

# Two mass effects in massive Deep Inelastic Scattering

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PARTICLEFACE: Case studies of analytical and numerical methods  
of multiloop calculations

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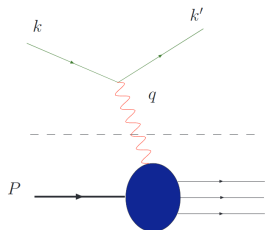
- ▶ Theory of deep inelastic scattering
- ▶ The variable flavor number scheme
- ▶ Two mass contribution to  $A_{gq,Q}^{(3)}$  and  $A_{qq,Q}^{(3),NS}$
- ▶ Two mass contribution to  $A_{Qq}^{PS,(3)}$
- ▶ Two mass contribution to  $A_{gg,Q}^{(3)}$
- ▶ Summary and Outlook

Based on:

- Ablinger, Blümlein, De Freitas, Goedicke Schneider, Wißbrock; Nucl.Phys. B921 (2017) 585-688
- Ablinger, Blümlein, De Freitas, Schneider, Schönwald; Nucl.Phys. B927 (2018) 339-367
- Ablinger, Blümlein, De Freitas, Goedicke Schneider, Schönwald; Nucl.Phys. B932 (2018) 129-240
- Blümlein, De Freitas, Schneider, Schönwald; Phys.Lett. B782 (2018) 362-366



# Theory of deep inelastic scattering



- ▶ Kinematic invariants:

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

- ▶ The cross section factorizes into leptonic and hadronic tensor:

$$\frac{d^2\sigma}{dQ^2 dx} \sim L_{\mu\nu} W^{\mu\nu}$$

- ▶ The hadronic tensor can be expressed through two structure functions:

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

- ▶  $F_L$  and  $F_2$  contain contributions from both, charm and bottom quarks.



# Motivation

- ▶ Precision of DIS world data:  $\sim 1\%$  for  $F_2$   
→ requires  $\mathcal{O}(\alpha_s^3)$  corrections
  - ▶ Heavy quarks yield essential contributions to the structure functions  
 $\sim 20 - 30\%$  at small  $x$
  - ▶ Heavy quark contributions to the scaling violations have different shape than the massless ones
- ⇒ **NNLO** heavy quark contributions are important for a precise determination of
1. the strong coupling constant  $\alpha_s$
  2. the heavy quark masses  $m_c, m_b$
  3. parton distribution functions for the heavy quarks

# Aspects of the Light Cone Expansion

Hadronic tensor:

$$W_{\mu\nu} = (\dots)_{\mu\nu} F_L(x, Q^2, m) + (\dots)_{\mu\nu} F_2(x, Q^2, m)$$

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Hadronic tensor:

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Structure function:

$$F_2(x, Q^2, m) = x \sum_j C_{2,j}(x, Q^2, m) \otimes f_j(x, Q^2)$$

$C_{2,j}$  perturbative Wilson coefficients

$f_j$  non-perturbative parton distribution functions

convolution  $\otimes$ :

$$\{f \otimes g\}(x) = \int_0^1 dz_1 \int_0^1 dz_2 \delta(x - z_1 z_2) f(z_1) g(z_2)$$

# Aspects of the Light Cone Expansion

Hadronic tensor:

$$W_{\mu\nu} = (\dots)_{\mu\nu} F_L(x, Q^2, m) + (\dots)_{\mu\nu} F_2(x, Q^2, m)$$

Structure function:

$$F_2(N-1, Q^2, m) = \sum_j C_{2,j}(N, Q^2, m) \cdot f_j(N, Q^2)$$

We mainly work in Mellin space via the transformation:

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

Here many relations **simplify**:

$$M[\{f \otimes g\}(x)](N) = M[f(x)](N) \cdot M[g(x)](N)$$



# Aspects of the Light Cone Expansion

Structure function:

$$F_2(N-1, Q^2, m) = \sum_j C_{2,j}(N, Q^2, m) \cdot f_j(N, Q^2)$$

Wilson coefficient:

$$C_j(N, Q^2, m) = C_{2,j}(N, Q^2) + H_{2,j}(N, Q^2, m^2)$$

We split the Wilson coefficient into

$C_{2,j}$  the massless Wilson coefficient NNLO [Moch, Vermaseren, Vogt '05]

$H_{2,j}$  the heavy flavor Wilson coefficient



# Aspects of the Light Cone Expansion

Wilson coefficient:

$$C_j(N, Q^2, m) = C_{2,j}(N, Q^2) + H_{2,j}(N, Q^2, m^2)$$

- ▶ At  $Q^2 \gg m^2$  the heavy flavor part can be calculated via **massive operator matrix elements** (OMEs) of local Operators  $O_i$  between partonic states  $j$

$$H_{2,j}(N) = \sum_i A_{ij}(N) C_{2,i}(N),$$

with

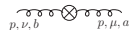
$$A_{ij} \left( \frac{m_c^2}{\mu^2}, \frac{m_b^2}{\mu^2}, N \right) = \langle j | O_i | j \rangle .$$

[Buza, Matiounine, Smith, van Neerven, Nucl.Phys. B472 (1996) 611-658]

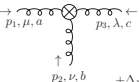
- Additional Feynman rules with local operator insertions for the partonic matrix elements



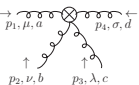
# Feynman rules for the local operator



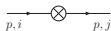
$$\frac{1+(-1)^N}{2} \delta^{ab} (\Delta \cdot p)^{N-2} \left[ g_{\mu\nu} (\Delta \cdot p)^2 - (\Delta_\mu p_\nu + \Delta_\nu p_\mu) \Delta \cdot p + p^2 \Delta_\mu \Delta_\nu \right], \quad N \geq 2$$



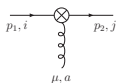
$$-ig \frac{1+(-1)^N}{2} f^{abc} \left( \left[ (\Delta_\nu g_{\lambda\mu} - \Delta_\lambda g_{\mu\nu}) \Delta \cdot p_1 + \Delta_\mu (p_{1,\nu} \Delta_\lambda - p_{1,\lambda} \Delta_\nu) \right] (\Delta \cdot p_1)^{N-2} + \Delta_\lambda \left[ \Delta \cdot p_1 p_{2,\mu} \Delta_\nu + \Delta \cdot p_2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



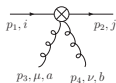
$$g^2 \frac{1+(-1)^N}{2} \left( f^{abc} f^{cde} O_{\mu\nu\lambda\sigma}(p_1, p_2, p_3, p_4) + f^{ace} f^{bde} O_{\mu\lambda\nu\sigma}(p_1, p_3, p_2, p_4) + f^{ade} f^{bce} O_{\mu\sigma\nu\lambda}(p_1, p_4, p_2, p_3) \right), \quad O_{\mu\nu\lambda\sigma}(p_1, p_2, p_3, p_4) = \Delta_\nu \Delta_\lambda \left\{ -g_{\mu\sigma} (\Delta \cdot p_3 + \Delta \cdot p_4)^{N-2} + [p_{4,\mu} \Delta_\sigma - \Delta \cdot p_4 g_{\mu\sigma}] \sum_{i=0}^{N-3} (\Delta \cdot p_3 + \Delta \cdot p_4)^i (\Delta \cdot p_4)^{N-3-i} - [p_{1,\sigma} \Delta_\mu - \Delta \cdot p_1 g_{\mu\sigma}] \sum_{i=0}^{N-3} (-\Delta \cdot p_1)^i (\Delta \cdot p_3 + \Delta \cdot p_4)^{N-3-i} + [\Delta \cdot p_1 \Delta \cdot p_4 g_{\mu\sigma} + p_1 \cdot p_4 \Delta_\mu \Delta_\sigma - \Delta \cdot p_4 p_{1,\sigma} \Delta_\mu - \Delta \cdot p_1 p_{4,\mu} \Delta_\sigma] \times \sum_{i=0}^{N-4} \sum_{j=0}^i (-\Delta \cdot p_1)^{N-4-i} (\Delta \cdot p_3 + \Delta \cdot p_4)^{i-j} (\Delta \cdot p_4)^j \right\} - \left\{ \begin{array}{l} p_1 \leftrightarrow p_2 \\ p_3 \leftrightarrow p_4 \\ \lambda \leftrightarrow \sigma \end{array} \right\} + \left\{ \begin{array}{l} p_1 \leftrightarrow p_2, p_3 \leftrightarrow p_4 \\ \mu \leftrightarrow \nu, \lambda \leftrightarrow \sigma \end{array} \right\}, \quad N \geq 2$$



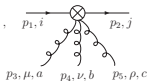
$$\delta^{ij} \Delta^\pm \gamma_\pm (\Delta \cdot p)^{N-1}, \quad N \geq 1$$



$$gt_{ji}^a \Delta^\mu \Delta^\nu \gamma_\pm \sum_{j=0}^{N-2} (\Delta \cdot p_1)^j (\Delta \cdot p_2)^{N-j-2}, \quad N \geq 2$$



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



$$g^3 \Delta_\mu \Delta_\nu \Delta_\rho \Delta_\sigma \gamma_\pm \sum_{j=0}^{N-4} \sum_{i=j+1}^{N-3} \sum_{m=i+1}^{N-2} (\Delta \cdot p_2)^j (\Delta \cdot p_1)^{N-m-2} \left[ (t^a t^b t^c)_{jii} (\Delta \cdot p_4 + \Delta \cdot p_5 + \Delta \cdot p_1)^{i-j-1} (\Delta \cdot p_5 + \Delta \cdot p_1)^{m-i-1} + (t^a t^c t^b)_{jii} (\Delta \cdot p_4 + \Delta \cdot p_5 + \Delta \cdot p_1)^{j-i-1} (\Delta \cdot p_4 + \Delta \cdot p_1)^{m-i-1} + (t^b t^a t^c)_{jii} (\Delta \cdot p_3 + \Delta \cdot p_5 + \Delta \cdot p_1)^{i-j-1} (\Delta \cdot p_5 + \Delta \cdot p_1)^{m-i-1} + (t^b t^c t^a)_{jii} (\Delta \cdot p_3 + \Delta \cdot p_5 + \Delta \cdot p_1)^{j-i-1} (\Delta \cdot p_3 + \Delta \cdot p_1)^{m-i-1} + (t^c t^a t^b)_{jii} (\Delta \cdot p_3 + \Delta \cdot p_4 + \Delta \cdot p_1)^{i-j-1} (\Delta \cdot p_4 + \Delta \cdot p_1)^{m-i-1} + (t^c t^b t^a)_{jii} (\Delta \cdot p_3 + \Delta \cdot p_4 + \Delta \cdot p_1)^{j-i-1} (\Delta \cdot p_3 + \Delta \cdot p_1)^{m-i-1} \right], \quad N \geq 4$$

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

# Operator Matrix Elements

- ▶ The OMEs can be split into parts which contain only contributions from **one heavy quark** and genuine **two mass contributions**

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

- ▶ Since the mass of the bottom quark  $m_b$  is not much larger than the charm mass  $m_c$

$$\eta = \frac{m_c^2}{m_b^2} \sim 0.1,$$

we have to take into account the contributions from both quarks simultaneously.

- ▶ Graphs with two massive quarks start contributing at  $\mathcal{O}(\alpha_s^3)$ , nevertheless two mass contributions can emerge from
  - ▶ reducible contributions
  - ▶ renormalization [Ablinger et al; Nucl.Phys. B921 (2017) 585-688]
  - ▶ scheme changes

⇒ this way two mass contributions even arise at  $\mathcal{O}(\alpha_s^2)$



# The variable flavor number scheme

- ▶ Matching conditions for parton distribution functions:

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

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

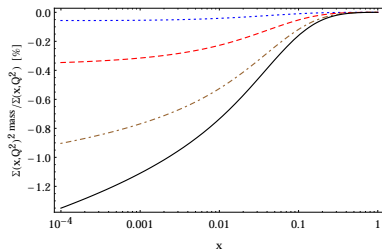
$$\Sigma(N_F + 2) = \left[ A_{qq,Q}^{NS} \left( N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) + A_{qq,Q}^{PS} \left( N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right. \\ \left. + A_{Qq}^{PS} \left( N_F + 2, \frac{m_1^2}{\mu^2}, \frac{m_2^2}{\mu^2} \right) \right] \cdot \Sigma(N_F)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

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

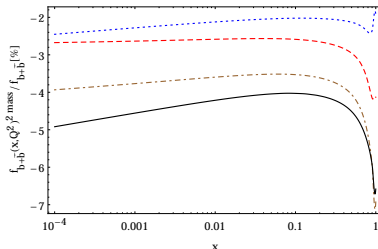


# The variable flavor number scheme at NLO

$$\Sigma(x, Q^2)^{2\text{-mass}} / \Sigma(x, Q^2)$$



$$f_{b+\bar{b}}(x, Q^2)^{2\text{-mass}} / f_{b+\bar{b}}(x, Q^2)$$



- ▶ The ratio of the 2-mass contributions to the singlet parton distribution  $\Sigma(x, Q^2)$  (left) and the heavy flavor parton distribution  $f_{b+\bar{b}}(x, Q^2)$  (right) over their full form in percent for  $m_c = 1.59$  GeV,  $m_b = 4.78$  GeV in the on-shell scheme. Dash-dotted line:  $Q^2 = 30$  GeV<sup>2</sup>; Dotted line:  $Q^2 = 30$  GeV<sup>2</sup>; Dashed red line:  $Q^2 = 100$  GeV<sup>2</sup>; Dash-dotted orange line:  $Q^2 = 1000$  GeV<sup>2</sup>; Full line:  $Q^2 = 10000$  GeV<sup>2</sup>.
- ▶ For the PDFs the NNLO variant of ABMP16 with  $N_f = 3$  flavors was used.  
Alekhin et al., Phys. Rev. D 96 (2017) 1



## Overview: Calculation

- ▶ No reduction to master integrals.
- ▶ Full Feynman parametrization of the diagrams.
- ▶ Integration of loop momenta can be achieved with standard formula.

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- To map to scalar integrals we can use the formulas

$$\int \frac{d^d k}{(2\pi)^d} k_{\mu_1} \dots k_{\mu_{2n}} f(k^2) = S_{\mu_1 \dots \mu_{2n}} \frac{2^{-n} \Gamma(d/2)}{\Gamma(d/2 + n)} \int \frac{d^d k}{(2\pi)^d} (k^2)^n f(k^2),$$

$$\int \frac{d^d k}{(2\pi)^d} (k \cdot p)^n (k \cdot \Delta + R_0 p \cdot \Delta)^N f(k^2) = (\Delta \cdot p)^N R_0^{N-n} \frac{2^{-n} \Gamma(d/2)}{\Gamma(d/2 + n)} \frac{\Gamma(N + 1)}{\Gamma(N - n + 1)} \int \frac{d^d k}{(2\pi)^d} (k^2)^n f(k^2),$$

where  $S_{\mu_1 \dots \mu_{2n}}$  is the symmetric tensor composed out of the metric and  $n \leq N$ .

- In the end only the one loop integral

$$\int \frac{d^d k}{(2\pi)^d} \frac{(k^2)^m}{(k^2 + R^2)^n} = \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(n - m - d/2)}{\Gamma(n)} \frac{\Gamma(m + d/2)}{\Gamma(d/2)} (R^2)^{m-n+d/2}$$

has to be done.

# Overview: Calculation

- ▶ No reduction to master integrals.
- ▶ Full Feynman parametrization of the diagrams.
- ▶ Integration of loop momenta can be achieved with standard formula.

We find representations like:

$$I = \Gamma\left(-\frac{3\varepsilon}{2}\right) \int_0^1 \left( \prod_{i=1}^7 dz_i \right) z_1^2 [z_2(1-z_2)]^{\frac{\varepsilon}{2}} z_3^2 [z_4(1-z_4)]^{\frac{\varepsilon}{2}} (1-z_5) [z_6(1-z_6)]^{\frac{\varepsilon}{2}} z_7^{1+\frac{\varepsilon}{2}} \\ \times (1-z_7)^2 [z_7(z_1 z_6 + z_3(1-z_6)) + z_5(1-z_7)]^{N-4} \left( \frac{z_6 m_a^2}{z_2(1-z_2)} + \frac{(1-z_6) m_b^2}{z_4(1-z_4)} \right)^{\frac{3\varepsilon}{2}}$$



# Overview: Calculation

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- ▶ The **masses** can be separated via a Mellin-Barnes integral:

$$\frac{1}{(r_1 m_a^2 + r_2 m_b^2)^s} = \frac{1}{2\pi i} \frac{1}{\Gamma(s)} (m_b^2)^{-s} \int_{-i\infty}^{+i\infty} d\sigma \left( \frac{m_a^2}{m_b^2} \right)^\sigma r_1^\sigma r_2^{-s-\sigma} \Gamma(-\sigma) \Gamma(\sigma + s)$$

- ▶ The **operator polynomial** can be split binomially:

$$(A + B)^N = \sum_{j=0}^N \binom{N}{j} A^j B^{N-j}$$



# Overview: Calculation

$$I = \frac{(m_b^2)^{\frac{3\varepsilon}{2}}}{2\pi i} \sum_{j=0}^{N-4} \sum_{i=0}^j \binom{N-4}{j} \binom{j}{i} \frac{\Gamma(3+i)\Gamma(3-i+j)\Gamma(N-j-3)}{\Gamma(4+i)\Gamma(4-i+j)\Gamma(N+1+\frac{\varepsilon}{2})}$$
$$\times \int_{-i\infty}^{+i\infty} d\sigma \left(\frac{m_a^2}{m_b^2}\right)^\sigma \left\{ \Gamma(-\sigma)\Gamma(-\frac{3\varepsilon}{2} + \sigma)\Gamma(1 - \frac{\varepsilon}{2} + i + \sigma)\Gamma(1 + \varepsilon - i + j - \sigma) \right.$$
$$\times \left. \frac{\Gamma(1 + \frac{\varepsilon}{2} - \sigma)\Gamma(3 + \frac{\varepsilon}{2} - \sigma)\Gamma(1 - \varepsilon - \sigma)\Gamma(3 - \varepsilon + \sigma)}{\Gamma(4 + \varepsilon - 2\sigma)\Gamma(4 - 2\varepsilon + 2\sigma)} \right\}$$

- ▶ The complex contour integral can be done by closing the integration contour and summing up residues.
- ⇒ The integration problem has been transformed into a (multi-)summation, which can be handled with the packages

[Sigma](#), [EvaluateMultiSums](#) [Schneider '07,'14], [SumProduction](#) [Ablinger, Blümlein, Hasselhuhn, Schneider '10, '14] and [HarmonicSums](#) [Ablinger, Blümlein, Schneider '10,'13].



# Overview: Mathematical Structures

$$A_{qq,Q}^{(3),NS}, A_{gq,Q}^{(3)}$$

## Harmonic Sums

[Vermaseren '98; Blümlein, Kurth '98]

$$\sum_{i=1}^N \frac{1}{i^3} \sum_{j=1}^i \frac{1}{j}$$

## HPLs

[Remiddi, Vermaseren '99]

$$\int_0^x \frac{d\tau_1}{1+\tau_1} \int_0^{\tau_1} \frac{d\tau_2}{1-\tau_2}$$

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

## Generalized harmonic and binomial sums

[Ablinger, Blümlein, Schneider '13]

[Ablinger, Blümlein, Raab, Schneider '14]

$$\sum_{i=1}^N \frac{4^i (1-\eta)^{-i}}{i \binom{2i}{i}} \sum_{j=1}^i \frac{(1-\eta)^j}{j^2}$$

## Iterated integrals over root and $\eta$ valued letters

[Ablinger, Blümlein, Raab, Schneider '14]

$$\int_0^x d\tau_1 \frac{\sqrt{\tau_1(1-\tau_1)}}{1-\tau_1(1-\eta)} \int_0^{\tau_1} \frac{d\tau_2}{\tau_2}$$

$$A_{Qq}^{(3),PS}$$

–

## Iterated integrals over root valued letters with restricted support

$$\theta(x - \eta_+) \int_0^{x(1-x)/\eta} d\tau \frac{\sqrt{1-4\tau}}{\tau}$$



# Two mass contributions to $A_{qq,Q}^{(3),NS}$ and $A_{gq,Q}^{(3)}$



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

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

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

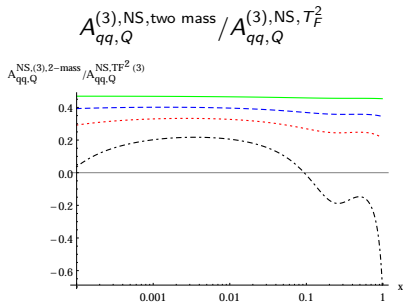
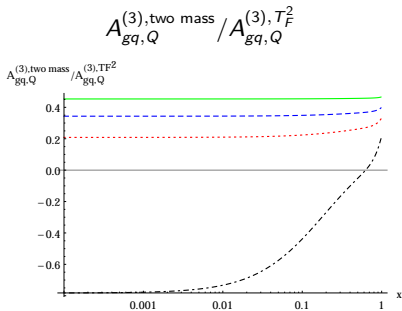
# Results: $A_{qq,Q}^{(3),NS}$

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

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



# Results: $A_{qq,Q}^{(3),NS}$ and $A_{gq,Q}^{(3)}$



- ▶ The ratio of the genuine 2-mass contributions to  $A_{qq,Q}^{(3),NS}$  and  $A_{gq,Q}^{(3)}$  to the respective complete  $T_F^2$ -part of massive 3-loop OMEs as a function of  $x$  and  $Q^2$ , for  $m_c = 1.59$  GeV,  $m_b = 4.78$  GeV in the on-shell scheme. Dash-dotted line:  $\mu^2 = 30$  GeV<sup>2</sup>; Dotted line:  $\mu^2 = 50$  GeV<sup>2</sup>; Dashed line:  $\mu^2 = 100$  GeV<sup>2</sup>; Full line:  $\mu^2 = 1000$  GeV<sup>2</sup>.

# Two mass contribution to $A_{Qq}^{PS,(3)}$



- ▶ In general the same steps as before are applicable.
- ▶ Problem: the recurrences for the  $N$ -space solution are not first order factorizable (i.e. 2nd order  $\leftrightarrow$  elliptic or even higher order)  
 $\Rightarrow$  The summation algorithms of [Sigma](#) cannot find the closed form solution
- ▶ Solution: aim directly for the  $x$ -space solution, which is first order factorizable

- ▶ Leaving one Feynman parameter unintegrated one obtains representations like:

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

- ▶ We now have two different cases for closing the contour:

- Case 1:  $\xi = \frac{1}{\eta x(1-x)}$

We can close the contour to the left, since  $\xi \geq 4/\eta$ .

- 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  $\eta_{\pm} = \frac{1}{2} (1 \pm \sqrt{1-\eta})$

- ▶ This shows that in momentum fraction space functions with different support contribute.



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

$$G(\{f_1(\tau), f_2(\tau), \dots, f_n(\tau)\}, z) = \int_0^z d\tau_1 f_1(\tau_1) G(\{f_2(\tau), \dots, f_n(\tau)\}, \tau_1)$$

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

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

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

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

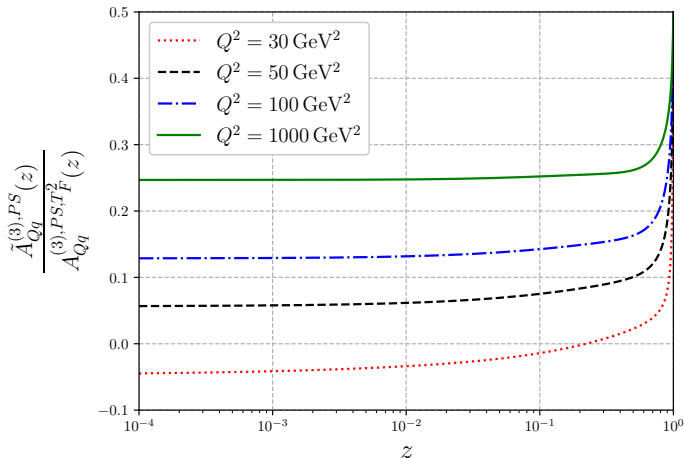
- For numerical evaluations we calculated all occurring iterated integrals as HPLs at involved and complex arguments, i.e.:

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

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



- The contribution to the whole  $T_F^2$ -term is given by:





- ▶ In general the structures in  $N$  and  $\eta$  do not factorize:

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

- ▶ The gluonic Feynman rules introduce large numerator structures
- single diagrams can lead to big expressions after taking all residues, the most involved diagram  $11b$  amounts to  $\sim 100\text{MB}$  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: $A_{gg,Q}^{(3)}$

$$\begin{aligned}
 \tilde{a}_{gg,Q}^{(3)}(N) &= \frac{1}{2} \left(1 + (-1)^N\right) \left\{ T_F^3 \left\{ \frac{32}{3} (L_1^3 + L_2^3) + \frac{64}{3} L_1 L_2 (L_1 + L_2) + 32 \zeta_2 (L_1 + L_2) + \frac{128}{9} \zeta_3 \right\} \right. \\
 &+ C_F T_F^2 \left\{ \dots + 32 \left( H_0^2(\eta) - \frac{1}{3} S_2 \right) S_1 + \frac{128}{3} S_{2,1} - \frac{64}{3} S_{1,1,1} \left( \frac{1}{1-\eta}, 1-\eta, 1, N \right) \right. \\
 &\quad - \frac{4P_{41}}{3(N-1)N^3(N+1)^2(N+2)(2N-3)(2N-1)} \left( \frac{\eta}{1-\eta} \right)^N \left[ H_0^2(\eta) \right. \\
 &\quad \left. \left. - 2H_0(\eta) S_1 \left( \frac{\eta-1}{\eta}, N \right) - 2S_2 \left( \frac{\eta-1}{\eta}, N \right) + 2S_{1,1} \left( \frac{\eta-1}{\eta}, 1, N \right) \right] + \dots \right\} \\
 &+ C_A T_F^2 \left\{ \dots + \left[ \frac{8P_{65}}{3645\eta(N-1)N^3(N+1)^3(N+2)(2N-3)(2N-1)} \right. \right. \\
 &\quad + \frac{8P_{37}H_0(\eta)}{45\eta(N-1)N^2(N+1)^2(N+2)} + \frac{2P_{23}H_0^2(\eta)}{9\eta(N-1)N(N+1)^2} + \frac{32}{27} H_0^3(\eta) + \frac{128}{9} H_{0,0,1}(\eta) \\
 &\quad \left. \left. + \frac{64}{9} H_0^2(\eta)H_1(\eta) - \frac{128}{9} H_0(\eta)H_{0,1}(\eta) \right] S_1 \right. \\
 &\quad + \frac{2^{-1-2N}P_{47}}{45\eta^2(N-1)N(N+1)^2(N+2)(2N-3)(2N-1)} \binom{2N}{N} \sum_{i=1}^N \frac{4^i \left( \frac{\eta}{\eta-1} \right)^i}{i \binom{2i}{i}} \left\{ \frac{1}{2} H_0^2(\eta) \right. \\
 &\quad \left. \left. S_{1,1} \left( \frac{\eta-1}{\eta}, 1, i \right) \right\} + \dots \right\}
 \end{aligned}$$



## 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 and subsequently solve it in terms of iterated integrals.
- ▶ We find i.e.

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

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

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

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

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



- ▶ 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 and subsequently solve it in terms of iterated integrals.
- ▶ For  $\tilde{A}_{gg,Q}^{(3)}$  we find the alphabet:

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

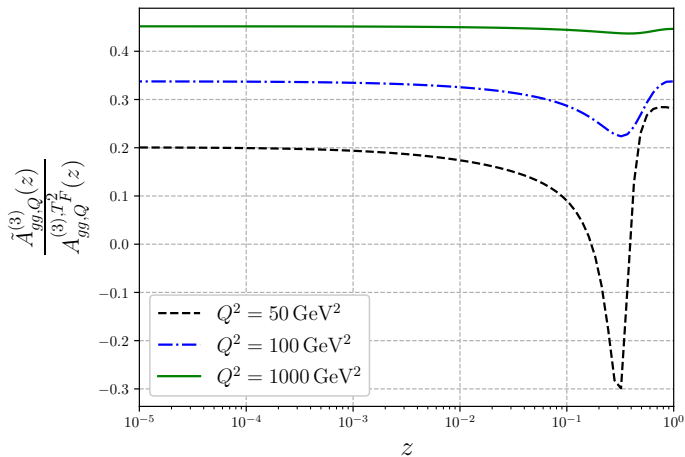
$$\frac{1}{\eta+x(1-\eta)}, \quad \frac{\sqrt{x(1-x)}}{1-x(1-\eta)}, \quad \frac{\sqrt{x(1-x)}}{x+\eta(1-x)}, \quad \frac{\sqrt{x(1-x)}}{\eta+x(1-\eta)}$$

- ▶ 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.



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

The two mass contributions over the whole  $T_F^2$ - contributions to the OME  $A_{gg,Q}^{(3)}$  for different values of  $Q^2$  look like:



# Summary and Outlook

- ▶ The 3-loop massive operator matrix elements  $A_{qq,Q}^{(3),NS}$ ,  $A_{qq,Q}^{(3),TR}$ ,  $A_{gq,Q}^{(3)}$ ,  $A_{Qq}^{(3),PS}$  and  $A_{gg,Q}^{(3)}$  with two heavy quarks have been calculated analytically.
- ▶ For  $A_{Qq}^{(3),PS}$  and  $A_{gg,Q}^{(3)}$  iterative integral representations over **square-root valued alphabets**, containing the mass ratio, are obtained.
- ▶ The contribution of these terms are of **comparable size** to the complete  $T_F^2 C_{F,A}$  contributions.
- ▶ Phenomenological implications have been studied to NLO. Here the **bottom quark** contributions receive the largest corrections of **up to 5%**.
- ▶ The calculation of  $A_{Qg}^{(3)}$  still needs to be completed in the single mass case (here elliptic and possibly more involved structures contribute). The two-mass calculation, expanding in the mass ratio, is under way.

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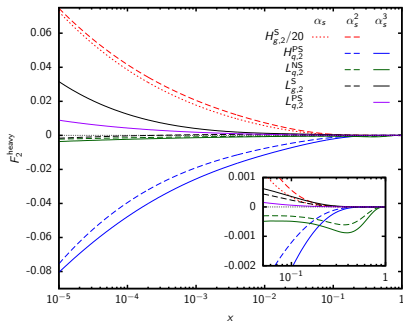
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# General Status of the Calculation

- ▶ A large number of Mellin moments (1000) is available for all OMEs in the **single mass** case, as well as all logarithmic contributions.
- ▶ All **single mass** contributions, but for  $A_{Qg}^{(3)}$ , have been completed; all 1st order factorizing terms to  $A_{Qg}^{(3)}$  are known.



- ▶ A series of moments is available for all OMEs in the **two-mass** case.
- ▶ The calculation of the **two-mass** OMEs for general  $N$  and  $x$  will be reported in the following.



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

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

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.

These are two of the functions:

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

$$\begin{aligned}
 h_3(\eta, y) = & (1-y)\left\{\frac{512}{9}(1-4\eta y(1-y))^{3/2}G\left(\left\{\frac{1}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}\right\}, \eta y(1-y)\right)\right. \\
 & + \frac{1024}{3}G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}\right\}, \eta y(1-y)\right) + \frac{512}{3}G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}, \frac{\sqrt{1-4\tau}}{\tau}, \frac{1}{\tau}\right\}, \eta y(1-y)\right) \\
 & + \left(\frac{512}{3}\zeta_2 - \frac{1024}{9}(4\eta y^2 - 4\eta y - 1)^2\right) \ln(\eta y(1-y)) + \frac{4096}{9}\eta y(1-y) + \frac{256}{9}\ln^3(\eta y(1-y)) \\
 & + \frac{1280}{9}\ln^2(\eta y(1-y)) + \frac{512}{9}\zeta_2(1-4\eta y(1-y))^{3/2} - \frac{512}{9}\zeta_2 \\
 & \left. + \left(\frac{512}{3}\zeta_2 - \frac{2}{9}(1-4\eta y(1-y))^{3/2}[2 + \ln(\eta y(1-y))]\right)G\left(\left\{\frac{\sqrt{1-4\tau}}{\tau}\right\}, \eta y(1-y)\right)\right\}
 \end{aligned}$$