# Higher order corrections to heavy flavor production in deep inelastic scattering

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Isabella Bierenbaum Higher order corrections to HF production in DIS

- Introduction
- 2 The Method
- The Calculation
- Results
- Somparison to former results
- Conclusion

## 1. Introduction

Deep-Inelastic Scattering (DIS):



Heavy-flavor production: LO-process: photon-gluon fusion



Hadronic Tensor for heavy quark production via single photon exchange:

$$\begin{split} W^{Q\bar{Q}}_{\mu\nu}(q,P,s) &= \frac{1}{4\pi} \int d^{4}\xi \exp(iq\xi) \langle P,s \mid [J^{em}_{\mu}(\xi), J^{em}_{\nu}(0)] \mid P,s \rangle_{Q\bar{Q}} \\ &= \frac{1}{2x} \left( g_{\mu\nu} - \frac{q_{\mu}q_{\nu}}{q^{2}} \right) F^{Q\bar{Q}}_{L}(x,Q^{2}) \\ &+ \frac{2x}{Q^{2}} \left( P_{\mu}P_{\nu} + \frac{q_{\mu}P_{\nu} + q_{\nu}P_{\mu}}{2x} - \frac{Q^{2}}{4x^{2}}g_{\mu\nu} \right) F^{Q\bar{Q}}_{2}(x,Q^{2}) \\ &- \frac{M}{2Pq} \varepsilon_{\mu\nu\alpha\beta}q^{\alpha} \left[ s^{\beta}g^{Q\bar{Q}}_{1}(x,Q^{2}) + \left( s^{\beta} - \frac{sq}{Pq}p^{\beta} \right) g^{Q\bar{Q}}_{2}(x,Q^{2}) \right] \end{split}$$

Collinear parton model  $\implies$  parton longitudinal momentum fraction: p = zP.

## Need for the Calculation

- Heavy flavor (charm) contributions to DIS structure functions are rather large [20-40 % at lower values of x].
- Need: Increase accuracy of the perturbative description of DIS structure functions.
- $\iff$  QCD analysis and determination of  $\Lambda_{\text{QCD}}$  from DIS data.
- $\iff$  Precise determination of the gluon and sea quark Distributions.



Calculation of the heavy flavor Wilson coefficients to higher orders for  $Q^2 \geq 25 \, \text{GeV}^2$  [sufficient in many applications] .

## 1. Introduction





Unpolarized DIS :

- LO : [Witten, 1976; Babcock & Sivers, 1978; Shifman, Vainshtein, Zakharov 1978; Leveille & Weiler, 1979]
- NLO : [Laenen, Riemersma, Smith, van Neerven, 1993, 1995] asymptotic : [Buza, Matiounine, Smith, Migneron, van Neerven, 1996]

Polarized DIS :

- LO : [Watson, 1982; Glück, Reya, Vogelsang, 1991; Vogelsang, 1991]
- NLO : asymptotic: [Buza, Matiounine, Smith, van Neerven, 1997]

Mellin-Space Expressions: [Alekhin, Blümlein, 2003].

massless RGE and Light–Cone Expansion in Bjørken–Limit  $\{Q^2, \nu\} \rightarrow \infty, x$  fixed:

$$\lim_{\xi^2 \to 0} \left[ J(\xi), J(0) \right] \propto \sum_{i,N,\tau} c_{i,\tau}^N(\xi^2, \mu^2) \xi_{\mu_1} ... \xi_{\mu_N} O_{i,\tau}^{\mu_1 ... \mu_m}(0, \mu^2)$$

Operators: flavour non-singlet, singlet & pure singlet; consider leading twist-2 operators

factorization between Wilson coefficients and parton densities;

$$F_{i}(x,Q^{2}) = \sum_{j} \underbrace{C_{i}^{j}\left(x,\frac{Q^{2}}{\mu^{2}}\right)}_{\text{perturbative}} \otimes \underbrace{f_{j}(x,\mu^{2})}_{\text{non-perturbative}}$$
  
with  $[f \otimes g](z) = \int_{0}^{1} dz_{1} \int_{0}^{1} dz_{2} \quad \delta(z-z_{1}z_{2}) \ f(z_{1})g(z_{2}) \ .$ 

(massless) RGE: Altarelli–Parisi (DGLAP) evolution equation for pdfs ( $\mu^2 = Q^2$ ):

$$\frac{d}{d \log Q^2} f_g(x, Q) = \frac{\alpha_s(Q^2)}{\pi} \int_x^1 \frac{dz}{z} \left\{ P_{g \leftarrow q}(z) \sum_f \left[ f_f(\frac{x}{z}, Q) + f_{\overline{f}}(\frac{x}{z}, Q) \right] + P_{g \leftarrow g}(z) f_g(\frac{x}{z}, Q) \right\}$$

 $P_{i\leftarrow j}$  are the splitting functions.

Heavy quark contribution: heavy quark Wilson coefficient,  $H_{(2,L),i}^{S,NS}\left(\frac{Q^2}{m^2},\frac{m^2}{m^2}\right)$ 

In limit  $Q^2 \gg m_0^2$ : massive RGE, derivative  $m^2 \partial / \partial m$ : all terms but power corrections, calculable through partonic operator matrix elements,  $\langle i|A_{l}|j\rangle$ , which are process independent objects!



holds for polarized and unpolarized case.

OMEs obey expansion

$$A_{k,i}^{\mathrm{S,NS}}\left(\frac{m^2}{\mu^2}\right) = \langle i|O_k^{\mathrm{S,NS}}|i\rangle = \delta_{k,i} + \sum_{l=1}^{\infty} a_s^l A_{k,i}^{\mathrm{S,NS},(l)}\left(\frac{m^2}{\mu^2}\right), \quad i = q, g$$

[Buza, Matiounine, Migneron, Smith, van Neerven, 1996; Buza, Matiounine, Smith, van Neerven, 1997.]

Expansion up to  $O(\alpha_s^2)$  of unpolarized Heavy Flavor Wilson Coefficient  $H_2$ :

$$\begin{split} H^{\rm S}_{2,g} \left( \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) &= a_s \left[ A^{(1)}_{Qg} \left( \frac{m^2}{\mu^2} \right) + \widehat{C}^{(1)}_{2,g} \left( \frac{Q^2}{\mu^2} \right) \right] \\ &+ a_s^2 \left[ A^{(2)}_{Qg} \left( \frac{m^2}{\mu^2} \right) + A^{(1)}_{Qg} \left( \frac{m^2}{\mu^2} \right) \otimes C^{(1)}_{2,q} \left( \frac{Q^2}{\mu^2} \right) + \widehat{C}^{(2)}_{2,g} \left( \frac{Q^2}{\mu^2} \right) \right] , \\ H^{\rm PS}_{2,q} \left( \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) &= a_s^2 \left[ A^{\rm PS}_{Qq} (2 \left( \frac{m^2}{\mu^2} \right) + \widehat{C}^{\rm PS}_{2,q} \left( \frac{Q^2}{\mu^2} \right) \right] , \\ H^{\rm NS}_{2,q} \left( \frac{Q^2}{m^2}, \frac{m^2}{\mu^2} \right) &= a_s^2 \left[ A^{\rm NS}_{Qq} (2 \left( \frac{m^2}{\mu^2} \right) + \widehat{C}^{\rm NS}_{2,q} \left( \frac{Q^2}{\mu^2} \right) \right] , \end{split}$$

Polarized and longitudinal Heavy Wilson coefficients obey similar expansion.

For H<sub>L</sub>, O(a<sup>2</sup><sub>s</sub>) contributions have been derived recently.
 [J. Blümlein, A. De Freitas, W. van Neerven, S. Klein, 2006].

The universal massive operator matrix elements have the same structure in the polarized and unpolarized case  $[F_2 \text{ vs. } g_1]$ . Up to  $O(a_s^2)$  they are given by:

$$\begin{split} A_{Qg}^{(1)} &= -\frac{1}{2} \widehat{P}_{qg}^{(0)} \ln\left(\frac{m^2}{\mu^2}\right) \\ A_{Qg}^{(2)} &= \frac{1}{8} \left\{ \widehat{P}_{qg}^{(0)} \otimes \left[ P_{qq}^{(0)} - P_{gg}^{(0)} + 2\beta_0 \right] \right\} \ln^2\left(\frac{m^2}{\mu^2}\right) - \frac{1}{2} \widehat{P}_{qg}^{(1)} \ln\left(\frac{m^2}{\mu^2}\right) \\ &+ \overline{a}_{Qg}^{(1)} \otimes \left[ P_{qq}^{(0)} - P_{gg}^{(0)} + 2\beta_0 \right] + a_{Qg}^{(2)} \\ A_{Qq}^{\mathrm{PS},(2)} &= -\frac{1}{8} \widehat{P}_{qg}^{(0)} \otimes P_{gq}^{(0)} \ln^2\left(\frac{m^2}{\mu^2}\right) - \frac{1}{2} \widehat{P}_{qq}^{\mathrm{PS},(1)} \ln\left(\frac{m^2}{\mu^2}\right) + a_{Qq}^{\mathrm{PS},(2)} + \overline{a}_{Qg}^{(1)} \otimes P_{gq}^{(0)} \\ A_{qq,Q}^{\mathrm{NS},(2)} &= -\frac{\beta_{0,Q}}{4} P_{qq}^{(0)} \ln^2\left(\frac{m^2}{\mu^2}\right) - \frac{1}{2} \widehat{P}_{qq}^{\mathrm{NS},(1)} \ln\left(\frac{m^2}{\mu^2}\right) + a_{qq,Q}^{\mathrm{NS},(2)} + \frac{1}{4} \beta_{0,Q} \zeta_2 P_{qq}^{(0)} \end{split}$$

- $\overline{a}_{Qg}^{(1)}$ :  $O(\varepsilon)$  of the OME  $A_{Qg}^{(1)}$  in the  $\overline{\text{MS}}$ -scheme. Enters  $A_{Qg}^{(2)}$  through renormalization.
- Renormalization of  $A_{Qg}^{(3)}$ :  $\overline{a}_{Qg}^{(2)}$  is needed  $(O(\varepsilon)$ -term of  $A_{Qg}^{(2)})$ .

## Operator Insertions in Light-Cone Expansion

E.g. singlet heavy quark operator:

$$O_Q^{\mu_1...,\mu_N}(z) = \frac{1}{2} i^{N-1} \overline{q}(z) \gamma^{\{\mu_1} D^{\mu_2} ... D^{\mu_N\}} q(z) - \text{trace terms} .$$



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

$$p_{1}, i$$
  
 $p_{2}, j$   
 $p_{3}, \mu, a$   
 $p_{4}, \nu, b$ 

$$\begin{split} g^2 \Delta^{\mu} \Delta^{\nu} &\Delta \gamma_{\pm} \sum_{0 \leq j < l}^{N-2} \left[ (\Delta p_1)^{N-l-2} (\Delta p_1 + \Delta p_4)^{l-j-1} (\Delta p_2)^j (t^a t^b)_{ji} \right. \\ & \left. + (\Delta p_1)^{N-l-2} (\Delta p_1 + \Delta p_3)^{l-j-1} (\Delta p_2)^j (t^b t^a)_{ji} \right] \,, \end{split}$$

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

Diagrams contributing to the gluonic OME  $\hat{A}_{Qg}^{(2)}$ :



Pure singlet:





 $\Rightarrow$  In general, two types of diagrams:

• 2-loop diagrams with 2-point 1-loop insertions



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### 3. The Calculation

Calculation in Mellin-space:

$$\Rightarrow \quad F(N) = \mathbf{M}[f, N] = \int_0^1 x^{N-1} f(x) \, dx$$

Convolution: 
$$[f \otimes g](x) = \int_0^1 dx_1 \int_0^1 dx_2 \ \delta(x - x_1 x_2) \ f(x_1)g(x_2) ,$$

 $\Rightarrow$  Product:

 $\mathsf{M}[f\otimes g,N]=\mathsf{M}[f,N]\:\mathsf{M}[g,N]\:=F(N)\:G(N).$ 

$$\begin{aligned} F_2^{Q\overline{Q}} &= \sum_{k=1}^{n_f} e_k^2 \left[ f_{k-\overline{k}}(N,\mu^2) H_{2,q}^{NS}\left(N,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\right) \right] \\ &+ e_Q^2 \left[ \Sigma(N,\mu^2) H_{2,q}^{PS}\left(N,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\right) + G(N,\mu^2) H_{2,q}^S\left(N,\frac{Q^2}{m^2},\frac{Q^2}{\mu^2}\right) \right] \end{aligned}$$

light-quark densities:

$$\begin{split} f_{k-\overline{k}}(N,\mu^2) &= f_k(N,\mu^2) - f_{\overline{k}}(N,\mu^2), \\ \Sigma(N,\mu^2) &= \sum_{k=1}^{n_f} f_{k+\overline{k}}(N,\mu^2). \end{split}$$

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Our calculation:

• use of Mellin-Barnes integrals

$$\frac{1}{(A+B)^{\nu}} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} d\sigma A^{\sigma} B^{-\nu-\sigma} \frac{\Gamma(-\sigma)\Gamma(\nu+\sigma)}{\Gamma(\nu)}$$

 $\rightsquigarrow$  numerical check & some analytic results

• use of hypergeometric functions for general analytic results

$${}_{P}F_{Q}\left[\begin{array}{c}(a_{1})...(a_{P})\\(b_{1})...(b_{Q})\end{array};z\right]=\sum_{i=0}^{\infty}\frac{(a_{1})_{i}...(a_{P})_{i}}{(b_{1})_{i}...(b_{Q})_{i}}\frac{z^{i}}{\Gamma(i+1)},\quad (c)_{i}=\frac{\Gamma(c+i)}{\Gamma(c)}.$$



### 3. The Calculation

Calculating scalar Feynman diagrams by Mellin-Barnes integrals:

[I.B., S. Weinzierl, 2003 (massless case); I.B., J. Blümlein and S. Klein, 2006]



$$I_{e,\nu_{1}} = \frac{(\Delta p)^{N-1}}{(4\pi)^{D}(2\pi i)^{2}} \frac{(m^{2})^{D-\nu_{12345}(-1)^{\nu_{12345}+1}}}{\Gamma(\nu_{2})\Gamma(\nu_{3})\Gamma(\nu_{5})\Gamma(D-\nu_{235})} \int_{\gamma_{1}-i\infty}^{\gamma_{1}+i\infty} d\sigma \int_{\gamma_{2}-i\infty}^{\gamma_{2}+i\infty} d\tau \, \Gamma(-\sigma)\Gamma(\nu_{3}+\sigma)$$

$$\times \frac{\Gamma(-\sigma+\nu_{4}+N-1)}{\Gamma(-\sigma+\nu_{4})}\Gamma(-\tau)\Gamma(\nu_{2}+\tau) \frac{\Gamma(\sigma+\tau+\nu_{235}-D/2)\Gamma(\sigma+\tau+\nu_{5})}{\Gamma(\sigma+\tau+\nu_{23})}$$

× 
$$\Gamma(-\sigma - \tau + D - \nu_{23} - 2\nu_5) \frac{\Gamma(-\sigma - \tau + \nu_{14} - D/2)}{\Gamma(-\sigma - \tau + \nu_{14} + N - 1)}$$

| N         | 2        | 3        | 4        | 5        |
|-----------|----------|----------|----------|----------|
| $I_{e,1}$ | +0.49999 | +0.31018 | +0.21527 | +0.16007 |
| $I_{e,2}$ | -0.09028 | -0.04398 | -0.02519 | -0.01596 |

[Mathematica package MB, M. Czakon, 2006] Hypergeometric functions: Example, scalar Diagram e:



$$I_{e,1} := \iint \frac{d^D q \ d^D k}{(2\pi)^{2D}} \frac{(\Delta q)^{N-1}}{[q^2 - m^2]^a [(q-p)^2 - m^2][k^2 - m^2][(k-p)^2 - m^2][(k-q)^2]}$$

$$I_{e,1} := \frac{(\Delta \rho)^{N-1} \Gamma(1-\varepsilon)}{N(N+1)(4\pi)^{4+\varepsilon} (m^2)^{1-\varepsilon}} \\ \int_0^1 dz \int_0^1 dw \, \frac{w^{-1-\varepsilon/2}(1-z)^{\varepsilon/2} z^{-\varepsilon/2}}{(z+w-wz)^{1-\varepsilon}} \left[ 1 - w^{N+1} - (1-w)^{N+1} \right] \,,$$

$$\int_{0}^{1} dz \int_{0}^{1} dw \frac{(1-w)^{a} w^{b} z^{c} (1-z)^{d}}{(z+w-zw)^{e}}$$
  
=  $B(d+1,c+1) B(a+1,b+1) {}_{3}F_{2} \begin{bmatrix} e,d+1,a+1\\ 2+c+d,2+a+b \end{bmatrix};1$ 

$$\begin{split} I_{e,1} &= \frac{S_{\varepsilon}^2}{(4\pi)^4 (m^2)^{1-\varepsilon}} \frac{(\Delta p)^{N-1}}{N(N+1)} \exp\left\{\sum_{i=2}^{\infty} \zeta_i \frac{\varepsilon^i}{i}\right\} \left\{ B(\varepsilon/2+1, 1-\varepsilon/2) B(1, -\varepsilon/2) \,_3F_2 \left[\begin{array}{c} 1-\varepsilon, 1, 1+\varepsilon/2\\ 2, 1-\varepsilon/2 \end{array}; 1\right] \\ &- B(\varepsilon/2+1, 1-\varepsilon/2) B(1, N+1-\varepsilon/2) \,_3F_2 \left[\begin{array}{c} 1-\varepsilon, 1, 1+\varepsilon/2\\ 2, N+2-\varepsilon/2 \end{array}; 1\right] \\ &- B(\varepsilon/2+1, 1-\varepsilon/2) B(N+2, -\varepsilon/2) \,_3F_2 \left[\begin{array}{c} 1-\varepsilon, N+2, 1+\varepsilon/2\\ 2, N+2-\varepsilon/2 \end{array}; 1\right] \right\} \end{split}$$

$$\begin{split} \Psi(x) &= \frac{1}{\Gamma(x)} \frac{d}{dx} \Gamma(x) \qquad \Psi(N+1) = S_1(N) - \gamma \ , \quad N \in \mathbb{N} \\ \Psi^k(N+1) &= (-1)^k \Gamma(k+1) \left[ S_{k+1}(N) - \zeta(k+1) \right] \ , \quad k > 1 \end{split}$$

harmonic sums: [Vermaseren, 1999; Blümlein, Kurth, 1999]

$$S_{a_1,\ldots,a_m}(N) = \sum_{n_1=1}^N \sum_{n_2=1}^{n_1} \cdots \sum_{n_m=1}^{n_{m-1}} \frac{(\operatorname{sign}(a_1))^{n_1}}{n_1^{|a_1|}} \frac{(\operatorname{sign}(a_2))^{n_2}}{n_2^{|a_2|}} \cdots \frac{(\operatorname{sign}(a_m))^{n_m}}{n_m^{|a_m|}}$$

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$$\begin{split} I_{e,1} &= \frac{-S_{\varepsilon}^2}{(4\pi)^4 (m^2)^{1-\varepsilon}} \frac{(\Delta p)^{N-1}}{N(N+1)} \sum_{s=1}^{\infty} \left\{ -\frac{1}{s^2} + \frac{S_1(s)}{s} - \frac{S_1(N+s)}{s} + \frac{B(N+1,s)}{s} \right\} + O(\varepsilon) \\ &= \frac{S_{\varepsilon}^2}{(4\pi)^4 (m^2)^{1-\varepsilon}} (\Delta p)^{N-1} \left\{ \frac{S_1^2(N) + 3S_2(N)}{2N(N+1)} + \frac{S_1^3(N) + 3S_1(N)S_2(N) + 8S_3(N)}{12N(N+1)} \varepsilon \right\} \end{split}$$

More complicated sums  $\rightarrow$  partly solved with C. Schneider's mathematica package SIGMA [I.B., J. Blümlein, S. Klein, C. Schneider, 2007].

|         |       |       |           | <i>c</i> |            | 12         |           |
|---------|-------|-------|-----------|----------|------------|------------|-----------|
| Linnola | rizod | CASA  | avamnlac  | tor      | Individual | diagrame - | - numeric |
| Ulipula | nzeu. | Case, | evaluates | 101      | munitudai  | ulagiailis | numenc.   |
|         |       |       |           |          |            |            |           |

| Diagram | Ν | $1/\varepsilon^2$ | $1/\varepsilon$ | 1        | ε        | $\varepsilon^2$ |
|---------|---|-------------------|-----------------|----------|----------|-----------------|
| ь       | 2 | -8                | 4.66666         | -8.82690 | 2.47728  | -5.69523        |
|         | 6 | -7.73333          | 0.81936         | -8.89777 | -1.84111 | -7.25674        |
| с       | 2 | -8                | 39.6            | -7.23431 | 34.66217 | 6.52891         |
|         | 6 | -2.66666          | 16.53968        | -2.68048 | 14.25224 | 2.77564         |
| d       | 2 | -8                | 7.86666         | -6.34542 | 4.71236  | -2.18586        |
|         | 6 | -2.66666          | -0.69523        | -2.60657 | -1.74990 | -2.37611        |
| е       | 2 | 8.88889           | -11.2593        | 9.82824  | -12.8921 | 2.39145         |
|         | 6 | 2.93878           | -4.24257        | 3.39094  | -4.3892  | 0.826978        |
| f       | 2 | 5.33333           | -9.77777        | 18.34139 | -2.52360 | 16.20210        |
|         | 6 | 3.31428           | -6.87289        | 12.25672 | -1.63790 | 10.86956        |
| g       | 2 | 2.66666           | -9.55555        | 4.59662  | -8.92015 | 1.07313         |
|         | 6 | 0.57142           | -2.00204        | 1.04814  | -1.89142 | 0.32219         |

$$\begin{split} &A_e^{Qg} \\ &= T_R \left[ C_F - \frac{C_A}{2} \right] \left\{ \frac{1}{\varepsilon^2} \frac{16(N+3)}{(N+1)^2} + \frac{1}{\varepsilon} \left[ -\frac{8(N+2)}{N(N+1)} S_1(N) - 8 \frac{3N^3 + 9N^2 + 12N + 4}{N(N+1)^3(N+2)} \right] \\ &+ \left[ -2 \frac{9N^4 + 40N^3 + 71N^2 - 12N - 36}{N(N+1)^2(N+2)(N+3)} S_2(N) - 2 \frac{N^3 - N^2 - 8N - 36}{N(N+1)(N+2)(N+3)} S_1^2(N) \right. \\ &+ 4 \frac{(N+3)}{(N+1)^2} \zeta_2 + 4 \frac{P_{e4}}{N^2(N+1)^2(N+2)(N+3)} S_1(N) + \frac{4P_4(N)}{N^2(N+1)^4(N+2)^2(N+3)} \right] \\ &+ \varepsilon \left[ -2 \frac{N+2}{N(N+1)} \left( 2S_{2,1}(N) + S_1(N) \zeta_2 \right) - \frac{2}{3} \frac{13N^4 + 60N^3 + 111N^2 + 4N - 36}{N(N+1)^2(N+2)(N+3)} S_3(N) \right. \\ &- \frac{1}{3} \frac{N^3 - N^2 - 8N - 36}{N(N+1)(N+2)(N+3)} \left( 3S_2(N)S_1(N) + S_1^3(N) \right) - 2 \frac{3N^3 + 9N^2 + 12N + 4}{N(N+1)^3(N+2)} \zeta_2 \\ &+ \frac{P_{e1}}{N^2(N+1)^3(N+2)(N+3)} S_2(N) + \frac{4N^5 + 11N^4 + 15N^3 - 86N^2 - 92N - 24}{N^2(N+1)^2(N+2)(N+3)} S_1(N) - 2 \frac{P_{e3}}{N^2(N+1)^2(N+2)(N+3)} + \frac{4}{3} \frac{N+3}{(N+1)^2} \zeta_3 \right] \bigg\} \end{split}$$

Results to order O(1): [I.B., J. Blümlein, S. Klein, 2006 & 2007]

## Unpolarized case, Singlet $O(\varepsilon)$

$$\begin{split} \overline{a}_{Qg}^{(2)} &= T_R C_F \left\{ \frac{2}{3} \frac{(N^2 + N + 2)(3N^2 + 3N + 2)}{N^2 (N + 1)^2 (N + 2)} \zeta_3 + \frac{P_1}{N^3 (N + 1)^3 (N + 2)} S_2 + \frac{N^4 - 5N^3 - 32N^2 - 18N - 4}{N^2 (N + 1)^2 (N + 2)} S_1^2 \right. \\ &+ \frac{N^2 + N + 2}{N (N + 1) (N + 2)} \left( 16S_{2,1,1} - 8S_{3,1} - 8S_{2,1}S_1 + 3S_4 - \frac{4}{3}S_3S_1 - \frac{1}{2}S_2^2 - S_2S_1^2 - \frac{1}{6}S_1^4 + 2\zeta_2S_2 - 2\zeta_2S_1^2 - \frac{8}{3}\zeta_3S_1 \right) \\ &- 8\frac{N^2 - 3N - 2}{N^2 (N + 1) (N + 2)} S_{2,1} + \frac{2}{3}\frac{3N + 2}{N^2 (N + 2)} S_1^3 + \frac{2}{3}\frac{3N^4 + 48N^3 + 43N^2 - 22N - 8}{N^2 (N + 1)^2 (N + 2)} S_3 + 2\frac{3N + 2}{N^2 (N + 1)^2 (N + 2)} S_2S_1 + 4\frac{S_1}{N^2} \zeta_2 \\ &+ \frac{N^5 + N^4 - 8N^3 - 5N^2 - 3N - 2}{N^3 (N + 1)^3} \zeta_2 - 2\frac{2N^5 - 2N^4 - 11N^3 - 19N^2 - 44N - 12}{N^2 (N + 1)^3 (N + 2)} S_1 + \frac{P_2}{N^5 (N + 1)^5 (N + 2)} \right\} \\ &+ T_R C_A \left\{ \frac{N^2 + N + 2}{(N + 1) (N + 2)} \left( 16S_{-2,1,1} - 4S_{2,1,1} - 8S_{-3,1} - 8S_{-2,2} - 4S_{3,1} - \frac{2}{3}\beta''' + 9S_4 - 16S_{-2,1}S_1 \right. \\ &+ \frac{40}{3}S_1S_3 + 4\beta''S_1 - 8\beta'S_2 + \frac{1}{2}S_2^2 - 8\beta'S_1^2 + 5S_1^2S_2 + \frac{1}{6}S_1^4 - \frac{10}{3}S_1\zeta_3 - 2S_2\zeta_2 - 2S_1^2\zeta_2 - 4\beta'\zeta_2 - \frac{17}{5}\zeta_2^2 \right) \\ &+ \frac{4(N^2 - N - 4)}{(N + 1)^2 (N + 2)^2} \left( -4S_{-2,1} + \beta'' - 4\beta'S_1 \right) - \frac{2}{3}\frac{N^3 + 8N^2 + 11N + 2}{N (N + 1)^2 (N + 2)^2}S_1^3 + 8\frac{N^4 + 2N^3 + 7N^2 + 22N + 20}{(N + 1)^3 (N + 2)^3}\beta' \\ &+ 2\frac{3N^3 - 12N^2 - 27N - 2}{N (N + 1)^2 (N + 2)^2} S_2S_1 - \frac{16}{3}\frac{N^5 + 10N^4 + 9N^3 + 3N^2 + 7N + 6}{(N - 1)N^2 (N + 1)^2 (N + 2)^2}S_3 - 8\frac{N^2 + N - 1}{(N + 1)^2 (N + 2)^2}\zeta_2S_1 \\ &- \frac{2}{3}\frac{9N^5 - 10N^4 - 11N^3 + 68N^2 + 24N + 16}{(N - 1)N^2 (N + 1)^2 (N + 2)^2}S_3 - 8\frac{N^2 + N - 1}{(N - 1)N^3 (N + 1)^3 (N + 2)^3}S_2 - \frac{2P_4}{(N - 1)N^3 (N + 1)^3 (N + 2)^3}\zeta_2 \\ &- \frac{P_5}{N (N + 1)^3 (N + 2)^3}S_1^2 + \frac{2P_6}{N (N + 1)^4 (N + 2)^4}S_1 - \frac{2P_7}{(N - 1)N^5 (N + 1)^5 (N + 2)^5} \right\}.$$

Unpolarized case, pure-singlet and non-singlet,  $O(\varepsilon)$ 

$$\begin{split} \overline{a}_{Qq}^{\mathrm{PS},(2)} &= C_F T_R \left\{ -2 \frac{(5N^3 + 7N^2 + 4N + 4)(N^2 + 5N + 2)}{(N-1)N^3(N+1)^3(N+2)^2} \Big( 2S_2(N) + \zeta_2 \Big) \right. \\ &\left. - \frac{4}{3} \frac{(N^2 + N + 2)^2}{(N-1)N^2(N+1)^2(N+2)} \Big( 3S_3(N) + \zeta_3 \Big) + 2 \frac{P_9}{(N-1)N^5(N+1)^5(N+2)^4} \right\} \,. \end{split}$$

$$\begin{split} \bar{a}_{qq,Q}^{\mathrm{NS},(2)} &= C_F T_R \left\{ \frac{4}{3} S_4(N) + \frac{4}{3} S_2(N) \zeta_2 - \frac{8}{9} S_1(N) \zeta_3 - \frac{20}{9} S_3(N) - \frac{20}{9} S_1(N) \zeta_2 \right. \\ &+ 2 \frac{3N^2 + 3N + 2}{9N(N+1)} \zeta_3 + \frac{112}{27} S_2(N) + \frac{3N^4 + 6N^3 + 47N^2 + 20N - 12}{18N^2(N+1)^2} \zeta_2 \\ &- \frac{656}{81} S_1(N) + \frac{P_8}{648N^4(N+1)^4} \right\} \,. \end{split}$$

## 5. Comparison

First Calculation to O( $\alpha_{S}^{2}$ ): [Buza, Matiounine, Smith, Migneron, van Neerven, 1996]

- $\rightsquigarrow$  Integration-by-parts method
- → direct integration of individual Feynman-parameter integrals in z-space

combinations of Nielsen integrals: 
$$S_{p,n}(x) = \frac{(-1)^{n+p-1}}{(n-1)!p!} \int_0^1 \frac{dz}{z} \ln^{n-1}(z) \ln^p(1-zx)$$

| $\delta(1 - x)$                             | 1                                      | $\ln(x)$                                | $\ln^2(x)$                          | $\ln^3(x)$                                   | $\ln(1 - x)$                           |
|---|--|---|-------------------------------------|--|--|
| $\ln^2(1 - x)$                              | $\ln^{3}(1 - x)$                       | $\ln(x)\ln(1-x)$                        | $\ln(x) \ln^2(1-x)$                 | $\ln^2(x)\ln(1-x)$                           | $\ln(1+x)$                             |
| $\ln(x)\ln(1+x)$                            | $\ln^2(x)\ln(1+x)$                     | $Li_2(1 - x)$                           | $\ln(x) \operatorname{Li}_2(1 - x)$ | $\ln(1 - x) \operatorname{Li}_2(1 - x)$      | $Li_{3}(1 - x)$                        |
| $S_{1,2}(1-x)$                              | $S_{1,2}(-x)$                          | $\frac{1}{1 - x}$                       | $\frac{1}{1+x}$                     | $\frac{\ln(x)}{1 - x}$                       | $\frac{\ln^2(x)}{1-x}$                 |
| $\frac{\ln^3(x)}{1-x}$                      | $\frac{\ln(x)}{1+x}$                   | $\frac{\ln^2(x)}{1+x}$                  | $\frac{\ln^3(x)}{1+x}$              | $\frac{\ln(1+x)}{1+x}$                       | $\frac{\ln(x)\ln(1+x)}{1+x}$           |
| $\frac{\ln(x)\ln^2(1+x)}{1+x}$              | $\frac{\ln^2(x)\ln(1+x)}{1+x}$         | $\frac{\ln(x)\ln(1-x)}{1-x}$            | $\frac{\ln(x)\ln^2(1-x)}{1-x}$      | $\frac{\ln(1-x)\operatorname{Li}_2(x)}{1-x}$ | $\frac{\operatorname{Li}_2(1-x)}{1-x}$ |
| $\frac{\ln(x)Li_2(1 - x)}{1 - x}$           | $\frac{\ln(x)\mathrm{Li}_2(1-x)}{1+x}$ | $\frac{\ln(1+x)\mathrm{Li}_2(-x)}{1+x}$ | $\ln(1+x)\operatorname{Li}_2(-x)$   | $\operatorname{Li}_2(-x)$                    | $\frac{\operatorname{Li}_2(-x)}{1+x}$  |
| $\frac{\ln(x)\operatorname{Li}_2(-x)}{1+x}$ | $\frac{\text{Li}_3(1-x)}{1-x}$         | $\frac{\text{Li}_3(-x)}{1 + x}$         | $\frac{S_{1,2}(1-x)}{1-x}$          | $\frac{S_{1,2}(1-x)}{1+x}$                   | $\frac{S_{1,2}(-x)}{1+x}$              |

## 5. Comparison

| Complexity of the results in Mellin space, | unpolarized | case to | order C | $(\varepsilon)$ | ): |
|--|-------------|---------|---------|-----------------|----|
|--|-------------|---------|---------|-----------------|----|

| Diag   | $S_1$                         | $S_2$ | $S_3$ | $S_4$ | $S_{-2}$ | $S_{-3}$ | $S_{-4}$ | $S_{2,1}$ | $S_{-2,1}$ | $S_{-2,2}$ | $S_{3,1}$ | $S_{-3,1}$ | $S_{2,1,1}$ | $S_{-2,1,1}$ |
|--------|-------------------------------|-------|-------|-------|----------|----------|----------|-----------|------------|------------|-----------|------------|-------------|--------------|
| а      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| b      | ++                            | ++    | ++    | +     |          |          |          | ++        |            |            | +         |            | +           |              |
| с      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| d      | ++                            | ++    | +     |       |          |          |          | +         |            |            |           |            |             |              |
| е      | ++                            | ++    | +     |       |          |          |          | +         |            |            |           |            |             |              |
| f      | ++                            | ++    | ++    | +     |          |          |          | ++        |            |            |           |            | +           |              |
| g      | ++                            | ++    | +     |       |          |          |          | +         |            |            |           |            |             |              |
| h      | ++                            | ++    | +     |       |          |          |          | +         |            |            |           |            |             |              |
| i      | ++                            | ++    | ++    | +     | ++       | ++       | +        | ++        | ++         | +          | +         | +          | +           | +            |
| j      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| k      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| 1      | ++                            | ++    | ++    | +     |          |          |          | ++        |            |            | +         |            | +           |              |
| m      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| n      | ++                            | ++    | ++    | +     | ++       | ++       | +        | ++        | ++         | +          | +         | +          | +           | +            |
| 0      | ++                            | ++    | ++    | +     |          |          |          | ++        |            |            | +         |            | +           |              |
| р      | ++                            | ++    | ++    | +     |          |          |          | ++        |            |            | +         |            | +           |              |
| s      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| t      |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| $PS_a$ |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| $PS_b$ |                               | ++    | +     |       |          |          |          |           |            |            |           |            |             |              |
| $NS_a$ |                               |       |       |       |          |          |          |           |            |            |           |            |             |              |
| $NS_b$ | ++                            | ++    | ++    | +     |          |          |          |           |            |            |           |            |             |              |
| Σ      | ++                            | ++    | ++    | +     | ++       | ++       | +        | +         | ++         | +          | +         | +          | +           | +            |
| + = 0  | $+ = O(1) + = O(\varepsilon)$ |       |       |       |          |          |          |           |            |            |           |            |             |              |

unpolarized case and polarized case: van Neerven et al. to O(1): unpolarized: 48 basic functions polarized: 24 basic functions

 $O(1): \qquad \{S_1, S_2, S_3, S_{-2}, S_{-3}\}, \qquad S_{-2,1} \Longrightarrow 2 \text{ basic objects.}$ 

$$\{S_1, S_2, S_3, S_4, S_{-2}, S_{-3}, S_{-4}\}, S_{2,1}, S_{-2,1}, S_{-3,1}, S_{2,1,1}, S_{-2,1,1}$$

$$O(\varepsilon): S_{-2,2} \text{ depends on } S_{-2,1}, S_{-3,1}$$

$$S_{3,1} \text{ depends on } S_{2,1}$$

$$\implies 6 \text{ basic objects}$$

$$\begin{split} \beta(N+1) &= (-1)^N [S_{-1}(N) + \ln(2)] ,\\ \beta^{(k)}(N+1) &= \Gamma(k+1)(-1)^{N+k} [S_{-k-1}(N) + (1-2^{-k})\zeta_{k+1}] , \ k \geq 2 ,\\ \mathsf{M}\Big[\frac{\mathrm{Li}_2(x)}{1+x}\Big](N+1) - \zeta_2 \beta(N+1) &= (-1)^{N+1} [S_{-2,1}(N) + \frac{5}{8}\zeta_3] \end{split}$$

harmonic sums with index {-1} cancel (holds even for each diagram) [cf. Blümlein, 2004; Blümlein and Ravindran, 2005; Blümlein and Moch, in preparation]. Calculation of quark–mass effects in QCD Wilson–coefficients in asymptotic regime  $Q^2 \gg m^2$ 

- Calculation in Mellin space
  - $\rightarrow$  essential for simplification of calculation
- Use of Mellin–Barnes integrals (mainly numerical checks) and generalized hypergeometric functions
- Results in term of nested harmonic sums → use of algebraic relations of harmonic sums for simplification of results
- Calculation of the constant term of the Operator Matrix Elements → full agreement with results of van Neerven et al.
- New: Calculation of the O( $\varepsilon$ ) term of the two-loop OMEs complete, necessary for the calculation of the Heavy Wilson coefficients up to O( $\alpha_s^2$ )