# 3-Loop Heavy Flavor Corrections to DIS: an Update

PDF4LHC meeting Geneva, CH

Johannes Blümlein | November 14, 2023

DESY

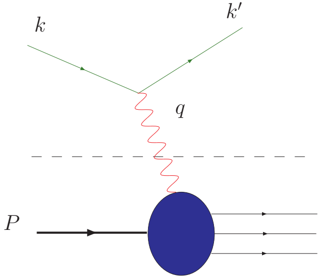
Based on:

- A. Behring, J.B., and K. Schönwald, The inverse Mellin transform via analytic continuation, JHEP **06** (2023) 62.
- J. Ablinger et al., The first-order factorizable contributions to the three-loop massive operator matrix elements $A_{Qg}^{(3)}$ and $\Delta A_{Qg}^{(3)}$, 2311.00644 [hep-ph]

In collaboration with:

J. Ablinger, A. Behring, A. De Freitas, A. von Manteuffel, C. Schneider, K. Schönwald

# Unpolarized Deep–Inelastic Scattering (DIS):




$\longrightarrow \quad L_{\mu\nu}$

$\longrightarrow \quad W_{\mu\nu}$

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

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

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

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

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 $Q^2 \gtrsim 10m^2$ 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).
- **What is known:**
  Single mass: $A_{qq,Q}^{\rm NS}, A_{qg,Q}, A_{qq,Q}^{\rm PS}, A_{gq,Q}, A_{Qq}^{\rm PS}, A_{gg,Q}, A_{Qg}$ to 3-loop order; $A_{Qg}$ to 2-loop order;
  Two-mass case to 3-loop order $A_{qq,Q}^{\rm NS}, A_{Qq}^{\rm PS}, A_{gq,Q}, A_{gg,Q}$; $A_{Qg}$ to 2-loop order.
- The same OMEs are also known in the polarized case.
- Objective of this talk: First non-logarithmic results in calculating $A_{Qg}$.
- $\Longrightarrow$ The necessary master integrals
- $\Longrightarrow$ The first-order factorizable contributions to $(\Delta)A_{Qg}$

# 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.

$$F(N) = \int_0^1 dx x^{N-1}[f(x) + (-1)^{N-1} g(x)]$$

$$\tilde{F}(t) = \sum_{N=1}^{\infty} t^N F(N)$$

$$f(x) + (-1)^{N-1} g(x) = \frac{1}{2\pi i}\left[\mathrm{Disc}_x \tilde{F}\left(\frac{1}{x}\right) + (-1)^{N-1} \mathrm{Disc}_x \tilde{F}\left(-\frac{1}{x}\right)\right]. \qquad (1)$$

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

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

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

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

Example:

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

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

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

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

# Square root valued alphabets

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

Monodromy also through:

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

$$F_7(x) = \frac{1}{\pi} \mathrm{Im} \frac{1}{t} \mathrm{G}\left(4; \frac{1}{t}\right) = 1 - \frac{2(1-x)(1+2x)}{\pi}\sqrt{\frac{1-x}{x}} - \frac{8}{\pi}\mathrm{G}(5;x),$$
$$F_8(x) = \frac{1}{\pi} \mathrm{Im} \frac{1}{t} \mathrm{G}\left(4,2; \frac{1}{t}\right) = -\frac{1}{\pi}\left[4\frac{(1-x)^{3/2}}{\sqrt{x}} + 2(1-x)(1+2x)\sqrt{\frac{1-x}{x}}[\mathrm{H}_0(x)+\mathrm{H}_1(x)] \right.$$
$$\left. +8[\mathrm{G}(5,2;x)+\mathrm{G}(5,1;x)]\right],$$

# 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 $3 \times 3$ system of this kind.
- The system is connected to that occurring in the case of $\rho$ 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:

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

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

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

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

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

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

- 1009 of 1233 contributing Feynman diagrams
- Solved: $N_F$-terms, $\zeta_2, \zeta_4$ and $B_4$ terms, unpolarized and polarized.
- Contributions to the rational and $\zeta_3$ terms:
  - The sum of the contributions vanishes for $N \rightarrow \infty$, while the individual terms $\propto 1$ and $\propto \zeta_3$ do strongly diverge.
  - Dynamical generation of a factor of $\zeta_3$.
  - 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 $N \rightarrow \infty$: $\propto 2^N, 4^N$ 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.

# Structure in $x$ space of the 1st order reducible terms

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 $x = 1/2$:

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

Wide double precision overlaps of the expansions around $x = 2/10$ and $x = 7/10$ by using 100 expansion terms.

# Structure in $x$ space

- The analytic results on the expansion coefficients contain iterated integrals over up to root-valued letters at main argument $x = 1$.
- One may rationalize the letters of these constants and switch to linear representations.
- This results into enormous numbers of Kummer-Poincaré integrals, which are calculated to 100 digits.

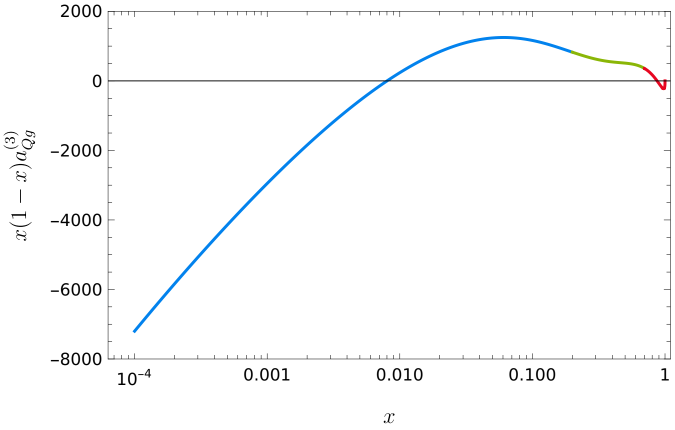
Unpolarized case:

- $\zeta_2$ term of the predicted $\ln(x)/x$ small $x$ expansion confirmed Catani, Ciafaloni, Hautmann, 1991

Polarized case:

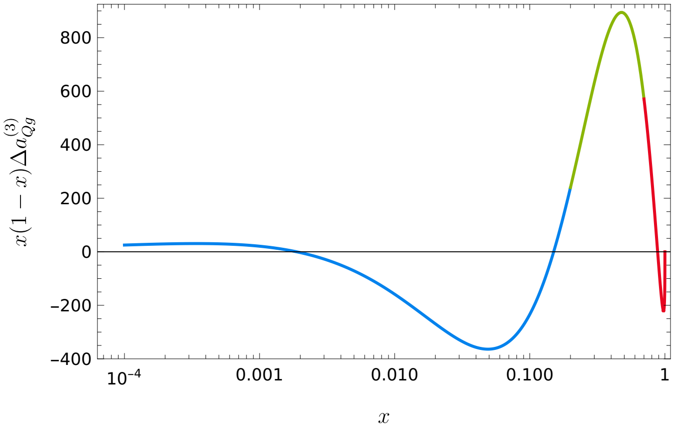
- Evanescent $\ln(x)/x$ and $1/x$ terms occur.
- One has to show their cancellation. Many special constants are involved here.
- New $\ln^5(x)$ term $\propto N_F$ found.

# $a_{Qg}^{(fact.,3)}$




The first order factorizable contributions to $a_{Qg}^{(3)}(N)$. Full line (blue): $x < 0.2$; Full line (green): $0.2 < x < 0.7$; Full line (blue): $0.7 < x < 1$ for $m_c = 1.59$ GeV and $N_F = 3$.

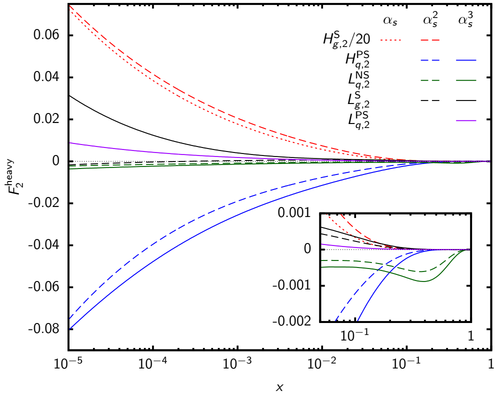
# $\Delta a_{Qg}^{(fact.,3)}$




The first order factorizable contributions to $\Delta a_{Qg}^{(3)}(N)$. Full line (blue): $x < 0.2$; Full line (green): $0.2 < x < 0.7$; Full line (blue): $0.7 < x < 1$ for $m_c = 1.59$ GeV and $N_F = 3$.

# Current summary on $F_2^{charm}$

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




for $Q^2 = 100$ GeV$^2$.

Allows to strongly reduce the current theory error on $m_c$.

Started $\sim$ 2009; will be completed soon.

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

# Conclusions

- All unpolarized and polarized single and two-mass OMEs, except the ones for $A_{Qg}^{(3)}$, and the associated massive Wilson coefficients for $Q^2 \gg m_Q^2$ have been calculated, including also the logarithmic contributions.
- Various new mathematical and technological steps were performed to prepare the calculation of $(\Delta)A_{Qg}^{(3)}$.
- Recently all elliptic base master integrals necessary to complete the calculation for $(\Delta)A_{Qg}^{(3)}$ were computed analytically.
- We have calculated already all the first-order factorizing contributions to $(\Delta)A_{Qg}^{(3)}$.
- The completion of $(\Delta)A_{Qg}^{(3)}$ is underway and will allow new precision analyses of the world DIS-data to measure $\alpha_s(M_Z)$ and $m_c$ at higher precision.
- In the small $x$ region BFKL approaches fail to present the physical result due to quite a lot of subleading terms, substantially correcting the LO behaviour. The growth of $F_2$ at small $x$ is a consequence of the shape of the non-perturbative PDFs and complete fixed order evolution at twist 2.