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Two–Loop Massive Operator Matrix Elements for Unpolarized Heavy Flavor Production to $O(\epsilon)$

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Abstract

We calculate the $O(\alpha_s^2)$ massive operator matrix elements for the twist–2 operators, which contribute to the heavy flavor Wilson coefficients in unpolarized deeply inelastic scattering in the region $Q^2 \gg m^2$, up to the $O(\varepsilon)$ contributions. These terms contribute through the renormalization of the $O(\alpha_s^3)$ heavy flavor Wilson coefficients of the structure function $F_2(x, Q^2)$. The calculation has been performed using light–cone expansion techniques without using the integration-by-parts method. We represent the individual Feynman diagrams by generalized hypergeometric structures, the ε–expansion of which leads to infinite sums depending on the Mellin variable N. These sums are finally expressed in terms of nested harmonic sums using the general summation techniques implemented in the `Sigma` package.

1 Introduction

The heavy flavor corrections to deeply inelastic scattering constitute an important part of the structure functions in the lower x region, cf. [1]. The current world data for the nucleon structure functions $F_2^{p,d}(x,Q^2)$ reached the precision of a few per cent over a wide kinematic region. Therefore both for the determination of the QCD scale $\Lambda_{\rm QCD}$ and the detailed shapes of the partonic distribution functions the analysis at the level of the $O(\alpha_s^3)$ corrections is required to control the theory-errors on the level of the experimental accuracy and below [2]. In a recent non–singlet analysis [3] errors for $\alpha_s(M_Z^2)$ of $O(1.5\ \%)$ were obtained extending the analysis effectively to N^{3}LO. In the flavor singlet case the yet unknown 3–loop heavy flavor Wilson coefficients prevent a consistent 3–loop analysis. Due to the large statistics in the lower x region one may hope to eventually improve the accuracy of $\alpha_s(M_Z^2)$ beyond the above value.

The heavy flavor corrections to $F_2^{p,d}(x,Q^2)$ were calculated to 2–loop order in the whole kinematic domain in a semi-analytic way in x-space in Refs. [4]. A fast implementation for complex N–space was given in [5]. In the range of higher values of Q^2 one may calculate the heavy flavor Wilson coefficients to the structure functions $F_2(x,Q^2)$ and $F_L(x,Q^2)$ in analytic form. For $F_2(x,Q^2)$ this calculation has been performed to 2–loop order in [6,7] and for $F_L(x,Q^2)$ to 3–loop order in [8]. In the region $Q^2 \gg m^2$ the heavy flavor Wilson coefficients for deep–inelastic scattering factorize into massive operator matrix elements $A_{ij}(\mu^2/m^2)$ and the massless Wilson coefficients $C_k(Q^2/\mu^2)$ [9–11] for all but the power suppressed contributions. The massive operator matrix elements are universal and contain all the mass dependence in the logarithmic orders and the constant term. The process dependence is due to the massless Wilson coefficients. In the case of the structure function $F_2(x,Q^2)$ the asymptotic heavy flavor contributions become quantitatively very close to those obtained in the complete calculation [4, 12] at LO and NLO already for $Q^2 \gtrsim 10\ m^2$. These scales are sufficiently low and match with the region analyzed in deeply inelastic scattering.

In the present paper we perform a first step towards the 3–loop heavy flavor Wilson coefficients for the structure function $F_2(x,Q^2)$. The renormalization of the massive operator matrix elements to 3–loop order encounters also the contributions of $O(\varepsilon)$ at $O(\alpha_s^2)$, which have not yet been calculated before. [1] The 2–loop $O(\varepsilon)$ terms form finite contributions to the $O(a_s^3)$ matrix elements with the single pole terms emerging at 1st order. We extend the work presented previously in Ref. [7]. For the calculation of the $O(\varepsilon)$ 2–loop contributions our representation which is based on hypergeometric integrals was extended straightforwardly. However, many more infinite nested sums, which contain the Mellin variable N, had to be evaluated for the first time, since other available techniques [15–17] could not be used for this purpose. We applied both suitable integral representations and the summation package `Sigma` [18], which solves these sums in $\Pi\Sigma$–fields. In the result all sums can be expressed in terms of nested harmonic sums [15, 19].

The paper is organized as follows. In section 2 the structure of the heavy flavor contributions to the deeply inelastic structure function is summarized for the kinematic region $Q^2 \gg m^2$. The renormalization of the massive operator matrix elements to 3–loop order is described in section 3. In section 4 the $O(\varepsilon)$ contributions to the 2–loop operator matrix elements are calculated. Section 5 contains the conclusions. In the appendices we present details of the calculation, newly derived infinite sums and related functions depending on the Mellin parameter N, and a further check on our result comparing the Abelian part of the first moment with the corresponding part

[1] In the massless case the off–shell operator matrix elements were calculated to this order for space–like momenta in the $\overline{\rm MS}$–scheme for unpolarized and polarized deeply inelastic scattering in [13,14], which are needed in the calculation of the 3–loop anomalous dimensions.

of the on–shell photon propagator,

2 Basic Formalism

In the twist–2 approximation, the deep–inelastic nucleon structure functions $F_n(x,Q^2),\ n = 2, L$, are described as Mellin convolutions between the parton densities $f_j(x,\mu^2)$ and the Wilson coefficients $\mathsf{C}_i^j(x,Q^2/\mu^2)$

$$F_n(x,Q^2) \;=\; \sum_j \mathsf{C}_n^j\left(x,\frac{Q^2}{\mu^2}\right) \otimes f_j(x,\mu^2) \tag{1}$$

to all orders in perturbation theory due to the factorization theorem. Here μ^2 denotes the factorization scale and the Mellin convolution is given by the integral

$$[A\otimes B](x) = \int_0^1 dx_1 \int_0^1 dx_2 \;\; \delta(x-x_1x_2)\; A(x_1)B(x_2)\;. \tag{2}$$

The distributions f_j refer to massless partons and the heavy flavor effects are contained in the Wilson coefficients only. As was shown in Ref. [6] in the region $Q^2 \gg m^2$ all non–power contributions to the heavy quark Wilson coefficients obey

$$H_{n;i}^{\mathsf{fl}}\left(\frac{Q^2}{m^2},\frac{m^2}{\mu^2},x\right) = C_{n;k}^{\mathsf{fl}}\left(\frac{Q^2}{\mu^2},x\right)\otimes A_{k,i}^{\mathsf{fl}}\left(\frac{m^2}{\mu^2},x\right)\;, \tag{3}$$

where $C_{n;k}^{\mathsf{fl}}\left(Q^2/\mu^2,x\right)$ are the Wilson coefficients for massless partons and $A_{k,i}^{\mathsf{fl}}\left(m^2/\mu^2,x\right)$ are the massive operator matrix elements. Here μ refers to the factorization scale between the heavy and light contributions in C_n^j. In the convolution (3) only those terms are accounted for which contribute to the respective heavy flavor Wilson coefficient functions. The index fl denotes the flavor-decomposition and labels the pure–singlet and gluon contributions (PS,G) and three non-singlet ($\mathrm{NS}^{\pm}$, NS^{v}) combinations. Due to the fact that the diagrams considered here contain one heavy quark line, at $O(a_s)$ only A_{Qg} contributes. Beginning with $O(a_s^2)$ there is also the pure-singlet A_{Qq}^{PS} and the non-singlet term $A_{Qq}^{\mathrm{NS}^+}$, while at $O(a_s^3)$ also the two other non-singlet terms $A_{Qq}^{\mathrm{NS}^-}$ and $A_{Qq}^{\mathrm{NS}^{\mathrm{v}}}$ contribute. The corresponding combinations of quark distributions for the singlet and non-singlet terms are $\Sigma(x,Q^2)$ and $q^{\mathrm{NS}^{\mathrm{l}}}(x,Q^2)$ with

$$\Sigma(x,Q^2) \;=\; \sum_{k=1}^{N_l}\left[q_k(x,Q^2)-\overline{q}_k(x,Q^2)\right] \tag{4}$$

$$q_{mn}^{\mathrm{NS}^{\pm}}(x,Q^2) \;=\; \left[q_m(x,Q^2)\pm\overline{q}_m(x,Q^2)\right]-\left[q_n(x,Q^2)\pm\overline{q}_n(x,Q^2)\right] \tag{5}$$

$$q^{\mathrm{NS}^{\mathrm{v}}}(x,Q^2) \;=\; \sum_{k=1}^{N_f}\left[q_k(x,Q^2)-\overline{q}_k(x,Q^2)\right]\;. \tag{6}$$

N_l denotes the number of light quark flavors. The massless Wilson coefficients were calculated in [9–11] to 3–loop orders. The massive operator matrix elements are process independent quantities. The factorization (3) is a consequence of the renormalization group equation. In Mellin space the operator matrix elements $A_{k,i}^{\mathsf{fl}}$ and light flavor Wilson coefficients obey the

following expansions :

$$A_{k,i}^{\rm fl}\left(\frac{m^2}{\mu^2}\right) = \langle i|O_k|i\rangle = \delta_{k,i} + \sum_{l=1}^{\infty} a_s^l A_{k,i}^{{\rm fl},(l)}, \qquad i = q, g \tag{7}$$

$$C_{2;i}^{\rm fl}\left(\frac{Q^2}{\mu^2}\right) = \delta_{i,q} + \sum_{l=1}^{\infty} a_s^l C_{2,i}^{{\rm fl},(l)}, \qquad i = q, g \tag{8}$$

of the twist–2 flavor singlet, non–singlet and gluon operators $O_k^{\rm NS,S,g}$ between partonic states $|i\rangle$, which are related by collinear factorization to the initial–state nucleon states $|N\rangle$. The local operators are given by

$$O_{q,r}^{{\rm NS},\mu_1,\ldots,\mu_N}(z) = \frac{1}{2} i^{N-1} S\left[\overline{q}(z)\gamma^{\mu_1} D^{\mu_2}\ldots D^{\mu_N}\frac{\lambda_r}{2} q(z)\right] - \text{Trace Terms} \tag{9}$$

$$O_{q}^{{\rm S},\mu_1,\ldots,\mu_N}(z) = \frac{1}{2} i^{N-1} S\left[\overline{q}(z)\gamma^{\mu_1} D^{\mu_2}\ldots D^{\mu_N} q(z)\right] - \text{Trace Terms} \tag{10}$$

$$O_{g}^{\mu_1,\ldots,\mu_N}(z) = \frac{1}{2} i^{N-2} S\left[F_\alpha^{a,\mu_1}(z) D^{\mu_2}\ldots D^{\mu_{N-1}} F^{a,\alpha,\mu_N}(z)\right] - \text{Trace Terms}\ . \tag{11}$$

Here S denotes the operator which symmetrizes all Lorentz-indices and $D_{\mu_1} = \partial_{\mu_1} - g t_a A_{\mu_1}^a$ is the covariant derivative, $q(z)$, $\overline{q}(z)$ and $F^{a,\mu\nu}(z)$ denote the quark-, anti-quark field and the gluon field-strength operators, with $g = (4\pi\alpha_s)^{1/2} = (16\pi^2 a_s)^{1/2}$ the strong coupling constant, t_a the generators of $SU(3)_c$, and λ_r the Gell-Mann matrices of $SU(3)_F$. The Feynman rules for the operator insertions are given in [7, 20].

3 Renormalization of the Matrix Elements

The massive operator matrix elements contain ultraviolet and collinear singularities which have to be renormalized. Charge-, mass-, operator-, and wave function renormalization have to be performed. Collinear singularities appear in those parts of the diagrams with vertices which link only to massless lines, and are specific to the particular classes of diagrams. Since in the present case at least one closed fermion line is massive, collinear singularities appear only at $O(a_s^2)$. The un-renormalized massive operator matrix elements read

$$\hat{\hat{A}}_{ij} = \delta_{ij} + \sum_{k=0}^{\infty} \hat{a}_s^k \hat{\hat{A}}_{ij}^{(k)}\ . \tag{12}$$

Here $\hat{a}_s$ denotes the bare coupling constant. To 2–loop order, the corresponding diagrams were given in Ref. [6]. Here one has to distinguish one-particle irreducible and reducible diagrams, which both contribute in the calculation. We would like to remind the reader the background of this aspect.

If one evaluates the heavy-quark Wilson coefficients in an usual Feynman-diagram calculation, the matrix elements are given by diagrams of the type depicted in Figure 1. The incoming gluon is factorized from the nucleon, i.e. we assume the parton life-time τ_L being much longer than the interaction time τ_I of the virtual photon with the nucleon. As is well-known [21], this condition is fulfilled whenever $k_\perp^2 \ll Q^2$ and neither the Bjorken variable x is very small ($x \not\ll 1$) nor large ($x \not\approx 1$). This is the case performing the Bjorken limit and applying the collinear parton model, in which the incoming massless partons are dealt with as on–shell particles. Also in this case,

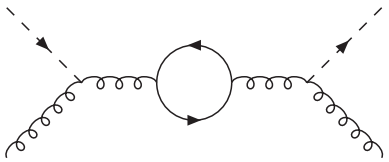

Figure 1: Massive quark self-energy correction to virtual scalar–gluon scattering

self-energy diagrams for the incoming parton lines are present. However, one may factorize these contributions into the non–perturbative parton densities at leading twist, resp. parton correlation functions at higher twist, since these contributions are virtual and are always present whatever hard scattering cross section is considered. They do not form a heavy quark signature which can be identified in a subspace of the complete final–state Fock–space emerging in deeply inelastic lepton–nucleon scattering. This procedure was adopted in Ref. [4]. One consequence is that at $O(a_s^2)$ there are no diagrams with two fermion lines, resp. at $O(a_s^3)$ none with three fermion lines in the general heavy flavor Wilson coefficients. The situation is different in case of the operator matrix elements obtained after the light–cone expansion is being performed. Here, the line between the two virtual photon- or weak gauge boson vertices is contracted. This line may contain virtual corrections, see e.g. Figure 1, which would be lost in the process of contraction. They have to be accounted for in attaching these self–energies to outer lines of the contracted diagram, see Figure 2. From the case of the fermion–fermion anomalous dimension at leading order these aspects are known for long [22–24].

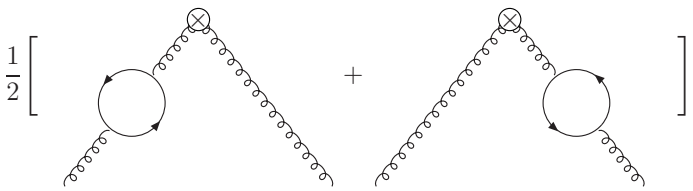

Figure 2: $O(a_s)$ Self-energy correction due to massive quarks for the operator matrix element $A_{gg}^{(1)}$.

In kinematic regions, where higher twist effects can be safely neglected [3, 25] and at sufficiently high scales Q^2, the scaling violations of deeply inelastic structure functions are due to the running coupling constant and heavy quark mass effects, after target mass effects [26] have been accounted for. We will further assume that we are in a region where power corrections due to heavy quarks are negligibly small, i.e., the heavy quark effects contribute logarithmically $\propto \ln^l(m^2/\mu^2)$, $l \geq 0$. In this region one may express the structure functions $F_i(N, Q^2)$ in Mellin space by

$$\begin{aligned} F_i(N,Q^2) &= \sum_{l=1}^{N_l} C_{i,q}(N, Q^2/\mu_f^2; a_s(\mu_r^2)) \cdot \left[q_l(N, \mu_f^2/\mu_0^2, a_s(\mu_r^2)) + \overline{q}_l(N, \mu_f^2/\mu_0^2, a_s(\mu_r^2))\right] \\ &\quad + C_{i,g}(N, Q^2/\mu_f^2; a_s(\mu_r^2)) \cdot g(N, \mu_f^2/\mu_0^2, a_s(\mu_r^2)) \end{aligned}$$

$$+\sum_{h=1}^{N_l} H_{i,q}(N,Q^2/\mu_f^2;a_s(\mu_r^2)) \cdot \left[q_l(N,\mu_f^2/\mu_0^2,a_s(\mu_r^2)) + \overline{q}_l(N,\mu_f^2/\mu_0^2,a_s(\mu_r^2))\right]$$
$$+H_{i,g}(N,Q^2/\mu_f^2;a_s(\mu_r^2)) \cdot g(N,\mu_f^2/\mu_0^2,a_s(\mu_r^2)) \ . \tag{13}$$

Here μ_r and μ_f denote the renormalization and factorization scales, respectively, μ_0 is a hadronic scale, and $q, \overline{q}$ and g denote the quark- and gluon distribution functions. Furthermore, the heavy quark Wilson coefficients factorize according to (3), which is described by the scale μ. In the following we identify all these scales $\mu = \mu_r = \mu_f$. Since the structure functions $F_i(N,Q^2)$ do not depend on these scales they obey the following renormalization group equation (RGE) [27]

$$\left[\mathcal{D} + 2\gamma_j\right] \ F_n(N,Q^2) = 0 \ , \tag{14}$$

where the differential operator $\mathcal{D}$ is defined by

$$\mathcal{D} = \mu^2 \frac{\partial}{\partial \mu^2} + \beta(a_s(\mu^2)) \frac{\partial}{\partial a_s(\mu^2)} - \gamma_m(a_s(\mu^2)) m^2(\mu^2) \frac{\partial}{\partial m^2(\mu^2)} \ . \tag{15}$$

$\beta(a_s)$ denotes the β-function, $\gamma_m(a_s)$ the mass anomalous dimension, and γ_j denote the anomalous dimensions of the quark fields. Here we discuss the case of conserved currents, which have vanishing anomalous dimensions. [2]

The RGE for the Wilson coefficients and the parton distributions read [23, 28]

$$\left[\mathcal{D}\ \delta_{kj} - \gamma_{kj}^N(a_s)\right] \mathsf{C}_n^j(N,Q^2/\mu^2) = 0 \tag{16}$$
$$\left[\left(\mathcal{D} + 2\gamma_j\right)\delta_{kk'} + \gamma_{kk'}^N(a_s)\right] f_{jk'}(N,\mu^2/\mu_0^2) = 0 \ , \tag{17}$$

with

$$f_{jk}(N,\mu^2/\mu_0^2) = \langle j|O_k|j\rangle \ . \tag{18}$$

In the following we describe the renormalization to $O(a_s^3)$.

3.1 Charge Renormalization

We perform the charge renormalization in the $\overline{\rm MS}$-scheme. This allows to compare the results obtained in the QCD analysis of deeply inelastic scattering data with analyzes of other data. The bare coupling constant $\hat{a}_s$ is expressed by the renormalized coupling a_s in the $\overline{\rm MS}$ scheme by

$$\begin{aligned}
\hat{a}_s(\varepsilon) &= Z_g^2(\varepsilon,\mu^2) a_s(\mu^2) \\
&= a_s(\mu^2)\left[1 + \delta a_{s,1} a_s(\mu^2) + \delta a_{s,2} a_s^2(\mu^2)\right] + O(a_s^4) && (19)\\
\delta a_{s,1} &= S_\varepsilon \frac{2\beta_0}{\varepsilon} && (20)\\
\delta a_{s,2} &= S_\varepsilon^2 \left[\frac{4\beta_0^2}{\varepsilon^2} + \frac{\beta_1}{\varepsilon}\right] \ , && (21)
\end{aligned}$$

with Z_g the Z–factor for the strong charge. Here the spherical factor S_ε is given by

$$S_\varepsilon = \exp\left[\frac{\varepsilon}{2}\left(\gamma_E - \ln(4\pi)\right)\right] \ , \tag{22}$$

[2] Calculating the evolution of the transversity structure function $h_1(x,Q^2)$ using the forward Compton amplitude, this is not the case, cf. [29].

with γ_E the Euler–Mascheroni number, $\varepsilon = D - 4$, and D the dimension of space–time. β_0 and β_1 [30] denote the first expansion coefficients of the β-function in the massless case

$$\frac{da_s(\mu^2)}{d\ln(\mu^2)} = \frac{1}{2}\varepsilon a_s(\mu^2) - \sum_{k=0}^{\infty} \beta_k a_s^{k+2}(\mu^2) \tag{23}$$

$$\beta_0 = \frac{11}{3}C_A - \frac{4}{3}T_F n_f \tag{24}$$

$$\beta_1 = \frac{34}{3}C_A^2 - 4\left(\frac{5}{3}C_A + C_F\right) T_F n_f \ . \tag{25}$$

The color factors for $SU(3)_c$ are $C_F = (N_c^2 - 1)/(2N_c) = 4/3, C_A = N_c = 3, T_F = 1/2$. n_f denotes the number of active flavors. The renormalized coupling constant is obtained absorbing Z_g into the bare coupling $\hat{g}$.

In [6] a slightly different point of view was taken, including mass effects in the evolution of $a_s(\mu^2)$ which usually means to choose another scheme, as e.g. the MOM-scheme [31]. To maintain the Slavnov-Taylor identities of QCD the calculation has to be performed using the background-field method [32] in [33]. [3] Since various mass scales contribute even in case power corrections can be disregarded, to treat a_s including mass effects is also somewhat non practical. We treat the corresponding mass effects explicitly, which is outlined in Section 3.4 below.

3.2 Mass Renormalization

We choose the on–mass–shell scheme for quarks. In case of the heavy quarks the bare mass $\hat{m}$ is related to the renormalized mass by

$$\hat{m} = m + \hat{a}_s \delta m_1 + \hat{a}_s^2 \delta m_2 + O(a_s^3) \tag{26}$$

$$\delta m_1 = C_F S_\varepsilon m \left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} \left[\frac{6}{\varepsilon} - 4 + \left(4 + \frac{3}{4}\zeta_2\right)\varepsilon\right] \tag{27}$$

$$\begin{aligned}\delta m_2 = {} & C_F S_\varepsilon^2 m \left(\frac{m^2}{\mu^2}\right)^{\varepsilon} \left[\frac{1}{\varepsilon^2}\left(18C_F + 22C_A - 8T_F(N_l + N_h)\right)\right. \\ & + \frac{1}{\varepsilon}\left(-\frac{45}{2}C_F + \frac{91}{2}C_A - 14T_F(N_l + N_h)\right) \\ & + C_F\left(\frac{199}{8} - \frac{51}{2}\zeta_2 + 48\ln(2)\zeta_2 - 12\zeta_3\right) + C_A\left(-\frac{605}{8} + \frac{5}{2}\zeta_2 - 24\ln(2)\zeta_2 + 6\zeta_3\right) \\ & \left. + T_F\left[N_l\left(\frac{45}{2} + 10\zeta_2\right) + N_h\left(\frac{69}{2} - 14\zeta_2\right)\right]\right]\end{aligned} \tag{28}$$

(27) is easily obtained. The pole terms to (28) were given in [35], after charge renormalization, and the constant term in [36], see also [37]. The 3–loop corrections were given in [38]. The renormalized mass is obtained absorbing Z_m into the bare mass $\hat{m}$. Heavy quark mass effects occur also for massless quark self-energies, see Section 3.4.

[3] Earlier calculations [26, 34] illustrated this reporting different expressions for Z_g depending on the vertex considered.

3.3 Operator Renormalization

The local operators which emerge in the light cone expansion contain ultraviolet divergences. These are renormalized by the following Z–factors for the flavor non-singlet (NS), singlet (S), and pure singlet (PS) contributions. The formulae are partly generic and have to be adapted, e.g. for the three flavor non–singlet contributions. Here we suppress the argument N in the anomalous dimensions $\gamma_{ij,k}$.

$$\begin{aligned}
Z_{\rm NS}(N,a_s,\varepsilon) &= 1 + a_s S_\varepsilon \frac{\gamma_{\rm NS,0}}{\varepsilon} + a_s^2 S_\varepsilon^2 \left[\frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{NS,0}^2 + \beta_0\gamma_{\rm NS,0}\right) + \frac{1}{2\varepsilon}\gamma_{\rm NS,1}\right] \\
&+ a_s^3 S_\varepsilon^3 \left[\frac{1}{\varepsilon^3}\left(\frac{1}{6}\gamma_{\rm NS,0}^3 + \beta_0\gamma_{\rm NS,0}^2 + \frac{4}{3}\beta_0^2\gamma_{\rm NS,0}\right)\right. \\
&\left. + \frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{\rm NS,0}\gamma_{\rm NS,1} + \frac{2}{3}\beta_0\gamma_{\rm NS,1} + \frac{2}{3}\beta_1\gamma_{\rm NS,0}\right) + \frac{1}{3\varepsilon}\gamma_{\rm NS,2}\right] \qquad (29) \\
Z_{qq}(N,a_s,\varepsilon) &= 1 + a_s S_\varepsilon \frac{\gamma_{qq,0}}{\varepsilon} + a_s^2 S_\varepsilon^2 \left\{\frac{1}{\varepsilon^2}\left[\frac{1}{2}\left(\gamma_{qq,0}^2 + \gamma_{qg,0}\gamma_{gq,0}\right) + \beta_0\gamma_{qq,0}\right] + \frac{1}{2\varepsilon}\gamma_{qq,1}\right\} \\
&+ a_s^3 S_\varepsilon^3 \left\{\frac{1}{\varepsilon^3}\left[\frac{1}{6}\left(\gamma_{qq,0}^3 + 2\gamma_{qq,0}\gamma_{qg,0}\gamma_{gq,0} + \gamma_{qg,0}\gamma_{gg,0}\gamma_{gq,0}\right) + \beta_0\left(\gamma_{qq,0}^2 + \gamma_{qg,0}\gamma_{gq,0}\right)\right.\right. \\
&\left. + \frac{4}{3}\beta_0^2\gamma_{qq,0}\right] + \frac{1}{\varepsilon^2}\left[\frac{1}{2}\gamma_{qq,0}\gamma_{qq,1} + \frac{1}{3}\gamma_{qg,0}\gamma_{gq,1} + \frac{1}{6}\gamma_{qg,1}\gamma_{gq,0} + \frac{2}{3}\left(\beta_0\gamma_{qq,1} + \beta_1\gamma_{qq,0}\right)\right] \\
&\left. + \frac{\gamma_{qq,2}}{3\varepsilon}\right\} \qquad (30) \\
Z_{qg}(N,a_s,\varepsilon) &= a_s S_\varepsilon \frac{\gamma_{qg,0}}{\varepsilon} + a_s^2 S_\varepsilon^2 \left\{\frac{1}{\varepsilon^2}\left[\frac{1}{2}\left(\gamma_{qg,0}\gamma_{gg,0} + \gamma_{qq,0}\gamma_{qg,0}\right) + \beta_0\gamma_{qg,0}\right] + \frac{1}{2\varepsilon}\gamma_{qg,1}\right\} \\
&+ a_s^3 S_\varepsilon^3 \left\{\frac{1}{\varepsilon^3}\left[\frac{1}{6}\left(\gamma_{qg,0}\gamma_{gg,0}^2 + \gamma_{qq,0}\gamma_{qg,0}\gamma_{gg,0} + \gamma_{qg,0}\gamma_{gq,0}\gamma_{qg,0}\right)\right.\right. \\
&\left. + \beta_0\left(\gamma_{qg,0}\gamma_{gg,0} + \gamma_{qq,0}\gamma_{qg,0}\right) + \frac{4}{3}\beta_0^2\gamma_{qg,0}\right] \\
&+ \frac{1}{\varepsilon^2}\left[\frac{1}{6}\left(\gamma_{qg,1}\gamma_{gg,0} + \gamma_{qq,1}\gamma_{qg,0} + 2\gamma_{qq,0}\gamma_{qg,1} + 2\gamma_{qg,0}\gamma_{gg,1}\right) + \frac{2}{3}\left(\beta_0\gamma_{qg,1} + \beta_1\gamma_{qg,0}\right)\right] \\
&\left. + \frac{\gamma_{qg,2}}{3\varepsilon}\right\} \qquad (31) \\
Z_{gq}(N,a_s,\varepsilon) &= a_s S_\varepsilon \frac{\gamma_{gq,0}}{\varepsilon} + a_s^2 S_\varepsilon^2 \left\{\frac{1}{\varepsilon^2}\left[\frac{1}{2}\left(\gamma_{gq,0}\gamma_{qq,0} + \gamma_{gg,0}\gamma_{gq,0}\right) + \beta_0\gamma_{gq,0}\right] + \frac{1}{2\varepsilon}\gamma_{gq,1}\right\} \\
&+ a_s^3 S_\varepsilon^3 \left\{\frac{1}{\varepsilon^3}\left[\frac{1}{6}\left(\gamma_{gq,0}\gamma_{qq,0}^2 + \gamma_{gg,0}\gamma_{gq,0}\gamma_{qq,0} + \gamma_{gq,0}\gamma_{qg,0}\gamma_{gq,0}\right)\right.\right. \\
&\left. + \beta_0\left(\gamma_{gq,0}\gamma_{qq,0} + \gamma_{gg,0}\gamma_{gq,0}\right) + \frac{4}{3}\beta_0^2\gamma_{gq,0}\right] \\
&+ \frac{1}{\varepsilon^2}\left[\frac{1}{6}\left(\gamma_{gq,1}\gamma_{qq,0} + \gamma_{gg,1}\gamma_{gq,0} + 2\gamma_{gg,0}\gamma_{gq,1} + 2\gamma_{gq,0}\gamma_{qq,1}\right) + \frac{2}{3}\left(\beta_0\gamma_{gq,1} + \beta_1\gamma_{gq,0}\right)\right] \\
&\left. + \frac{\gamma_{gq,2}}{3\varepsilon}\right\} \qquad (32)
\end{aligned}$$

$$
\begin{aligned}
Z_{gg}(N,a_s,\varepsilon) &= 1 + a_s S_\varepsilon \frac{\gamma_{gg,0}}{\varepsilon} + a_s^2 S_\varepsilon^2 \left\{ \frac{1}{\varepsilon^2} \left[\frac{1}{2} \left(\gamma_{gg,0}^2 + \gamma_{gq,0}\gamma_{qg,0} \right) + \beta_0 \gamma_{gg,0} \right] + \frac{1}{2\varepsilon} \gamma_{gg,1} \right\} \\
&+ a_s^3 S_\varepsilon^3 \left\{ \frac{1}{\varepsilon^3} \left[\frac{1}{6} \left(\gamma_{gg,0}^3 + 2\gamma_{gg,0}\gamma_{gq,0}\gamma_{qg,0} + \gamma_{gq,0}\gamma_{qg,0}\gamma_{gg,0} \right) + \beta_0 \left(\gamma_{gg,0}^2 + \gamma_{gq,0}\gamma_{qg,0} \right) \right. \right. \\
&\left. + \frac{4}{3}\beta_0^2 \gamma_{gg,0} \right] + \frac{1}{\varepsilon^2} \left[\frac{1}{2}\gamma_{gg,0}\gamma_{gg,1} + \frac{1}{3}\gamma_{gq,0}\gamma_{qg,1} + \frac{1}{6}\gamma_{gq,1}\gamma_{qg,0} + \frac{2}{3} \left(\beta_0 \gamma_{gg,1} + \beta_1 \gamma_{gg,0} \right) \right] \\
&\left. + \frac{\gamma_{gg,2}}{3\varepsilon} \right\} \qquad (33)
\end{aligned}
$$

The pure–singlet operator has the following Z–factor.

$$
\begin{aligned}
Z_{qq}^{\rm PS}(N,a_s,\varepsilon) &= a_s^2 S_\varepsilon^2 \left[\frac{1}{2\varepsilon^2} \gamma_{qg,0}\gamma_{gq,0} + \frac{1}{2\varepsilon} \gamma_{qq,1}^{\rm PS} \right] \\
&+ a_s^3 S_\varepsilon^3 \left[\frac{1}{6\varepsilon^3} \left(2\gamma_{qq,0}\gamma_{qg,0}\gamma_{gq,0} + \gamma_{qg,0}\gamma_{gg,0}\gamma_{gq,0} \right) + \frac{1}{6\varepsilon^2} \left(2\gamma_{qg,0}\gamma_{gq,1} + \gamma_{qg,1}\gamma_{gq,0} \right) \right. \\
&\left. + \frac{\gamma_{qq,2}^{\rm PS}}{3\varepsilon} \right] \qquad (34)
\end{aligned}
$$

The anomalous dimensions $\gamma_{ij,k}(N)$ are related to the splitting functions by

$$
\gamma_{ij,k}(N) = -\int_0^1 dz z^{N-1} P_{ij}^{(k)}(z) \ . \qquad (35)
$$

The renormalized operators are obtained absorbing $Z_{\rm NS}$, $Z_{ij,{\rm S}}$, and $Z_{qq}^{\rm PS}$, into the bare operators, resp. operator matrix elements.

3.4 Wave Function Renormalization

The external legs of the operator matrix elements are treated on–shell to be able to apply their factorization from the nucleon wave-functions in the light cone expansion as outlined above. Here the mass scale is set by a heavy quark mass. To the operator matrix elements also one-particle reducible diagrams contribute. If either the self-energy insertion on the external legs or the remainder diagram contain only massless lines, with the exception of the tree-level terms, the diagrams are vanishing since one of the factors has no scale. I.e. finite contributions are due to the self-energy insertions containing a massive line. The corresponding corrections are due to the massive contributions to the massless quark self–energy up to 3–loop order and the gluon self–energies up to 2–loop order. The former terms emerge in case of the flavor non–singlet terms $A_{qq,Q}^{{\rm NS}^{\rm l},(3)}$ and the latter in $A_{Qg}^{(3)}$, while the pure singlet contributions $A_{Qq}^{{\rm PS},(3)}$ obtain no corrections.

3.4.1 Massless External Quark Lines

The 2-loop correction reads

$$
\Sigma_{ij}^{(2)} = a_s^2 \delta_{ij} T_F C_F \left(\frac{m^2}{\mu^2} \right)^\varepsilon S_\varepsilon^2 \left\{ \frac{2}{\varepsilon} + \frac{5}{6} + \left[\frac{89}{72} + \frac{\zeta_2}{2} \right] \varepsilon + O(\varepsilon^2) \right\} \cdot i\not{p} \ . \qquad (36)
$$

At $O(a_s^2)$ this contribution implies, that the 1st moment of the non–singlet operator matrix element vanishes.

3.4.2 External Gluon Lines

The gluon vacuum polarization is given by

$$\Pi^{ab}_{\mu\nu}(q) \;=\; \left[-g_{\mu\nu}q^2 + q_\mu q_\nu\right]\Pi^{ab}(q^2)\;, \tag{37}$$

with a and b the color indices. The 1-loop and 2-loop corrections read

$$\Pi^{ab}_{(1)}(0) \;=\; -ia_s\delta^{ab}T_F S_\varepsilon \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon/2} \frac{4}{3}\left\{\frac{2}{\varepsilon} + \frac{\varepsilon}{4}\zeta_2 + O(\varepsilon^2)\right\} \tag{38}$$

$$\begin{aligned}\Pi^{ab}_{(2)}(0) \;=\; & -ia_s^2\delta^{ab}T_F S_\varepsilon^2 \left(\frac{\hat{m}^2}{\mu^2}\right)^{\varepsilon} \left\{C_F\left[\frac{12}{\varepsilon} + \frac{13}{3} + \left(\frac{35}{12} + 3\zeta_2\right)\varepsilon\right]\right. \\ & \left. + C_A\left[\frac{4}{\varepsilon^2} - \frac{5}{\varepsilon} - \left(\frac{13}{12} - \zeta_2\right) - \left(\frac{169}{144} + \frac{5}{4}\zeta_2 - \frac{\zeta_3}{3}\right)\varepsilon\right] + O(\varepsilon^2)\right\}\end{aligned} \tag{39}$$

The C_F-term can be compared with a corresponding contribution in the photon propagator, (180), before mass renormalization. At 2–loop order the diagrams u and v from [6] and the term $Z_{qg}^{-1,(1)}\hat{A}_{gg}^{(1)}$ combine to

$$\begin{aligned}\hat{A}_{Qg}^{(2)}\Big|_{u,v} + Z_{qg}^{-1,(1)}\hat{A}_{gg}^{(1)} \;&=\; -2\overline{a}_{Qg}^{(1)}\sum_{H=4}^{6}\beta_{0,H}\left(\frac{m_H^2}{\mu^2}\right)^{\varepsilon/2}\left(1 + \frac{\varepsilon^2}{8}\zeta_2\right) \\ &=\; T_F^2\frac{\zeta_2}{3}P_{qg}^{(0)}(N)\sum_{H=4}^{6}\left(\frac{m_H^2}{\mu^2}\right)^{\varepsilon/2}\left(1 + \frac{\varepsilon^2}{8}\zeta_2\right)\;,\end{aligned} \tag{40}$$

with

$$\beta_{0,H} = -\frac{4}{3}T_F\;. \tag{41}$$

(40) yields a finite contribution $\propto T_F^2$ in the $\overline{\rm MS}$ scheme. Our treatment differs from that in Ref. [6] as we do not include the mass effects of (40) into the running coupling, because we have chosen to define it in the $\overline{\rm MS}$–scheme. This is convenient for direct comparisons of the parton densities and the QCD–scale $\Lambda_{\rm QCD}$ measured in other analyzes of hard scattering cross sections.

3.5 Mass Factorization

The mass singularities are factored into the functions $\Gamma_{\rm NS}$, $\Gamma_{ij,\rm S}$ and $\Gamma_{qq,\rm PS}$, respectively. If all quarks were massless these functions were given by

$$\Gamma_{\rm NS} \;=\; Z_{\rm NS}^{-1} \tag{42}$$

$$\Gamma_{ij,\rm S} \;=\; Z_{ij,\rm S}^{-1} \tag{43}$$

$$\Gamma_{qq,\rm PS} \;=\; Z_{qq,\rm PS}^{-1}\;, \tag{44}$$

with

$$\Gamma_{\rm NS}(N,a_s,\varepsilon) \;=\; 1 - a_s S_\varepsilon\frac{\gamma_{\rm NS,0}}{\varepsilon} + a_s^2 S_\varepsilon^2\left[\frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{NS,0}^2 - \beta_0\gamma_{\rm NS,0}\right) - \frac{1}{2\varepsilon}\gamma_{\rm NS,1}\right] \tag{45}$$

$$\Gamma_{ij,\rm S}(N,a_s,\varepsilon) \;=\; \delta_{ij} - a_s S_\varepsilon\frac{\gamma_{ij,0}}{\varepsilon} + a_s^2 S_\varepsilon^2\left[\frac{1}{\varepsilon^2}\left(\frac{1}{2}\gamma_{ik,0}\gamma_{kj,0} - \beta_0\gamma_{ij,0}\right) - \frac{1}{2\varepsilon}\gamma_{ij,1}\right] \tag{46}$$

$$\Gamma_{qq,\rm PS}(N,a_s,\varepsilon) \;=\; -a_s^2 S_\varepsilon^2\left[\frac{1}{2\varepsilon^2}\gamma_{qg,0}\gamma_{gq,0} + \frac{1}{2\varepsilon}\gamma_{qq,\rm PS,1}\right]\;. \tag{47}$$

In the present calculation at least one quark line is massive in each diagram. Therefore the Γ–matrices (45–47) apply to the parts of the diagrams which contain massless lines only, which are at most 2–loop sub-graphs. The mass factorization is therefore different in various sub–classes of contributing Feynman diagrams. The functions $\Gamma_{\rm NS}, \Gamma_{ij,\rm S}$, and $\Gamma_{qq,\rm PS}$ do thus enter the renormalization of the operator matrix elements only in products with other functions. The singularities contained in $\Gamma_{\rm NS}, \Gamma_{ij,\rm S}$, and $\Gamma_{qq,\rm PS}$ are absorbed into the bare parton densities, which become scale–dependent in this way.

3.6 The renormalized operator matrix elements

The operator matrix element reads after charge and mass renormalization

$$\begin{aligned}\hat{A}_{ij} &= \delta_{ij} + a_s \hat{\hat{A}}_{ij}^{(1)} + a_s^2 \left[\hat{\hat{A}}_{ij}^{(2)} + \delta m_1 \frac{d}{dm} \hat{\hat{A}}_{ij}^{(1)} + \delta a_s^{(1)} \hat{\hat{A}}_{ij}^{(1)} \right] \\ &+ a_s^3 \left[\hat{\hat{A}}_{ij}^{(3)} + \delta m_1 \frac{d}{dm} \hat{\hat{A}}_{ij}^{(2)} + \delta m_2 \frac{d}{dm} \hat{\hat{A}}_{ij}^{(1)} + \delta m_1^2 \frac{1}{2} \frac{d^2}{dm^2} \hat{\hat{A}}_{ij}^{(1)} + \delta a_s^{(2)} \hat{\hat{A}}_{ij}^{(1)} + \delta a_s^{(1)} \hat{\hat{A}}_{ij}^{(2)} \right] . \end{aligned} \tag{48}$$

The renormalized operator matrix elements are obtained removing the ultraviolet singularities and collinear singularities of the operator matrix elements,

$$A_{ij} = Z_{ik}^{-1} \hat{A}_{kl} \Gamma_{lj}^{-1} = \delta_{ij} + a_s A_{ij}^{(1)} + a_s^2 A_{ij}^{(2)} + a_s^3 A_{ij}^{(3)} . \tag{49}$$

Here self energy insertions containing massive lines in the external legs of the operator matrix elements have to be kept.

4 The $O(\varepsilon)$ Contributions

The $O(\varepsilon)$ contributions to $A_{Qg}, A_{Qq}^{\rm PS}$ and $A_{qq,Q}^{\rm NS}$ at $O(a_s^2)$ contribute to these quantities at $O(a_s^3)$ in combination with the various single pole terms emerging at 1–loop, as outlined in Section 3. The diagrams to be evaluated are shown in [6, 7]. The results for the individual un-renormalized diagrams in $O(\varepsilon)$ are given in Appendix A. As outlined before in Ref. [7], we calculate the massive operator matrix elements performing the Feynman-parameter integrals directly, i.e., without using the integration-by-parts method [39] which was applied in [6] up to the terms $O(\varepsilon^0)$ before. We obtain representations in terms of generalized hypergeometric functions [40], which may be expanded to the desired order in ε. With increasing depth in ε, more and more involved nested infinite sums are obtained, which depend on the Mellin–parameter N. These sums can be summed applying analytic methods, as integral representations, and general summation methods, as encoded in the `Sigma` package [18]. We applied both methods to evaluate the sums which emerge at $O(\varepsilon)$. The underlying algorithms of `Sigma` are based on a refined version [41] of Karr's difference field theory of $\Pi\Sigma$-fields [42]. In this algebraic setting one can represent completely algorithmically indefinite nested sums and products without introducing any algebraic relations between them. Note that this general class of sum expressions covers as special cases, e.g., the harmonic sums [15, 19] or generalized nested harmonic sums cf. [43–46]. Given such an optimal representation, by introducing as less sums as possible, various summation principles are available in `Sigma`. In this article we applied the following strategy which has been generalized from the the hypergeometric case [47] to the $\Pi\Sigma$-field setting.

1. Given a definite sum that involves an extra parameter N, for typical sums see the Appendix B. We compute a recurrence relation in N that is fulfilled by the input sum. The underlying difference field algorithms exploit Zeilberger's creative telescoping principle [47].

2. Then we solve the derived recurrence in terms of the so-called d'Alembertian solutions [47]. Since this class covers the harmonic sums, we find all solutions in terms of harmonic sums.

3. Taking the initial values of the original input sum, we can combine the solutions found from step 2 in order to arrive at a closed form representation in terms of harmonic sums.

A detailed example for the sum (120) with all its computation steps has been carried out in [48]. In Appendix B we present the details for the calculation of a further example, Eq. (151), in section (B.8).

The results for new sums contributing are listed in Appendix B. In the calculation also more well-known sums are occurring which were found before in [7] or can be easily solved using the `FORM`–code [49] `summer` [15].

The $O(\varepsilon)$ contribution to $A_{Qg}^{(2)}$ reads :

$$
\begin{aligned}
\overline{a}_{Qg}^{(2)}(N) &= T_F C_F \left\{ \frac{N^2+N+2}{N(N+1)(N+2)} \Big(16 S_{2,1,1} - 8 S_{3,1} - 8 S_{2,1} S_1 + 3 S_4 - \frac{4}{3} S_3 S_1 - \frac{1}{2} S_2^2 - S_2 S_1^2 \right. \\
&- \frac{1}{6} S_1^4 + 2 \zeta_2 S_2 - 2 \zeta_2 S_1^2 - \frac{8}{3} \zeta_3 S_1 \Big) - 8 \frac{N^2-3N-2}{N^2(N+1)(N+2)} S_{2,1} + \frac{2}{3} \frac{3N+2}{N^2(N+2)} S_1^3 \\
&+ \frac{2}{3} \frac{3N^4+48N^3+43N^2-22N-8}{N^2(N+1)^2(N+2)} S_3 + 2 \frac{3N+2}{N^2(N+2)} S_2 S_1 + 4 \frac{S_1}{N^2} \zeta_2 \\
&+ \frac{2}{3} \frac{(N^2+N+2)(3N^2+3N+2)}{N^2(N+1)^2(N+2)} \zeta_3 + \frac{P_1}{N^3(N+1)^3(N+2)} S_2 \\
&+ \frac{N^4-5N^3-32N^2-18N-4}{N^2(N+1)^2(N+2)} S_1^2 - \frac{5N^6+15N^5+36N^4+51N^3+25N^2+8N+4}{N^3(N+1)^3(N+2)} \zeta_2 \\
&\left. - 2 \frac{2N^5-2N^4-11N^3-19N^2-44N-12}{N^2(N+1)^3(N+2)} S_1 - \frac{P_2}{N^5(N+1)^5(N+2)} \right\} \\
&+ T_F C_A \left\{ \frac{N^2+N+2}{N(N+1)(N+2)} \right. \\
&\times \Big(16 S_{-2,1,1} - 4 S_{2,1,1} - 8 S_{-3,1} - 8 S_{-2,2} - 4 S_{3,1} - \frac{2}{3} \beta''' + 9 S_4 \\
&- 16 S_{-2,1} S_1 + \frac{40}{3} S_1 S_3 + 4 \beta'' S_1 - 8 \beta' S_2 + \frac{1}{2} S_2^2 - 8 \beta' S_1^2 + 5 S_1^2 S_2 + \frac{1}{6} S_1^4 - \frac{10}{3} S_1 \zeta_3 \\
&- 2 S_2 \zeta_2 - 2 S_1^2 \zeta_2 - 4 \beta' \zeta_2 - \frac{17}{5} \zeta_2^2 \Big) + \frac{4(N^2-N-4)}{(N+1)^2(N+2)^2} \Big(-4 S_{-2,1} + \beta'' - 4 \beta' S_1 \Big) \\
&- \frac{16}{3} \frac{N^5+10N^4+9N^3+3N^2+7N+6}{(N-1)N^2(N+1)^2(N+2)^2} S_3 + 2 \frac{3N^3-12N^2-27N-2}{N(N+1)^2(N+2)^2} S_2 S_1 \\
&- \frac{2}{3} \frac{N^3+8N^2+11N+2}{N(N+1)^2(N+2)^2} S_1^3 - 8 \frac{N^2+N-1}{(N+1)^2(N+2)^2} \zeta_2 S_1 \\
&- \frac{2}{3} \frac{9N^5-10N^4-11N^3+68N^2+24N+16}{(N-1)N^2(N+1)^2(N+2)^2} \zeta_3 + 8 \frac{N^4+2N^3+7N^2+22N+20}{(N+1)^3(N+2)^3} \beta'
\end{aligned}
$$

$$-\frac{P_3}{(N-1)N^3(N+1)^3(N+2)^3}S_2 - \frac{2P_4}{(N-1)N^3(N+1)^3(N+2)^2}\zeta_2$$

$$-\frac{P_5}{N(N+1)^3(N+2)^3}S_1^2 + \frac{2P_6}{N(N+1)^4(N+2)^4}S_1$$
$$-\frac{2P_7}{(N-1)N^5(N+1)^5(N+2)^5}\Bigg\} . \tag{50}$$

Here the argument N of the harmonic sums, and $(N+1)$ in the function

$$\beta(N) = \frac{1}{2}\left[\psi\left(\frac{N+1}{2}\right) - \psi\left(\frac{N}{2}\right)\right] \tag{51}$$
$$S_{-1}(N) = (-1)^N\beta(N+1) - \ln(2) \tag{52}$$

and in the polynomials $P_i(N)$ was omitted as well as the factor

$$S_\varepsilon^2 a_s^2 \left(\frac{m^2}{\mu^2}\right)^\varepsilon . \tag{53}$$

In the gluon and pure–singlet case we did not write the overall factor

$$\frac{1+(-1)^N}{2} .$$

It does not emerge generically in the non–singlet case. In accordance with the light–cone expansion only even integer moments contribute in the present case. The polynomials in Eq. (50) are

$$P_1 = 3N^6 + 30N^5 + 15N^4 - 64N^3 - 56N^2 - 20N - 8 , \tag{54}$$
$$P_2 = 24N^{10} + 136N^9 + 395N^8 + 704N^7 + 739N^6 + 407N^5 + 87N^4 + 27N^3 + 45N^2 + 24N + 4 ,$$
$$P_3 = N^9 + 21N^8 + 85N^7 + 105N^6 + 42N^5 + 290N^4 + 600N^3 + 456N^2 + 256N + 64 \tag{55}$$
$$P_4 = (N^3 + 3N^2 + 12N + 4)(N^5 - N^4 + 5N^2 + N + 2) , \tag{56}$$
$$P_5 = N^6 + 6N^5 + 7N^4 + 4N^3 + 18N^2 + 16N - 8 , \tag{57}$$
$$P_6 = 2N^8 + 22N^7 + 117N^6 + 386N^5 + 759N^4 + 810N^3 + 396N^2 + 72N + 32 , \tag{58}$$
$$P_7 = 4N^{15} + 50N^{14} + 267N^{13} + 765N^{12} + 1183N^{11} + 682N^{10} - 826N^9 - 1858N^8 \tag{59}$$
$$-1116N^7 + 457N^6 + 1500N^5 + 2268N^4 + 2400N^3 + 1392N^2 + 448N + 64 . \tag{60}$$

The flavor non-singlet and pure-singlet contributions read :

$$\overline{a}_{qq,Q}^{\mathrm{NS},(2)} = T_F C_F \Bigg\{ \frac{4}{3}S_4 + \frac{4}{3}S_2\zeta_2 - \frac{8}{9}S_1\zeta_3 - \frac{20}{9}S_3 - \frac{20}{9}S_1\zeta_2 + 2\frac{3N^2+3N+2}{9N(N+1)}\zeta_3 + \frac{112}{27}S_2$$
$$+\frac{3N^4+6N^3+47N^2+20N-12}{18N^2(N+1)^2}\zeta_2 - \frac{656}{81}S_1 + \frac{P_8}{648N^4(N+1)^4}\Bigg\} . \tag{61}$$
$$P_8 = 1551N^8 + 6204N^7 + 15338N^6 + 17868N^5 + 8319N^4$$
$$+944N^3 + 528N^2 - 144N - 432 . \tag{62}$$

$$\overline{a}_{Qq}^{\rm PS,(2)} = T_F C_F \Biggl\{ -2 \frac{(5N^3+7N^2+4N+4)(N^2+5N+2)}{(N-1)N^3(N+1)^3(N+2)^2} \Bigl(2S_2+\zeta_2\Bigr) - \frac{4}{3} \frac{(N^2+N+2)^2}{(N-1)N^2(N+1)^2(N+2)} \Bigl(3S_3+\zeta_3\Bigr) + 2 \frac{P_9}{(N-1)N^5(N+1)^5(N+2)^4} \Biggr\}. \tag{63}$$

$$P_9 = 5N^{11}+62N^{10}+252N^9+374N^8-400N^6+38N^7-473N^5 -682N^4-904N^3-592N^2-208N-32\ . \tag{64}$$

The harmonic sums contributing to the individual diagrams, see Appendix A, are listed in Table 1.

Table 1: Complexity of the results in Mellin space for the individual diagrams in the unpolarized case, cf. [7], up to $O(\varepsilon)$

Diagram	S_1	S_2	S_3	S_4	S_{-2}	S_{-3}	S_{-4}	$S_{2,1}$	$S_{-2,1}$	$S_{-2,2}$	$S_{3,1}$	$S_{-3,1}$	$S_{2,1,1}$	$S_{-2,1,1}$
A		+	+											
B	+	+	+	+				+			+		+	
C		+	+											
D	+	+	+					+						
E	+	+	+					+						
F	+	+	+	+				+					+	
G	+	+	+					+						
H	+	+	+					+						
I	+	+	+	+	+	+	+	+	+	+	+	+	+	+
J		+	+											
K		+	+											
L	+	+	+	+				+			+		+	
M		+	+											
N	+	+	+	+	+	+	+	+	+	+	+	+	+	+
O	+	+	+	+				+			+		+	
P	+	+	+	+				+			+		+	
S		+	+											
T		+	+											
PS_a		+	+											
PS_b		+	+											
NS_a														
NS_b	+	+	+	+										

Here we have already made use of the algebraic relations [50]. Moreover, two of the sums, $S_{-2,2}(N)$ and $S_{3,1}(N)$, can be related by structural relations [51] to other harmonic sums, i.e., they lie in corresponding equivalence classes and may be obtained by either rational argument

relations and/or differentiation w.r.t. N. Reference to these equivalence classes is useful since the representation of these sums for $N \epsilon \mathbf{C}$ needs not to be derived newly, except of differentiation which is easily carried out. Therefore the two–loop massive operator matrix elements to $O(\varepsilon)$ depend on six basic harmonic sums.

diagram/order	$1/\varepsilon^2$	$1/\varepsilon$	1	ε	ε^2
B N = 2	−8	4.66666	−8.82690	2.47728	−5.69523
N = 6	−7.73333	0.81936	−8.89777	−1.84111	−7.25674
C N = 2	−4	19.8	−3.61715	17.33108	3.26445
N = 6	−1.33333	8.26984	−1.34024	7.12612	1.38782
D N = 2	−8	7.86666	−6.34542	4.71236	−2.18586
N = 6	−2.66666	−0.69523	−2.60657	−1.74990	−2.37611
E N = 2	8.88889	−11.2593	9.82824	−12.8921	2.39145
N = 6	2.93878	−4.24257	3.39094	−4.3892	0.826978
F N = 2	2.66667	−4.88889	9.1707	−1.2618	8.10105
N = 6	1.65714	−3.43645	6.12836	−0.81895	5.43478
G N = 2	2.66666	−9.55555	4.59662	−8.92015	1.07313
N = 6	0.57142	−2.00204	1.04814	−1.89142	0.32219
H N = 2	−2.66666	3.55555	−3.76328	4.57782	−2.02934
N = 6	−0.57143	0.83061	−0.9478	1.08896	−0.55443
I N = 2	0	0	0	0	0
N = 6	$0.34285\,C_A$ $+0.C_F$	$-0.38979\,C_A$ $+0.30793\,C_F$	$0.45862\,C_A$ $-0.00949\,C_F$	$-0.33621\,C_A$ $+0.32243\,C_F$	$0.27344\,C_A$ $+0.10405\,C_F$
L N = 2	22.22222	−8.07407	21.63853	−1.09400	14.38017
N = 6	9.42675	0.69179	9.99619	4.12879	8.49503
M N = 2	−0.44444	−1.66666	−0.25375	−2.19775	−0.72592
N = 6	0.09977	−0.21941	0.12862	−0.23387	0.03250
N N = 2	5.77778	−1.70370	4.24641	−0.06679	2.27892
N = 6	4.26462	0.17238	4.61023	1.71768	3.87767
O N = 2	−4.44444	3.14815	−4.96659	2.01274	−3.0498
N = 6	−1.03605	0.56098	−1.12332	0.27406	−0.73034

Table 2: Numerical values for the moments $N = 2, 6$ for the the expansion of the un-renormalized matrix element A_{Qg}^2 for the terms $O(1/\varepsilon^2)$ to $O(\varepsilon^2)$ for individual diagrams.

In the complex Mellin-N plane these functions, up to more simple terms due to the soft- and virtual corrections, are meromorphic functions with poles at the non–positive integers, which

possess both an analytic regular asymptotic representation and recursion relations, through which they may be calculated. To apply the results obtained in the present calculation in Mellin space in a QCD–analysis of deeply inelastic structure functions, their scale evolution is first evaluated in Mellin space, incorporating the heavy flavor Wilson coefficients for complex values of N. This requires analytic continuations of the corresponding harmonic sums as worked out in [52]. The result in x–space is obtained by a single, fast numeric Mellin-inversion performed by a contour integral around the singularities of the problem located at the real axis left to some value r. In case one wants to include small–x resummations as well, this can be done in a similar way, see [53].

We performed an independent check on our calculation evaluating fixed moments in N for the un-renormalized diagrams using the Mellin-Barnes method [54, 55]. Here we use an extension of a method developed for massless propagators in [56] to massive on–shell operator matrix elements [57]. The Mellin-Barnes integrals are evaluated numerically using the package `MB` [58]. In Table 2, we present the moments $N = 2$ and $N = 6$ for the more difficult two–loop diagrams, cf. [7], for the $O(1/\varepsilon^2)$ to the $O(\varepsilon^2)$ terms.

A further test for the Abelian part of the first moment of the un-renormalized massive operator matrix element $A_{Qg}^{(2)}$ after mass renormalization, i.e., the term $\propto T_F C_F$, can be performed after analytic continuation of even values of N. This term is related to a corresponding contribution of the on–shell photon polarization function as noted in [6]. We apply this method to the $O(\varepsilon)$ term in Appendix C and find agreement.

5 Conclusions

We calculated the $O(\varepsilon)$ contributions to the massive operator matrix elements at $O(a_s^2)$ which contribute to the heavy flavor Wilson coefficients in deeply inelastic scattering to the non power-suppressed contributions. In the renormalization of the heavy flavor Wilson coefficients to 3–loop order they contribute together with with the single pole terms at $O(a_s)$. These terms, and the $O(a_s^2\varepsilon)$ contributions to the operator matrix element $A_{gg}(N)$ to be published soon, form all but the constant terms of the 3–loop heavy flavor unpolarized operator matrix elements needed to describe the 3–loop heavy flavor Wilson coefficients, together with the known 3–loop massless Wilson coefficients [11], in the region $Q^2 \gg m^2$. In the calculation, we made use of the representation of the Feynman–parameter integrals in terms of generalized hypergeometric functions in a direct calculation, without applying the integration-by-parts method. The ε–expansion leads to new infinite sums which had to be solved by analytic and advanced algebraic methods. We checked our results for finite values of N, using the Mellin-Barnes method, and for a series of diagrams by a second program. Here, the calculation can be extended to higher corrections in ε. For $N = 1$, one may compare in addition the terms $\propto T_F C_F$ in $\overline{a}_{Qg}^{(2)}$ with the corresponding contribution in the 2–loop on–shell photon propagator. The terms $\overline{a}^{(2)}(N)$ can be expressed in terms of polynomials of the basic nested harmonic sums up to weight $\mathsf{w} = 4$ and derivatives thereof. They belong to the complexity-class of the general two-loop Wilson coefficients or hard scattering cross sections in massless QED and QCD found for space– and time–like unpolarized and polarized anomalous dimensions, massless Wilson coefficients for deeply inelastic scattering, parton fragmentation, the Drell–Yan process, hadronic Higgs– and pseudoscalar Higgs production in the heavy mass limit as well as the soft- and virtual contribution to Bhabha-scattering, cf. [60], and are described by six basic functions and their derivatives in Mellin space. Their analytic continuation to complex values of N is known in explicit form.

The package `Sigma` [18] proved to be a useful tool to solve the sums occurring in the present problem and was extended accordingly. One advantage to seek for solutions of the recurrences emerging in $\Pi\Sigma$-fields consists in finding irreducible structures for the representation. In the present calculation these were nested harmonic sums. In even more complicated single scale problems in higher orders, this needs not to be the case. The new basis elements, however, would be uniquely found applying the present procedure.

A The $O(\varepsilon)$ Terms for the Individual Diagrams

In the following we list the results for the individual diagrams for comparisons and to illustrate the analytic structures emerging in the calculation. The calculation is performed in Feynman gauge. Again we suppress the factor (53) and the argument N in the sums and polynomials.

$$\overline{A}_a^{Qg} = T_F C_F \left\{ 4\frac{3S_3+\zeta_3}{3N^2(N+1)} + 2\frac{2N^3-N-2}{N^3(N+1)^2(N+2)}\Big(2S_2+\zeta_2\Big) - \frac{2\hat{P}_1}{N^5(N+1)^4(N+2)^3} \right\} , \quad (65)$$

$$\hat{P}_1 = 2N^9 - 16N^8 - 89N^7 - 166N^6 - 135N^5 - 6N^4 + 85N^3 + 94N^2 + 44N + 8 \; .$$

$$\begin{aligned}\overline{A}_b^{Qg} = T_F C_F \Bigg\{ & \frac{1}{N}\Big(8S_{2,1,1} - 8S_{3,1} + 11S_4 - 8S_{2,1}S_1 - \frac{4}{3}S_3S_1 + \frac{7}{2}S_2^2 - S_2S_1^2 - \frac{1}{6}S_1^4 + 6S_2\zeta_2 \\ & -2S_1^2\zeta_2 - \frac{8}{3}S_1\zeta_3 + \frac{8}{3}\zeta_3\Big) + \frac{N^2+7N+2}{N(N+1)(N+2)}\Big(8S_{2,1} + 2S_2S_1 + \frac{2}{3}S_1^3 + 4S_1\zeta_2\Big) \\ & -4\frac{N^5+3N^4+19N^3+37N^2+16N+4}{N^2(N+1)^2(N+2)^2}S_2 - 4\frac{N^3+9N^2+8N+4}{N^2(N+2)^2}S_1^2 \\ & -8\frac{N^2+5N+2}{N(N+1)(N+2)}\zeta_2 + \frac{4}{3}\frac{N^2-17N+2}{N(N+1)(N+2)}S_3 + \frac{16\hat{P}_2}{N^2(N+1)^3(N+2)^3}S_1 \\ & -\frac{16\hat{P}_3}{N(N+1)^4(N+2)^3}\Bigg\} , \end{aligned} \quad (66)$$

$$\hat{P}_2 = N^7 + 14N^6 + 65N^5 + 153N^4 + 197N^3 + 134N^2 + 44N + 8 \; ,$$

$$\hat{P}_3 = 2N^7 + 27N^6 + 130N^5 + 306N^4 + 385N^3 + 266N^2 + 100N + 16 \; .$$

$$\begin{aligned}\overline{A}_c^{Qg} = T_F C_F \Bigg\{ & \frac{2}{N}\Big(5S_3 - \frac{1}{3}\zeta_3\Big) - 2\frac{7N^3+29N^2+15N+2}{N^2(N+1)(N+2)}S_2 \\ & +\frac{13N^4+82N^3+82N^2+N-6}{N^2(N+1)(N+2)(N+3)}\zeta_2 + \frac{\hat{P}_4}{N^4(N+1)^3(N+2)^3(N+3)}\Bigg\} , \end{aligned} \quad (67)$$

$$\begin{aligned}\hat{P}_4 = {} & 32N^{10} + 448N^9 + 2177N^8 + 5123N^7 + 6312N^6 + 3863N^5 + 902N^4 \\ & +9N^3 - 74N^2 - 68N - 24 \; . \end{aligned}$$

$$\begin{aligned}\overline{A}_d^{Qg} = T_F C_F \Bigg\{ & \frac{1}{N}\Big(-4S_{2,1} - \frac{2}{3}S_3 - S_2S_1 - \frac{1}{3}S_1^3 - 2S_1\zeta_2 - \frac{4}{3}\zeta_3\Big) \\ & +\frac{N^4+8N^3+43N^2+36N+12}{N^2(N+1)^2(N+2)}\Big(S_2+S_1^2\Big) + 2\frac{N^3+10N^2+59N+42}{N(N+1)(N+2)(N+3)}\zeta_2 \\ & -\frac{4\hat{P}_5}{N^2(N+1)^3(N+2)^2}S_1 + \frac{4\hat{P}_6}{N(N+1)^4(N+2)^3(N+3)}\Bigg\} , \end{aligned} \quad (68)$$

$$\hat{P}_5 = N^6 + 8N^5 + 79N^4 + 207N^3 + 205N^2 + 96N + 20 \; ,$$

$$\hat{P}_6 = 2N^8 + 24N^7 + 262N^6 + 1371N^5 + 3514N^4 + 4775N^3 + 3544N^2 + 1404N + 240 \; .$$

$$\begin{aligned}\overline{A}_e^{Qg} = T_F \left[C_F - \frac{C_A}{2}\right] \Bigg\{ & -2\frac{N+2}{N(N+1)}\Big(2S_{2,1} + S_1\zeta_2\Big) - \frac{2}{3}\frac{13N^4+60N^3+111N^2+4N-36}{N(N+1)^2(N+2)(N+3)}S_3 \\ & -\frac{1}{3}\frac{N^3-N^2-8N-36}{N(N+1)(N+2)(N+3)}\Big(3S_2S_1 + S_1^3\Big) + \frac{4}{3}\frac{N+3}{(N+1)^2}\zeta_3 - 2\frac{3N^3+9N^2+12N+4}{N(N+1)^3(N+2)}\zeta_2 \end{aligned}$$

$$+\frac{\hat{P}_7}{N^2(N+1)^3(N+2)(N+3)}S_2+\frac{4N^5+11N^4+15N^3-86N^2-92N-24}{N^2(N+1)^2(N+2)(N+3)}S_1^2$$
$$-2\frac{\hat{P}_8}{N^2(N+1)^3(N+2)^2(N+3)}S_1-2\frac{\hat{P}_9}{N^3(N+1)^5(N+2)^3(N+3)}\Bigg\}\;, \tag{69}$$

$$\hat{P}_7 = 20N^6+119N^5+290N^4+105N^3-290N^2-212N-24\;,$$
$$\hat{P}_8 = 8N^7+62N^6+181N^5+127N^4-226N^3-404N^2-296N-96\;,$$
$$\hat{P}_9 = 38N^{10}+394N^9+1775N^8+4358N^7+6323N^6+5788N^5+3626N^4+1462N^3$$
$$+100N^2-184N-48\;.$$

$$\overline{A}_f^{Qg} = T_F\left[C_F-\frac{C_A}{2}\right]\Bigg\{\frac{4}{N}\Big(2S_{2,1,1}-2S_4-S_2^2-\zeta_2S_2\Big)+\frac{16(S_1-1)\zeta_3}{3(N+1)(N+2)}$$
$$-8\frac{2N^2-5N-2}{N^2(N+1)(N+2)}S_{2,1}+\frac{4}{3}\frac{26N^2-33N-10}{N^2(N+1)(N+2)}S_3$$
$$+\frac{2}{3}\frac{2N^2-3N+2}{N^2(N+1)(N+2)}\Big(3S_2S_1+S_1^3\Big)+4\frac{5N+2}{N^2(N+1)(N+2)}S_1\zeta_2$$
$$-2\frac{2N^3+15N^2+12N-4}{N(N+1)^2(N+2)^2}S_1^2+2\frac{14N^3+85N^2+132N+52}{N(N+1)^2(N+2)^2}S_2$$
$$+4\frac{2N^5+18N^4+25N^3+10N^2+44N+56}{N(N+1)^3(N+2)^3}S_1-\frac{8\zeta_2}{(N+1)^2(N+2)}$$
$$-8\frac{6N^5+52N^4+178N^3+309N^2+264N+84}{(N+1)^4(N+2)^3}\Bigg\}\;. \tag{70}$$

$$\overline{A}_g^{Qg} = T_FC_F\Bigg\{\frac{12S_{2,1}-58S_3+3S_2S_1+S_1^3+6\zeta_2S_1+8\zeta_3}{3(N+1)(N+2)}+\frac{(9N+8)(5N^2+9N-1)}{N(N+1)^2(N+2)^2}S_2$$
$$-\frac{3N^3+31N^2+45N+8}{N(N+1)^2(N+2)^2}S_1^2-2\frac{17N^2+47N+28}{(N+1)^2(N+2)^2}\zeta_2$$
$$+2\frac{6N^5+104N^4+376N^3+514N^2+277N+48}{N(N+1)^3(N+2)^3}S_1-\frac{2\hat{P}_{10}}{(N+1)^4(N+2)^4}\Bigg\}\;, \tag{71}$$

$$\hat{P}_{10} = 74N^6+722N^5+2697N^4+4960N^3+4700N^2+2143N+368\;.$$

$$\overline{A}_h^{Qg} = T_F\left[C_F-\frac{C_A}{2}\right]\Bigg\{\frac{4(N+3)}{N(N+1)(N+2)}\Big(2S_{2,1}+S_1\zeta_2\Big)-\frac{4}{3}\frac{N^2-26N+9}{N(N+1)(N+2)(N+3)}S_3$$
$$-\frac{2}{3}\frac{N^2-2N+9}{N(N+1)(N+2)(N+3)}\Big(3S_2S_1+S_1^3\Big)-\frac{8\zeta_3}{3(N+1)(N+2)}$$
$$-2\frac{N^2+7N+8}{(N+1)^2(N+2)^2}\zeta_2-\frac{N^4+115N^3+335N^2+265N+84}{N(N+1)^2(N+2)^2(N+3)}S_2$$
$$+\frac{7N^4+N^3-31N^2-37N-36}{N(N+1)^2(N+2)^2(N+3)}S_1^2$$
$$-\frac{2\hat{P}_{11}}{N(N+1)^3(N+2)^3(N+3)}S_1+\frac{2\hat{P}_{12}}{(N+1)^4(N+2)^4(N+3)}\Bigg\}\;, \tag{72}$$

$$\hat{P}_{11} = 10N^6+38N^5-43N^4-533N^3-1267N^2-1269N-456\;,$$

$$
\begin{aligned}
\hat{P}_{12} &= 36N^7 + 344N^6 + 1287N^5 + 2143N^4 + 818N^3 - 2153N^2 - 2795N - 960 \ . \\
\overline{A}_i^{Qg} &= T_F C_A \Bigg\{ \frac{8}{N+2} \Big(4S_{-2,1,1} - 2S_{-3,1} - 2S_{-2,2} - 4S_{-2,1}S_1 + S_{-4} + 2S_{-3}S_1 \\
&+ 2S_{-2}S_2 + 2S_{-2}S_1^2 + S_{-2}\zeta_2 \Big) + 8\frac{N^2-N-4}{(N+1)(N+2)^2} \Big(2S_{-2,1} - S_{-3} - 2S_{-2}S_1 \Big) \\
&+ \frac{1}{(N+1)(N+2)} \Bigg(4(4N+7)S_{2,1,1} - 4(6N+7)S_{3,1} - 4(4N+5)S_{2,1}S_1 + \frac{32N+27}{2}S_4 \\
&+ \frac{2}{3}(36N+35)S_3S_1 - \frac{16N+25}{4}S_2^2 + \frac{16N+15}{2}S_2S_1^2 - \frac{1}{12}S_1^4 \\
&- S_1^2\zeta_2 + \frac{4}{3}S_1\zeta_3 + (4N+3)S_2\zeta_2 \Bigg) + 2\frac{N^3+9N^2+17N+8}{N(N+1)^2(N+2)^2}S_1\zeta_2 \\
&+ 4\frac{2N^4+N^3-N^2+9N+8}{N(N+1)^2(N+2)^2}S_{2,1} - \frac{2}{3}\frac{18N^4+3N^3-67N^2-39N+8}{N(N+1)^2(N+2)^2}S_3 \\
&- \frac{8N^4-3N^3-47N^2-29N+8}{N(N+1)^2(N+2)^2}S_2S_1 + \frac{1}{3}\frac{3N^3+7N^2-3N-8}{N(N+1)^2(N+2)^2}S_1^3 \\
&- \frac{4(N+4)\zeta_3}{3(N+1)(N+2)^2} + 8\frac{N^4+2N^3+7N^2+22N+20}{(N+1)^2(N+2)^3}S_{-2} + \frac{\hat{P}_{13}S_2}{N(N+1)^3(N+2)^3} \\
&- \frac{6N^5+40N^4+92N^3+94N^2+49N+16}{N(N+1)^3(N+2)^3}S_1^2 - 2\frac{2N^3+8N^2+19N+16}{(N+1)^2(N+2)^3}\zeta_2 \\
&+ \frac{2\hat{P}_{14}}{N(N+1)^4(N+2)^4}S_1 - \frac{2\hat{P}_{15}}{(N+1)^4(N+2)^5} \Bigg\} \\
&+ T_F C_F \Bigg\{ \frac{1}{(N+1)(N+2)} \Big(-32S_{2,1,1} + 16S_{3,1} - 6S_4 + \frac{8}{3}S_3S_1 + 16S_{2,1}S_1 \\
&+ S_2^2 + 2S_2S_1^2 + \frac{1}{3}S_1^4 - 4S_2\zeta_2 + 4S_1^2\zeta_2 + 32\zeta_2 + 224 \Big) - 16\frac{2S_{2,1}+S_1\zeta_2}{N(N+2)} \\
&- \frac{4}{3}\frac{3N-2}{N(N+1)(N+2)} \Big(3S_2S_1 + S_1^3 \Big) + \frac{16}{3}\frac{3N+1}{N(N+1)(N+2)}S_3 \\
&- 8\frac{2N^2+2N-1}{N(N+1)^2(N+2)}S_2 + 8\frac{3N^2+3N+1}{N(N+1)^2(N+2)}S_1^2 \\
&- 8\frac{11N^3+33N^2+38N+14}{N(N+1)^3(N+2)}S_1 \Bigg\} \ , \qquad (73) \\
\hat{P}_{13} &= 4N^6 + 10N^5 + 12N^4 + 8N^3 - 18N^2 - 37N - 16 \ , \\
\hat{P}_{14} &= 10N^7 + 114N^6 + 533N^5 + 1374N^4 + 2144N^3 + 2027N^2 + 1057N + 224 \ , \\
\hat{P}_{15} &= 20N^7 + 236N^6 + 1202N^5 + 3384N^4 + 5688N^3 + 5720N^2 + 3195N + 768 \ . \\
\overline{A}_j^{Qg} &= T_F C_A \Bigg\{ -\frac{2}{3}\frac{4N^2+4N-5}{N^2(N+1)^2} \Big(3S_3 + \zeta_3 \Big) + \frac{\hat{P}_{16}}{N^5(N+1)^5(N+2)^3} \\
&+ \frac{4N^5+22N^4+11N^3+13N^2+35N+10}{N^3(N+1)^3(N+2)} \Big(2S_2 + \zeta_2 \Big) \Bigg\} \ , \qquad (74)
\end{aligned}
$$

$$\hat{P}_{16} = 28N^{10} + 148N^9 + 342N^8 + 285N^7 - 212N^6 - 114N^5 + 1117N^4 + 1587N^3 + 826N^2 + 260N + 40 \; .$$

$$\overline{A}_k^{Qg} = T_F C_A \left\{ \frac{2}{3} \frac{3N^2 - 23N - 20}{(N-1)N(N+1)^2(N+2)} \Big(3S_3 + \zeta_3 \Big) - \frac{\hat{P}_{17}}{(N-1)N(N+1)^5(N+2)^4} \right.$$
$$\left. - \frac{10N^4 + 7N^3 + 51N^2 + 172N + 112}{(N-1)N(N+1)^3(N+2)^2} \Big(2S_2 + \zeta_2 \Big) \right\} , \tag{75}$$

$$\hat{P}_{17} = 14N^8 + 70N^7 + 96N^6 - 375N^5 - 1493N^4 - 1056N^3 + 2392N^2 + 4192N + 1792 \; . \tag{76}$$

$$\overline{A}_l^{Qg} = T_F C_A \left\{ \frac{1}{N} \Big(-4S_{2,1,1} + 4S_{3,1} + \frac{5}{2} S_4 + 4S_{2,1} S_1 + \frac{2}{3} S_3 S_1 + \frac{9}{4} S_2^2 + \frac{1}{2} S_2 S_1^2 + S_2 \zeta_2 + \frac{1}{12} S_1^4 \right.$$
$$\left. + S_1^2 \zeta_2 + \frac{4}{3} S_1 \zeta_3 \Big) + \frac{2}{N(N+1)} \Big(-4S_{2,1} - S_2 S_1 - \frac{1}{3} S_1^3 - 2S_1 \zeta_2 \Big) \right.$$
$$- \frac{2}{3} \frac{6N^3 + 5N^2 - 4N - 6}{N^2(N+1)^2} S_3 + \frac{8N^5 + 18N^4 + 11N^3 + N^2 + 6N + 4}{N^3(N+1)^3} S_2$$
$$- \frac{(N+2)(2N+1)}{N^2(N+1)^2} S_1^2 + 2 \frac{7N^3 + 15N^2 + 7N + 4}{N^2(N+1)^3} S_1 + \frac{2}{3} \frac{2N^3 + 5N^2 + 4N + 2}{N^2(N+1)^2} \zeta_3$$
$$\left. - \frac{\hat{P}_{18} \zeta_2}{N^3(N+1)^3(N+2)} - \frac{\hat{P}_{19}}{N^5(N+1)^5(N+2)} \right\} , \tag{77}$$

$$\hat{P}_{18} = 4N^6 + 30N^5 + 55N^4 + 38N^3 + 4N^2 - 10N - 4 \; ,$$

$$\hat{P}_{19} = 16N^{10} + 152N^9 + 454N^8 + 628N^7 + 447N^6 + 180N^5 + 52N^4 - 10N^3 - 28N^2 - 18N - 4 \; ,$$

$$\overline{A}_m^{Qg} = T_F C_A \left\{ \frac{2}{3} \frac{N^2 - 2N - 2}{N^2(N+1)^2} \Big(3S_3 + \zeta_3 \Big) - \frac{2N^5 + 11N^4 + 12N^3 + 2N^2 + 6N + 4}{N^3(N+1)^3(N+2)} \Big(2S_2 + \zeta_2 \Big) \right.$$
$$\left. - \frac{6N^8 + 28N^7 + 53N^6 + 30N^5 - 14N^4 + 2N^3 + 18N^2 + 14N + 4}{N^5(N+1)^5(N+2)} \right\} , \tag{78}$$

$$\overline{A}_n^{Qg} = T_F C_A \left\{ \frac{4(N-1)}{N(N+1)} \Big(-4S_{-2,1,1} + 2S_{-3,1} + 2S_{-2,2} - S_{-4} + 4S_{-2,1} S_1 - 2S_{-3} S_1 - 2S_{-2} S_2 \right.$$
$$\left. - 2S_{-2} S_1^2 - S_{-2} \zeta_2 \Big) + \frac{2N^2 + 3N + 2}{24N(N+1)(N+2)} \Big(S_1^4 + 12 S_1^2 \zeta_2 + 16 \zeta_3 S_1 \Big) \right.$$
$$- 2 \frac{6N^2 + 7N - 6}{N(N+1)(N+2)} \Big(S_{2,1,1} - S_{2,1} S_1 \Big) + 2 \frac{8N^2 + 9N - 10}{N(N+1)(N+2)} S_{3,1} - \frac{54N^2 + 97N - 10}{4N(N+1)(N+2)} S_4$$
$$- \frac{34N^2 + 33N - 74}{3N(N+1)(N+2)} S_3 S_1 + \frac{2N^2 - 37N - 78}{8N(N+1)(N+2)} S_2^2 - \frac{14N^2 + 13N - 34}{4N(N+1)(N+2)} S_2 S_1^2$$
$$- \frac{10N^2 + 21N + 6}{2N(N+1)(N+2)} S_2 \zeta_2 + 8 \frac{N^2 - N - 4}{(N+1)^2(N+2)} \Big(-2S_{-2,1} + S_{-3} + 2S_{-2} S_1 \Big)$$
$$- 2 \frac{5N^5 + 10N^4 - 20N^3 - 62N^2 - 40N - 8}{N^2(N+1)^2(N+2)^2} S_{2,1} - \frac{2N(N+3)}{3(N+1)^2(N+2)} \zeta_3$$
$$+ \frac{35N^5 + 66N^4 - 118N^3 - 294N^2 - 152N - 40}{3N^2(N+1)^2(N+2)^2} S_3$$
$$- \frac{N^5 + 6N^4 + 4N^3 - 30N^2 - 40N - 8}{N^2(N+1)^2(N+2)^2} \zeta_2 S_1$$

$$
\begin{aligned}
&+\frac{15N^5+10N^4-100N^3-98N^2+40N+8}{2N^2(N+1)^2(N+2)^2}S_2S_1\\
&-\frac{N^5+6N^4+4N^3-30N^2-40N-8}{6N^2(N+1)^2(N+2)^2}S_1^3-8\frac{N^4+2N^3+7N^2+22N+20}{(N+1)^3(N+2)^2}S_{-2}\\
&-\frac{\hat{P}_{20}S_2-\hat{P}_{21}S_1^2}{2N(N+1)^3(N+2)^3}+\frac{2N^4+11N^3+15N^2+12N+8}{(N+1)^3(N+2)^2}\zeta_2\\
&-\frac{\hat{P}_{22}S_1}{N(N+1)^4(N+2)^4}+\frac{\hat{P}_{23}}{(N+1)^5(N+2)^4}\Bigg\}\,, \qquad (79)
\end{aligned}
$$

$$
\begin{aligned}
\hat{P}_{20} &= 6N^6+36N^5+60N^4-99N^3-390N^2-316N-40\,,\\
\hat{P}_{21} &= 2N^6+20N^5+40N^4-45N^3-170N^2-100N+8\,,\\
\hat{P}_{22} &= 4N^8+50N^7+224N^6+544N^5+927N^4+1140N^3+712N^2-64N-208\,,\\
\hat{P}_{23} &= 8N^8+86N^7+370N^6+805N^5+807N^4-16N^3-772N^2-568N-96\,.
\end{aligned}
$$

$$
\begin{aligned}
\overline{A}_o^{Qg} &= T_FC_A\Bigg\{\frac{1}{2N(N+2)}\Big(8S_{2,1,1}-8S_{3,1}-5S_4-8S_1S_{2,1}-\frac{4}{3}S_3S_1-\frac{9}{2}S_2^2-S_2S_1^2\\
&-\frac{1}{6}S_1^4-2S_2\zeta_2-2S_1^2\zeta_2-\frac{8}{3}S_1\zeta_3\Big)+\frac{2N^2+9N+12}{2N(N+1)(N+2)^2}\Big(4S_{2,1}+S_2S_1+\frac{1}{3}S_1^3+2S_1\zeta_2\Big)\\
&-\frac{2}{3}\frac{N^2+7N+8}{(N+1)^2(N+2)^2}\zeta_3\\
&+\frac{1}{3}\frac{14N^3+41N^2+51N+36}{N(N+1)^2(N+2)^2}S_3-\frac{12N^5+124N^4+472N^3+817N^2+641N+176}{2N(N+1)^3(N+2)^3}S_2\\
&+\frac{4N^4+16N^3-4N^2-61N-48}{2N(N+1)^2(N+2)^3}S_1^2+\frac{N(11N^3+56N^2+92N+49)}{(N+1)^3(N+2)^3}\zeta_2\\
&-\frac{\hat{P}_{24}S_1}{N(N+1)^3(N+2)^4}+\frac{\hat{P}_{25}}{(N+1)^5(N+2)^5}\Bigg\}\,, \qquad (80)
\end{aligned}
$$

$$
\begin{aligned}
\hat{P}_{24} &= 16N^6+101N^5+194N^4+4N^3-421N^2-501N-192\,,\\
\hat{P}_{25} &= 62N^8+668N^7+3073N^6+7849N^5+12052N^4+11127N^3+5640N^2+1065N-128\,.
\end{aligned}
$$

$$
\begin{aligned}
\overline{A}_p^{Qg} &= T_FC_A\Bigg\{\frac{N-4}{2N(N+1)(N+2)}\Big(4S_{2,1,1}-4S_{3,1}-4S_{2,1}S_1-\frac{2}{3}S_3S_1-\frac{1}{2}S_2S_1^2-\frac{1}{12}S_1^4-S_1^2\zeta_2\\
&-\frac{4}{3}S_1\zeta_3\Big)+\frac{N^3-17N^2-41N-16}{2N(N+1)^2(N+2)^2}\Big(4S_{2,1}+S_2S_1+\frac{1}{3}S_1^3+2S_1\zeta_2\Big)\\
&+\frac{11N+20}{4N(N+1)(N+2)}S_4\\
&+\frac{7N+36}{8N(N+1)(N+2)}S_2^2+\frac{3N+4}{2N(N+1)(N+2)}S_2\zeta_2-\frac{1}{3}\frac{11N^3+17N^2-N+16}{N(N+1)^2(N+2)^2}S_3\\
&-\frac{2}{3}\frac{N+4}{(N+1)(N+2)^2}\zeta_3+\frac{10N^5+48N^4+122N^3+222N^2+213N+64}{2N(N+1)^3(N+2)^3}S_2\\
&+\frac{2N^5+48N^4+174N^3+242N^2+161N+64}{2N(N+1)^3(N+2)^3}S_1^2+\frac{4N^3+26N^2+51N+32}{(N+1)^2(N+2)^3}\zeta_2\\
&-\frac{\hat{P}_{26}S_1}{N(N+1)^4(N+2)^4}+\frac{\hat{P}_{27}}{(N+1)^4(N+2)^5}\Bigg\}\,, \qquad (81)
\end{aligned}
$$

$$\hat{P}_{26} = 8N^7 + 120N^6 + 595N^5 + 1538N^4 + 2432N^3 + 2419N^2 + 1329N + 256 \; ,$$
$$\hat{P}_{27} = 22N^7 + 266N^6 + 1360N^5 + 3826N^4 + 6400N^3 + 6376N^2 + 3515N + 832 \; .$$
$$\overline{A}_s^{Qg} = T_F C_A \left\{ -\frac{2}{3}\frac{3S_3+\zeta_3}{N^2(N+1)^2} + \frac{2N^3+N^2-3N-1}{N^3(N+1)^3}\Big(2S_2+\zeta_2\Big) + \frac{\hat{P}_{28}}{N^5(N+1)^5(N+2)^2}\right\} , \tag{82}$$
$$\hat{P}_{28} = 4N^9 + 8N^8 + 6N^7 + 35N^6 + 66N^5 - 6N^4 - 85N^3 - 61N^2 - 24N - 4 \; .$$
$$\overline{A}_t^{Qg} = T_F C_A \left\{ \frac{2}{3}\frac{N^2+3N+4}{(N-1)N(N+1)^2(N+2)}\Big(3S_3+\zeta_3\Big) - \frac{2N^4+5N^3-3N^2-20N-16}{(N-1)N(N+1)^3(N+2)^2}\Big(2S_2+\zeta_2\Big) - \frac{\hat{P}_{29}}{(N-1)N(N+1)^5(N+2)^4}\right\} , \tag{83}$$
$$\hat{P}_{29} = 2N^8 + 10N^7 + 28N^6 + 91N^5 + 213N^4 + 160N^3 - 248N^2 - 512N - 256 \; . \tag{84}$$
$$A_u^{Qg} = a_s^2 S_\varepsilon^2 \left\{ \frac{8}{3\varepsilon} T_F \Big(1+\frac{\zeta_2}{8}\varepsilon^2\Big) \sum_{i=1}^{3} \left(\frac{m_i^2}{\mu^2}\right)^{\varepsilon/2} \right\} \left\{ -8 T_F \left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} \left(\frac{1}{\varepsilon}\frac{N^2+3N+2}{N(N+1)(N+2)} - \frac{1}{(N+1)(N+2)} + \varepsilon\Big(\frac{1}{2(N+1)(N+2)} + \frac{\zeta_2}{8N}\Big)\right)\right\} , \tag{85}$$
$$A_v^{Qg} = a_s^2 S_\varepsilon^2 \left\{ \frac{8}{3\varepsilon} T_F \Big(1+\frac{\zeta_2}{8}\varepsilon^2\Big) \sum_{i=1}^{3} \left(\frac{m_i^2}{\mu^2}\right)^{\varepsilon/2} \right\} \left\{ 16 T_F \left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} \times \left(\frac{1}{\varepsilon} - \frac{1}{2} + \varepsilon\left(\frac{1}{4}+\frac{\zeta_2}{8}\right)\right)\frac{1}{(N+1)(N+2)}\right\} . \tag{86}$$

Note that for diagram u and v the sum runs over all heavy quark flavors.

The diagrams contributing to the pure singlet contributions yield

$$\overline{A}_a^{Qq} = T_F C_F \left\{ -\frac{4}{3}\frac{(N+2)(N-1)}{N^2(N+1)^2}\Big(3S_3+\zeta_3\Big) - 2\frac{5N^3-5N^2-16N-4}{N^3(N+1)^3(N+2)}\Big(2S_2+\zeta_2\Big) + \frac{2\hat{P}_{30}}{N^5(N+1)^5(N+2)^3}\right\} , \tag{87}$$
$$\hat{P}_{30} = 5N^9 + 25N^8 - 35N^7 - 229N^6 - 107N^5 + 481N^4 + 688N^3 + 360N^2 + 112N + 16 \; .$$
$$\overline{A}_b^{Qq} = T_F C_F \left\{ -\frac{32}{3}\frac{3S_3+\zeta_3}{(N-1)N(N+1)(N+2)} - 32\frac{2N+3}{(N-1)N(N+1)^2(N+2)^2}\Big(2S_2+\zeta_2\Big) + 32\frac{(2N+3)(N^4+6N^3+5N^2-12N-16)}{N(N-1)(N+1)^4(N+2)^4}\right\} . \tag{88}$$

The flavor non–singlet contributions are given by

$$\begin{aligned}
\overline{A}_a^{qq,Q} &= T_F C_F \left\{ -\frac{2}{9}\frac{(N+2)(N-1)}{N(N+1)}\zeta_3 - \frac{2}{9}\frac{N^4+2N^3-10N^2-5N+3}{N^2(N+1)^2}\zeta_2 \right. \\
&\left. -\frac{2}{81}\frac{\hat{P}_{31}}{N^4(N+1)^4} \right\}, \qquad (89) \\
\hat{P}_{31} &= 49N^8+196N^7-83N^6-533N^5-374N^4-59N^3-33N^2+9N+27. \\
\overline{A}_b^{qq,Q} &= T_F C_F \left\{ \frac{4}{3}S_4 + \frac{4}{3}S_2\zeta_2 - \frac{8}{9}S_1\zeta_3 - \frac{20}{9}S_3 - \frac{20}{9}S_1\zeta_2 + \frac{8}{9}\zeta_3 + \frac{112}{27}S_2 + \frac{8}{9}\zeta_2 \right. \\
&\left. -\frac{656}{81}S_1 + \frac{392}{81} \right\}, \qquad (90) \\
\overline{A}_c^{qq,Q} &= T_F C_F \left\{ -\frac{\zeta_2}{2} - \frac{89}{72} \right\}. \qquad (91)
\end{aligned}$$

B Infinite Sums

In this appendix we list a series of infinite sums which were needed in the present analysis and are newly calculated. In addition we made use of the sums in [7]. σ_1 is a symbol for $\sum_{k=1}^{\infty}(1/k)$ and the corresponding sums are divergent. The calculation was partly performed using integral representations, solving difference equations and using the summation package `Sigma`, see also [48].

B.1 Weighted Beta functions

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+2)^3} = (-1)^N\left[\frac{4S_{1,-2}(N+2)+2S_{-3}(N+2)+2\zeta_2S_1(N+2)+2\zeta_3}{N(N+1)(N+2)} + \frac{-6S_{-2}(N+2)-3\zeta_2}{N(N+1)(N+2)}\right] + \frac{1}{N(N+1)(N+2)^2}\ , \tag{92}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+3)^2} = 6(-1)^N\frac{2S_{-2}(N+3)+\zeta_2}{N(N+1)(N+2)(N+3)} + \frac{N^4+5N^3+13N^2+18N+13}{N(N+1)^2(N+2)^2(N+3)^2}\ , \tag{93}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+4)^2} = 24(-1)^N\frac{2S_{-2}(N+4)+\zeta_2}{N(N+1)(N+2)(N+3)(N+4)} + \frac{N^6+11N^5+54N^4+143N^3+213N^2+178N+100}{N(N+1)^2(N+2)^2(N+3)^2(N+4)^2}\ , \tag{94}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+1)^2} = \frac{-1+2N}{N} + (1-N)S_{1,2}(N) + \frac{-1+N+N^2}{N}S_2(N) + \left(\frac{1-N-N^2}{N} + (-1+N)S_1(N)\right)\zeta_2 + (1-N)\zeta_3 \tag{95}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+4)} = -\frac{-144+300N-415N^2+241N^3-63N^4+6N^5}{144N^2} + \frac{(N-1)(N-2)(N-3)(N-4)}{24}\left(\zeta_2-S_2(N)\right)\ . \tag{96}$$

B.2 Weighted Beta functions and harmonic sums

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{i+1}S_1(i) = (N-1)S_3(N-1)-(N-1)\zeta_3-S_2(N-1)+\zeta_2\ , \tag{97}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{i+2}S_1(i) = \left(\zeta_3-S_3(N-1)\right)\frac{(N-1)(N-2)}{2} + \left(\zeta_2-S_2(N-1)\right)\frac{N^2-3N+3}{2} + \frac{2-N}{2}\ , \tag{98}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{i+3}S_1(i) = \left(-\zeta_3+S_3(N-1)\right)\frac{(N-1)(N-2)(N-3)}{6}$$

$$-\Big(\zeta_2 - S_2(N-1)\Big)\frac{3N^3-18N^2+33N-22}{12} + \frac{(6N-13)(N-3)}{24}\;, \tag{99}$$

$$\begin{aligned}\sum_{i=1}^{\infty}\frac{B(N,i)}{i+4}S_1(i) &= -\frac{-864+2040N^2-3746N^3+2453N^4-675N^5+66N^6}{864N^3}\\ &+\frac{300-550N+385N^2-110N^3+11N^4}{144}\Big(\zeta_2 - S_2(N)\Big)\\ &+\frac{(N-1)(N-2)(N-3)(N-4)}{24}\Big(\zeta_3 - S_3(N)\Big)\end{aligned} \tag{100}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{i+N+3}S_1(i) = \frac{\zeta_2 - S_2(N+2)}{N+3} + \frac{3N^6+15N^5+36N^4+51N^3+52N^2+36N+8}{N^3(N+1)^3(N+2)^3}\;, \tag{101}$$

$$\begin{aligned}\sum_{i=1}^{\infty}\frac{B(N,i)}{i+N+4}S_1(i) &= \frac{\zeta_2 - S_2(N+3)}{N+4} + 2\frac{2N^9+24N^8+129N^7+408N^6+854N^5+1270N^4}{N^3(N+1)^3(N+2)^3(N+3)^3}\\ &+2\frac{1405N^3+1158N^2+594N+108}{N^3(N+1)^3(N+2)^3(N+3)^3}\;,\end{aligned} \tag{102}$$

$$\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+1)^2}S_1(i) = (-1)^N\frac{2S_{1,-2}(N)+S_{-3}(N)+\zeta_2 S_1(N)+\zeta_3}{N(N+1)} + \frac{\zeta_2 - S_2(N)}{(N+1)^2}\;, \tag{103}$$

$$\begin{aligned}\sum_{i=1}^{\infty}\frac{B(N,i)}{i+1}S_1(i+N) &= (N-1)\Big(2S_3(N)+S_1(N)S_2(N)-\zeta_2 S_1(N)-2\zeta_3\Big)\\ &-\frac{N-1}{N}\Big(S_2(N)-\zeta_2\Big)+\frac{1-N+N^2}{N^2}S_1(N)+\frac{1}{N^3}\end{aligned} \tag{104}$$

$$\begin{aligned}\sum_{i=1}^{\infty}\frac{B(N,i)}{i+2}S_1(i+N) &= \frac{(N-1)(N-2)}{2}\Big(-2S_3(N)-S_1(N)S_2(N)+\zeta_2 S_1(N)+2\zeta_3\Big)\\ &+\frac{(N-2)(2N-1)}{2N}\Big(S_2(N)-\zeta_2\Big)-\frac{-4+6N-7N^2+2N^3}{4N^2}S_1(N)\\ &+\frac{2-2N^2+N^3}{2N^3}\;.\end{aligned} \tag{105}$$

$$\begin{aligned}\sum_{i=1}^{\infty}\frac{B(N,i)}{i+3}S_1(i+N) &= \frac{(N-1)(N-2)(N-3)}{6}\Big(2S_3(N)+S_1(N)S_2(N)-\zeta_2 S_1(N)-2\zeta_3\Big)\\ &-\frac{(N-3)(3N^2-6N+2)}{6N}\Big(S_2(N)-\zeta_2\Big)\\ &-\frac{-12+21N^2-19N^3+4N^4}{12N^3}\\ &+\frac{36-66N+85N^2-39N^3+6N^4}{36N^2}S_1(N)\end{aligned} \tag{106}$$

$$\begin{aligned}\sum_{i=1}^{\infty}\frac{B(N,i)}{i+4}S_1(i+N) &= \frac{144-340N^2+397N^3-150N^4+18N^5}{144N^3}\\ &-\frac{-144+300N-415N^2+241N^3-63N^4+6N^5}{144N^2}S_1(N)\end{aligned}$$

$$
\begin{aligned}
&+\Big\{-\frac{(N-4)(2N-3)(1-3N+N^2)}{12N}\\
&+\frac{(N-1)(N-2)(N-3)(N-4)}{24}S_1(N)\Big\}\Big(\zeta_2-S_2(N)\Big)\\
&+\frac{(N-1)(N-2)(N-3)(N-4)}{12}\Big(\zeta_3-S_3(N)\Big) \qquad (107)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+1)^2}S_1(i+N) &= \frac{(-1)^{N+1}}{N(N+1)}\Big(4S_{1,-2}(N+1)-2S_{-3}(N+1)\\
&-2S_1(N+1)S_{-2}(N+1)+\zeta_2S_1(N+1)-\zeta_3-2S_{-2}(N+1)\\
&-\zeta_2\Big)+\frac{S_1(N+1)}{N(N+1)^2}+\frac{1}{N(N+1)^3}\ , \qquad (108)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+2)^2}S_1(i+N) &= \frac{(-1)^{N+1}}{N(N+1)(N+2)}\Big(8S_{1,-2}(N+2)-4S_{-3}(N+2)\\
&-4S_1(N+2)S_{-2}(N+2)+2\zeta_2S_1(N+2)-2\zeta_3\\
&-10S_{-2}(N+2)-5\zeta_2\Big)+\frac{1+N+N^2}{N(N+1)^2(N+2)^2}S_1(N+2)\\
&-\frac{1+7N+6N^2+N^3}{N(N+1)^3(N+2)^3}\ , \qquad (109)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+3)}S_1(i+N) &= \frac{16N^3+12+40N+30N^2+6N^4+N^5}{N^3(N+1)^2(N+2)^2(N+3)}\\
&+\frac{85N^2+36+66N+69N^3+34N^4+9N^5+N^6}{N^2(N+1)^2(N+2)^2(N+3)^2}S_1(N)\\
&-6(-1)^N\left(\frac{\zeta(2)+2S_{-2}(N)}{N(N+1)(N+2)(N+3)}\right)\ , \qquad (110)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i=1}^{\infty}\frac{B(N,i)}{(i+N+4)}S_1(i+N) &= \frac{144+564N+564N^2+361N^3+180N^4+62N^5+12N^6+N^7}{N^3(N+1)^2(N+2)^2(N+3)^2(N+4)}\\
&+\frac{424N^5+110N^6+16N^7+N^8}{N^2(N+1)^2(N+2)^2(N+3)^2(N+4)^2}S_1(N)\\
&+\frac{576+1200N+1660N^2+1576N^3+1013N^4}{N^2(N+1)^2(N+2)^2(N+3)^2(N+4)^2}S_1(N)\\
&-24(-1)^N\left(\frac{\zeta(2)+2S_{-2}(N)}{N(N+1)(N+2)(N+3)(N+4)}\right)\ , \qquad (111)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i=1}^{\infty}B(N,i)S_1(i+N)^2 &= \frac{-2+5N-2N^2+N^3}{(N-1)^3N^3}+2\frac{(1-N+N^2)S_1(N)}{(N-1)^2N^2}+\frac{S_1(N)^2}{N-1}\\
&+2\frac{(-1)^NS_{-2}(N)}{(N-1)N}+\frac{(-1)^N\zeta_2}{(N-1)N} \qquad (112)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{i=1}^{\infty}\frac{B(N,i)}{i}S_1(i+N)^2 &= \frac{2}{N^4}+2\frac{S_1(N)}{N^3}+\frac{S_1^2(N)}{N^2}-S_1^2(N)S_2(N)-4S_1(N)S_3(N)\\
&-3S_4(N)-2\frac{(-1)^NS_{-2}(N)}{N^2}+2S_{-2}^2(N)-\frac{(-1)^N\zeta_2}{N^2}
\end{aligned}
$$

$$+S_1^2(N)\zeta_2 + 2S_{-2}(N)\zeta_2 + \frac{17}{10}\zeta_2^2 + 4S_1(N)\zeta_3 \ , \tag{113}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N} S_1(i+N)^2 = \frac{(-1)^{N+1}}{N^2}\Big(\zeta_2 + 2S_{-2}(N)\Big) + \frac{S_1(N)^2}{N^2} + 2\frac{S_1(N)}{N^3} + \frac{2}{N^4} \tag{114}$$

$$\begin{aligned}\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N+1} S_1(i+N)^2 &= \frac{(-1)^N}{N(N+1)}\Big(-6S_{-2,1}(N-1) + 2S_{-2}(N-1)S_1(N-1) \\ &+S_{-3}(N-1) + \zeta_2 S_1(N-1) - 3\zeta_3 - 2S_{-2}(N-1) - \zeta_2\Big) \\ &+\frac{1+N+N^2}{N^2(N+1)^2} S_1(N-1)^2 + 2\frac{1+2N}{N^2(N+1)^2} S_1(N-1) \\ &+\frac{2+3N}{N^3(N+1)^2} \ ,\end{aligned} \tag{115}$$

$$\begin{aligned}\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N+2} S_1(i+N)^2 &= \frac{(-1)^N}{N(N+1)(N+2)}\Big(-12S_{-2,1}(N-1) + 4S_{-2}(N-1)S_1(N-1) \\ &+2S_{-3}(N-1) + 2\zeta_2 S_1(N-1) - 6\zeta_3 + 2(N-1)S_{-2}(N-1) \\ &+(N-5)\zeta_2\Big) + \frac{4+6N+7N^2+4N^3+N^4}{N^2(N+1)^2(N+2)^2} S_1(N-1)^2 \\ &+4\frac{3+3N+N^2}{N^2(N+1)(N+2)^2} S_1(N-1) + \frac{4+11N+5N^2}{N^3(N+1)(N+2)^2} \ ,\end{aligned} \tag{116}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N} S_1(i)^2 = \frac{S_{1,2}(N-1) - 2S_3(N-1) - \zeta_2 S_1(N-1) + 3\zeta_3}{N} \ , \tag{117}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N+1} S_1(i)^2 = \frac{S_{1,2}(N) - 2S_3(N) - \zeta_2 S_1(N) + 3\zeta_3}{N+1} - \frac{S_2(N) - \zeta_2}{N^2} + \frac{2}{N^4} \ , \tag{118}$$

$$\begin{aligned}\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N+2} S_1(i)^2 &= \frac{S_{1,2}(N+1) - 2S_3(N+1) - \zeta_2 S_1(N+1) + 3\zeta_3}{N+2} \\ &-\frac{2N^2+N+1}{N^2(N+1)^2}\Big(S_2(N+1) - \zeta_2\Big) \\ &+\frac{5N^4+8N^3+13N^2+8N+2}{N^4(N+1)^4} \ ,\end{aligned} \tag{119}$$

$$\begin{aligned}\sum_{i=1}^{\infty} \frac{B(N,i)}{i+N+2} S_1(i) S_1(N+i) &= \frac{(-1)^N}{N(N+1)(N+2)}\Bigg(4S_{-2,1}(N) - 6S_{-3}(N) - 4S_{-2}(N)S_1(N) \\ &-2\zeta_2 S_1(N) - 2\zeta_3 - 2\frac{\zeta_2}{(N+1)} - 4\frac{S_{-2}(N)}{(N+1)}\Bigg) - 2\frac{S_3(N)}{N+2} \\ &-\frac{S_1(N)S_2(N)}{N+2} + \frac{\zeta_2 S_1(N)}{N+2} + \frac{2\zeta_3}{N+2} \\ &+\frac{2+7N+7N^2+5N^3+N^4}{N^3(N+1)^3(N+2)} S_1(N)\end{aligned}$$

$$+2\frac{2+7N+9N^2+4N^3+N^4}{N^4(N+1)^3(N+2)}\;, \tag{120}$$

$$\sum_{i=1}^{\infty} B(N,i)S_2(N+i) = \frac{1}{(N-1)N^2} + \frac{S_2(N)}{N-1} - 2\frac{(-1)^N S_{-2}(N)}{(N-1)N} - \frac{(-1)^N\zeta_2}{(N-1)N} \tag{121}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{i}S_2(N+i) = -3S_4(N) - 2S_{-2}(N)^2 - S_2(N)^2 - 2S_{-2}(N)\zeta_2 + S_2(N)\zeta_2 + \frac{7}{10}\zeta_2^2$$
$$+(-1)^N\frac{\zeta(2)+2S_{-2}(N)}{N^2} + \frac{S_2(N)}{N^2}\;, \tag{122}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{N+i}S_2(N+i) = (-1)^N\frac{\zeta(2)+2S_{-2}(N)}{N^2} + \frac{S_2(N)}{N^2}\;, \tag{123}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{N+i+1}S_2(N+i) = \frac{1+N+N^2}{N^2(N+1)^2}S_2(N) + (-1)^N\left[-\frac{2S_{1,-2}(N)}{N(N+1)} + \frac{2S_{-2}(N)}{N^2}\right.$$
$$\left.-\frac{S_{-3}(N)}{N(N+1)} + \frac{\zeta_2}{N^2} - \frac{S_1(N)\zeta_2}{N(N+1)} - \frac{\zeta_3}{N(N+1)}\right]\;, \tag{124}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{N+i+2}S_2(N+i) = \frac{N^4+4N^3+7N^2+6N+4}{N^2(N+1)^2(N+2)^2}S_2(N) + \frac{2}{N(N+1)^2(N+2)}$$
$$+(-1)^N\left[-\frac{4S_{1,-2}(N)}{N(N+1)(N+2)} - \frac{2(N-2)S_{-2}(N)}{N^2(N+2)}\right.$$
$$-\frac{2S_{-3}(N)}{N(N+1)(N+2)} + \zeta_2\Big(-\frac{2S_1(N)}{N(N+1)(N+2)} - \frac{N-2}{N^2(N+2)}\Big)$$
$$\left.-\frac{2\zeta_3}{N(N+1)(N+2)}\right]\;, \tag{125}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{N+i+2}S_2(i) = \frac{S_{1,2}(N)}{N+2} - \frac{S_1(N)\zeta_2}{N+2} + \frac{\zeta_3}{N+2} - \frac{(2+3N+4N^2+N^3)S_2(N)}{N^2(N+1)^2(N+2)}$$
$$+\frac{(2+3N+4N^2+N^3)\zeta_2}{N^2(N+1)^2(N+2)} + \frac{2}{N(N+1)^4(N+2)}\;, \tag{126}$$

$$\sum_{i=1}^{\infty} \frac{B(N,i)}{(N+i+2)^2}S_1(i) = \frac{-8+N+3N^2}{N(N+1)^4(N+2)^2} - \frac{S_2(N)}{(N+2)^2} + \frac{\zeta_2}{(N+2)^2}$$
$$+\Big(\frac{2\zeta_2}{N(1+N)^2(N+2)} + \frac{2S_1(N)\zeta_2}{N(N+1)(N+2)}$$
$$+\frac{2\zeta_3}{N(N+1)(N+2)} + \frac{4S_{-2}(N)}{N(N+1)^2(N+2)}$$
$$+\frac{2S_{-3}(N)}{N(N+1)(N+2)} + \frac{4S_{1,-2}(N)}{N(N+1)(N+2)}\Big)(-1)^N\;, \tag{127}$$

B.3 Weighted Harmonic Sums

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+N)}{i+N} = \frac{\sigma_1^3 - \zeta_3 - S_1^3(N) - 2S_3(N)}{3} + \frac{S_1^2(N) + S_2(N)}{N} - S_1(N)S_2(N) \ , \quad (128)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+N)}{i+N+1} = \frac{\sigma_1^3 - 4\zeta_3}{3} + \frac{S_3(N) - S_1^3(N)}{3} - S_1(N)\zeta_2 \ , \quad (129)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+N)}{i+N+2} = \frac{\sigma_1^3 - 4\zeta_3}{3} + \frac{S_3(N) - S_1^3(N)}{3} - \frac{S_1^2(N)}{N+1} - S_1(N)\zeta_2 - \frac{\zeta_2}{N+1}$$
$$-\frac{(N+2)}{(N+1)^2}S_1(N) - \frac{1}{(N+1)^2} \ , \quad (130)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+N)}{i+3} = \frac{\sigma_1^3 - \zeta_3}{3} + S_{1,1,1}(N) - \frac{3N^2 - 6N + 2}{N(N-1)(N-2)}S_{1,1}(N) + \frac{13N - 19}{4(N-1)(N-2)}$$
$$-\frac{(N+1)(7N-6)}{4N(N-1)}S_1(N) \ , \quad (131)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+N)}{i+4} = \frac{1}{3}\sigma_1^3 - \frac{(N+1)(132 - 232N + 85N^2)}{36(N-2)(N-1)N}S_1(N) - \frac{1}{3}\zeta_3 + S_{1,1,1}(N)$$
$$-2\frac{(-3+2N)(1-3N+N^2)}{(N-3)(N-2)(N-1)N}S_{1,1}(N) + \frac{809 - 909N + 232N^2}{36(N-3)(N-2)(N-1)} \quad (132)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i+N)S_1^2(i)}{i} = \frac{\sigma_1^4}{4} + \frac{43}{20}\zeta_2^2 + 3S_1(N)\zeta_3 + \frac{S_1^2(N) - S_2(N)}{2}\zeta_2 - S_1(N)S_{2,1}(N)$$
$$+\frac{S_1^2(N)S_2(N)}{2} + \frac{2}{3}S_1(N)S_3(N) - \frac{S_2^2(N)}{4} + \frac{S_1^4(N)}{12} \ , \quad (133)$$

$$\sum_{i=1}^{\infty} \frac{S_1^2(i+N)S_1(i)}{i} = \frac{\sigma_1^4}{4} + \frac{43}{20}\zeta_2^2 + 5S_1(N)\zeta_3 + \frac{3S_1^2(N) - S_2(N)}{2}\zeta_2 - 2S_1(N)S_{2,1}(N)$$
$$+S_1^2(N)S_2(N) + S_1(N)S_3(N) - \frac{S_2^2(N)}{4} + \frac{S_1^4(N)}{4} \ , \quad (134)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_2(i+N)}{i} = \frac{\sigma_1^2}{2}\zeta_2 - \frac{1}{5}\zeta_2^2 - S_1(N)\zeta_3 - \frac{S_1^2(N) - 3S_2(N)}{2}\zeta_2 - 2S_{3,1}(N) + \frac{1}{2}S_4(N)$$
$$+\frac{S_1^2(N)S_2(N)}{2} + S_1(N)S_3(N) \ , \quad (135)$$

$$\sum_{i=1}^{\infty} \frac{S_1(i+N)S_2(i)}{i} = \frac{\sigma_1^2}{2}\zeta_2 - \frac{\zeta_2^2}{5} + S_1(N)\zeta_3 + \frac{S_1^2(N) - S_2(N)}{2}\zeta_2 + 2S_{1,1,2}(N)$$
$$-2S_{1,3}(N) + S_1(N)S_{2,1}(N) - S_1^2(N)S_2(N) + \frac{S_4(N) - S_2^2(N)}{2} \ , \quad (136)$$

$$\sum_{i=1}^{\infty} \frac{S_{1,1}(i+N)S_1(i)}{i+N} = \frac{\sigma_1^4}{8} + \frac{\sigma_1^2}{4}\zeta_2 - \frac{9}{40}\zeta_2^2 - 3\frac{S_4(N)}{4} + \frac{S_1^3(N)}{2N} - \frac{S_1^4(N)}{8} - 3\frac{S_1^2(N)S_2(N)}{4}$$
$$-3\frac{S_2^2(N)}{8} + S_1(N)\Big(3\frac{S_2(N)}{2N} - S_3(N)\Big) + \frac{S_3(N)}{N} \ , \quad (137)$$

$$\sum_{i=1}^{\infty} \frac{S_{1,1}(i+N)S_1(i)}{i} = \frac{\sigma_1^4}{8} + \frac{\sigma_1^2\zeta_2}{4} + \frac{39}{40}\zeta_2^2 + 2S_1(N)\zeta_3 + \frac{S_1^2(N)+S_2(N)}{2}\zeta_2 - S_{3,1}(N)$$
$$+3\frac{S_1^2(N)S_2(N)}{4} + \frac{S_1^4(N)}{8} - \frac{S_2^2(N)}{8} + S_1(N)\Big(-S_{2,1}(N) + S_3(N)\Big)$$
$$+\frac{S_4(N)}{4} \; . \tag{138}$$

$$\sum_{i=1}^{\infty} \frac{S_1(i)S_2(i+N)}{i+N} = \frac{\sigma_1^2}{2}\zeta_2 - \frac{9}{10}\zeta_2^2 + \Big(-\frac{S_1(N)}{N} + \frac{S_1^2(N)}{2} + \frac{S_2(N)}{2}\Big)\zeta_2 - S_1^2(N)S_2(N)$$
$$-\frac{S_2^2(N)}{2} - \frac{S_{2,1}(N)}{N} + S_1(N)\Big(2\frac{S_2(N)}{N} + S_{2,1}(N) - 2S_3(N)\Big)$$
$$+2\frac{S_3(N)}{N} + S_{3,1}(N) - \frac{3S_4(N)}{2} \; , \tag{139}$$

$$\sum_{i=1}^{\infty} \frac{S_2(i)S_1(i+N)}{i+N} = \frac{\sigma_1^2}{2}\zeta_2 - \frac{7}{10}\zeta_2^2 + \Big(\frac{2}{N} - 2S_1(N)\Big)\zeta_3 + \Big(\frac{S_1(N)}{N} - \frac{S_1^2(N)}{2} - \frac{S_2(N)}{2}\Big)\zeta_2$$
$$-\frac{S_1^2(N)}{N^2} - \frac{S_2(N)}{N^2} + \frac{S_2^2(N)}{2} - \frac{S_{2,1}(N)}{N} + S_1(N)S_{2,1}(N) + S_{3,1}(N)$$
$$+\frac{S_4(N)}{2} \; , \tag{140}$$

$$\sum_{i=1}^{\infty} \frac{S_1(i+N)S_1(i)}{(i+N)^2} = \frac{6}{5}\zeta_2^2 + \Big(-\frac{2}{N} + 2S_1(N)\Big)\zeta_3 + \frac{S_1^2(N)}{N^2} + \frac{S_2(N)}{N^2} - \frac{S_2^2(N)}{2} + \frac{S_{2,1}(N)}{N}$$
$$-S_1(N)S_{2,1}(N) - S_{3,1}(N) - \frac{S_4(N)}{2} \; , \tag{141}$$

$$\sum_{i=1}^{\infty} \frac{S_1(i+N)S_1^2(i)}{i+N} = \frac{\sigma_1^4}{4} - \frac{3\zeta_2^2}{4} + \Big(\frac{2}{N} - 2S_1(N)\Big)\zeta_3 + \Big(\frac{S_1(N)}{N} - \frac{S_1^2(N)}{2} - \frac{S_2(N)}{2}\Big)\zeta_2$$
$$+\frac{S_1^3(N)}{N} - \frac{S_1^4(N)}{4} + S_1^2(N)\Big(-\frac{1}{N^2} - \frac{3S_2(N)}{2}\Big) - \frac{S_2(N)}{N^2} - \frac{S_2^2(N)}{4}$$
$$-\frac{S_{2,1}(N)}{N} + S_1(N)\Big(3\frac{S_2(N)}{N} + S_{2,1}(N) - 2S_3(N)\Big) + 2\frac{S_3(N)}{N} + S_{3,1}(N)$$
$$-S_4(N) \; , \tag{142}$$

B.4 Harmonic Sums

$$\sum_{i=1}^{\infty} S_3(i+N) - S_3(i) = S_2(N) - (N+1)S_3(N) + N\zeta_3 \; , \tag{143}$$

$$\sum_{i=1}^{\infty} (S_3(i+N) - S_3(i))i = \frac{S_1(N) - S_2(N) + N(N+1)S_3(N) - N(N+1)\zeta_3}{2}$$
$$-NS_2(N) + N\zeta_2 \; , \tag{144}$$

$$\sum_{i=1}^{\infty} \Big(S_1(i+N) - S_1(i)\Big)^3 = -\frac{3}{2}S_1^2(N) - S_1^3(N) - \frac{1}{2}S_2(N) + 3NS_{2,1}(N) - NS_3(N)$$
$$+N\zeta_3 \; , \tag{145}$$

$$\sum_{i=1}^{\infty}\Big(S_1(i+N)-S_1(i)\Big)^3 i = \frac{N}{2}\Big(-(N+1)\zeta_3 - 3(N+1)S_{2,1}(N) + (N+1)S_3(N) + (3N-1)\zeta_2\Big) + \frac{1+2N+6N^2}{4}S_2(N) + \frac{3}{4}S_1^2(N) + \frac{2-6N}{4}S_1(N)\ , \tag{146}$$

$$\sum_{i=1}^{\infty}\Big(S_1(i+N)-S_1(i)\Big)S_2(i) = -\frac{1}{2}S_1^2(N) - \frac{1}{2}S_2(N) + NS_{2,1}(N) + N\zeta_2 - NS_1(N)\zeta_2 + N\sigma_1\zeta_2 - 2N\zeta_3\ , \tag{147}$$

$$\sum_{i=1}^{\infty}\Big(S_1(i+N)-S_1(i)\Big)S_2(i+N) = -(1+S_1(N))S_2(N) + NS_3(N) - NS_1(N)\zeta_2 + N(\zeta_2 + \sigma_1\zeta_2 - \zeta_3)\ , \tag{148}$$

B.5 Miscellaneous Sums

$$\sum_{k=0}^{l-1}\frac{B(k+2,\varepsilon/2)}{k+1} = \frac{4}{\varepsilon^2} - \frac{2}{\varepsilon}B(1+l,\varepsilon/2)\ , \tag{149}$$

$$\sum_{l=0}^{N-1}\binom{N-1}{l}(-1)^l B(l+1-\varepsilon/2,2-\varepsilon/2) = B(1-\varepsilon/2,N+1-\varepsilon/2)\ . \tag{150}$$

B.6 Double and Other Sums

$$\sum_{i,j=1}^{\infty}\frac{S_1(i)S_1(i+j+N)}{i(i+j)(j+N)} = 6\frac{S_1(N)}{N}\zeta_3 + \zeta_2\Big(2\frac{S_1^2(N)}{N} + \frac{S_2(N)}{N}\Big) + \frac{S_1^4(N)}{6N} + \frac{S_1^2(N)S_2(N)}{N} - \frac{S_2^2(N)}{N} + 4\frac{S_{2,1,1}(N)}{N} + S_1(N)\Big(-3\frac{S_{2,1}(N)}{N} + 4\frac{S_3(N)}{3N}\Big) - 2\frac{S_{3,1}(N)}{N} - \frac{S_4(N)}{2N}\ , \tag{151}$$

$$\sum_{k=1}^{\infty}\frac{B(k+\varepsilon/2,N)}{N+k} = \frac{1}{N^2} + \frac{\varepsilon}{2}\left\{(-1)^N\frac{2S_{-2}(N)+\zeta_2}{N} - \frac{S_1(N)}{N^2}\right\} + \varepsilon^2\left\{-(-1)^N\frac{S_{-2,1}(N)}{N} + (-1)^N\frac{2S_{-3}(N)-\zeta_3}{4N} + (-1)^N\frac{2S_{-2}(N)+\zeta_2}{4N}S_1(N) + \frac{S_1^2(N)+S_2(N)}{8N^2}\right\}$$

$$
\begin{aligned}
&+ \frac{\varepsilon^3}{48N}\Biggl\{\frac{12}{5}(-1)^N\zeta_2^2 - 6(-1)^N S_1(N)\zeta_3 + \zeta_2\Biggl(3(-1)^N S_1^2(N) \\
&+3(-1)^N S_2(N)\Biggr) + 48(-1)^N S_{-2,1,1}(N) - 24(-1)^N S_{-3,1}(N) \\
&-24(-1)^N S_{-2,2}(N) + 12(-1)^N S_{-4}(N) + 6(-1)^N S_1^2(N) S_{-2}(N) \\
&+6(-1)^N S_2(N) S_{-2}(N) - 2\frac{S_3(N)}{N} - \frac{S_1^3(N)}{N} \\
&+S_1(N)\Biggl(-3\frac{S_2(N)}{N} - 24(-1)^N S_{-2,1}(N) + 12(-1)^N S_{-3}(N)\Biggr)\Biggr\} \\
&+O(\varepsilon^4)\ . \qquad (152)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{k=1}^{\infty}\frac{B(N+1,k+\varepsilon/2)}{N+k} &= (-1)^N\sum_{j=1}^{N}(-1)^j\left(\sum_{k=1}^{\infty}\frac{B(j,k+\varepsilon/2)}{j+k} + \frac{B(j,1+\varepsilon/2)}{j}\right) \\
&+(-1)^N\sum_{k=1}^{\infty}\frac{B(1,k+\varepsilon/2)}{k}\ , \qquad (153)
\end{aligned}
$$

$$
\begin{aligned}
\sum_{k=1}^{\infty}\frac{B(k+\varepsilon/2,N+1)}{N+k} &= (-1)^N\Bigl[2S_{-2}(N) + \zeta_2\Bigr] \\
&+ \frac{\varepsilon}{2}(-1)^N\Bigl[-\zeta_3 + \zeta_2 S_1(N) + 2S_{1,-2}(N) - 2S_{-2,1}(N)\Bigr] \\
&+ \frac{\varepsilon^2}{4}(-1)^N\Biggl[\frac{2}{5}\zeta_2^2 - \zeta_3 S_1(N) + \zeta_2 S_{1,1}(N) \\
&+2\Bigl\{S_{1,1,-2}(N) + S_{-2,1,1}(N) - S_{1,-2,1}(N)\Bigr\}\Biggr] \\
&+ \varepsilon^3(-1)^N\Biggl[-\frac{\zeta_5}{8} + \frac{S_1(N)}{20}\zeta_2^2 - \frac{S_{1,1}(N)}{8}\zeta_3 + \frac{S_{1,1,1}(N)}{8}\zeta_2 \\
&+\frac{S_{1,-2,1,1}(N) + S_{1,1,1,-2}(N) - S_{-2,1,1,1}(N) - S_{1,1,-2,1}(N)}{4}\Biggr] \\
&+O(\varepsilon^4)\ . \qquad (154)
\end{aligned}
$$

B.7 Expansion of harmonic sums for small argument

One may expand nested harmonic sums into Taylor series w.r.t. the outer argument, using the corresponding differentiation rules [51]. In the present calculation we made use of the following relations.

$$
\begin{aligned}
S_1(\varepsilon) &= \zeta_2\varepsilon - \zeta_3\varepsilon^2 + \frac{2}{5}\zeta_2^2\varepsilon^3 - \zeta_5\varepsilon^4 + O(\varepsilon^5)\ , \qquad (155) \\
S_2(\varepsilon) &= 2\zeta_3\varepsilon - \frac{6}{5}\zeta_2^2\varepsilon^2 + 4\zeta_5\varepsilon^3 - \frac{8}{7}\zeta_2^3\varepsilon^4 + O(\varepsilon^5)\ , \qquad (156) \\
S_3(\varepsilon) &= \frac{6}{5}\zeta_2^2\varepsilon - 6\zeta_5\varepsilon^2 + \frac{16}{7}\zeta_2^3\varepsilon^3 - 15\zeta_7\varepsilon^4 + O(\varepsilon^5)\ , \qquad (157)
\end{aligned}
$$

$$S_4(\varepsilon) = 4\zeta_5\varepsilon - \frac{16}{7}\zeta_2^3\varepsilon^2 + 20\zeta_7\varepsilon^3 - \frac{24}{5}\zeta_2^4\varepsilon^4 + O(\varepsilon^5) \; , \tag{158}$$

$$S_{2,1}(\varepsilon) = \frac{7}{10}\zeta_2^2\varepsilon + \left(2\zeta_3\zeta_2 - \frac{11}{2}\zeta_5\right)\varepsilon^2 + O(\varepsilon^3) \; , \tag{159}$$

$$S_{3,1}(\varepsilon) = \left(\frac{9}{2}\zeta_5 - \zeta_3\zeta_2\right)\varepsilon + O(\varepsilon^2) \; , \tag{160}$$

$$S_{2,1,1}(\varepsilon) = \left(\frac{11}{2}\zeta_5 - 2\zeta_3\zeta_2\right)\varepsilon + O(\varepsilon^2) \; . \tag{161}$$

These relations can be obtained expanding the representation of the sums in terms of Mellin transforms of Nielsen integrals weighted by $1/(1 \pm x)$. In case of the single harmonic sums the expansions result from Euler's ψ–function and its derivatives.

B.8 Sample Calculation for one of the Sum

In the following we illustrate the calculation of sum (151) in using the `Sigma` package :

$$\sum_{j=1}^{\infty} \frac{1}{j+N} \sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+j+N)}{i(i+j)}. \tag{162}$$

First, we treat the inner sum for N fixed,

$$F(j) = \sum_{i=1}^{\infty} \frac{S_1(i)S_1(i+j+N)}{i(i+j)} \; . \tag{163}$$

By `Sigma`'s creative telescoping algorithm we compute the recurrence relation

$$\begin{aligned} -(j+N+1)j^2F(j) + (j+1)\left(3j^2+3Nj+7j+2N+4\right)F(j+1) \\ -(j+2)\left(3j^2+3Nj+11j+4N+10\right)F(j+2) \\ +(j+2)(j+3)(j+N+3)F(j+3) &= A(j) + B(j)S_1(j+N) \end{aligned} \tag{164}$$

where

$$\begin{aligned} A(j) &= \frac{1}{\left(j^2+3j+2\right)\left(j^2+(2N+3)j+N^2+3N+2\right)^2} \\ &\quad \times\Big(3j^5+(9N+26)j^4+\left(10N^2+63N+86\right)j^3+\left(5N^3+49N^2+156N+137\right)j^2 \\ &\quad +\left(N^4+12N^3+74N^2+163N+106\right)j+5N^3+34N^2+61N+32\Big), \end{aligned} \tag{165}$$

$$B(j) = \frac{3j^3+(4N+13)j^2+\left(-N^2+11N+18\right)j-N^3-2N^2+7N+8}{(j+1)(j+2)(j+N+1)(j+N+2)}. \tag{166}$$

Next, we apply `Sigma`'s recurrence solver and obtain three linearly independent solutions of the homogeneous version of the recurrence:

$$\frac{1}{j}, \quad \frac{S_1(j+N)}{j}, \quad \frac{-jS_1(j)+jS_1(j+N)+1}{j^2(N+1)}$$

and one solution of the recurrence itself:

$$\begin{aligned}
p(j) &= \frac{S_1(j+N)^3}{6j} - \frac{S_1(j+N)^2}{2j^2} + \left(-\frac{S_2(N)}{2j} + \frac{S_2(j+N)}{2j} + \frac{3}{Nj+j}\right) S_1(j+N) - \frac{S_3(N)}{3j} \\
&+ \frac{S_1(N)^2}{2Nj+2j} + \frac{3N+2}{j^2(N+1)^2} + \frac{(j-2(N+1))S_1(N)}{2j^2(N+1)^2} + \frac{S_2(N)}{2j^2} - \frac{S_2(j+N)}{2j^2} + \frac{S_3(j+N)}{3j} \\
&+ \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{i^2}}{j} - \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{i}}{j^2} - \frac{\sum_{i=1}^{j} \frac{S_1(i)S_1(i+N)}{i}}{j} + \frac{\sum_{i=1}^{j} \frac{S_2(i+N)}{i}}{2j} + \frac{\sum_{i=1}^{j} \frac{S_1(i+N)^2}{i}}{2j} \\
&+ S_1(j)\left(\frac{-3N-2}{j(N+1)^2} + \frac{S_1(N)}{Nj+j} - \frac{S_2(N)}{2j} + \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{i}}{j}\right) - \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{(i+N)^2}}{j}. \qquad (167)
\end{aligned}$$

The function $F(j)$ is given by

$$F(j) = a_1 \frac{1}{j} + a_2 \frac{S_1(j+N)}{j} + a_3 \frac{-jS_1(j) + jS_1(j+N) + 1}{j^2(N+1)} + p(j) \qquad (168)$$

for some properly chosen constants a_1, a_2 and a_3 which are free of j. Looking at the initial values for $j = 1, 2, 3$ of $F(j)$ we can conclude that

$$a_1 = -\frac{1}{6}S_1(N)^3 - \frac{S_1(N)^2}{2N+2} + \left(-\frac{1}{2}S_2(N) - \frac{1}{2(N+1)^2}\right) S_1(N) - S_{2,1}(N) + 2\zeta_3, \qquad (169)$$

$$a_2 = \frac{1}{2}\left(- S_1(N)^2 - \frac{2S_1(N)}{N+1} + S_2(N) + \frac{2\left((N+1)^2\zeta_2 - 1\right)}{(N+1)^2}\right), \qquad (170)$$

$$a_3 = \frac{1}{2}(N+1)S_1(N)^2 + S_1(N) - \frac{3N+2}{N+1}. \qquad (171)$$

One obtains

$$\begin{aligned}
F(j) &= -\frac{S_1(N)^3}{6j} + \frac{S_1(N)^2}{2j^2} + \left(\frac{1}{2jN^2} - \frac{S_2(N)}{2j}\right) S_1(N) + \frac{S_1(j+N)^3}{6j} - \frac{S_1(j+N)^2}{2j^2} \\
&+ S_1(j)^2\left(-\frac{S_1(j+N)}{2j} - \frac{1}{2jN}\right) + \frac{S_2(N)}{2j^2} - \frac{S_2(j+N)}{2j^2} - \frac{S_3(N)}{3j} + \frac{S_3(j+N)}{3j} \\
&- \frac{S_{2,1}N)}{j} + \frac{\sum_{i=1}^{j} \frac{S_1(i)^2}{i+N}}{2j} + \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{i^2}}{2j} - \frac{(j+N)\sum_{i=1}^{j} \frac{S_1(i+N)}{i}}{j^2 N} - \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{(i+N)^2}}{j} \\
&+ S_1(j)\left(-\frac{S_1(N)^2}{2j} + \frac{S_1(j+N)}{jN} - \frac{S_2(N)}{2j} + \frac{\sum_{i=1}^{j} \frac{S_1(i+N)}{i}}{j} + \frac{1}{2jN^2}\right) \\
&+ \frac{\sum_{i=1}^{j} \frac{S_1(i+N)^2}{i}}{2j} + \frac{\sum_{i=1}^{j} \frac{S_2(i+N)}{i}}{2j} + S_1(j+N)\left(\frac{S_2(j+N)}{2j} - \frac{\frac{1}{N^2} - 2\zeta_2}{2j}\right) + \frac{2\zeta_3}{j}. \qquad (172)
\end{aligned}$$

Finally, we look at the indefinite nested sum

$$S(N, a) = \sum_{j=1}^{a} \frac{F(j)}{j+N} \qquad (173)$$

with

$$\lim_{a\to\infty} S(N,a) = \sum_{j=1}^{a}\sum_{j=1}^{\infty} \frac{S_1(i)S_1(i+j+N)}{i(i+j)(j+N)}. \tag{174}$$

At this point we emphasize that the sum expression (173) with the derived sum representation of $F(j)$ fits into the input class of `Sigma`. Hence, we can apply `Sigma`'s machinery again and arrive for $S(a,N)$ at the following sum representation

$$\begin{aligned}
S(a,N) \;=\; & -\frac{S_1(N)^4}{8N} + \frac{S_1(a+N)S_1(N)^3}{6N} + \left(\frac{S_2(a)}{4N} - \frac{S_2(N)}{4N} + \frac{\zeta_2}{2N}\right) S_1(N)^2 \\
& + \left(S_1(a+N)\left(\frac{S_2(N)}{2N} - \frac{1}{2N^3}\right) - \frac{S_{2,1}(N)}{N} + \frac{2\zeta_3}{N}\right) S_1(N) - \frac{S_1(a+N)^4}{24N} \\
& + \frac{S_2(N)^2}{8N} - \frac{S_2(a+N)^2}{8N} + \frac{\left(\sum_{i=1}^{a} \frac{S_1(i+N)}{i}\right)^2}{2N} + S_1(a)^3\left(-\frac{S_1(a+N)}{3N} - \frac{1}{3N^2}\right) \\
& + S_1(a)^2\left(-\frac{S_1(N)^2}{4N} + \frac{S_1(a+N)}{2N^2} - \frac{S_2(N)}{4N} + \frac{1}{4N^3}\right) + S_2(a)\left(\frac{S_2(N)}{4N} + \frac{1}{12N^3}\right) \\
& + \frac{S_3(N)}{3N^2} - \frac{S_3(a+N)}{3N^2} + \frac{S_4(N)}{4N} - \frac{S_4(a+N)}{4N} - \frac{\sum_{i=1}^{a} \frac{S_1(i)}{(i+N)^3}}{3N} - \frac{\sum_{i=1}^{a} \frac{S_1(i)^2}{(i+N)^2}}{2N} \\
& + \left(\frac{S_1(a)}{2N} - \frac{S_1(a+N)}{2N} + \frac{1}{2N^2}\right)\sum_{i=1}^{a} \frac{S_1(i)^2}{i+N} - \frac{\sum_{i=1}^{a} \frac{S_1(i)^3}{i+N}}{6N} - \frac{\sum_{i=1}^{a} \frac{S_1(i+N)}{i^3}}{6N} \\
& + \left(\frac{S_1(a)}{2N} - \frac{S_1(a+N)}{2N}\right)\sum_{i=1}^{a} \frac{S_1(i+N)}{i^2} \\
& + \left(-\frac{S_1(a)}{N} + \frac{S_1(a+N)}{N} + \frac{1}{N^2}\right)\sum_{i=1}^{a} \frac{S_1(i+N)}{(i+N)^2} \\
& + \frac{\sum_{i=1}^{a} \frac{S_1(i+N)}{(i+N)^3}}{N} - \frac{\sum_{i=1}^{a} \frac{S_1(i)S_1(i+N)}{i^2}}{2N} + \frac{\sum_{i=1}^{a} \frac{S_1(i)S_1(i+N)}{(i+N)^2}}{N} + \frac{\sum_{i=1}^{a} \frac{S_1(i)^2S_1(i+N)}{i+N}}{N} \\
& + \left(\frac{S_1(a)}{2N} - \frac{S_1(a+N)}{2N} - \frac{1}{N^2}\right)\sum_{i=1}^{a} \frac{S_1(i+N)^2}{i} - \frac{\sum_{i=1}^{a} \frac{S_1(i+N)^2}{(i+N)^2}}{N} \\
& + \frac{2\sum_{i=1}^{a} \frac{S_1(i+N)^3}{i}}{3N} + \frac{\sum_{i=1}^{a} \frac{S_1(i+N)S_2(i)}{i}}{2N} + \left(\frac{S_1(a)}{2N} - \frac{S_1(a+N)}{2N}\right)\sum_{i=1}^{a} \frac{S_2(i+N)}{i} \\
& + \frac{\sum_{i=1}^{a} \frac{S_1(i)S_1(i+N)^2}{i}}{2N} - \frac{\sum_{i=1}^{a} \frac{S_1(i)S_2(i+N)}{i}}{2N} + \frac{\sum_{i=1}^{a} \frac{S_1(i+N)S_2(i+N)}{i}}{N} \\
& + \frac{S_2(a+N)\left(1-3N^2\zeta_2\right)}{6N^3} + \frac{S_2(N)\left(3N^2\zeta_2-1\right)}{6N^3} + \frac{S_1(a+N)}{N^2} \\
& + \left(\sum_{i=1}^{a} \frac{S_1(i+N)}{i}\right)\left(\frac{S_1(a)^2}{2N} + \left(-\frac{S_1(a+N)}{N} - \frac{1}{N^2}\right)S_1(a) - \frac{S_1(N)^2}{2N}\right. \\
& \left. - \frac{S_2(a)}{2N} - \frac{S_2(N)}{2N} + \frac{\zeta_2}{N} - \frac{1}{2N^3}\right) + S_1(a+N)^2\left(\frac{1-N^2\zeta_2}{2N^3} - \frac{S_2(a+N)}{4N}\right)
\end{aligned}$$

$$
\begin{aligned}
&+S_1(a+N)\left(\frac{S_3(N)}{3N}-\frac{S_3(a+N)}{3N}+\frac{S_{2,1}(N)}{N}-\frac{2\zeta_3}{N}\right)\\
&+S_1(a)\Bigg(-\frac{S_1(N)^3}{6N}+\frac{S_1(a+N)S_1(N)^2}{2N}+\left(\frac{1}{2N^3}-\frac{S_2(N)}{2N}\right)S_1(N)\\
&+S_1(a+N)\left(\frac{S_2(N)}{2N}-\frac{1}{2N^3}\right)-\frac{S_3(N)}{3N}+\frac{S_3(a+N)}{3N}-\frac{S_{2,1}(N)}{N}+\frac{2\zeta_3}{N}\Bigg). \qquad (175)
\end{aligned}
$$

We remark that all the sums in this expression are algebraically independent, i.e., no relations occur that could cancel some of the involved sums.

Finally, we send a to infinity in the last expression and note that the involved sum expressions can be simplified by the sum identities (128)–(142) and some additional identities of similar type. In the final expression divergences of the type σ_1^k being contained in some of the terms vanish. We find the right hand side of (151).

C The first moment of the operator matrix element

After the analytic continuation from the even values of N to $N \epsilon \mathbf{C}$ is performed one may consider the limit $N \to 1$. In this procedure the term $(1 + (-1)^N)/2$ equals to 1. At $O(a_s^2)$ the terms $\propto T_F C_A$ contain $1/z$ contributions in momentum fraction space and their first moment diverges. For the other contributions to the un–renormalized operator matrix element (after mass renormalization to 2–loop order), the first moment is related to the Abelian part of the transverse contribution to the gluon propagator $\Pi_V(p^2, m^2)|_{p^2=0}$, Figure 3, except the term $\propto T_F^2$

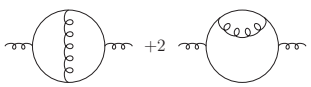

Figure 3: Abelian part of the gluon self-energy due to heavy quarks.

which results from wave function renormalization. This was shown in [6] up to the constant term in ε. One obtains

$$\Pi_V(p^2, m^2) = S_\varepsilon a_s T_F \Pi_V^{(1)}(p^2, m^2) + S_\varepsilon^2 a_s^2 C_F T_F \Pi_V^{(2)}(p^2, m^2) + O(a_s^3) \;, \tag{176}$$

with

$$\lim_{p^2 \to 0} \Pi_V^{(1)}(p^2, m^2) = \frac{1}{2} \hat{\hat{A}}_{Qg}^{(1),N=1} \tag{177}$$

$$\lim_{p^2 \to 0} \Pi_V^{(2)}(p^2, m^2) = \frac{1}{2} \hat{\hat{A}}_{Qg}^{(2),N=1}|_{C_F} \;. \tag{178}$$

Here we extend the relation to the linear terms in ε. For the first moment the double pole contributions in ε vanish in (177,178). From the corresponding QED-expressions $\Pi_T^{V(k)}$ given in [59] by asymptotic expansion of the photon propagator $(1/p^2)\tilde{\Pi}_V^{(k)}(p^2, m^2)$ in m^2/p^2 and adjusting the relative color factor for $k = 2$ to $1/4 = 1/(C_F C_A)$, due to the transition from QED to QCD, the comparison can be performed up to the constant term in ε. One obtains

$$\lim_{p^2 \to 0} \frac{1}{p^2} \tilde{\Pi}_V^{(1)}(p^2, m^2) = \frac{1}{2T_F} \hat{\hat{A}}_{Qg}^{(1),N=1} = -\left(\frac{m^2}{\mu^2}\right)^{\varepsilon/2} S_\varepsilon \left[\frac{8}{3\varepsilon} + \frac{\varepsilon}{3}\zeta_2\right] \tag{179}$$

$$\lim_{p^2 \to 0} \frac{1}{p^2} \tilde{\Pi}_V^{(2)}(p^2, m^2) = \frac{1}{2T_F C_F} \hat{\hat{A}}_{Qg}^{(2),N=1}|_{C_F} = \left(\frac{m^2}{\mu^2}\right)^{\varepsilon} \left[-\frac{4}{\varepsilon} + 15 - \left(\frac{31}{4} + \zeta_2\right)\varepsilon\right] \;. \tag{180}$$

The latter term is easily obtained using `MATAD` [61].

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