3 Loop unpolarized and polarized heavy flavor corrections to DIS: two mass contributions

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Introduction

Introduction

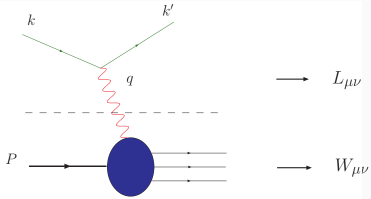
- The correct treatment of heavy quark masses is important for precision at the LHC.
- Often we want to describe data in different kinematic regimes:
  (a) $m^2 \sim Q^2$: low energies where power corrections are important
  (b) $m^2 \ll Q^2$: high energies, where large logarithms are produced

  $\Rightarrow$ 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:

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

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

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:

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

- 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. (S)-ACOT, FONLL:

[Aivazis, Collins, Olness, Tung '94;...; Guzzi, Nadolsky, Reina, Wackeroth, Xie '24] [Cacciari, Greco, Nason '98;...; Barontini, Candido, Hekhorn, Magni, Stegeman '24]

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

Two mass contributions

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

Option 1: $\boxed{Q^2 \gg m_b^2 \gg m_c^2}$

- 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: $\boxed{Q^2 \gg m_b^2 \sim m_c^2}$

- Decouple charm and bottom together.
- New OMEs with both massive quarks present simultaneously appear. [Ablinger, Blümlein, De Freitas, Hasselhuhn, Schneider, Wißbrock '17]

$$A_{ij}(N_F+2, m_c, m_b, \mu) = A_{ij}\left(N_F+1, \frac{m_c^2}{\mu^2}\right) + A_{ij}\left(N_F+1, \frac{m_b^2}{\mu^2}\right) + \tilde{A}_{ij}(N_F+2, m_c, m_b, \mu)$$

Matching conditions for parton distribution functions:

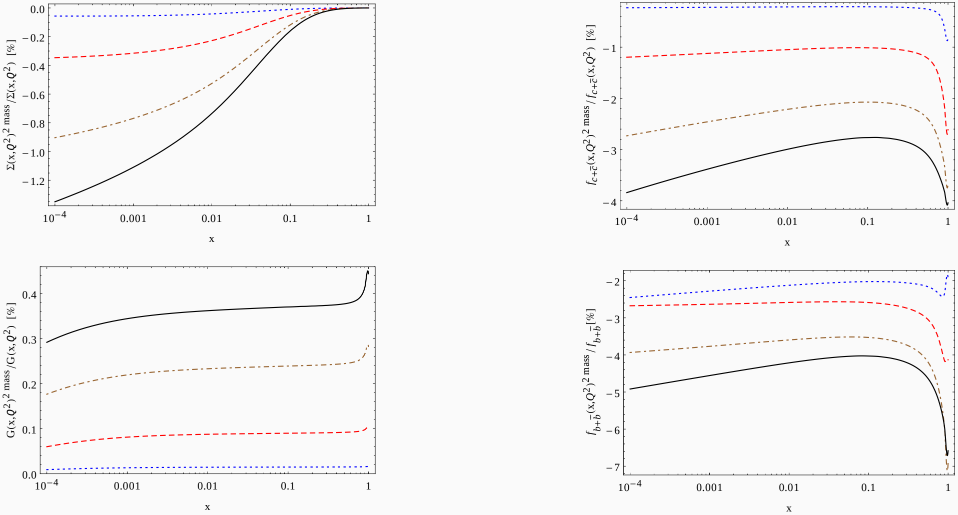
$$f_k(N_F+2) + f_{\overline{k}}(N_F+2) = A_{qq,Q}^{\rm NS}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) \cdot \left[f_k(N_F) + f_{\overline{k}}(N_F)\right]$$
$$+ \frac{1}{N_F} A_{qq,Q}^{\rm PS}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) \cdot \Sigma(N_F)$$
$$+ \frac{1}{N_F}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

$$\Sigma(N_F+2) = \left[A_{qq,Q}^{\rm NS}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) + A_{qq,Q}^{\rm PS}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) + A_{Qq}^{\rm PS}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right)\right] \cdot \Sigma(N_F)$$
$$+ \left[A_{qg,Q}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) + A_{Qg}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right)\right] \cdot G(N_F) \,,$$
$$G(N_F+2) = A_{gq,Q}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) \cdot \Sigma(N_F) + A_{gg,Q}\left(N_F+2, \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}\right) \cdot G(N_F) \,.$$

The Variable Flavor Number Scheme at NLO

[Blümlein, De Freitas, Schneider, Schönwald, '18]

Illustration of two mass effects at NLO ($Q^2 = 30\text{GeV}^2$, 50GeV^2, 100GeV^2, 1000GeV^2):



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

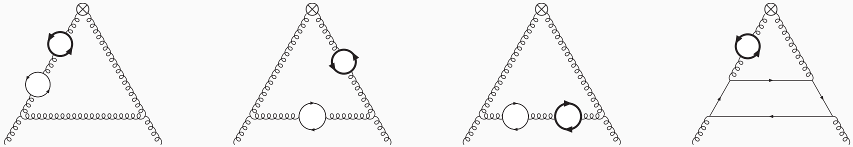
Computing Massive Operator Matrix Elements

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

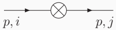
$$O^{\rm NS}_{q,r;\mu_1,\ldots,\mu_N} = i^{N-1} \mathcal{S} \left[\bar{\psi} \gamma_{\mu_1} D_{\mu_2} \ldots D_{\mu_N} \frac{\lambda_r}{2} \psi \right] - \text{trace terms} \; ,$$
$$O^{\rm S}_{q,r;\mu_1,\ldots,\mu_N} = i^{N-1} \mathcal{S} \left[\bar{\psi} \gamma_{\mu_1} D_{\mu_2} \ldots D_{\mu_N} \psi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

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

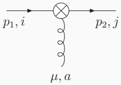
- The operator insertions introduce Feynman rules which depend on the Mellin variable N.



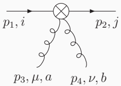
The OMEs are calculated using the QCD Feynman rules together with the following operator insertion Feynman rules:



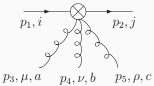
$$\delta^{ij}\not\Delta\gamma_\pm(\Delta\cdot p)^{N-1}\,, \quad N\ge 1$$



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



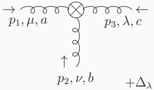
$$g^2\Delta^\mu\Delta^\nu\not\Delta\gamma_\pm\sum_{j=0}^{N-3}\sum_{l=j+1}^{N-2}(\Delta p_2)^j(\Delta p_1)^{N-l-2} \Big[(t^at^b)_{ji}(\Delta p_1+\Delta p_4)^{l-j-1}+(t^bt^a)_{ji}(\Delta p_1+\Delta p_3)^{l-j-1}\Big]\,, \quad N\ge 3$$



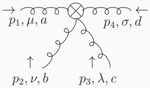
$$\begin{aligned} &g^3\Delta_\mu\Delta_\nu\Delta_\rho\not\Delta\gamma_\pm\sum_{j=0}^{N-4}\sum_{l=j+1}^{N-3}\sum_{m=l+1}^{N-2}(\Delta.p_2)^j(\Delta.p_1)^{N-m-2} \\ &\Big[\ (t^at^bt^c)_{ji}(\Delta.p_4+\Delta.p_5+\Delta.p_1)^{l-j-1}(\Delta.p_5+\Delta.p_1)^{m-l-1} \\ &\ +(t^at^ct^b)_{ji}(\Delta.p_4+\Delta.p_5+\Delta.p_1)^{l-j-1}(\Delta.p_4+\Delta.p_1)^{m-l-1}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

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

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



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

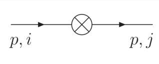


$$\begin{aligned} &g^2\frac{1+(-1)^N}{2}\Bigg(f^{abe}f^{cde}O_{\mu\nu\lambda\sigma}(p_1,p_2,p_3,p_4) \\ &+f^{ace}f^{bde}O_{\mu\lambda\nu\sigma}(p_1,p_3,p_2,p_4)+f^{ade}f^{bce}O_{\mu\sigma\nu\lambda}(p_1,p_4,p_2,p_3)\Bigg)\,, \end{aligned}$$

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

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]
- γ_5 is treated in the Larin scheme: [Larin, 1993]
- Color algebra: `Color` [van Ritbergen, Schellekens, Vermaseren, 1999]
- IBP reduction: `Reduze 2` [von Manteuffel, Studerus 2009,2012]

$\Rightarrow$ 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

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

$$\updownarrow$$

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

$$\updownarrow$$

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

$$\updownarrow$$

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

- $\hat{f}(t) \to \tilde{f}(N)$: 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` [Schneider, '07,'13,...] and `HarmonicSums` [Ablinger, '09,'12,...]

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

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

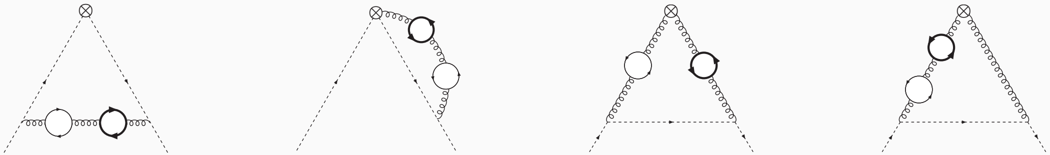
  and obtain recurrences for the expansion coefficients.
- **Method 1:** Solve the recurrences directly with advanced methods implemented in `Sigma` [Schneider, '07,'13] .
- **Method 2:** Obtain a large number of moments [Blümlein, Schneider, '17] and guess a recurrence [Kauers et al. '09] of the final 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 $t > 0$.

Two mass contributions to $A_{qq,Q}^{\mathrm{NS},(3)}$ and $A_{gq}^{(3)}$ [Nucl.Phys.B 921 (2017), Nucl.Phys.B 964 (2021)]



- After introducing Feynman parameters the integrals can be represented as:

$$I \sim \mathcal{C}(\varepsilon, N) \int_{-i\infty}^{+i\infty} d\sigma \eta^{\sigma} \Gamma \left[\begin{matrix} g_1(\varepsilon)+\sigma, g_2(\varepsilon)+\sigma, g_3(\varepsilon)+\sigma, g_4(\varepsilon)-\sigma, g_5(\varepsilon)-\sigma \\ g_6(\varepsilon)+\sigma, g_7(\varepsilon)-\sigma \end{matrix} \right].$$

- The η and N dependence completely factorizes, and after closing the integration contour and summing residues a linear combination of hypergeometric ${}_4F_3$-functions is obtained

$$I = \sum_j \mathcal{C}_j(\varepsilon, N)\, {}_4F_3 \left[\begin{matrix} a_1(\varepsilon), a_2(\varepsilon), a_3(\varepsilon), a_4(\varepsilon) \\ b_1(\varepsilon), b_2(\varepsilon), b_3(\varepsilon) \end{matrix}, \eta \right]$$

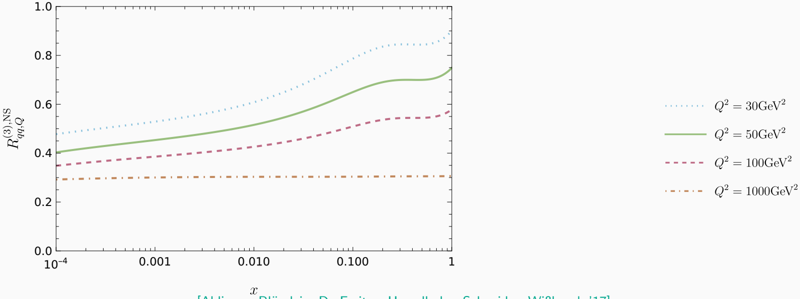
- The ε-expansion gives rise to (poly)logarithmic functions with argument η, $\sqrt{\eta}$ and $-\sqrt{\eta}$.

Two mass contributions to $A_{qq,Q}^{\mathsf{NS},(3)}$

- We use the following ratio to visualize the size of the two mass contributions:

$$(\Delta)R_{ij} = \frac{(\Delta)\tilde{A}_{ij}^{(3)}(m_c^2, m_b^2, Q^2)}{(\Delta)\tilde{A}_{ij}^{(3)}(m_c^2, m_b^2, Q^2) + (\Delta)A_{ij}^{(3),T_F^2+T_F^3}(m_c^2, Q^2) + (\Delta)A_{ij}^{(3),T_F^2+T_F^3}(m_b^2, Q^2)} \xrightarrow{m_c=m_b} \frac{1}{2}$$

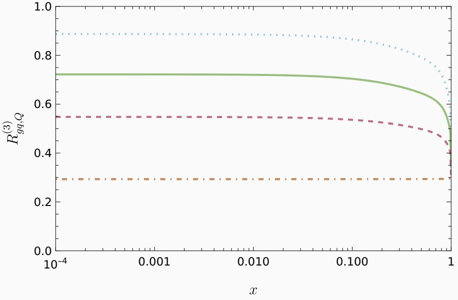
$$m_c = 1.59\text{GeV}, \qquad m_b = 4.78\text{GeV}, \qquad \frac{m_c}{m_b} \sim 0.333\ldots$$



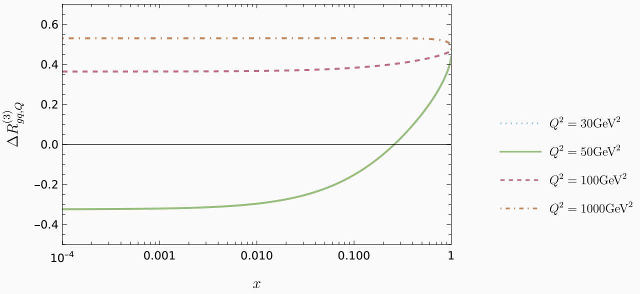
[Ablinger, Blümlein, De Freitas, Hasselhuhn, Schneider, Wißbrock '17]

Two mass contributions to $A_{gq}^{(3)}$

$m_c = 1.59\text{GeV}, \qquad m_b = 4.78\text{GeV}, \qquad \frac{m_c}{m_b} \sim 0.333...$

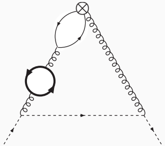


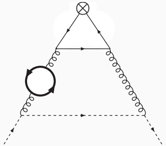
[Ablinger, Blümlein, De Freitas, Hasselhuhn, Schneider, Wißbrock '17]



[Behring, Blümlein, De Freitas, von Manteuffel, Schönwald, Schneider '21]

Two mass contribution to $A_{Qq}^{\mathsf{PS},(3)}$ [Nucl.Phys.B 927 (2018), Nucl.Phys.B 952 (2020)]





- After introducing Feynman parameters the integrals can be represented as:

$$I \sim r(N) \int_0^1 \mathrm{d}x \, x^N f(x) \int_{-i\infty}^{+i\infty} \mathrm{d}\sigma \, \xi^\sigma \, g(\sigma)$$

- Problem: the sums for the N-space solution are not first order factorizable
  $\Rightarrow$ Summation algorithms of `Sigma` cannot find the closed form solution
- Solution: aim directly for the solution in momentum fraction space, which is first order factorizable

Details: $A_{Qq}^{(3),\mathrm{PS}}$

- After introducing Feynman parameters the integrals can be represented as:

$$I \sim r(N) \int_0^1 \mathrm{d}x\, x^N f(x) \int_{-i\infty}^{+i\infty} \mathrm{d}\sigma\, \xi^\sigma g(\sigma)$$

- We now have two different cases for closing the contour:
- o Case 1: $\xi = \frac{1}{\eta x(1-x)}$
  We can close the contour to the left, since $\xi \geq 4/\eta$.
- o Case 2: $\xi = \frac{\eta}{x(1-x)}$
  We have to split the integration region into the three regions:
  1: $x \in (0, \eta_-)$: close to the left
  2: $x \in (\eta_-, \eta_+)$: close to the right
  3: $x \in (\eta_+, 1)$: close to the left
  with $\eta_\pm = \frac{1}{2}\left(1 \pm \sqrt{1-\eta}\right)$
- This shows that in momentum fraction space functions with different support contribute.

Results: $A_{Qq}^{(3),\mathbf{PS}}$

$$
\begin{aligned}
a_{Qq}^{(3),\mathrm{PS}}(N) \quad = \quad & \int_0^1 dx\, x^{N-1} \Big\{ K(\eta,x) + \big(\theta(\eta_- - x) + \theta(x-\eta_+)\big) x\, g_0(\eta,x) \\
& + \theta(\eta_+ - x)\theta(x-\eta_-) \left[x\, f_0(\eta,x) - \int_{\eta_-}^{x} dy \left(f_1(\eta,y) + \frac{y}{x} f_2(\eta,y) + \frac{x}{y} f_3(\eta,y) \right) \right] \\
& + \theta(\eta_- - x) \int_x^{\eta_-} dy \left(g_1(\eta,y) + \frac{y}{x} g_2(\eta,y) + \frac{x}{y} g_3(\eta,y) \right) \\
& - \theta(x-\eta_+) \int_{\eta_+}^{x} dy \left(g_1(\eta,y) + \frac{y}{x} g_2(\eta,y) + \frac{x}{y} g_3(\eta,y) \right) \\
& + x\, h_0(\eta,x) + \int_x^1 dy \left(h_1(\eta,y) + \frac{y}{x} h_2(\eta,y) + \frac{x}{y} h_3(\eta,y) \right) \\
& + \theta(\eta_+ - x) \int_{\eta_-}^{\eta_+} dy \left(f_1(\eta,y) + \frac{y}{\eta_+ x} f_2(\eta,y) + \eta_+ \frac{x}{y} f_3(\eta,y) \right) \\
& + \int_{\eta_+}^{1} dy \left(g_1(\eta,y) + \frac{y}{x} g_2(\eta,y) + \frac{x}{y} g_3(\eta,y) \right) \Big\}
\end{aligned}
$$

The function $a_{Qq}^{(3),\mathrm{PS}}(x)$ is continuous.

The integrals $\int_{\eta_-}^{x} dy$, $\int_{\eta_+}^{x} dy$, $\int_{x}^{1} dy$, $\int_{\eta_-}^{\eta_+} dy$ and $\int_{\eta_+}^{1} dy$ arise from the absorption of N dependant factors.

E.g. we find:

$$
\begin{aligned}
f_2(\eta, y) \quad = \quad & -\frac{64 P_1 \left(\eta + 4y^2 - 4y\right)^{3/2}}{9\eta^{3/2}(1-y)y^2} G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, \frac{\eta}{y(1-y)}\right) \\
& + G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\}, \frac{\eta}{y(1-y)}\right) \left\{\frac{128}{3}(1-y) G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, \frac{\eta}{y(1-y)}\right)\right. \\
& \left. -\frac{32 P_1 \left(\eta + 4y^2 - 4y\right)^{3/2}}{9\eta^{3/2}(1-y)y^2} \left[1 - 2\ln\left(\frac{\eta}{y(1-y)}\right)\right]\right\} + \frac{1280}{9}(1-y)\ln^2\left(\frac{\eta}{y(1-y)}\right) \\
& - \frac{128}{3}(1-y) G\left(\left\{\frac{1}{\tau}, \sqrt{4-\tau}\sqrt{\tau}, \sqrt{4-\tau}\sqrt{\tau}\right\}, \frac{\eta}{y(1-y)}\right) - \frac{256}{9}(1-y)\ln^3\left(\frac{\eta}{(1-y)y}\right) \\
& + \frac{32}{3}(1-y)\left[1 - 2\ln\left(\frac{\eta}{y(1-y)}\right)\right] G\left(\left\{\sqrt{4-\tau}\sqrt{\tau}\right\}, \frac{\eta}{y(1-y)}\right)^2 + \frac{4P_2}{9(1-y)^3 y^4} \\
& - \left(\frac{16 P_3}{9(1-y)^3 y^4} + \frac{512}{3}(1-y)\zeta_2\right) \ln\left(\frac{\eta}{y(1-y)}\right) + \frac{2560}{9}(1-y)\zeta_2 - \frac{1024}{3}(1-y)\zeta_3
\end{aligned}
$$

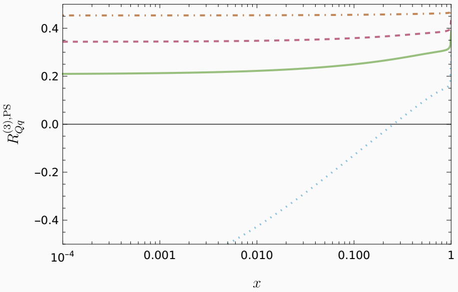
- For numerical evaluations we calculated a long list of iterated integrals as HPLs at involved and complex arguments, i.e.:

$$
\begin{aligned}
G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau},\frac{1}{\tau}\right\},\xi_1\right) &= \omega_1\left(-4-4\ln(2)+2\ln\left(4\xi_1\right)\right)+\ln^2\left(1-\omega_1\right)-\frac{1}{2}\ln^2\left(4\xi_1\right)\\
&-4\ln\left(1-\omega_1\right)-2\ln(2)\ln\left(1-\omega_1\right)+2\ln\left(4\xi_1\right)+2\ln(2)\ln\left(4\xi_1\right)-2\mathrm{Li}_2\left(\frac{1-\omega_1}{2}\right)+4-\ln^2(2),\\
G\left(\left\{\frac{1}{\tau},\frac{\sqrt{1-4\tau}}{\tau},\frac{1-\sqrt{4\tau}}{\tau}\right\},\xi_1\right) &= -\Big(\ln\left(1-\omega_1\right)\left(2\ln\left(4\xi_1\right)-4\right)-\ln^2\left(4\xi_1\right)\Big)\ln(2)\\
&-\left(2-2\ln\left(1-\omega_1\right)+\ln\left(4\xi_1\right)\right)\ln^2(2)-\ln^2\left(1-\omega_1\right)\left(-5\ln\left(4\xi_1\right)-6\right)-\Bigg(8-4\mathrm{Li}_2\left(\frac{1-\omega_1}{2}\right)\\
&-8\omega_1+8\ln\left(4\xi_1\right)+2\ln^2\left(4\xi_1\right)+4\zeta_2\Bigg)\ln\left(1-\omega_1\right)-\left(-4+2\mathrm{Li}_2\left(\frac{1-\omega_1}{2}\right)+4\omega_1-2\zeta_2\right)\ln\left(4\xi_1\right)\\
&-2\left(-4-\mathrm{Li}_3\left(\frac{1+\omega_1}{\omega_1-1}\right)+2\mathrm{Li}_2\left(\frac{1-\omega_1}{2}\right)+4\omega_1+4\xi_1\right)\\
&-\frac{10}{3}\ln^3\left(1-\omega_1\right)+\frac{1}{6}\ln^3\left(4\xi_1\right)+2\ln^2\left(4\xi_1\right)
\end{aligned}
$$

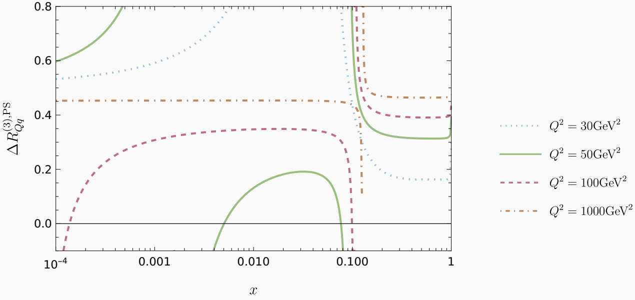
with $\omega_1=\sqrt{1-4\xi_1}$.

Result: $A_{Qq}^{(3),\mathrm{PS}}$

$$m_c = 1.59\text{GeV}, \qquad m_b = 4.78\text{GeV}, \qquad \frac{m_c}{m_b} \sim 0.333\ldots$$



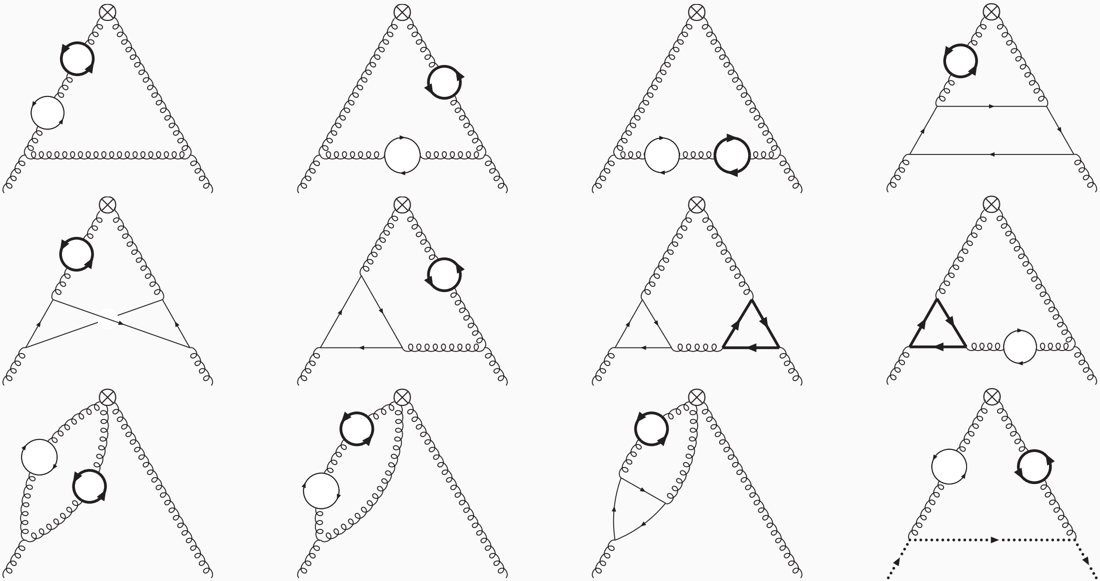
[Ablinger, Blümlein, De Freitas, Schneider, Schönwald '17]



[Ablinger, Blümlein, De Freitas, Saragnese, Schneider, Schönwald '19]

Two mass contribution to $A_{gg,Q}^{(3)}$

[Nucl.Phys.B 932 (2018), Nucl.Phys.B 955 (2020)]



Details: $A_{gg,Q}^{(3)}$

- In general the structures in N and η do not factorize:

$$I \sim C(\epsilon, N) \int_{-\infty}^{+\infty} \eta^{\sigma} \Gamma \left[\begin{matrix} (2+\frac{\varepsilon}{2}-\sigma)^2, \varepsilon-\sigma, -\sigma, \sigma-\frac{3\varepsilon}{2}, (2-\varepsilon+\sigma)^2, N-\frac{\varepsilon}{2}+\sigma \\ N+2+\frac{\varepsilon}{2}, 4+\varepsilon-2\sigma, 4-2\varepsilon+2\sigma \end{matrix} \right]$$

- The gluonic Feynman rules introduce large numerator structures

$\rightarrow$ single diagrams can lead to big expressions after taking all residues, the most involved diagram $11b$ amounts to $\sim$ 100MB disk space

- Our approach to tackle these sums:
  1. Crunch the expressions to a few master sums using `SumProduction`.
  2. Solve these master sums independently using the refined algorithms implemented in `EvaluateMultiSums` using `HarmonicSums` for limiting procedures.
  3. Reduce the occurring sums from the master sums to a smaller set of independent sums.
- This way the summation of diagram $11b$ can be tackled in $\sim$ 78 days and $\sim$ 33 days are needed to reduce the occurring sums to a basis
- The full summation amounted to around 5 months of calculation.

Results: $A_{gg,Q}^{(3)}$

$$
\begin{aligned}
\tilde{a}_{gg,Q}^{(3)}(N) \quad = \quad & \frac{1}{2}\left(1+(-1)^N\right)\Bigg\{ T_F^3 \left\{ \frac{32}{3}\left(L_1^3+L_2^3\right) + \frac{64}{3} L_1 L_2 \left(L_1+L_2\right) + 32\zeta_2\left(L_1+L_2\right) + \frac{128}{9}\zeta_3 \right\} \\
+ \quad & C_F T_F^2 \Bigg\{ \cdots + 32\left(\mathrm{H}_0^2(\eta) - \frac{1}{3} S_2\right) S_1 + \frac{128}{3} S_{2,1} - \frac{64}{3} S_{1,1,1}\left(\frac{1}{1-\eta}, 1-\eta, 1, N\right) \\
& - \frac{4P_{41}}{3(N-1)N^3(N+1)^2(N+2)(2N-3)(2N-1)} \left(\frac{\eta}{1-\eta}\right)^N \Bigg[\mathrm{H}_0^2(\eta) \\
& - 2\mathrm{H}_0(\eta) S_1\left(\frac{\eta-1}{\eta}, N\right) - 2S_2\left(\frac{\eta-1}{\eta}, N\right) + 2S_{1,1}\left(\frac{\eta-1}{\eta}, 1, N\right)\Bigg] + \ldots \Bigg\} \\
+ \quad & C_A T_F^2 \Bigg\{ \cdots + \Bigg[\frac{8P_{65}}{3645\eta(N-1)N^3(N+1)^3(N+2)(2N-3)(2N-1)} \\
& + \frac{8P_{37}\mathrm{H}_0(\eta)}{45\eta(N-1)N^2(N+1)^2(N+2)} + \frac{2P_{23}\mathrm{H}_0^2(\eta)}{9\eta(N-1)N(N+1)^2} + \frac{32}{27}\mathrm{H}_0^3(\eta) + \frac{128}{9}\mathrm{H}_{0,0,1}(\eta) \\
& + \frac{64}{9}\mathrm{H}_0^2(\eta)\mathrm{H}_1(\eta) - \frac{128}{9}\mathrm{H}_0(\eta)\mathrm{H}_{0,1}(\eta)\Bigg] S_1 \\
& + \frac{2^{-1-2N} P_{47}}{45\eta^2(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)} \binom{2N}{N} \sum_{i=1}^{N} \frac{4^i \left(\frac{\eta}{\eta-1}\right)^i}{i\binom{2i}{i}} \Bigg\{ \frac{1}{2}\mathrm{H}_0^2(\eta) \\
& S_{1,1}\left(\frac{\eta-1}{\eta}, 1, i\right)\Bigg\} + \ldots \Bigg\}
\end{aligned}
$$

Details: $A_{gg,Q}^{(3)}$

- The Mellin-inversion of the binomial sum structures can be handled with an improved algorithm implemented in HarmonicSums.
- The general idea is based on deriving a differential equation for the x-space solution nad subsequently solve it in terms of iterated integrals.
- We find i.e.

$$\sum_{i_1=1}^{N} \frac{2^{-2i_1}\binom{2i_1}{i_1}}{i_1} \sum_{i_2=1}^{i_1} \frac{2^{2i_2}}{\binom{2i_2}{i_2} i_2^2} \sum_{i_3=1}^{i_2} \frac{1}{i_3} =$$

$$\int_0^1 \mathrm{d}x \frac{(x^N-1)\sqrt{x}(4x-2)}{\sqrt{1-x}} \left[\pi \ln(2) - 8G\left(\left\{\sqrt{1-\tau}\sqrt{\tau}, \frac{1}{1-\tau}\right\}, x\right) - 4G\left(\left\{\sqrt{1-\tau}\sqrt{\tau}\right\}, x\right) - \frac{7\zeta_3}{2\pi}\right]$$

$$+\int_0^1 \mathrm{d}x \frac{x^N-1}{1-x} \left[\frac{-21x^2+32x^3-18x^4}{12} + 8G\left(\left\{\sqrt{1-\tau}\sqrt{\tau}, \sqrt{1-\tau}\sqrt{\tau}\right\}, x\right)\right.$$

$$+\frac{x-5x^2+8x^3-4x^4}{2} G\left(\left\{\frac{1}{1-\tau}\right\}, x\right) + 16G\left(\left\{\sqrt{1-\tau}\sqrt{\tau}, \sqrt{1-\tau}\sqrt{\tau}, \frac{1}{1-\tau}\right\}, x\right)$$

$$\left. -\frac{2\pi^2\ln(2) - 7\zeta_3}{\pi} G\left(\left\{\sqrt{1-\tau}\sqrt{\tau}\right\}, x\right)\right]$$

Details: $A_{gg,Q}^{(3)}$

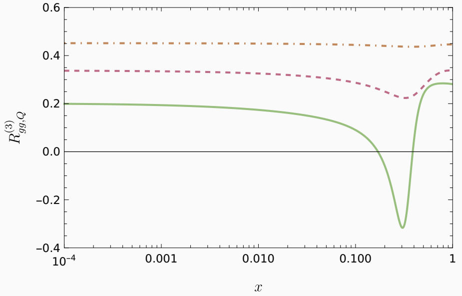
- The Mellin-inversion of the binomial sum structures can be handled with an improved algorithm implemented in HarmonicSums.
- The general idea is based on deriving a differential equation for the x-space solution nad subsequently solve it in terms of iterated integrals.
- For $\tilde{A}_{gg,Q}^{(3)}$ we find the alphabet:

$$\frac{1}{x}\,,\quad \frac{1}{1+x}\,,\quad \frac{1}{1-x}\,,\quad \sqrt{x(1-x)}\,,\quad \frac{1}{x+\eta(1-x)}\,,\quad \frac{1}{1-x(1-\eta)}$$
$$\frac{1}{\eta+x(1-\eta)}\,,\quad \frac{\sqrt{x(1-x)}}{1-x(1-\eta)}\,,\quad \frac{\sqrt{x(1-x)}}{x+\eta(1-x)}\,,\quad \frac{\sqrt{x(1-x)}}{\eta+x(1-\eta)}$$

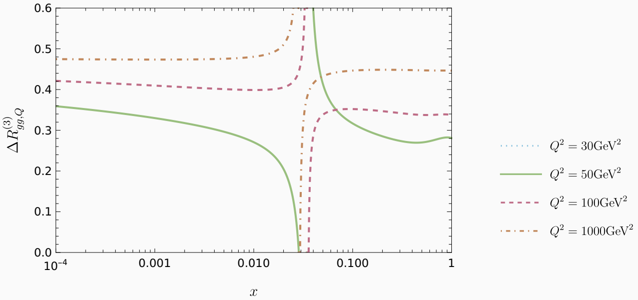
- Rational prefactors in N have to be included by convolution integrals.
- For numerical evaluations we calculated all occurring iterated integrals as HPLs at involved and complex arguments.

Two mass contribution to $A_{gg,Q}^{(3)}$

$$m_c = 1.59\text{GeV}, \qquad m_b = 4.78\text{GeV}, \qquad \frac{m_c}{m_b} \sim 0.333\ldots$$

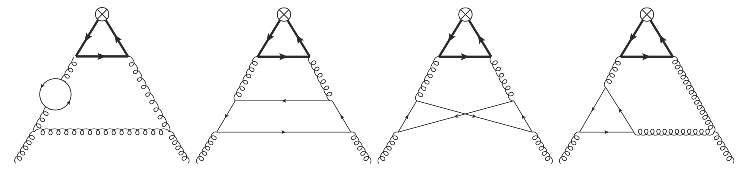


[Ablinger, Blümlein, De Freitas, Schneider, Schönwald '18]



[Ablinger, Blümlein, Goedicke, De Freitas, Saragnese, Schneider, Schönwald '20]

Two mass contributions to $A_{Qg}^{(3)}$



The calculation of $\tilde{A}_{Qg}^{(3)}$ is the biggest challenge:

- $A_{Qg}^{(3)}$ in the single mass case is already elliptic, the function space gets more complicated including a second mass.
- However, the physical value of $m_c/m_b \sim 0.3$ provides a natural expansion variable.

⇒ Idea: Obtain results in an expansion around $\eta \to 0$!

Two mass contributions to $A_{Qg}^{(3)}$: $\eta \ll 1$

- Use $\eta = m_c^2/m_b^2$ as expansion parameter similar do $\epsilon = d - 4$.
- Calculate a large number of moments ($\mathcal{O}(3000)$) of the master integrals with the methods of arbitrary high moments utilizing the differential equation.
- Boundary conditions at fixed N, which can be computed for arbitrary η.
- Use guessing techniques to reconstruct the all-N solution of the amplitude.

Unpolarized case					
Coefficient	# moments	rec. order	rec. degree	N_0	poles
$C_A T_F^2$	2622	26	513	2	
$C_A T_F^2 \eta$	2080	23	400	4	2
$C_A T_F^2 \eta^2$	1548	20	311	4	2
$C_A T_F^2 \eta^3$	1457	17	324	6	2,4

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Problems:

- Closed solutions only for $N > N_0$.
- N_0 increases with higher orders in the expansion in η.
- More poles appear for $N < N_0$ leading to an unphysical behavior of the x-space solution.

Two mass contributions to $A_{Qg}^{(3)}$: $\eta \sim 1$

- Inspiration from semileptonic $b \to c$ decay [Fael, Schönwald, Steinhauser '21] :
  - Expansion in $m_c/m_b \ll 1$ very complicated.
  - Expansion in $\delta = 1 - m_c/m_b$ much simpler and good convergence for physical point.
- Expand master integrals in $\delta = 1 - m_c/m_b$ using the differential equation in m_c.
- The boundaries for the expansion are the masters for $m_c = m_b$:
  We can reuse the solution of the master integrals in the single mass case.

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- The boundaries for the expansion are the masters for $m_c = m_b$:
  We can reuse the solution of the master integrals in the single mass case.

Success! We can find solutions, which can approximate the OMEs over all x!

Two mass contributions to $A_{Qg}^{(3)}$: $\eta \sim 1$

Convergence of the expansion (setting $m_b = 4.78$, $m_c/m_b = 1/3$, $Q^2 = 30\text{GeV}^2$):

$$\begin{aligned}
\tilde{A}_{Qg}^{(3)}(N=10) &= -74.21586397318846267\ldots \\
&\approx 4.69095\ldots - 52.87648\ldots\chi - 13.51460\ldots\chi^2 - 5.77578\ldots\chi^3 - 2.91093\ldots\chi^4 \\
&- 1.58651\ldots\chi^5 - 0.90329\ldots\chi^6 - 0.52844\ldots\chi^7 - 0.31488\ldots\chi^8 - 0.19014\ldots\chi^9 \\
&- 0.11599\ldots\chi^{10} - 0.07134\ldots\chi^{11} - 0.04417\ldots\chi^{12} - 0.02750\ldots\chi^{13} - 0.01720\ldots\chi^{14} \\
&- 0.01081\ldots\chi^{15} - 0.00681\ldots\chi^{16} - 0.00431\ldots\chi^{17} - 0.00273\ldots\chi^{18} - 0.00174\ldots\chi^{19} + \ldots \\
&= -74.21277466475527301\ldots\ ,
\end{aligned}$$

setting $\delta = 2/3\chi$.

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&= -74.21277466475527301 8\ldots\,,
\end{aligned}$$

setting $\delta = 2/3\chi$. Using one step of the sum acceleration we get:

$$\tilde{A}_{Qg}^{(3),\text{approx}}(N=10) \approx -74.21581659848 2\ldots$$

Difference: 0.00006%

Two mass contributions to $A_{Qg}^{(3)}$: Results

$$(\Delta)r(N) = \frac{\tilde{A}_{Qg}^{\text{exact}}(N) - \tilde{A}_{Qg}^{\text{approx}}(N)}{\tilde{A}_{Qg}^{\text{exact}}(N)}$$

N	$\tilde{A}_{Qg}^{\text{exact}}(N)$	$r(N)[\%]$	N	$\Delta\tilde{A}_{Qg}^{\text{exact}}(N)$	$\Delta r(N)[\%]$
2	-4236.5	0.00004	1	0	(0.00004)
6	-3091.6	0.00005	5	-2988.0	0.00008
12	-1970.7	0.00005	11	-2026.4	0.00008

Two mass contributions to $A_{Qg}^{(3)}$: Results

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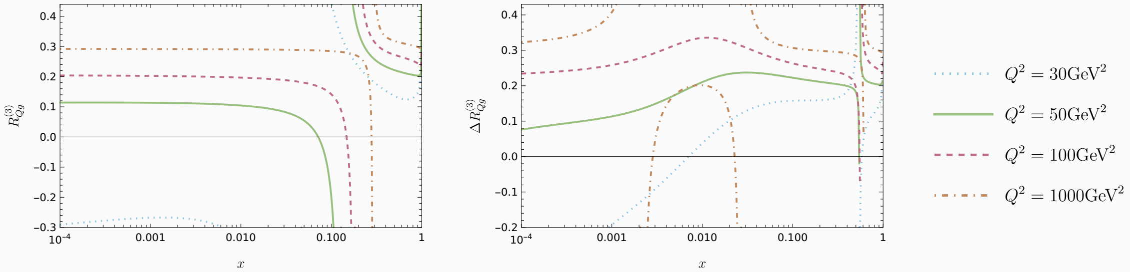

Summary and Outlook

Summary and Outlook

Summary

- Two mass corrections can make up 20%-50% of the respective color factors of the OMEs.
- 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 is 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 analytic solution of the two mass contributions to A_{Qg} is even more involved.
- A fully consistent NNLO precision analysis of the DIS World Data to determine α_s and m_c can now be carried out.

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

Backup

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

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

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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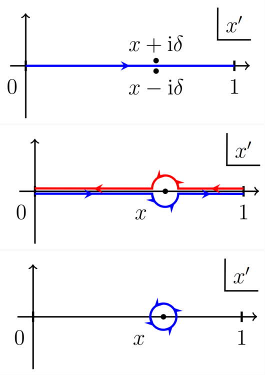
Therefore:

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



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 $x \in (0, 1)$.

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The x-space representation

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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.

Variable Flavor Number Scheme

FFNS

- Fixed order in perturbation theory and fixed number of light partons in the proton.
- The heavy quarks are produced extrinsically only.
- The large logarithmic terms in the heavy quark coefficient functions entirely determine the charm component of the structure function for large values of Q^2.

VFNS

- Define a threshold above which the heavy quark is treated as light, thereby obtaining a parton density.
- Absorb mass singular terms from the asymptotic heavy quark coefficient functions and absorb them into parton densities.
- Resum large logarithms involving the mass.
- Provide heavy flavor initial state parton desities for the LHC, e.g. for $c\bar{s} \to W^+$.

Important:

- The VFNS is derived from the FFNS directly.
- New parton densities for the heavy quarks appear, which are now treated as light.
- Only universal (not power-supressed) terms are absorbed into the parton densities.

Results: $A_{qq,Q}^{(3),\mathrm{NS}}$

$$
\begin{aligned}
\tilde{a}_{qq,Q}^{(3),\mathrm{NS}} = \; & C_F T_F^2 \Bigg\{ \left(\frac{4}{9} S_1 - \frac{3N^2+3N+2}{9N(N+1)} \right) \Bigg[-24 \left({L_1}^3 + {L_2}^3 + (L_1 L_2 + 2\zeta_2 + 5)(L_1 + L_2) \right) \\
& + \frac{\eta+1}{\eta^{3/2}} \left(5\eta^2 + 22\eta + 5 \right) \left(-\frac{1}{4} \ln^2(\eta) \ln\left(\frac{1+\sqrt{\eta}}{1-\sqrt{\eta}} \right) + 2\ln(\eta) \mathrm{Li}_2\left(\sqrt{\eta}\right) - 4\mathrm{Li}_3\left(\sqrt{\eta}\right) \right) \\
& + \frac{\left(\sqrt{\eta}+1\right)^2}{2\eta^{3/2}} \left(-10\eta^{3/2} + 5\eta^2 + 42\eta - 10\sqrt{\eta} + 5 \right) \left[\mathrm{Li}_3(\eta) - \ln(\eta) \mathrm{Li}_2(\eta) \right] + \frac{64}{3} \zeta_3 \\
& + \frac{8}{3} \ln^3(\eta) - 16 \ln^2(\eta) \ln(1-\eta) + 10 \frac{\eta^2-1}{\eta} \ln(\eta) \Bigg] + \frac{16\left(405\eta^2 - 3238\eta + 405\right)}{729\eta} S_1 \\
& + \frac{4}{3} \left(\frac{3N^4+6N^3+47N^2+20N-12}{3N^2(N+1)^2} - \frac{40}{3} S_1 + 8 S_2 \right) \left[\frac{4}{3}\zeta_2 + (L_1 + L_2)^2 \right] \\
& + \frac{8}{9} \left(\frac{130N^4+84N^3-62N^2-16N+24}{3N^3(N+1)^3} - \frac{52}{3} S_1 + \frac{80}{3} S_2 - 16 S_3 \right) (L_1 + L_2) \\
& + \left[-\frac{R_1}{18N^2(N+1)^2\eta} + \frac{2\left(5\eta^2+2\eta+5\right)}{9\eta} S_1 + \frac{32}{9} S_2 \right] \ln^2(\eta) - \frac{4R_2}{729N^4(N+1)^4\eta} \\
& + \frac{3712}{81} S_2 - \frac{1280}{81} S_3 + \frac{256}{27} S_4 \Bigg\}
\end{aligned}
$$

The R_i's are polynomials in N and η. For $\tilde{a}_{gq,Q}^{(3)}$ and $\tilde{a}_{qq,Q}^{(3),\mathrm{NS,\,Tr}}$ one finds similar expressions.

Details: $A_{Qq}^{(3),\mathrm{PS}}$

- The residue sums can be done with Sigma, EvaluateMultiSums and HarmonicSums in terms of generalized iterated integrals and there special values

$$G\left(\{f_1(\tau), f_2(\tau), \cdots, f_n(\tau)\}, z\right) = \int_0^z d\tau_1 \; f_1(\tau_1) G\left(\{f_2(\tau), \cdots, f_n(\tau)\}, \tau_1\right)$$

- Rational prefactors in N can be absorbed via integration by parts identities or convolution integrals, i.e.

$$\frac{1}{N+l}\int_a^b \mathrm{d}x \; x^{N-1} \; f(x) = \frac{b^{N+l}}{N+l}\int_a^b \mathrm{d}y \; \frac{f(y)}{y^{l+1}} - \int_a^b \mathrm{d}x \; x^{N+l-1} \int_a^x \mathrm{d}y \; \frac{f(y)}{y^{l+1}}.$$

- The alphabet of the occurring iterated integrals contains only two new letters:

$$\frac{1}{x}, \qquad \frac{1}{1+x}, \qquad \frac{1}{1-x}, \qquad \sqrt{4-x}\sqrt{x}, \qquad \frac{\sqrt{1-4x}}{x}$$