t) \right] + \frac{992 - 368t + 75t^2 - 27t^3}{144t} + (1-t) \left(\frac{(43+10t+t^2)}{12t} H_1(t) + \frac{(4-t)}{4t} \right. \\
& \quad \left. \times H_{0,1}(t) + \frac{3\zeta_2}{4t} H_1(t) \right) + (1-t) g_1(t) \left(\frac{31 \ln(2)}{16} + \frac{1}{144} (265 + 31\pi(-3i + \sqrt{3})) \dots \right)
\end{aligned}$$

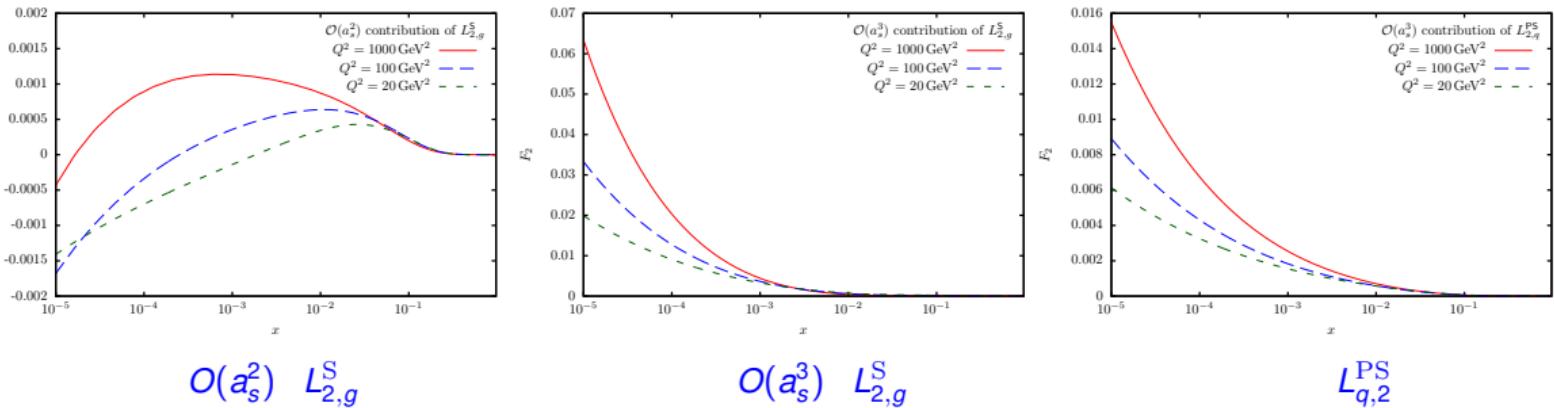
Essential step for calculating $a_{Qg}^{(3)}$ completely.

First-order factorizable contributions



- All contributions to the amplitude in t - and x -space can be represented by G -functions over at most square-root valued alphabets.
- Singularities in $x \in [0, 1]$ in individual terms have to be removed first.
- The resulting functions can all be rationalized.
- Further, they can be mapped to Kummer-Poincaré integrals over alphabets with many letters and even many more special numbers.
- One may now perform formal analytic Taylor expansions around $x = 0$ and $x = 1$, which are usually log-modulated.
- Because of the limited range of convergence of these series, a few more expansions inside $[0, 1]$ are needed.
- The coefficients of these expansions are Kummer-Poincaré constants, i.e. G -functions at argument $x = 1$. They can all be calculated using the Hölder convolution to high precision [[Borwein, Bradley, Broadhurst, Lisonek 2001](#); [Weinzierl, Vollinga, 2005](#)].
- The amount of these coefficients is huge.

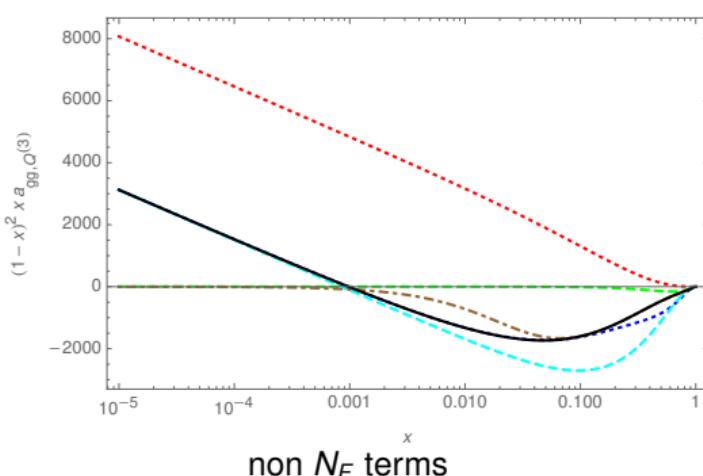
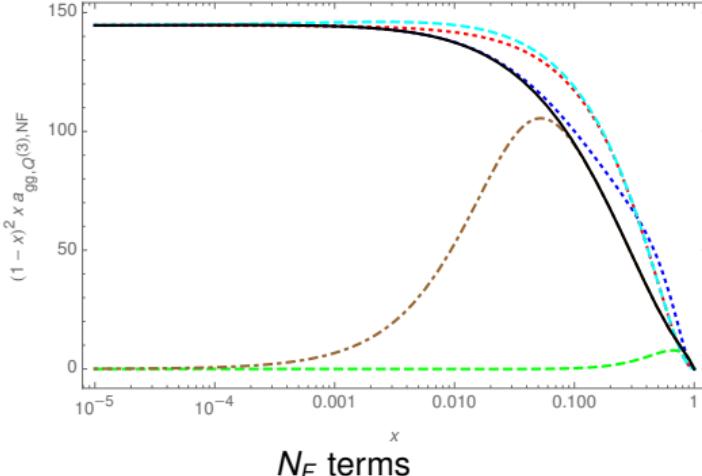
Numerical Results : $L_{g,2}^S$ and $L_{q,2}^{PS}$



$O(a_s^2) \quad L_{2,g}^S$

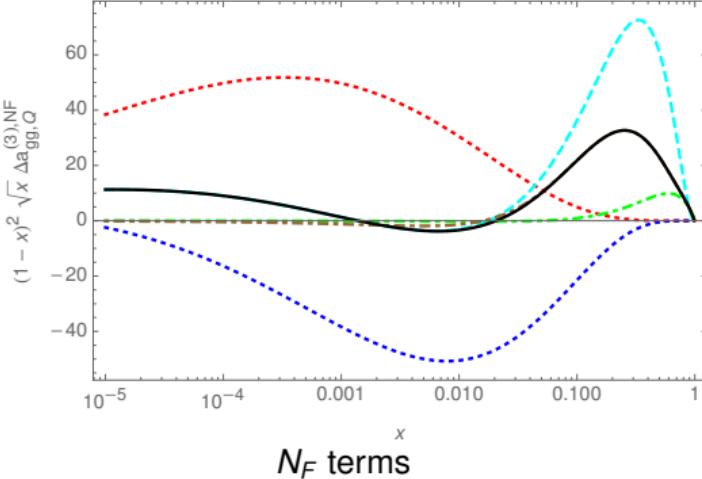
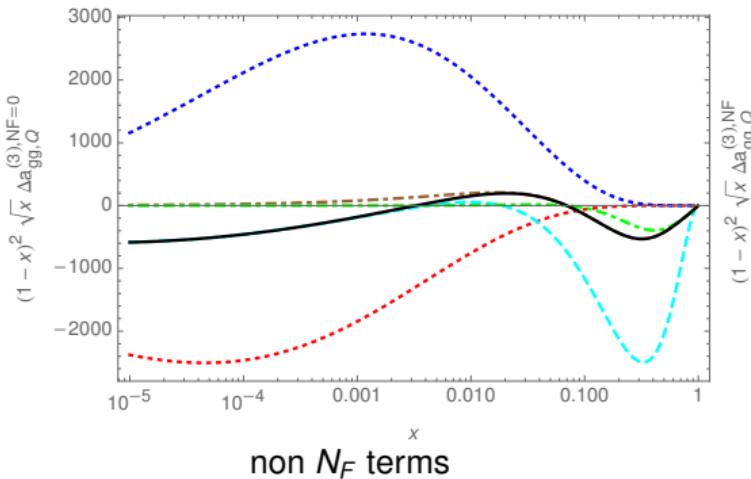
$O(a_s^3) \quad L_{2,g}^S$

$L_{q,2}^{PS}$

non N_F terms N_F terms

Left panel: 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 $\propto \ln(x)/x$; 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. Right panel: the same for the N_F contribution.

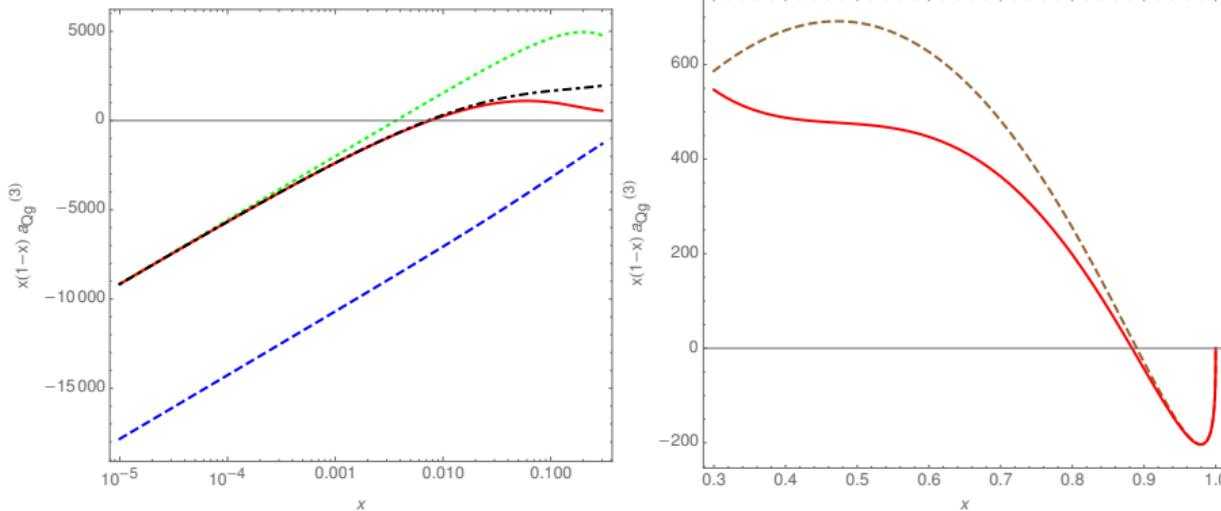
$\Delta a_{gg}^{(3)}$



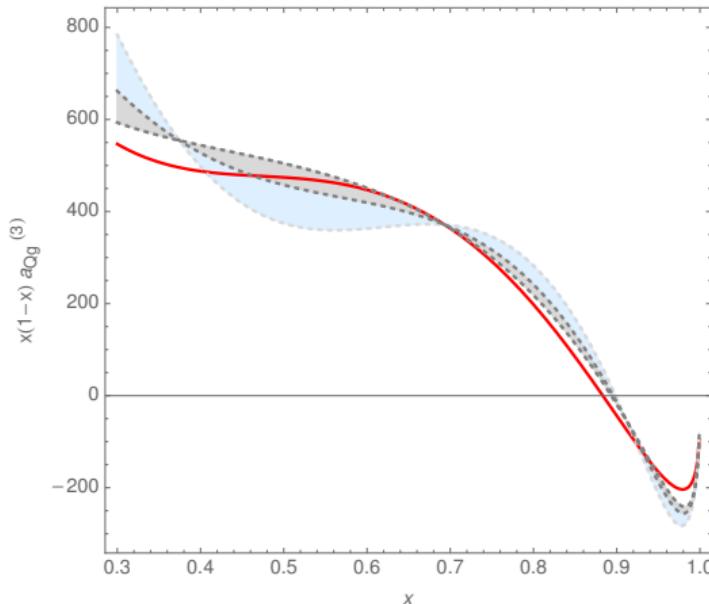
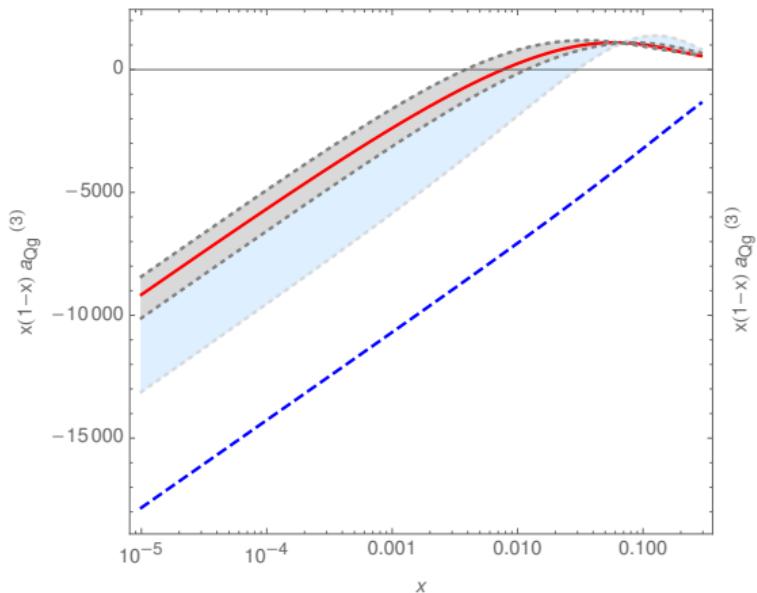
The non- N_F terms of $\Delta a_{gg,Q}^{(3)}(N)$ (rescaled) as a function of x . Full line (black): complete result; lower dotted line (red): term $\ln^5(x)$; upper dotted line (blue): small x terms $\propto \ln^5(x)$ and $\ln^4(x)$; upper dashed line (cyan): small x terms including all $\ln(x)$ terms up to the constant term; lower dash-dotted line (green): large x contribution up to the constant term; dash-dotted line (brown): full large x contribution. Right panel: the same for the N_F contribution.

$a_{Qg}^{(3)}$ 

1009 of the total 1233 Feynman diagrams have first-order factorizing contributions only and are given by G -functions up to root-values letters. The letters for all constants can be rationalized.

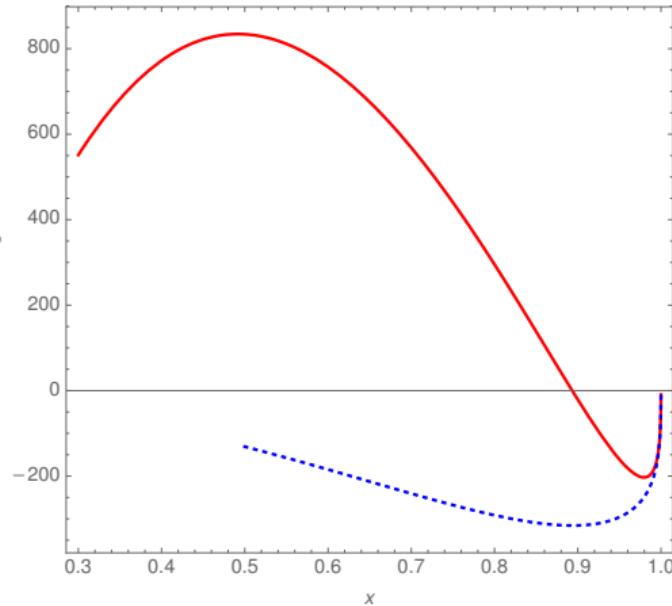
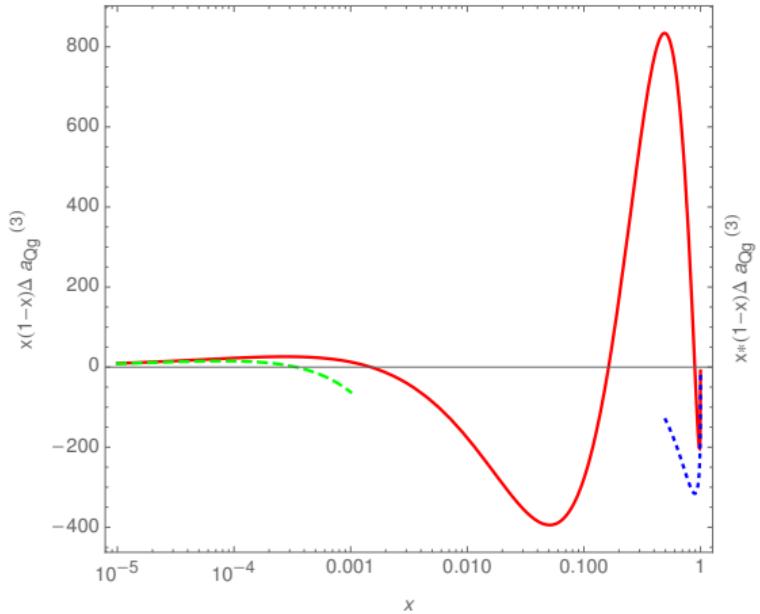


$a_{Qg}^{(3)}(x)$ as a function of x , rescaled by the factor $x(1 - x)$. Left panel: smaller x region. Full line (red): $a_{Qg}^{(3)}(x)$; dashed line (blue): leading small- x term $\propto \ln(x)/x$ [Catani, Ciafaloni, Hautmann, 1990]; dotted line (green): $\ln(x)/x$ and $1/x$ term; dash-dotted line (black): all small- x terms, including also $\ln^k(x)$, $k \in \{1, \dots, 5\}$. Right panel: larger x region. Full line (red): $a_{Qg}^{(3)}(x)$; dashed line (brown): leading large- x terms up to the terms $\propto (1 - x)$, covering the logarithmic contributions of $O(\ln^k(1 - x))$, $k \in \{1, 4\}$.

$a_{Qg}^{(3)}$ 

$a_{Qg}^{(3)}(x)$ as a function of x , rescaled by the factor $x(1 - x)$. Left panel: smaller x region. Full line (red): $a_{Qg}^{(3)}(x)$; dashed line (blue): leading small- x term $\propto \ln(x)/x$ [Catani, Ciafaloni, Hautmann, 1990]; light blue region: estimates of [Kawamura et al., 2012]; gray region: estimates of [ABMP 2017]. Right panel: larger x region. Full line (red): $a_{Qg}^{(3)}(x)$; light blue region: estimates of [Kawamura et al., 2012] gray region: estimates of [ABMP 2017].

$\Delta a_{Qg}^{(3)}$

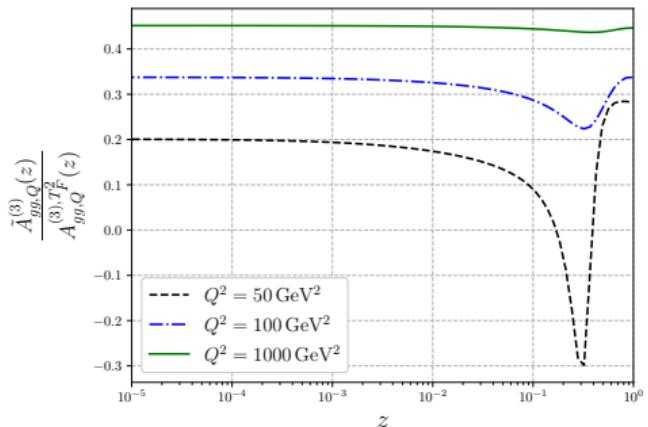


$\Delta a_{Qg}^{(3)}(x)$ as a function of x , rescaled by the factor $x(1 - x)$. Left panel: full line (red): $\Delta a_{Qg}^{(3)}(x)$; dashed line (green): the small- x terms $\ln^k(x)$, $k \in \{1, \dots, 5\}$; dotted line (blue): the large- x terms $\ln^l(1 - x)$, $l \in \{1, \dots, 4\}$. Right panel: larger x region. Full line (red): $\Delta a_{Qg}^{(3)}(x)$; dotted line (blue): the large- x terms $\ln^l(1 - x)$, $l \in \{1, \dots, 4\}$.

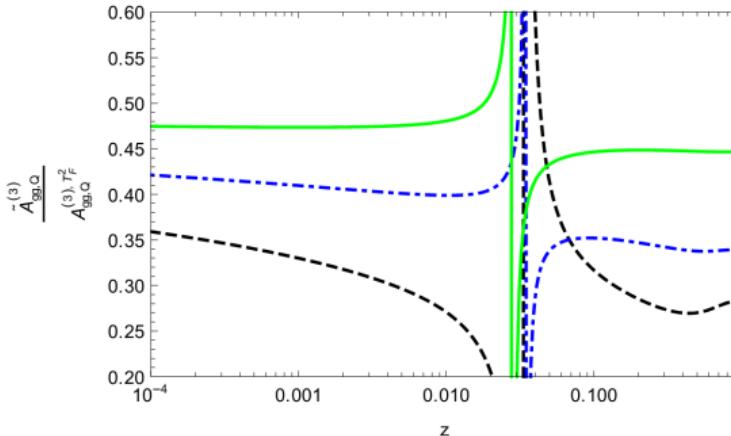
Two-mass Results: $\tilde{A}_{gg,Q}^{(3)}$



The two mass contributions over the whole T_F^2 -contributions to the OME $\tilde{A}_{gg,Q}^{(3)}$:



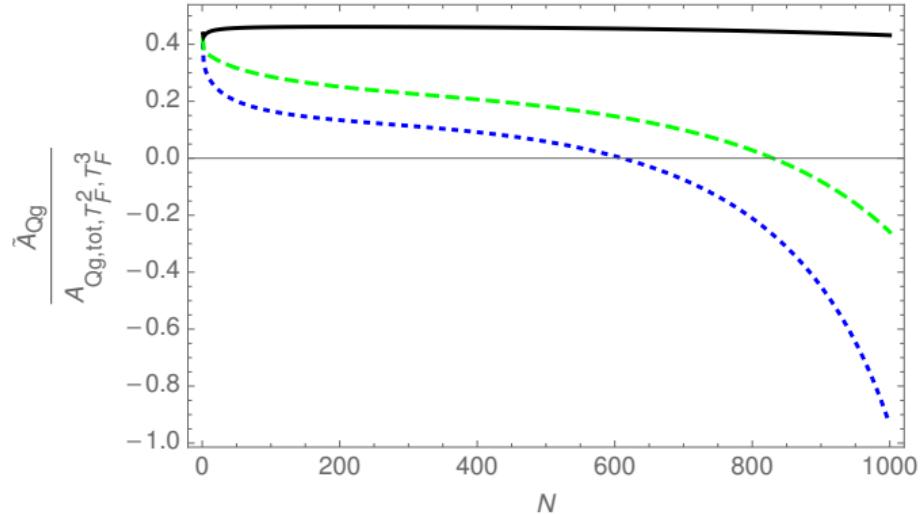
unpolarized



polarized

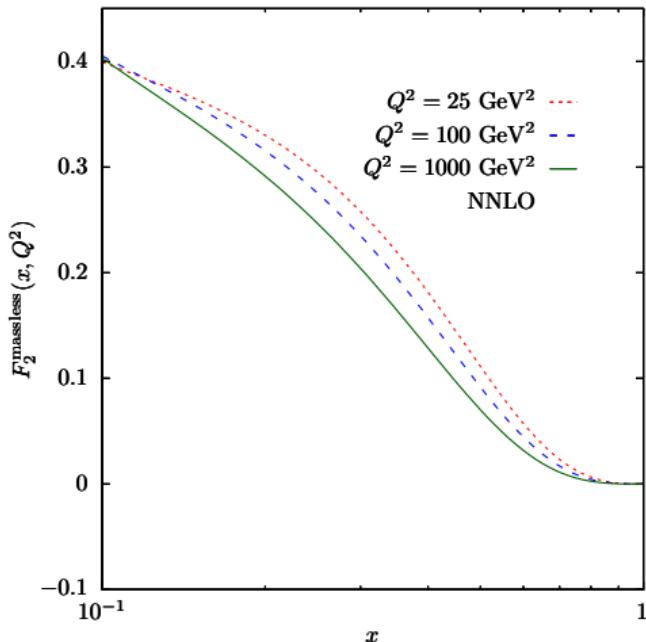
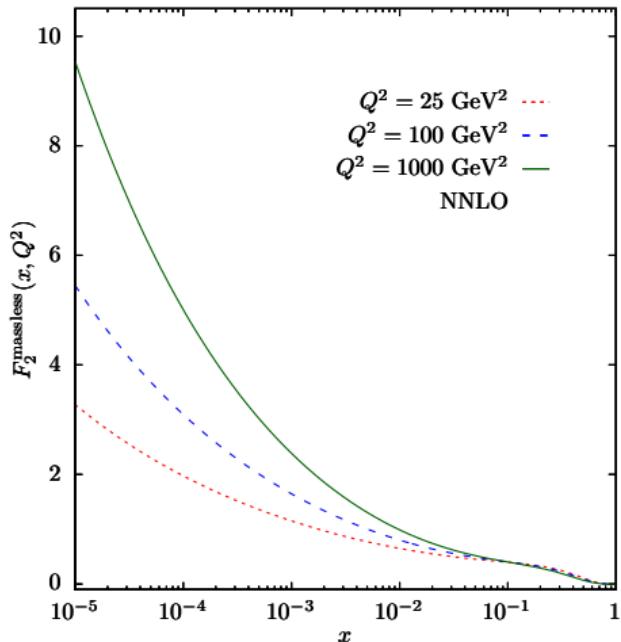


Relative contribution of $\tilde{A}_{Qg}^{(3)}(N)$



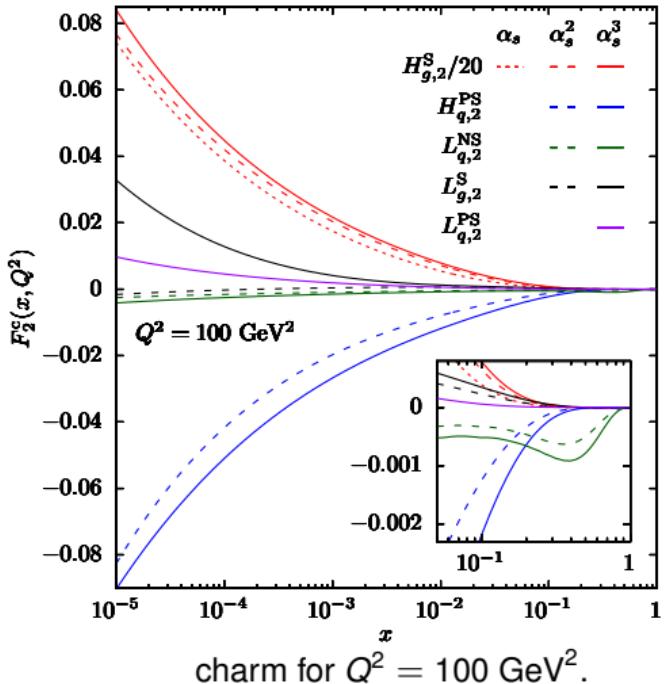
$Q^2 = 30 \text{ GeV}^2$: dotted line; $Q^2 = 10^2 \text{ GeV}^2$: dashed line; $Q^2 = 10^4 \text{ GeV}^2$: full line.

The massless contributions to F_2

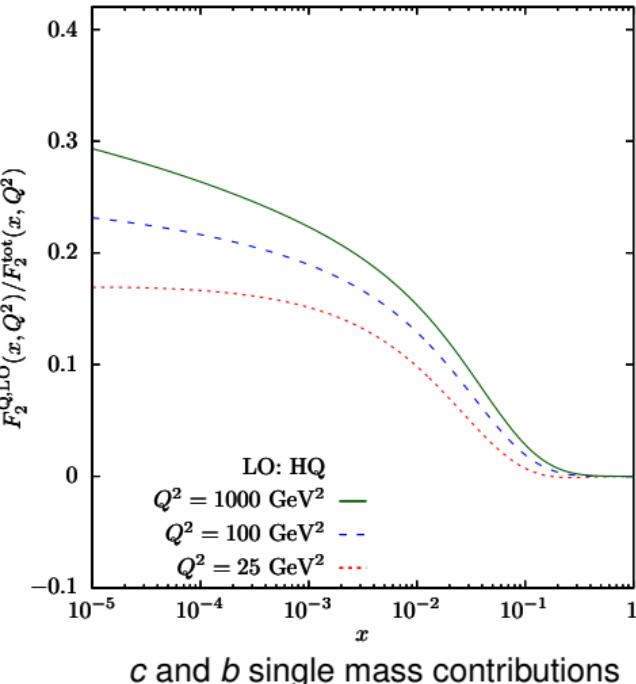


$N_F = 3$ massless quarks.

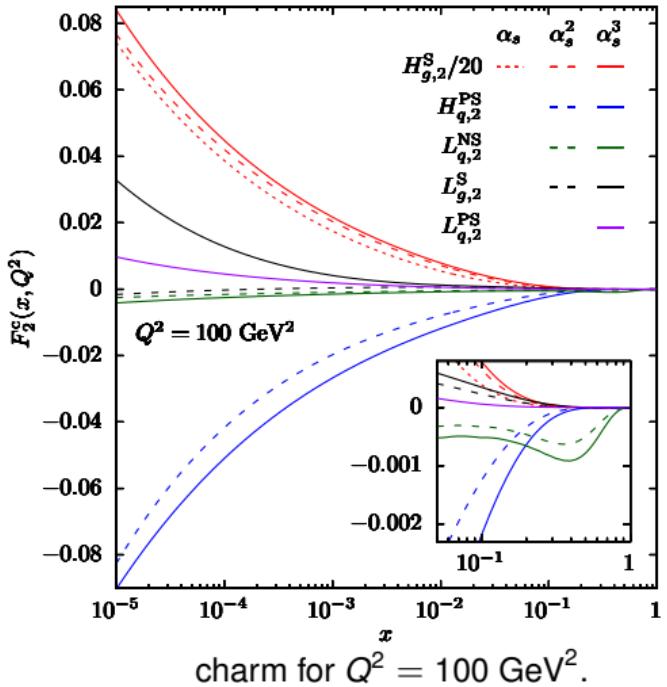
Single-mass contributions to $F_2^{c,b}$



Allows to strongly reduce the current theory error on m_c .

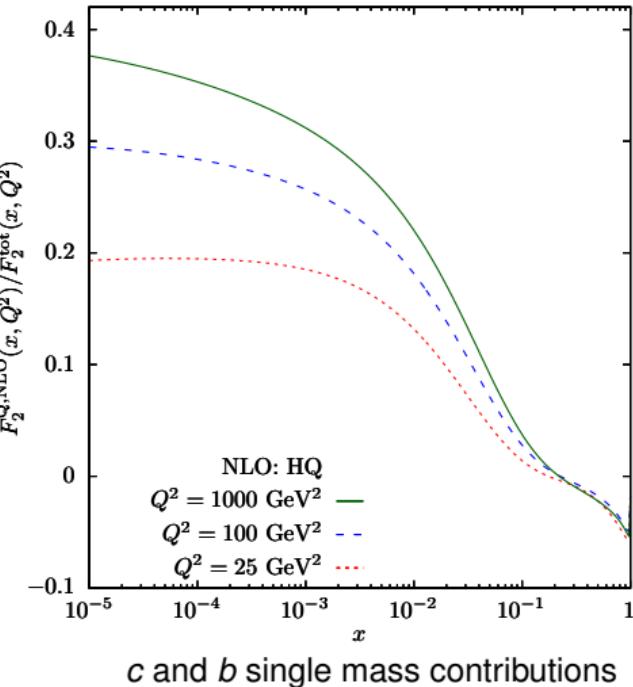


Single-mass contributions to $F_2^{c,b}$



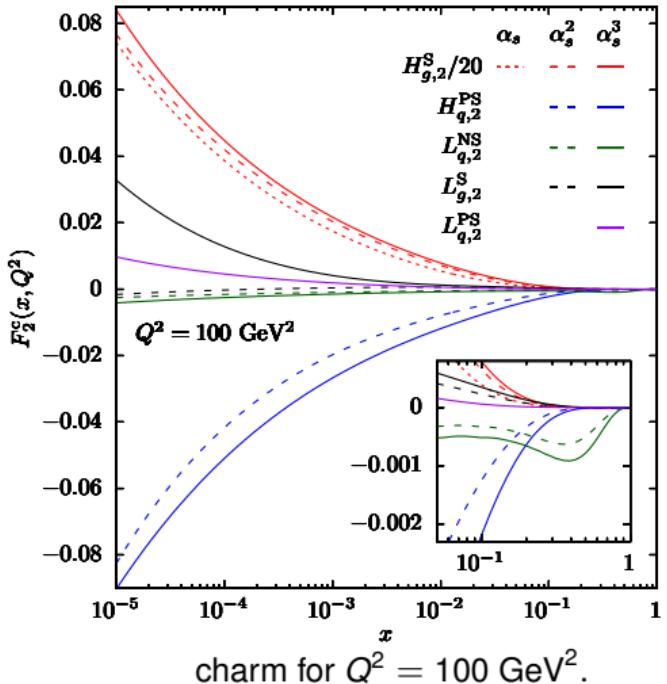
charm for $Q^2 = 100 \text{ GeV}^2$.

Allows to strongly reduce the current theory error on m_c .

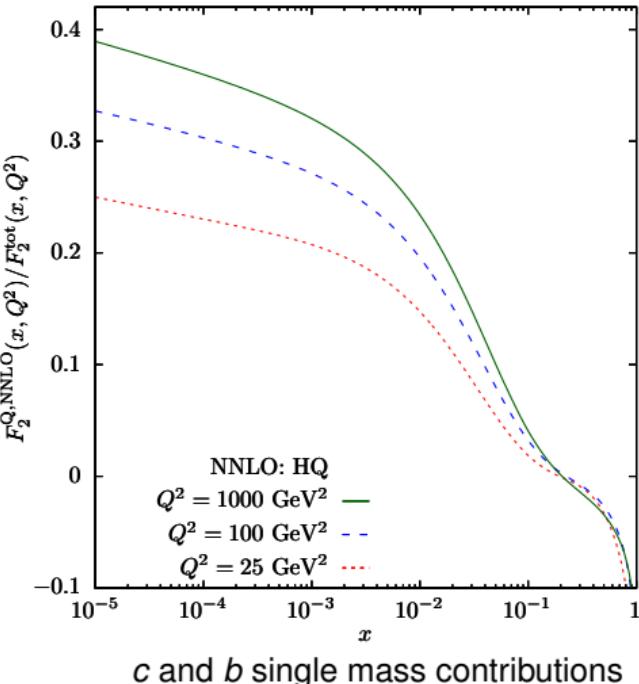


c and b single mass contributions

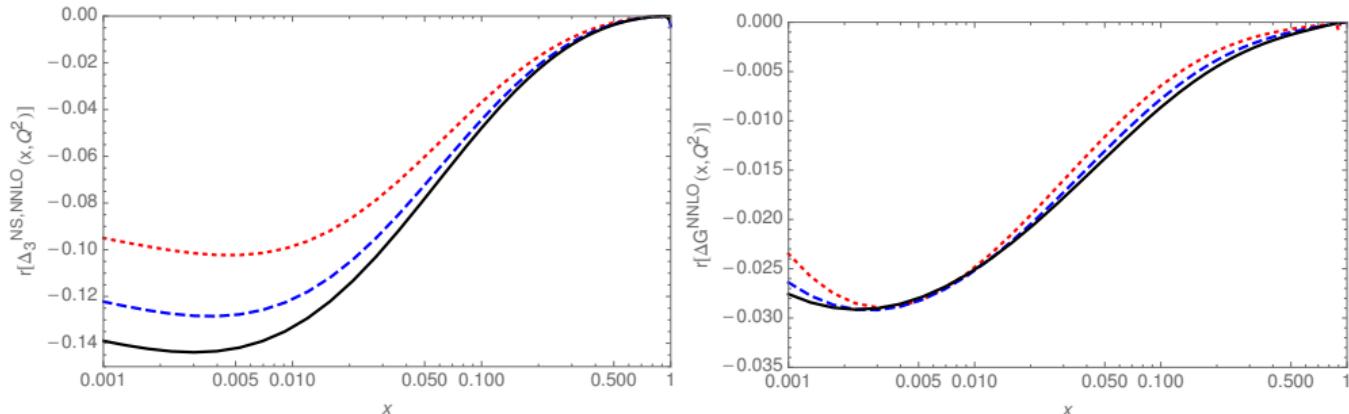
Single-mass contributions to $F_2^{c,b}$



Allows to strongly reduce the current theory error on m_c .



Polarized PDF evolution in the Larin Scheme



[Dotted line: $Q^2 = 100 \text{ GeV}^2$, dashed line: $Q^2 = 1000 \text{ GeV}^2$, full line: $Q^2 = 10000 \text{ GeV}^2$]

$$r(x, Q^2) = \frac{f^L(x, Q^2)}{f^M(x, Q^2)} - 1$$

The pdfs are necessary to match HO Larin-scheme calculations.



Conclusions

- All unpolarized and polarized **single-mass OMEs** and the associated massive Wilson coefficients for $Q^2 \gg m_Q^2$ have been calculated. The unpolarized and **polarized massless three-loop Wilson coefficients** were calculated and contribute to the present results.
- The calculation of all unpolarized and polarized **two-mass OMEs**, except for $(\Delta)A_{Qg}^{(3)}$, are finished and the remaining OMEs will be available very soon.
- Various new **mathematical and technological methods** were developed during the present project. They are available for use in further single- and two-mass calculations in other QFT projects.
- Very soon new precision analyses of the world DIS-data to measure $\alpha_s(M_Z)$ and m_c at higher precision can be carried out.
- Both the single- and two-mass **VFNS at 3-loop** order will be available in form of a numerical program, to be used e.g. in applications at hadron colliders.
- The results in the **polarized case** prepare the analysis of the precision data, which will be taken at the **EIC** starting at the end of this decade.
- For all sub-processes it turned out that the small x **BFKL approaches fail** to present the physical result due to quite a series of missing subleading terms, which substantially correct the LO behaviour. The correct description requires the full calculation.