Heavy quark production and the variable-flavor-number-scheme at NNLO

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Introduction

Introduction

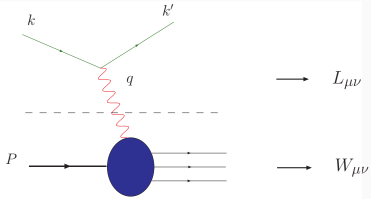
- The correct treatment of heavy quark masses is important for precision at the LHC.
- Often we want to describe data in different kinematic regimes:
  (a) $m^2 \sim Q^2$: low energies where power corrections are important
  (b) $m^2 \ll Q^2$: high energies, where large logarithms are produced

  $\Rightarrow$ Heavy flavor effects need to be consistently treated over wide energy ranges.

In this talk:

- Heavy flavor production in deep-inelastic-scattering.
- Asymptotic heavy mass effects via operator matrix elements.
- Treating more than one heavy quark.

Theory of Deep Inelastic Scattering



- Kinematic invariants:

$$Q^2 = -q^2, \qquad x = \frac{Q^2}{2P.q}$$

- The cross section factorizes into leptonic and hadronic tensor:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}Q^2\mathrm{d}x} \sim L_{\mu\nu} W^{\mu\nu}$$

- The hadronic tensor can be expressed through structure functions:

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

- F_L, F_2, g_1 and g_2 contain contributions from both, charm and bottom quarks.

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

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

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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

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

[Buza, Matiounine, Smith, van Neerven (Nucl.Phys.B (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

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

The heavy flavor Wilson coefficients in the asymptotic limit:

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

$$L^{\rm NS}_{q,(2,L)}(N_F+1) = a_s^2\left[A^{(2),\rm NS}_{qq,Q}(N_F+1)\delta_2 + \hat{C}^{(2),\rm NS}_{q,(2,L)}(N_F)\right] + a_s^3\left[A^{(3),\rm NS}_{qq,Q}(N_F+1)\delta_2 + A^{(2),\rm NS}_{qq,Q}(N_F+1)C^{(1),\rm NS}_{q,(2,L)}(N_F+1) + \hat{C}^{(3),\rm NS}_{q,(2,L)}(N_F)\right]$$

$$L^{\rm PS}_{q,(2,L)}(N_F+1) = a_s^3\left[A^{(3),\rm PS}_{qq,Q}(N_F+1)\delta_2 + N_F A^{(2),\rm NS}_{gq,Q}(N_F)\tilde{C}^{(1),\rm NS}_{g,(2,L)}(N_F+1) + N_F \hat{\tilde{C}}^{(3),\rm PS}_{q,(2,L)}(N_F)\right]$$

$$L^{\rm S}_{g,(2,L)}(N_F+1) = a_s^2 A^{(1)}_{gg,Q}(N_F+1)N_F\tilde{C}^{(2)}_{g,(2,L)}(N_F+1) + a_s^3\left[A^{(3)}_{qg,Q}(N_F+1)\delta_2 + A^{(1)}_{gg,Q}(N_F+1)N_F\tilde{C}^{(2)}_{g,(2,L)}(N_F+1)\right.$$
$$\left. + A^{(2)}_{gg,Q}(N_F+1)N_F\tilde{C}^{(1)}_{g,(2,L)}(N_F+1) + A^{(1)}_{Qg}(N_F+1)N_F\tilde{C}^{(2),\rm PS}_{q,(2,L)}(N_F+1) + N_F\hat{\tilde{C}}^{(3)}_{g,(2,L)}(N_F)\right]$$

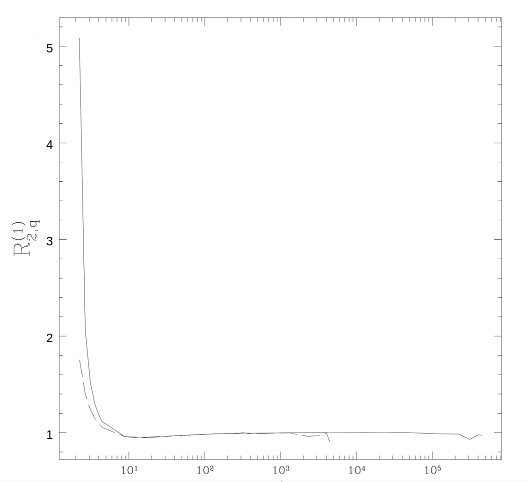
$$H^{\rm PS}_{q,(2,L)}(N_F+1) = a_s^2\left[A^{(2),\rm PS}_{Qq}(N_F+1)\delta_2 + \tilde{C}^{(2),\rm PS}_{q,(2,L)}(N_F+1)\right]$$
$$+ a_s^3\left[A^{(3),\rm PS}_{Qq}(N_F+1)\delta_2 + A^{(2)}_{gq,Q}(N_F+1)\tilde{C}^{(2)}_{g,(1,L)}(N_F+1) + A^{(2),\rm PS}_{Qq}(N_F+1)\tilde{C}^{(1),\rm NS}_{q,(2,L)}(N_F+1) + \tilde{C}^{(3),\rm PS}_{q,(2,L)}(N_F+1)\right]$$

$$H^{\rm S}_{g,(2,L)}(N_F+1) = a_s\left[A^{(1)}_{Qg}(N_F+1)\delta_2 + \tilde{C}^{(1)}_{g,(2,L)}(N_F+1)\right]$$
$$+ a_s^2\left[A^{(2)}_{Qg}(N_F+1)\delta_2 + A^{(1)}_{Qg}(N_F+1)\tilde{C}^{(1)}_{q,(2,L)}(N_F+1) + A^{(1)}_{gg,Q}(N_F+1)\tilde{C}^{(1)}_{g,(2,L)}(N_F+1) + \tilde{C}^{(2)}_{g,(2,L)}(N_F+1)\right]$$
$$+ a_s^3\left[A^{(3)}_{Qg}(N_F+1)\delta_2 + A^{(2)}_{Qg}(N_F+1)\tilde{C}^{(1)}_{q,(2,L)}(N_F+1) + A^{(2)}_{gg,Q}(N_F+1)\tilde{C}^{(1)}_{g,(2,L)}(N_F+1)\right.$$
$$\left. + A^{(1)}_{Qg}(N_F+1)\tilde{C}^{(2),\rm S}_{q,(2,L)}(N_F+1) + A^{(1)}_{gg,Q}(N_F+1)\tilde{C}^{(1)}_{g,(2,L)}(N_F+1) + \tilde{C}^{(3)}_{g,(2,L)}(N_F+1)\right]$$

- Light flavor Wilson coefficients are known up to $\mathcal{O}(\alpha_s^3)$. [Moch, Vermaseren, Vogt '04–'05]
  [Blümlein, Marquard, Schneider, Schönwald '22]

Validity of the Asymptotic Limit

- The corrections to $\mathcal{O}(\alpha_s^2)$ have been calculated numerically.
  [Laenen, Riemersma, Smith, Neerven '93]
- The comparison to the exact $\mathcal{O}(\alpha_s^2)$ calculation shows:
  - $F_2^{c\bar{c}}$ needs $Q^2/m^2 \geq 10$
  - $F_L^{c\bar{c}}$ needs $Q^2/m^2 \geq 1000$



Q^2/m^2

Comparison of the asymptotic and exact two loop contributions. [Buza, Matiounine, Smith, Migneron, Neerven '96]

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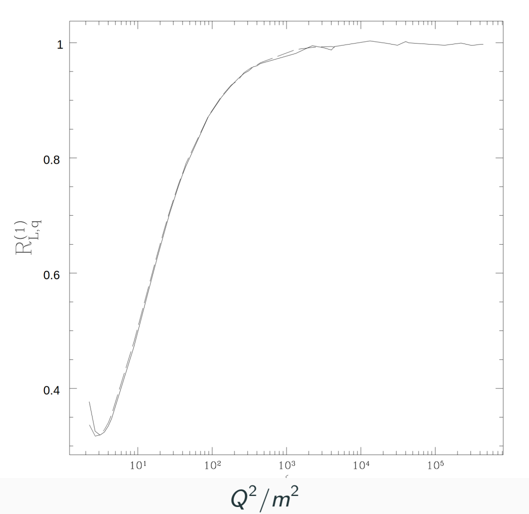
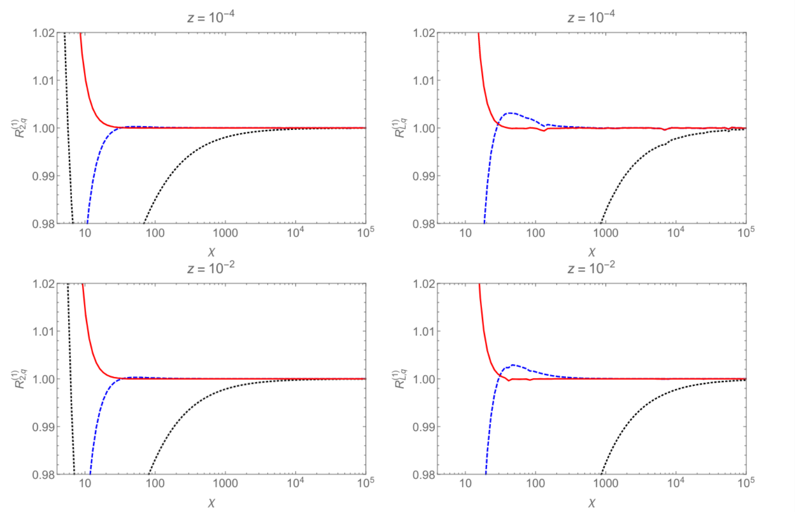


Comparison of the asymptotic and exact two loop contributions. [Buza, Matiounine, Smith, Migneron, Neerven '96]

Massive Wilson Coefficients – Pure-Singlet

[Blümlein, De Freitas, Raab, Schönwald ’19]



The ratio of the full over the asymptotic results including terms of:
$\mathcal{O}\left((m^2/Q^2)^0\right)$, $\mathcal{O}\left((m^2/Q^2)^1\right)$, $\mathcal{O}\left((m^2/Q^2)^2\right)$.

Variable Flavor Number Scheme

- **Idea:** When $Q^2 \gg m^2$ we can treat the heavy quark effectively as massless.
- Demand for the structure functions in the asymptotic limit:

$$F_i(n_f, Q^2) + F_i^{c\bar{c},asymp}(n_f, Q^2, m^2) \overset{Q^2 \gg m^2}{=} F_i^{VFNS}(n_f + 1, Q^2)$$

- By comparing both sides of the equation we can define new parton densities, which become dependent on the heavy quark mass.
- **General-Mass VFNS:** interpolate between fixed flavor number scheme and asymptotic representation, e.g. FONLL, (S)-ACOT:

[Forte, Laenen, Nason, Rojo '10;...; Barontini, Candido, Hekhorn, Magni, Stegeman '24]

[Aivazis, Collins, Olness, Tung '94;...; Guzzi, Nadolsky, Reina, Wackeroth, Xie '24]

$$\mathbb{C}_i = \mathbb{C}_i^{VFNS}(n_f + 1, Q^2) + \left[\mathbb{C}_i\left(n_f, Q^2, m^2\right) - \mathbb{C}_i\left(n_f, Q^2, m^2\right)\Big|_{Q^2 \gg m^2}\right]$$

Variable Flavor Number Scheme

Matching conditions for parton distribution functions:

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

$$f_Q(N_F+1) + f_{\overline{Q}}(N_F+1) = A_{Qq}^{\text{PS}}\left(N_F+1, \frac{m^2}{\mu^2},\right) \cdot \Sigma(N_F) + A_{Qg}\left(N_F+1, \frac{m^2}{\mu^2}\right) \cdot G(N_F)\ ,$$

$$\Sigma(N_F+1) = \left[A_{qq,Q}^{\text{NS}}\left(N_F+1, \frac{m^2}{\mu^2}\right) + A_{qq,Q}^{\text{PS}}\left(N_F+1, \frac{m^2}{\mu^2}\right) + A_{Qq}^{\text{PS}}\left(N_F+1, \frac{m^2}{\mu^2}\right)\right] \cdot \Sigma(N_F)$$
$$+ \left[A_{qg,Q}\left(N_F+1, \frac{m^2}{\mu^2}\right) + A_{Qg}\left(N_F+1, \frac{m^2}{\mu^2}\right)\right] \cdot G(N_F)\ ,$$

$$G(N_F+1) = A_{gq,Q}\left(N_F+1, \frac{m^2}{\mu^2}\right) \cdot \Sigma(N_F) + A_{gg,Q}\left(N_F+1, \frac{m^2}{\mu^2}\right) \cdot G(N_F)\ .$$

Massive Operator Matrix Elements at $\mathcal{O}(\alpha_s^3)$

Status of the Operator Matrix Element

Leading Order: [Witten (1976); Babcock, Sivers, Wolfram (1978); Shifman, Vainshtein, Zakharov (1978); Leveille, Weiler (1979); Glück, Reya (1979); Glück, Hoffmann, Reya (1982)]

Next-to-Leading Order:

full m dependence (numeric) [Laenen, van Neerven, Riemersma, Smith (1993)]

$Q^2 \gg m^2$: via IBP [Buza, Matiounine, Smith, Migneron, van Neerven (1996)]

Compact results via ${}_pF_q$'s [Bierenbaum, Blümlein, Klein (2007)]

$O(\alpha_s^2 \varepsilon)$ (for general N) [Bierenbaum, Blümlein, Klein (2008, 2009)]

Next-to-Next-to-Leading Order: $Q^2 \gg m^2$

- Moments (using `MATAD` [Steinhauser (2000)]):
  - F_2: $N = 2, ..., 10(14)$ [Bierenbaum, Blümlein, Klein (2009)]
  - transversity: $N = 1, ..., 13$
  - Two masses $m_1 \neq m_2 \rightarrow$ Moments N $= 2,4,6$ [Blümlein, Wißbrock (2011)]
- Analytic solutions for $A_{qq,Q}^{\rm NS}$, $A_{qg,Q}$, $A_{gq,Q}$, $A_{qq,Q}^{\rm PS}$, $A_{Qq}^{\rm PS}$, $A_{gg,Q}$ [Blümlein et al (2010-2023)] , with recent extension to polarized scattering.
- Precise semi-analytic solution for A_{Qg} [Blümlein et al (2023-2024)] .
- Analytic two mass solutions for $A_{qq,Q}^{\rm NS}$, $A_{qg,Q}$, $A_{gq,Q}$, $A_{qq,Q}^{\rm PS}$, $A_{Qq}^{\rm PS}$, $A_{gg,Q}$ [Blümlein et al (2017-2020)] , with recent extension to polarized scattering.

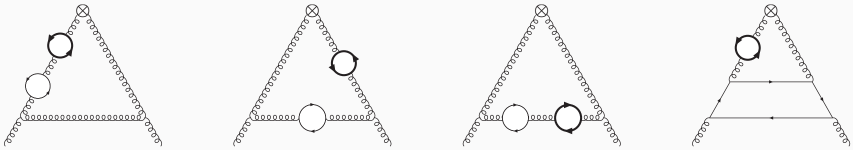
Computing Massive Operator Matrix Elements

- We want to calculate massive operator matrix elements: $A_{ij} = \langle i | O_j | i \rangle$, with the operators

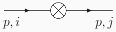
$$O^{\mathrm{NS}}_{q,r;\mu_1,\ldots,\mu_N} = i^{N-1} \mathcal{S} \left[\bar{\psi} \gamma_{\mu_1} D_{\mu_2} \ldots D_{\mu_N} \frac{\lambda_r}{2} \psi \right] - \text{trace terms} \,,$$
$$O^{\mathrm{S}}_{q,r;\mu_1,\ldots,\mu_N} = i^{N-1} \mathcal{S} \left[\bar{\psi} \gamma_{\mu_1} D_{\mu_2} \ldots D_{\mu_N} \psi \right] - \text{trace terms} \,,$$
$$O^{\mathrm{S}}_{g,r;\mu_1,\ldots,\mu_N} = 2 i^{N-2} \mathcal{S} \left[F^{a}_{\mu_1 \alpha} D_{\mu_2} \ldots D_{\mu_N} F^{\alpha,a}_{\mu_N} \right] - \text{trace terms}$$

  and on-shell external partons $i = q, g$.

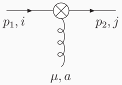
- The operator insertions introduce Feynman rules which depend on the Mellin variable N.



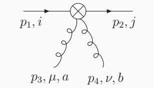
The OMEs are calculated using the QCD Feynman rules together with the following operator insertion Feynman rules:



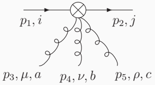
$$\delta^{ij}\not\Delta\gamma_\pm(\Delta\cdot p)^{N-1}\,, \quad N\geq 1$$



$$g t^a_{ji}\Delta^\mu\not\Delta\gamma_\pm\sum_{j=0}^{N-2}(\Delta\cdot p_1)^j(\Delta\cdot p_2)^{N-j-2}\,, \quad N\geq 2$$



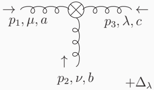
$$g^2\Delta^\mu\Delta^\nu\not\Delta\gamma_\pm\sum_{j=0}^{N-3}\sum_{l=j+1}^{N-2}(\Delta p_2)^j(\Delta p_1)^{N-l-2}\Big[(t^at^b)_{ji}(\Delta p_1+\Delta p_4)^{l-j-1}+(t^bt^a)_{ji}(\Delta p_1+\Delta p_3)^{l-j-1}\Big]\,,\quad N\geq 3$$



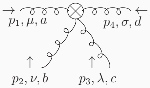
$$\begin{aligned}
&g^3\Delta_\mu\Delta_\nu\Delta_\rho\not\Delta\gamma_\pm\sum_{j=0}^{N-4}\sum_{l=j+1}^{N-3}\sum_{m=l+1}^{N-2}(\Delta.p_2)^j(\Delta.p_1)^{N-m-2}\\
&\Big[\ (t^at^bt^c)_{ji}(\Delta.p_4+\Delta.p_5+\Delta.p_1)^{l-j-1}(\Delta.p_5+\Delta.p_1)^{m-l-1}\\
&\quad+(t^at^ct^b)_{ji}(\Delta.p_4+\Delta.p_5+\Delta.p_1)^{l-j-1}(\Delta.p_4+\Delta.p_1)^{m-l-1}\\
&\quad+(t^bt^at^c)_{ji}(\Delta.p_3+\Delta.p_5+\Delta.p_1)^{l-j-1}(\Delta.p_5+\Delta.p_1)^{m-l-1}\\
&\quad+(t^bt^ct^a)_{ji}(\Delta.p_3+\Delta.p_5+\Delta.p_1)^{l-j-1}(\Delta.p_3+\Delta.p_1)^{m-l-1}\\
&\quad+(t^ct^at^b)_{ji}(\Delta.p_3+\Delta.p_4+\Delta.p_1)^{l-j-1}(\Delta.p_4+\Delta.p_1)^{m-l-1}\\
&\quad+(t^ct^bt^a)_{ji}(\Delta.p_3+\Delta.p_4+\Delta.p_1)^{l-j-1}(\Delta.p_3+\Delta.p_1)^{m-l-1}\Big]\,,\\
&\qquad N\geq 4
\end{aligned}$$

$$\gamma_+=1\,,\quad \gamma_-=\gamma_5\,.$$

$$\frac{1+(-1)^N}{2}\delta^{ab}(\Delta\cdot p)^{N-2}\Big[g_{\mu\nu}(\Delta\cdot p)^2-(\Delta_\mu p_\nu+\Delta_\nu p_\mu)\Delta\cdot p+p^2\Delta_\mu\Delta_\nu\Big]\,,\quad N\geq 2$$



$$\begin{aligned}
&-ig\frac{1+(-1)^N}{2}f^{abc}\Bigg(\\
&\Big[(\Delta_\nu g_{\lambda\mu}-\Delta_\lambda g_{\mu\nu})\Delta\cdot p_1+\Delta_\mu(p_{1,\nu}\Delta_\lambda-p_{1,\lambda}\Delta_\nu)\Big](\Delta\cdot p_1)^{N-2}\\
&+\Delta_\lambda\Big[\Delta\cdot p_1 p_{2,\mu}\Delta_\nu+\Delta\cdot p_2 p_{1,\nu}\Delta_\mu-\Delta\cdot p_1\Delta\cdot p_2 g_{\mu\nu}-p_1\cdot p_2\Delta_\mu\Delta_\nu\Big]\\
&\times\sum_{j=0}^{N-3}(-\Delta\cdot p_1)^j(\Delta\cdot p_2)^{N-3-j}\\
&+\left\{\begin{smallmatrix}p_1\to p_2\to p_3\to p_1\\ \mu\to\nu\to\lambda\to\mu\end{smallmatrix}\right\}+\left\{\begin{smallmatrix}p_1\to p_3\to p_2\to p_1\\ \mu\to\lambda\to\nu\to\mu\end{smallmatrix}\right\}\Bigg)\,,\quad N\geq 2
\end{aligned}$$

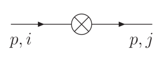


$$\begin{aligned}
&g^2\frac{1+(-1)^N}{2}\Bigg(f^{abe}f^{cde}O_{\mu\nu\lambda\sigma}(p_1,p_2,p_3,p_4)\\
&+f^{ace}f^{bde}O_{\mu\lambda\nu\sigma}(p_1,p_3,p_2,p_4)+f^{ade}f^{bce}O_{\mu\sigma\nu\lambda}(p_1,p_4,p_2,p_3)\Bigg)\,,
\end{aligned}$$

$$\begin{aligned}
&O_{\mu\nu\lambda\sigma}(p_1,p_2,p_3,p_4)=\Delta_\nu\Delta_\lambda\Bigg\{-g_{\mu\sigma}(\Delta\cdot p_3+\Delta\cdot p_4)^{N-2}\\
&+[p_{4,\mu}\Delta_\sigma-\Delta\cdot p_4 g_{\mu\sigma}]\sum_{i=0}^{N-3}(\Delta\cdot p_3+\Delta\cdot p_4)^i(\Delta\cdot p_4)^{N-3-i}\\
&-[p_{1,\sigma}\Delta_\mu-\Delta\cdot p_1 g_{\mu\sigma}]\sum_{i=0}^{N-3}(-\Delta\cdot p_1)^i(\Delta\cdot p_3+\Delta\cdot p_4)^{N-3-i}\\
&+[\Delta\cdot p_1\Delta\cdot p_4 g_{\mu\sigma}+p_1\cdot p_4\Delta_\mu\Delta_\sigma-\Delta\cdot p_4 p_{1,\sigma}\Delta_\mu-\Delta\cdot p_1 p_{4,\mu}\Delta_\sigma]\\
&\quad\times\sum_{i=0}^{N-4}\sum_{j=0}^{i}(-\Delta\cdot p_1)^{N-4-i}(\Delta\cdot p_3+\Delta\cdot p_4)^{i-j}(\Delta\cdot p_4)^j\Bigg\}\\
&-\left\{\begin{smallmatrix}p_1\leftrightarrow p_2\\ \mu\leftrightarrow\nu\end{smallmatrix}\right\}-\left\{\begin{smallmatrix}p_3\leftrightarrow p_4\\ \lambda\leftrightarrow\sigma\end{smallmatrix}\right\}+\left\{\begin{smallmatrix}p_1\leftrightarrow p_2,\ p_3\leftrightarrow p_4\\ \mu\leftrightarrow\nu,\ \lambda\leftrightarrow\sigma\end{smallmatrix}\right\}\,,\quad N\geq 2
\end{aligned}$$

Calculation methods

- Resum operator insertions into propagator insertions:



$$\sim \quad (\Delta.k)^N \quad \rightarrow \quad \sum_{N=0}^{\infty} t^N (\Delta.k)^N = \frac{1}{1 - t\ \Delta.k}$$

- 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]

⇒ We obtain the amplitudes in terms of master integrals $\vec{M}$ and their associated system of differential equations in t:

$$\frac{d}{dt}\vec{M} = A(\epsilon, t) \cdot \vec{M}$$

Relation between the different spaces

$$\hat{f}(t) = \sum_{N=1}^{\infty} t^N \, \tilde{f}(N)$$

$$\updownarrow$$

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x \, x^{N-1} \, f(x)$$

$$\updownarrow$$

$$f(x) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} x^{-N} \tilde{f}(N) \mathrm{d}N$$

$$\updownarrow$$

$$f(x) = \frac{i}{2\pi} \underset{x}{\mathrm{Disc}} \hat{f}\left(t = \frac{1}{x}\right)$$

- $\hat{f}(t) \to \tilde{f}(N)$: find ans solve a recurrence starting from the differential equation in t
- $f(x) \to \tilde{f}(N)$: find ans solve a recurrence starting from the differential equation in x
- $\tilde{f}(N) \to f(x)$: find and solve a differential equations starting from the recurrence in N
- $\hat{f}(t) \to f(x)$: analytic continuation to $t > 1$.
  [Behring, Blümlein, Schönwald '23]
- algorithms implemented in public packages `Sigma` and `HarmonicSums`

BUT: Algorithmic solutions are only possible if the recurrences or differential equations factorize to first order.

$$\frac{d}{dt}\vec{M} = A(\epsilon, t) \cdot \vec{M}$$

N-space calculations:

- Insert a formal power series into the differential equation

$$\vec{M} = \sum_{i=0}^{\infty} \vec{c}_i \, t^i$$

  and obtain recurrences for the expansion coefficients.
- **Method 1:** Solve the recurrences directly with advanced methods implemented in `Sigma` [Schneider, 2007,2013] .
- **Method 2:** Obtain a large number of moments [Blümlein, Schneider, 2017] and guess a recurrence [Kauers et al. '09] of the final quantity to compute and solve with `Sigma`.

$$\frac{d}{dt}\vec{M} = A(\epsilon, t) \cdot \vec{M}$$

x-**space calculations:**

- **Method 1:** Solve the differential equation analytically in t and compute the Nth derivative symbolically and do the inverse Mellin transform (algorithms implemented in `HarmonicSums` [Ablinger '09-]).
- **Method 2:** Use analytic series expansions and numerical matching to obtain semi-analytic results for all values of t. The x-space solution can be found through the imaginary part for $t > 0$.

First order factorizable sector – The function spaces

Sums

Harmonic Sums

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

gen. Harmonic Sums

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

Cycl. Harmonic Sums

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

Binomial Sums

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

Integrals

Harmonic Polylogarithms

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

gen. Harmonic Polylogarithms

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

Cycl. Harmonic Polylogarithms

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

root-valued iterated integrals

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

Special Numbers

multiple zeta values

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

gen. multiple zeta values

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

cycl. multiple zeta values

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

associated numbers

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

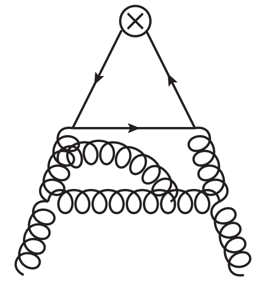
shuffle, stuffle, and various structural relations $\Longrightarrow$ algebras

The OME A_{Qg}

First order factorizable contributions – A_{Qg}

[Ablinger, Behring, Blümlein, De Freitas, Manteuffel, Schneider, Schönwald '24]

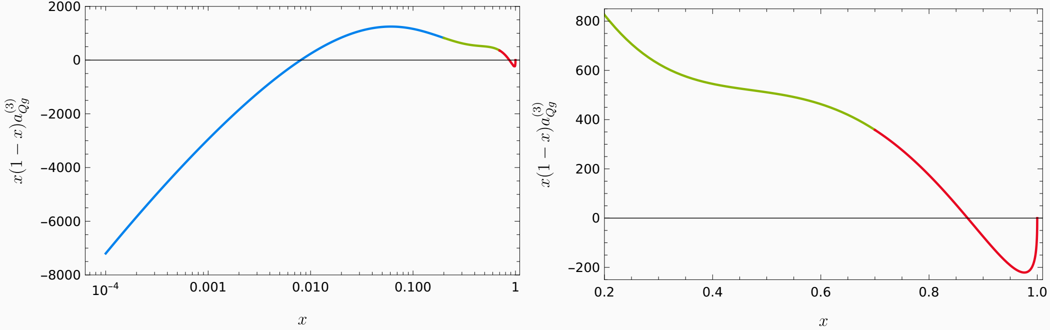
- 468 out of 666 **master integrals** solved analytically.
- 1009 out of 1233 contributing **Feynman diagrams** solved.
- Solved via the method of large moments: N_F, ζ_2, ζ_4 and B_4.
- Inverse Mellin transform via analytic continuation from t-space.
- Alphabet of the iterated integrals:



$$\left\{\frac{1}{t}, \frac{1}{1\pm t}, \frac{1}{2\pm t}, \frac{1}{4\pm t}, \frac{1}{1\pm 2t}, \sqrt{t(4\pm t)}, \frac{\sqrt{t(4\pm t)}}{1\pm t}, \frac{\sqrt{t(4\pm t)}}{1\mp t}, \frac{\sqrt{t(4\pm t)}}{1\mp 2t}\right\}$$

First order factorizable contributions – A_{Qg}

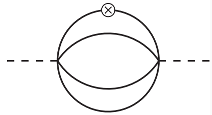
[Ablinger, Behring, Blümlein, De Freitas, Manteuffel, Schneider, Schönwald '23]



First order factorizable contributions to $a_{Qg}^{(3)}$. The colors show that expansions around $x = 0$, $x = 1/2$ and $x = 1$ are used.

The elliptic sector – A_{Qg}

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



$$\begin{aligned} R_1(t,\varepsilon) &= \frac{1}{t(1-t)\varepsilon^3}\left[16 - \frac{68}{3}\varepsilon + \left(\frac{59}{3} + 6\zeta_2\right)\varepsilon^2 + \left(-\frac{65}{12} - \frac{17}{2}\zeta_2 + 2\zeta_3\right)\varepsilon^3\right] + O(\varepsilon), \\ R_2(t,\varepsilon) &= \frac{1}{t(1-t)\varepsilon^3}\left[8 - \frac{16}{3}\varepsilon + \left(\frac{4}{3} + 3\zeta_2\right)\varepsilon^2 + \left(\frac{14}{3} - 2\zeta_2 + \zeta_3\right)\varepsilon^3\right] + O(\varepsilon), \\ R_3(t,\varepsilon) &= \frac{1}{12t(8+t)\varepsilon^3}\left[-192 + 8\varepsilon - 8(4 + 9\zeta_2)\varepsilon^2 + (68 + 3\zeta_2 - 24\zeta_3)\varepsilon^3\right] + O(\varepsilon). \end{aligned}$$

Full solution

- We find:

$$F_3(t) = \frac{1}{\epsilon^2}\left[\frac{10}{3} - \frac{t}{6}\right] + \frac{1}{\epsilon}\left[-\frac{31}{6} + \frac{3t}{8} - \left(\frac{1}{3} - \frac{1}{6t} - \frac{t}{6}\right) H_1(t)\right] + \left[\frac{3}{4}\ln(2) g_1(t) + \frac{1}{12}(10 + \pi(-3i + \sqrt{3}))g_1(t) - \frac{g_2(t)}{3} + \frac{25}{54}\left[g_1(t)G(13;t) - g_2(t)G(7;t)\right] + \frac{28}{27}\left[g_2(t)G(8;t) - g_1(t)G(14;t)\right] + \frac{1}{3}\left[g_1(t)G(16;t) - g_2(t)G(10;t)\right]\right]\zeta_2 + \ldots$$

with $\left[f(t) = -\frac{27t}{(1-t)^2(8+t)}\right]$

$$g_1(t) = \frac{2}{(1-t)^{2/3}(8+t)^{1/3}}\,{}_2F_1\left[\begin{matrix}\frac{1}{3}, \frac{4}{3}\\ 2\end{matrix}; f(t)\right], \quad g_2(t) = \frac{9\sqrt{3}\Gamma^2(1/3)}{8\pi}\frac{1}{(1-t)^{2/3}(8+t)^{1/3}}\,{}_2F_1\left[\begin{matrix}\frac{1}{3}, \frac{4}{3}\\ \frac{2}{3}\end{matrix}; 1 - f(t)\right],$$

and the alphabet:

$$A = \{1, 2, \ldots, 17\} = \left\{\frac{1}{t}, \frac{1}{1-t}, \frac{1}{8+t}, g_1, g_2, \frac{g_1}{t}, \frac{g_1}{1-t}, \frac{g_1}{8+t}, \frac{g_1'}{t}, \frac{g_1'}{1-t}, \frac{g_1'}{8+t}, \frac{g_2}{t}, \frac{g_2}{1-t}, \frac{g_2}{8+t}, \frac{g_2'}{t}, \frac{g_2'}{1-t}, \frac{g_2'}{8+t}, t\,g_1, t\,g_2\right\}$$

$G(w_1, \vec{w}; t) = \int_0^t \mathrm{d}t'\, A_{w_1}(t') G(\vec{w}; t')$, with the usual regularization at $t = 0$ understood implicitly

Semi-analytic calculation

[Ablinger, Behring, Blümlein, De Freitas, Manteuffel, Schneider, Schönwald '24]

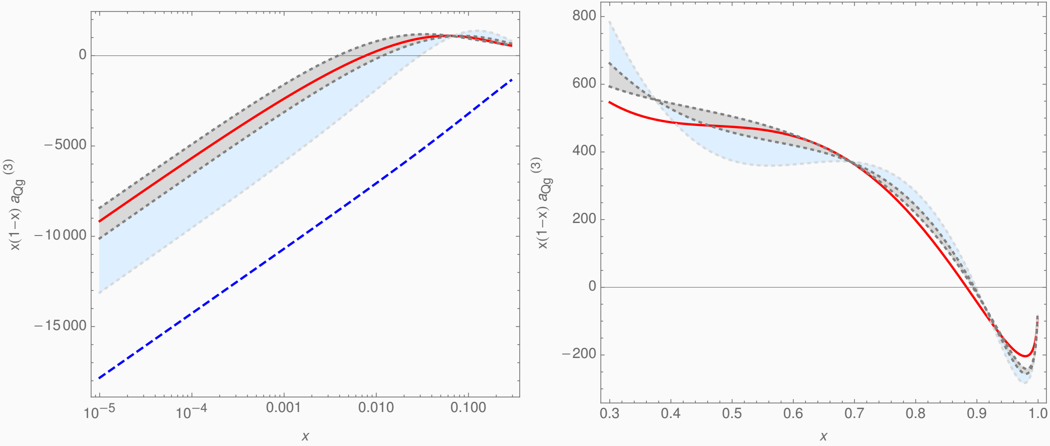
General idea:

- Evaluate the master integrals via series expansion around the point $t_0 = 0$.
- Calculate a second symbolic expansion around $t_1 > t_0$.
- Use the first series expansion at the point $(t_0 + t_1)/2$ as new boundary conditions.
- Continue until $t \in (0, \infty)$ is covered.

! The solution around $t \to 1^-$ is a power-log series, the analytic continuation of $\ln(1-t)$ for $t > 1$ provides the imaginary parts.

Full solution – A_{Qg}

[Ablinger, Behring, Blümlein, De Freitas, Manteuffel, Schneider, Schönwald '24]



Full line: our full result for $a_{Qg}^{(3)}(x)$

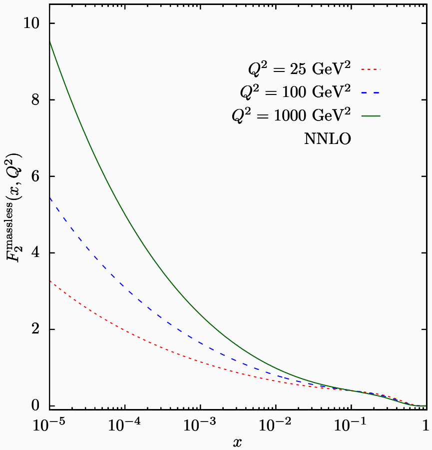
dashed line: leading small-x term $\propto \ln(x)/x$ [Catani, Ciafaloni, Hautmann, 1990]

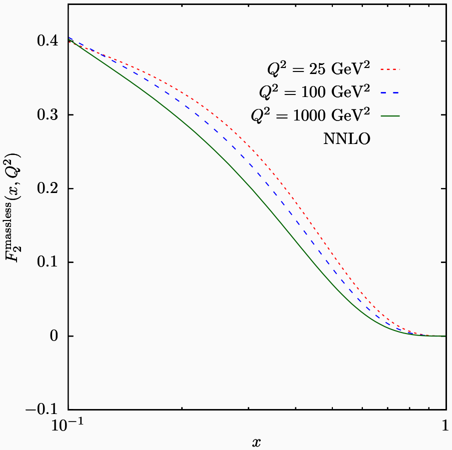
light blue region: estimates based on 5 moments [Kawamura et al., 2012]

gray region: estimates using relations to $a_{Qq}^{(3),\mathrm{PS}}$ [Alekhin, Blümlein, Moch, Placakyte, 2017]

Quantitative Results

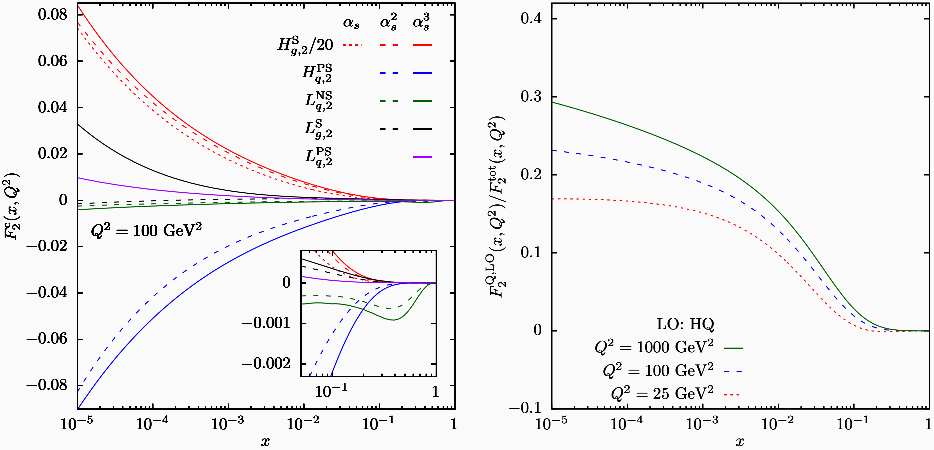
The massless contributions to F_2





Results for $N_F = 3$ massless quarks.

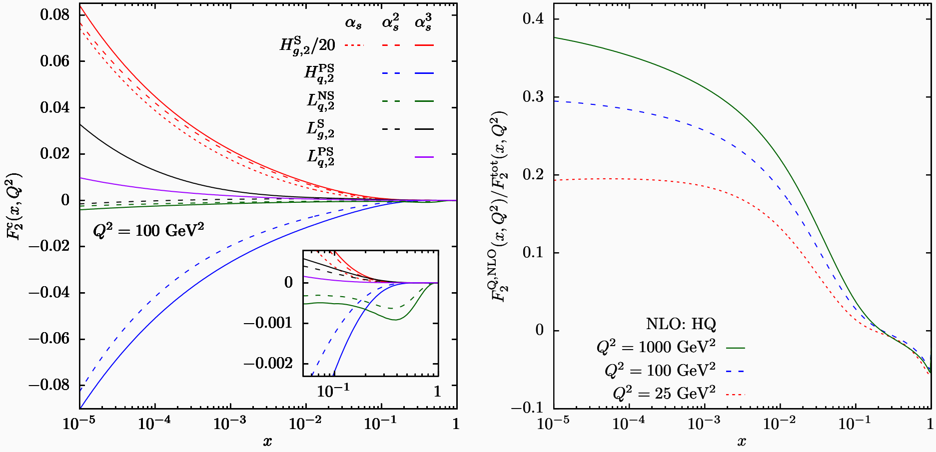
Single-mass contributions to F_2^c



left: charm contributions for $Q^2 = 100$ GeV^2

right: c quark contributions at **LO**

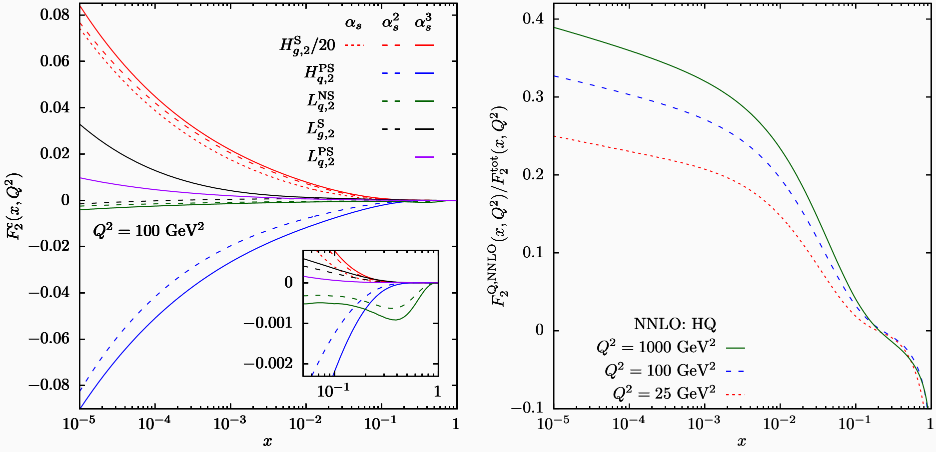
Single-mass contributions to F_2^c



left: charm contributions for $Q^2 = 100$ GeV^2

right: c quark contributions at **NLO**

Single-mass contributions to F_2^c



left: charm contributions for $Q^2 = 100$ GeV^2

right: c quark contributions at **NNLO**

Two mass contributions

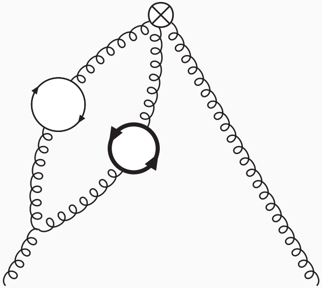
At high enough energies $Q^2 \gg m_c^2, m_b^2$, treat charm and bottom as massless:

Option 1: $Q^2 \gg m_b^2 \gg m_c^2$

- Decouple charm, then decouple bottom while considering the charm as massless.
- No new ingredients appear in the asymptotic representation.
- Universal power corrections in $\sqrt{\eta} = \frac{m_c}{m_b} \sim 0.3$ are not accounted for.

Option 2: $Q^2 \gg m_b^2 \sim m_c^2$

- Decouple charm and bottom together.
- New OMEs with both massive quarks present simultaneously appear.
- All two-mass OMEs exept A_{Qg} already calculated.



Two mass contributions

Mathematical Structures

- $\mathbf{A}_{\mathbf{qq},\mathbf{Q}}^{\mathbf{NS}}$: $S_1(n), \ldots; \; H_1(x), \ldots$
- $\mathbf{A}_{\mathbf{Qq}}^{\mathbf{PS}}$: no closed solution; $\theta(\eta_- - x) \int\limits_x^{\eta_-} \mathrm{d}y \int\limits_0^u \mathrm{d}t \frac{\sqrt{1-4t}}{t}, \ldots$
- $\mathbf{A}_{\mathbf{gg},\mathbf{Q}}$: $4^{-N} \sum\limits_{i=1}^{N} \left(\frac{4}{1-\eta}\right)^i \frac{1}{i\binom{2i}{i}}, \ldots; \; \int\limits_0^x \mathrm{d}t \frac{\sqrt{t(1-t)}}{1-t(1-\eta)}, \ldots$
- $\mathbf{A}_{\mathbf{Qg}}$: work in progress

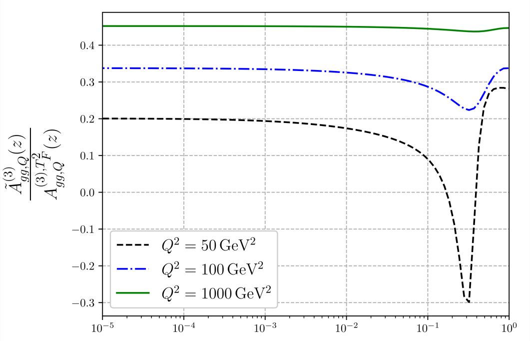


Illustration for the two mass cobtributions to $A_{gg,Q}^{(3)}$ normalized to the single mass T_F^2 contributions for different values of Q^2.

Summary and Outlook

Summary and Outlook

Summary

- Massive operator matrix elements are important for phenomenology.
  They can be used for:
  - the interpretation of DIS precision data.
  - the precise determination of parton distribution functions.
- At 3-loop order all OMEs for unpolarized and polarized scattering have been calculated.
- Together with the massless Wilson coefficients we can describe heavy quark production in DIS at large Q^2.
- The variable-flavor-number-scheme at 3-loop can be completed.
- During the project new methods and tools have been developed.
- Also power corrections in $\frac{m_c}{m_b}$ can be considered.

Summary and Outlook

Outlook

- All results will be implemented in a numerical program and released soon.
- The analytic solution of A_{Qg} depends on two elliptic sectors and is work in progress.
- The two mass contributions to A_{Qg} are work in progress.
- A reanalysis of DIS data to measure α_s and m_c can be carried out.

Summary and Outlook

Outlook

- All results will be implemented in a numerical program and released soon.
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- The two mass contributions to A_{Qg} are work in progress.
- A reanalysis of DIS data to measure α_s and m_c can be carried out.

$\Rightarrow$ Polarized results are directly applicable for EIC analysis in the future.

Backup

Massive Wilson Coefficients – Pure-Singlet

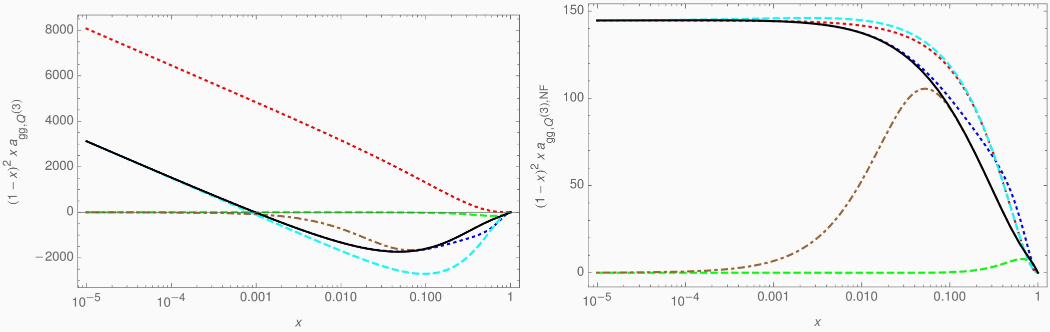
- We have analytically calculated the pure-singlet contributions in terms of iterated integrals (with involved letters). [Blümlein, De Freitas, Raab, Schönwald '19]
- The expression in terms of iterated integrals allows a systematic expansion in the asymptotic limit $Q^2 \gg m^2$.
- This can be compared to the prediction of the asymptotic limit:

$$H_{L,q}^{(2),\mathrm{PS}}\left(z, \frac{Q^2}{m^2}\right) = \tilde{C}_{q,L}^{(2),\mathrm{PS}}(N_F+1) + \mathcal{O}\left(\frac{m^2}{Q^2}\right) ,$$

$$H_{2,q}^{(2),\mathrm{PS}}\left(z, \frac{Q^2}{m^2}\right) = A_{Qq}^{(2),\mathrm{PS}}(N_F+1) + \tilde{C}_{q,2}^{(2),\mathrm{PS}}(N_F+1) + \mathcal{O}\left(\frac{m^2}{Q^2}\right)$$

$$
\begin{aligned}
H_{L,q}^{2,\mathrm{PS}} &= -32 C_F T_F \Biggl\{ \frac{(1-z)\bigl(1-2z+10z^2\bigr)}{9z} - (1+z)(1-2z)\mathrm{H}_0 - z\mathrm{H}_0^2 \\
&+ \frac{(1-z)\bigl(1-2z-2z^2\bigr)}{3z}\mathrm{H}_1 - z\mathrm{H}_{0,1} + z\zeta_2 + \frac{m^2}{Q^2}\Biggl[-\frac{(1-z)\bigl(2-z+2z^2\bigr)}{3z} \ln^2\left(\frac{m^2}{Q^2}\right) \\
&+ \frac{(1-z)\bigl(-22+4z+29z^2\bigr)}{9z} - \Biggl(\frac{(1-z)\bigl(20-7z-25z^2\bigr)}{9z} + \frac{2}{3}(3-6z \\
&-2z^2)\mathrm{H}_0 \Biggr) \ln\left(\frac{m^2}{Q^2}\right) + \Biggl(\frac{2}{9}(-6+3z+13z^2) + \frac{2(1+z)\bigl(-2+z+2z^2+2z^3\bigr)}{3z} \\
&\times \mathrm{H}_{-1} \Biggr) \mathrm{H}_0 - \frac{2}{3} z^3 \mathrm{H}_0^2 + \Biggl(-\frac{(1-z)^2(14+13z)}{9z} + \frac{4(1-z)\bigl(2-z+2z^2\bigr)}{3z}\mathrm{H}_0 \Biggr) \mathrm{H}_1 \\
&+ \frac{(1-z)\bigl(2-z+2z^2\bigr)}{3z}\mathrm{H}_1^2 - \frac{2\bigl(4-3z-4z^3\bigr)}{3z}\mathrm{H}_{0,1} \\
&+ \frac{2(1+z)\bigl(2-z-2z^2-2z^3\bigr)}{3z}\mathrm{H}_{0,-1} - \frac{2(1-z)\bigl(2-z+2z^2+2z^3\bigr)}{3z}\zeta_2 \Biggr]
\end{aligned}
$$

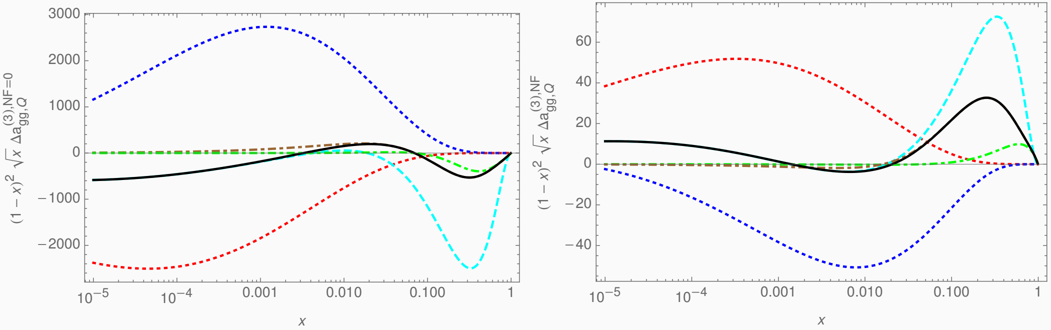
$a_{gg}^{(3)}$



non N_F terms $\qquad$ N_F terms

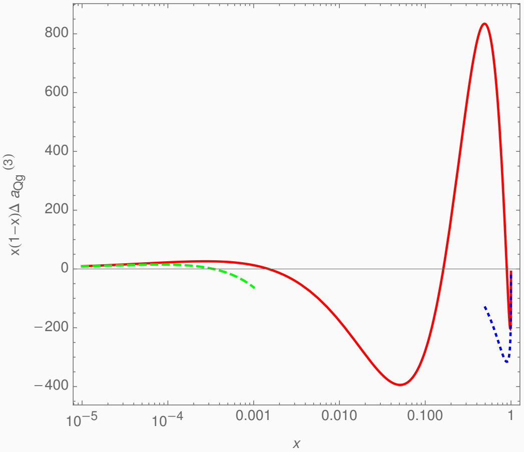
Left panel: The non–N_F terms of $a_{gg,Q}^{(3)}(N)$ (rescaled) as a function of x. Full line (black): complete result; upper dotted line (red): term $\propto \ln(x)/x$; lower dashed line (cyan): small x terms $\propto 1/x$; lower dotted line (blue): small x terms including all $\ln(x)$ terms up to the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

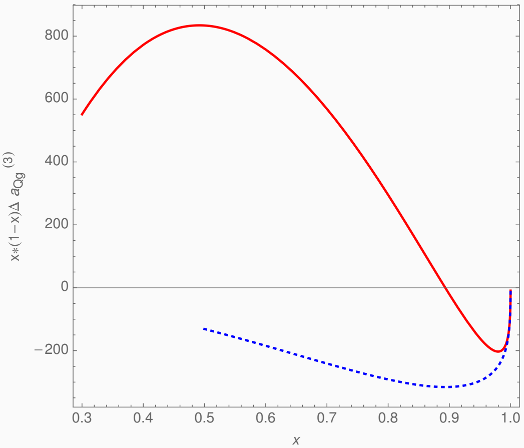
$\Delta a_{gg}^{(3)}$



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.

Full solution – A_{Qg}



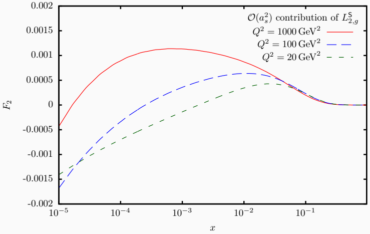


Full line: our full result for $\Delta a_{Qg}^{(3)}(x)$

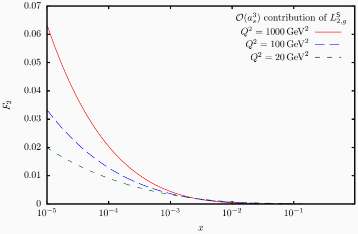
dashed line: leading small-x term $\propto \ln(x)$

dashed line: leading large-x term $\propto \ln(1-x)$

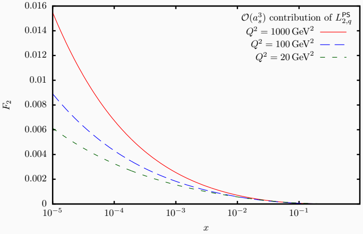
Numerical Results : $L_{g,2}^{\mathrm{S}}$ and $L_{q,2}^{\mathrm{PS}}$



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



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



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

Inverse Mellin transform via analytic continuation

[based on: Behring, Blümlein, Schönwald (JHEP (2023))]

$$\hat{f}(t) = \sum_{N=1}^{\infty} \tilde{f}(N) t^N = \sum_{N=1}^{\infty} \int_0^1 \mathrm{d}x' \; t^N {x'}^{N-1} f(x') = \int_0^1 \mathrm{d}x' \; \frac{t}{1-tx'} f(x')$$

Setting $t = \frac{1}{x}$ we obtain:

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{f(x')}{x-x'}$$

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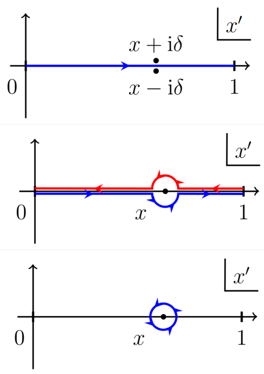

Setting $t = \frac{1}{x}$ we obtain:

$$\hat{f}\left(\frac{1}{x}\right) = \int_0^1 \mathrm{d}x' \frac{f(x')}{x - x'}$$

Therefore:

$$f(x) = \frac{i}{2\pi} \lim_{\delta \to 0} \oint_{|x - x'| = \delta} \frac{f(x')}{x - x'} = \frac{i}{2\pi} \operatorname*{Disc}_x \hat{f}\left(\frac{1}{x}\right)$$

Inverse Mellin transform via analytic continuation

The discussion before used some implicit assumptions.
The x-space representation

1. has no $(-1)^N$ term.
2. is regular and has now contributions from distributions.
3. has a support only on $x \in (0, 1)$.

Inverse Mellin transform via analytic continuation

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The x-space representation

1. has no $(-1)^N$ term.
2. is regular and has now contributions from distributions.
3. has a support only on $x \in (0,1)$.

For physical examples:

$$\tilde{f}(N) = \int_0^1 \mathrm{d}x\, x^{N-1} \left[f(x) + (-1)^N g(x) + \left(f_\delta + (-1)^N g_\delta\right) \delta(1-x)\right] + \int_0^1 \mathrm{d}x\, \frac{x^{N-1}-1}{1-x}, \left[f_+(x) + (-1)^N g_+(x)\right]$$

All of this can be lifted, but the discussion is more involved.